Thermally Driven Moisture Redistribution in Partially Saturated Porous Media

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ABSTRACT

Experimental and theoretical studies have been conducted to develop a quantitative understanding of the thermohydrologic phenomena induced by emplacement of high-level radioactive waste (HLW) in an unsaturated fractured porous media. A series of laboratory experiments was conducted in a variety of media to study the physics of thermally driven moisture redistribution. Principles of similarity theory were applied to develop dimensionless parameters to be used to predict thermohydrologic behavior at the field and repository scales from that observed at the laboratory scale. Numerical modeling of two-phase flow phenomena was used to evaluate the scaling theories and interpret the experimental results.

Eleven laboratory-scale experiments were conducted which are categorized according to: (i) the fluid phase that is the focus of study, (ii) temperature regime, (iii) geometry, and (iv) test medium. These experiments centered on nonisothermal liquid flow and considered sub-boiling and boiling regimes in both unconsolidated and consolidated porous media. A conceptual model was identified based on experimental results in which the thermal regime was characterized as having three distinct periods: (i) an initial heating period in which moisture is transported mostly as vapor, (ii) a transitional period when water moves as both liquid and vapor, and (iii) a cooling period during which water moves mostly as liquid only.

Specific heat and mass transfer mechanisms and phenomena were identified using experimental results. Three different expressions of dryout/condensation proximal to the heat source were observed in the experiments: (i) media with low permeability and a low air-entry value experienced a relatively narrow zone of moisture buildup immediately outside of the dryout zone, (ii) media with a relatively low permeability but with a large air-entry value experienced condensation over a broad area beyond the dryout zone, and (iii) media with a sufficiently high permeability did not experience a complete dryout zone nor an area of condensate buildup, even for heater temperatures as high as 170 °C. Resaturation rates measured in consolidated media during the cooling period were at least 10 times slower than drying rates measured during the heating period. Gas pressure buildup was observed in heated porous media, supporting the premise of the conceptual model that gas advection, and not buoyancy, will be the prominent water transport mechanism in media with sufficiently low permeability and with sufficiently high heat source temperatures.

The V-TOUGH computer code was used to simulate the heating, transitional, and cooling periods for three spatial scales: (i) laboratory (~cm); (ii) field (~m); and (iii) repository (~km). Calculations of the temperature, pressure, and saturation fields were used to evaluate the proposed scaling theories. The model simulations indicated that fluid flow fields near a heat source may be more complex than predicted by the numerical models. The occurrence of and the time at which the peak gas pressure occurred in laboratory-scale experiments were adequately simulated with the numerical model, although the magnitude of the peak gas pressure was not.

Through the application of dimensional analysis, a set of dimensionless parameters was derived to describe the characteristic thermohydrologic behavior for the heating and cooling periods. The dimensionless parameters of key importance are the advection numbers Ad_{gl} , for the gas (g) and liquid (l) phases, and characteristic time scales T_{gl} . The advection number indicates the relative importance of the pressure and buoyancy driving forces. Characteristic time scales provided estimates of the time when gas advection is the dominant water transport mechanism and the time necessary to rewet the region near the heat source for the three spatial scales investigated: laboratory, field and repository.

Results from the dimensional analyses indicated that dimensionless parameters are useful to design field-scale experiments so as to maximize the information gained from the experiment and to predict heat and mass transfer of larger scale porous media systems. Dimensional analysis did not prove to be useful in scaling systems containing discrete features such as faults or fractures. A major conclusion of this report is that conduct of a heater test at field scale is crucial to investigate and understand heat and mass transfer through partially saturated fractured, porous media at a meaningful scale. Continued investigation at the laboratory scale would be fruitful, however, conclusive understanding of heat and mass transfer through partially saturated fractured porous media would not be possible. Therefore, the final recommendation of this report is that the conduct of a field-scale heater test is imperative to understand thermally driven moisture through naturally occurring geologic media.

This report summarizes studies conducted over the past 2 yr and since the issuance of the last progress report on the Thermohydrology Research Project (Green et al., 1993b). The report summarizes the experimental data, theoretical developments, and evaluation of scaling relationships.

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NOMENCLATURE

Ad_g	= gas advection number (-)
Ad_l	= liquid advection number (-)
C_s	= specific heat of solid (J/kg-K)
d	= pore size (m)
D	= binary gas diffusion coefficient (m ² /s)
$\vec{e}_z$	= unit vector in z direction
g	= acceleration of gravity (m/s)
h	= fluid enthalpy per unit mass (J/kg)
h_{lg}	= change in enthalpy for water, from liquid to gas ($h_{lg} = 2,400$ kJ/kg at approximately 40 °C)
I	= gamma ray intensity (counts/s)
k	= permeability (m ²)
$k_{rel,i}$	= relative permeability (-)
K	= hydraulic conductivity (m/s)
L	= characteristic length scale (-)
$\dot{m}_{out}$	= gas flow out of the control volume (kg/m ³ -s)
$\dot{m}_{evap}$	= rate at which liquid water is evaporated per unit volume, negative if vapor is condensed (kg/m ³ -s)
$\dot{m}_v$	= rate of vapor generation of the control volume (kg/m ³ -s)
M	= mass contained in the control volume (kg)
n	= empirically determined parameter (van Genuchten n) (-)
p	= fluid pressure (Pa)
P_c	= suction (capillary pressure) (Pa)
P_v	= partial pressure of the vapor (Pa)
P_{sat}	= thermodynamic saturation pressure of the pure substance (Pa)
P_{lg}	= pressure difference between gas and liquid (Pa)
P_e	= Peclet number, $V_g L/D$, (-)
$\bar{q}_i$	= mass flux of the i th component (kg/m ² -s)
$\bar{q}_v$	= mass diffusion flux of the vapor through the gas mixture (kg/m ² -s)

NOMENCLATURE (Cont'd)

Q	= heat sink/source rate of energy addition per unit volume (W/m^3)
r_o	= reference radius of control volume (m)
R_g	= ideal gas constant for the pure substance (J/kg-K)
S	= saturation (-)
S_{eff}	= effective liquid saturation level, $(S_l - S_r)/(1 - S_r)$ (-)
S_g	= saturation level of gas (-)
S_r	= minimum saturation possible (residual saturation) (-)
S_{vo}	= characteristic vapor saturation (-)
t	= time (s)
T	= temperature (K)
ΔT_o	= temperature change from the reference condition (K)
u	= fluid internal energy per unit mass (J/kg)
$\vec{V}$	= fluid velocity (m/s)
$\vec{V}_g$	= Darcy velocity (advection) of the gas (m/s)
$\bar{V}$	= control volume (m^3)
w_a	= mass fraction of air in the gas mixture (-)
w_v	= mass fraction of water vapor in the gas mixture (-)

NOMENCLATURE (Cont'd)

Greek

- α_s = bulk thermal diffusivity of saturated medium (m^2/s)

$$\alpha_s \equiv \frac{\kappa}{\rho_s C_s}$$
 α = empirically determined parameter (van Genuchten α) (Pa^{-1})
 β_i = thermal expansion coefficient of the i^{th} component (K^{-1})
 κ = thermal conductivity of the gas-liquid-solid combination (w/m-k)
 ρ = fluid density (kg/m^3)
 ρ_g = density of gas (kg/m^3)
 ϕ = porosity (-)
 ρ_w = reference density (kg/m^3)
 ρ_s = density of the solid
 σ = surface tension (n/m)
 τ = tortuosity (-)
 θ = $\Delta T / \Delta T_o$, nondimensional temperature change (-)
 μ = fluid viscosity (Pa-s)
 μ_c = attenuation coefficient of cell (m^{-1})
 μ_m = attenuation coefficient of medium (m^{-1})
 μ_w = attenuation coefficient of water (m^{-1})
 ν = kinematic viscosity (m^2/s)

NOMENCLATURE (Cont'd)

Subscripts

a	= air
c	= cell, capillary
d	= dry or diffusive
e	= equilibrium
evap	= evaporation
F	= fluid
g	= gas
i	= fluid component
l	= liquid
m	= medium
o	= reference state
rel	= relative
s	= solid
v	= vapor
w	= water, wet

Also

^ denotes dimensionless quantity

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QUALITY OF DATA, ANALYSES, AND CODES

DATA: CNWRA-generated data contained in this report meet quality assurance requirements described in the CNWRA Quality Assurance Manual. Sources for other data cited in the report should be consulted for determining the level of quality for those data.

ANALYSES AND CODES: The V-TOUGH code is controlled under the CNWRA Software Configuration Procedure. The RETC code is not currently under software configuration management. Testing is underway to bring RETC into compliance with the software configuration management procedures.

LIST OF ABBREVIATIONS

ABBREVIATION	DESCRIPTION
1D, 2D, 3D	1-Dimensional, 2-Dimensional, 3-Dimensional
ALTS	Apache Leap Test Site
ASTM	American Society for Testing and Materials
CDMs	Compliance Determination Methods
CNWRA	Center for Nuclear Waste Regulatory Analyses
DAS	Data Acquisition System
DOE	U.S. Department of Energy
EBS	Engineered Barrier System
EPA	Environmental Protection Agency
FACs	Favorable Conditions
HLW	High-Level Radioactive Waste
KTUs	Key Technical Uncertainties
LARP	License Application Review Plan
LBT	Large Block Test
NRC	U.S. Nuclear Regulatory Commission
PACs	Potentially Adverse Conditions
SEM	Scanning Electron Microscope
SMU	Southern Methodist University
TSPAs	Total-System Performance Assessments
YM	Yucca Mountain

FOREWORD

This report was prepared by the Center for Nuclear Waste Regulatory Analyses as part of its Thermohydrology Research project managed by the Waste Management Branch in the Office of Nuclear Regulatory Research (Job Control Number B6666). The report describes laboratory-scale simulations of coupled thermal and hydrological interactions that may occur around heat-generating high-level radioactive waste disposed in unsaturated fractured rocks. The experiments are analyzed using a simple mathematical based on similitude considerations and a more detailed mathematical model of coupled thermal and hydrological interactions implemented in a modified version of the computer program TOUGH.

NUREG/CR-6348 is not a substitute for NRC regulations, and compliance is not required. The approaches and/or methods described in this report are provided for information only. Publication of this report does not necessarily constitute NRC approval of or agreement with the information contained herein.

1 INTRODUCTION

1.1 OVERVIEW

It is widely recognized that the decay heat produced by high-level radioactive waste (HLW) will likely have a significant impact on both the pre- and post-closure performance of the proposed repository at Yucca Mountain (YM), in southwest Nevada. The task of delineating which aspects of that impact are favorable to isolation performance and which are adverse is an extremely challenging technical undertaking because of such factors as the hydrothermal regimes involved, heterogeneity of the geologic media, and the time and space scales involved. This difficulty has motivated both the U.S. Department of Energy (DOE) and the U.S. Nuclear Regulatory Commission (NRC) to undertake multi-year thermohydrology research programs to examine the effects of decay heat on pre- and post-closure performance of the repository. Both of these organizations are currently pursuing laboratory and field experiments, as well as numerical modeling studies, to advance the state of knowledge of the thermohydrologic phenomena relevant to the proposed geologic repository.

One of the primary objectives of the DOE repository program (U.S. Department of Energy, 1994) is to develop a thermal loading strategy that makes constructive use (Ramspott, 1991; Nitao et al., 1992; Buscheck and Nitao, 1992, 1993, 1994; Wilder, 1993) of the thermohydrologic conditions to:

- Improve system and subsystem performance
- Protect the waste packages and other repository components from water contact
- Compensate, to the degree possible, for uncertainties in the current and future states of the repository system

Recent numerical modeling studies (Buscheck et al., 1993; Lichtner and Walton, 1994) suggest that the thermal evolution of a geologic HLW repository can be divided into three distinct periods: (i) heating, (ii) transitional, and (iii) cooling. During the heating period, radioactive decay of the waste causes a monotonic rise in temperature that may last several hundreds of years. During this period, the rise in temperature at the heat source vaporizes liquid water, which then moves away from the heat source due to gas-phase pressure gradients. Water movement occurs primarily as water vapor migrating away from the heat source, resulting in the drying of rock near the waste containers. Late in the thermal regime, after temperatures at the heat source have decreased, water transport occurs essentially only in the liquid phase. This is the cooling period in the repository thermal regime. A transitional period occurs between the heating and cooling periods during which water is transported as both vapor and liquid (referred to here as moisture), potentially in opposing directions. The three periods in the thermal evolution of a HLW repository form the basis of the conceptual model proposed in this document. Starting with this concept of the thermal evolution of a HLW repository, thermohydrologic modeling studies by DOE researchers (Buscheck and Nitao, 1992, 1993, 1994; Wilder, 1993) suggest that the proper selection of the thermal loading could potentially extend the time period that the waste packages remain dry. Preliminary findings from such studies have led the DOE to consider an extended-dry concept that could: (i) extend the period of radionuclide containment in the engineered barrier system (EBS), (ii) delay the period of controlled radionuclide release (and transport), and (iii) reduce the sensitivity of total-system performance to hydrologic variability.

The NRC research program is focused on developing an adequate scientific understanding of thermohydrologic phenomena for use in reviewing the DOE repository design and site characterization program as well as in conducting total-system and subsystem performance assessments. In addition, the NRC research activities are placing emphasis on probing potentially adverse conditions (PACs) that may arise as a result of thermohydrologic processes (Green et al., 1994) and associated coupled thermo-hydrologic-mechanical-chemical phenomena (Manteufel et al., 1993). One general concern is related to the possible adverse condition of rapid condensate drainage through fractures, which would result in significant moisture reflux through the repository. A prerequisite to addressing this and other important technical concerns, however, is the need to more fully understand the interrelationships among such processes as water vaporization, liquid and vapor flow, condensation, imbibition of liquid water into the tuff rock matrix, and partially saturated flow in discrete fractures.

The NRC-sponsored Thermohydrology Research Project, which was initiated in mid-1989 at the Center for Nuclear Waste Regulatory Analyses (CNWRA), began with the intent of addressing a broad spectrum of generic thermohydrologic questions. While some of these questions were answered in the conduct of the study, other new and challenging ones were encountered. Initial progress made in addressing those technical questions was documented in an interim progress report (Green et al., 1993d). Subsequent to that report, laboratory-scale experiments were designed to address four fundamental questions regarding thermohydrologic phenomena:

- What are the principal mechanisms controlling the redistribution of moisture?
- Under what hydrothermal conditions and time frames do individual mechanisms predominate?
- What driving mechanism is associated with a particular hydrothermal regime?
- What is the temporal and spatial scale of each hydrothermal regime?

Data from a series of laboratory experiments have been compiled and utilized to test scaling theories derived from similarity analyses. Within certain constraints, the scaling theories provide a vehicle for relating thermohydrologic behavior between laboratory, canister, and repository scale. This report presents the research results and findings obtained since issuance of the first progress report (Green et al., 1993).

1.2 REGULATORY NEED

The thermohydrologic conditions in the repository have implications regarding the two performance objectives in 10 CFR Part 60 for the EBS stated in 10 CFR 60.113(a)(1): (i) containment requirement for the HLW packages, and (ii) radionuclide release rate limit from the EBS. How well the EBS meets the containment time performance objective greatly depends on the hydrothermal conditions because the canister corrosion processes are a direct function of the presence of liquid water. Similarly, meeting the release rate performance objective will depend on the water flow rates past failed waste packages. In addition, thermohydrologic conditions are of key importance in addressing the regulatory uncertainties associated with the performance objective for the geologic barrier. For example, 10 CFR 60.113(a)(2) defines the groundwater travel time as a performance objective for the geologic barrier. Part of this regulation introduces terms such as disturbed zone which may include consideration of thermohydrologic effects.

The DOE currently predicts (Andrews et al., 1994) that the thermohydrologic conditions associated with the extended-dry concept could potentially enhance the compliance margin with the current cumulative radionuclide release requirements set in Table 1-1 of the 1985 version of 40 CFR Part 191. The DOE studies also suggest that a favorable compliance margin may exist even if the Environmental Protection Agency (EPA) standard is amended to include a numerical limit for dose-to-man. Such compliance margins, if achievable, may indeed provide a degree of robustness that reduces the sensitivity of total-system performance to spatial or temporal variations in the subsurface hydrologic conditions.

While a number of aspects of the extended-dry repository thermohydrologic environment appear beneficial to subsystem and total-system performance, detailed theoretical and experimental studies must be performed to ensure that a quantitative understanding of thermohydrologic effects is obtained. Additional justification for studying near-field thermohydrologic phenomena is derived from the fact that the NRC must be sufficiently knowledgeable about the potential impact of the DOE thermal loading strategy to conduct effective prelicensing activities, such as commenting on: (i) the DOE Total-System Performance Assessments (TSPAs) for YM, (ii) repository and EBS designs, and (iii) thermohydrologic field and laboratory experiments.

Another regulatory purpose for the NRC thermohydrology research program is the need to support the ongoing development of the NRC License Application Review Plan (LARP) (U.S. Nuclear Regulatory Commission, 1994). More specifically, Compliance Determination Methods (CDMs) are currently being developed for the LARP that will specify the approach and acceptance criteria that the NRC will use to judge compliance with the performance objectives and other regulatory requirements. Several of these CDMs contain various Key Technical Uncertainties (KTUs) that involve considerations of thermohydrologic conditions. Some of these KTUs, for example, delineate uncertainties associated with:

- Identifying which conceptual models adequately represent isothermal and nonisothermal liquid and vapor phase movement of water through unsaturated fractured rock at YM
- Confirming experimentally the basic physical concept of groundwater flow through unsaturated fractured rock
- Modeling groundwater flow through unsaturated fractured rock using codes that have not been tested against field and laboratory data
- Modeling the formation of perched zones caused by thermally driven flow

In addition, studies of thermohydrologic processes are relevant to CDMs associated with favorable conditions (FACs) and PACs.

1.3 PROJECT SCOPE AND OBJECTIVES

The broad programmatic objective of the Thermohydrology Research Project is to establish an adequate scientific understanding of thermohydrologic phenomena for use in conducting independent reviews of the DOE repository design and site characterization program. A subsidiary objective is to develop the laboratory facilities, experimental methods, measurement techniques, and analytical skills to address thermohydrologic issues that may arise in the repository program. The scope of the research activities can be grouped into three categories: (i) laboratory experiments, (ii) similarity analyses, and

(iii) mathematical modeling. Laboratory experiments have been pursued for the purpose of studying individual thermohydrologic mechanisms and providing data for testing mathematical models. Similarity analyses have been utilized to extend the range of applicability of data by developing scaling relationships. Mathematical modeling of heat transfer and two-phase fluid flow has been used as a tool to analyze and interpret experimental results as well as to evaluate alternate scaling theories.

The laboratory experiments were designed in such a manner that various effects could be studied separately. The scope of these experiments included examination of such factors as transient heating, gas pressure buildup, liquid redistribution, various thermal boundary conditions, heater configurations, and test media with contrasting hydraulic properties. Because of the inherent difficulty of conducting flow experiments under nonisothermal conditions, a number of initial scoping experiments were necessary in order to perfect instrumentation and measurement techniques, properly select and characterize test media, and systematically compile data on moisture and temperature fields. Results from the scoping and preliminary experiments are documented in an earlier report (Green et al., 1993b).

Similarity analyses were developed in this study to characterize the heating and cooling periods. Techniques of similitude theory were applied to the set of governing equations relevant to heat transfer and two-phase flow for the heating and cooling periods. A set of dimensionless parameters was derived that can be used to delineate thermo-fluid regimes in the context of scaling theories. An important technical objective of this work was the formulation of scaling theories that could be used to relate observations of thermohydrologic behavior at the laboratory scale to that of the field scale and, ultimately, to the repository scale.

Mathematical modeling of thermohydrologic phenomena was an integral component in the analysis of experimental results. For the most part, the basic purposes of the mathematical models have been to aid the analysis and interpretation of experimental results, to design various experiments, to test various hypotheses, and to evaluate proposed scaling theories. Simple analytical models, for example, were developed for use in describing gas pressure buildup as a function of temperature. Similarly, detailed simulations of selected laboratory experiments were made using the V-TOUGH code (Pruess, 1987; Nitao, 1990) to interpret the observed patterns of moisture redistribution and temperature variation. In addition, computer simulations were performed to test the scaling relationships developed through similarity analysis.

1.4 REPORT ORGANIZATION

In addition to this introductory chapter, this report covers the following topics:

- Chapter 2, Thermohydrologic Phenomena and Scaling Theory
- Chapter 3, Description of Laboratory Experiments
- Chapter 4, Heat and Mass Transfer Mechanisms Analyses
- Chapter 5, Assessment of Scaling Laws
- Chapter 6, Conclusions and Recommendations

A brief overview is presented in Chapter 2 that covers the relevant conservation principles (and associated mathematical theory) applied to two-phase flow in unsaturated media and the similarity analysis theory developed for thermohydrologic regimes. In Chapter 3, the laboratory experiments designed and used to study the relation between thermohydrologic driving forces and moisture redistribution and gas pressure buildup are described. In Chapter 4, interpretations of the experimental data are presented. In Chapter 5, the proposed scaling laws are assessed. In Chapter 6, the broad conclusions drawn from this research project are listed and explained. Chapter 6 also presents ideas for possible further experimental research.

2 THERMOHYDROLOGIC PHENOMENA AND SCALING THEORY

2.1 MATHEMATICAL THEORY OF TWO-PHASE FLOW

A brief description of the physical mechanisms that control two-phase flow in unsaturated porous media is presented. The mathematical framework used to describe the dynamics of these mechanisms is then developed.

2.1.1 Physical Mechanisms of Two-Phase Flow

Flow of a two-component (water and air), two-phase (liquid and gas) fluid in a partially saturated, fractured, porous medium involves many diverse and coupled physical processes. In some situations, certain mechanisms are controlling, while others are relatively unimportant; in other situations, all the mechanisms may play equally important roles. Thus, in this study, the approach taken was to begin by investigating the individual processes separately and then, after an understanding was obtained, embarking upon investigations of the coupled processes. These experimental and mathematical investigations were guided by idealized conceptual models that were used to develop similitude requirements in the form of dimensionless parameters. The dimensionless parameters also provided insight into the relative importance of various physical mechanisms to the experimental and numerical cases of interest and permitted laboratory- and field-scale test results to be interpreted in terms of the anticipated responses of the HLW repository. As an introduction to two-phase phenomena, the theory of single-phase flow in saturated media is first briefly reviewed.

2.1.1.1 Flow in Saturated Media

Fluid flow in a fully saturated porous medium is one-component and single-phase (liquid or gas). Mathematical models of such flows are based on well understood and plausible physical mechanisms. The fluid is conceptualized to be transported through a multitude of interconnected capillary-like channels of varying length and diameter, under the combined action of pressure difference, laminar viscous stresses, and gravity (Batchelor, 1967; Bear, 1972; Freeze and Cherry, 1979; Domenico and Schwartz, 1990). Instead of attempting to describe the geometry of the flow channels in detail, the mathematical theory of porous flow characterizes the medium as a continuum with certain parameters such as porosity ϕ and saturated permeability k . The porosity is defined as the percentage of void space in the solid matrix per unit volume. The permeability incorporates other geometric details (such as pore diameter, channel length and connectivity, etc.) of the medium; it can best be understood by its use in the relation between the flow and the net driving force:

$$\vec{V} = -\frac{k}{\mu}(\nabla p + \rho g \vec{e}_z) \quad (2-1)$$

where the symbols are defined as:

$\vec{V}$ = fluid velocity (m/s)

p = fluid pressure (Pa)

- k = permeability (m^2)
- μ = fluid viscosity (Pa-s)
- ρ = fluid density (kg/m^3)
- g = acceleration of gravity (m/s^2)
- z = vertical coordinate, positive upward (m)
- $\bar{e}_z$ = unit vector in z direction

Equation (2-1) is Darcy's law and $\bar{V}$ is the Darcy velocity, defined as the fluid volumetric flow rate divided by the total cross-sectional area. Darcy's law is theoretically exact for creeping flows in which fluid inertia is small, and it can be derived from the general Navier-Stokes equations for simple geometries such as bundles of capillaries or spheres. In general, the permeability must be inferred from measurements of flow and pressure drop for a given porous medium. If the medium contains fractures, the inferred k is a volume-average, and probably does not represent the permeability of either the porous matrix or the fractures separately.

It should be noted that solutes and marker particles in the fluid are not transported at the Darcy velocity, but at a velocity equal to the larger velocity of the fluid in the flow channels. For steady-state conditions, the mass flux of solute or marker particles past a given location is, however, the same when computed by either the Darcy or the interstitial velocity. This is also approximately true for the slowly time-varying flows of interest here. The time of first arrival of the solute or particles at a specific location does depend on the interstitial velocity.

When a saturated porous medium is heated to temperatures below the boiling point of the liquid, buoyancy forces can induce a natural convection motion. The mathematical description of such a flow is complicated in detail, but experiments show that the flow is similar to that of liquid confined in a volume of the same shape that contains no porous material (Kulacki and Emara, 1975; Wooding, 1956). For example, Figure 2-1 shows the predicted flow streamlines in a two dimensional (2D), saturated, permeable area bounded by relatively impermeable zones, which simulates a geothermal reservoir at Wairakei, New Zealand (Wooding, 1956). This is the same kind of general recirculation pattern that would occur for a heated body of fluid in a cavity. Small-scale experiments can thus be interpreted in terms of large-scale responses through the relevant Rayleigh, Prandtl, and Reynolds dimensionless numbers (Keyhani et al., 1981).

2.1.1.2 Flow in Partially Saturated Media

A partially saturated porous medium contains two or more fluid components or phases. Compared to the case of a saturated medium, the flow of several components or phases presents a difficult challenge to model (Narasimhan, 1982; Wang and Narasimhan, 1986; Rasmussen and Evans, 1989). The flow is strongly influenced by surface forces at the interfaces between the liquid and gas phases. In addition, the phases may not be distributed as continuous bodies throughout the medium. If one of the phases is distributed as a series of isolated pockets, that phase is essentially immobile (although the discontinuities can be cleared by a high-velocity flow of the continuous phase). If both phases are mobile, they must be connected throughout the medium in a complicated three-dimensional (3D) pattern. Figure 2-2, which is a schematic illustration of a 2D slice through a 3D unsaturated medium, shows the need for these 3D connections (i.e., above or below the section shown) in order to make the various liquid regions (or gas regions) into a continuous body. Therefore, the flow of each phase is inherently 3D. The

Figure 2-1. Buoyancy-induced flow streamlines in a heated, saturated porous medium (Wooding, 1956)

Figure 2-2. Cross-section through a partially saturated porous medium showing continuous and discontinuous bodies of liquid and gas

modeling difficulties are accentuated for a fractured medium such as the host rock of the YM repository because the widely different permeability of the matrix and the fractures sometimes, but not always, segregates the flow of the two components—liquid through the matrix and gas through the fractures. Some of the important effects of two-component, two-phase flow in a porous medium are discussed in the following subsection.

Liquid Suction Pressure. When the liquid saturation is small, liquid in the form of thin layers adheres to the solid surfaces of the medium by molecular forces. The effective capillary or suction pressure of these layers may be 10^5 kPa or greater for sufficiently tight, low-permeability matrices, even for saturations of 50 percent or more. Figure 2-3 shows, for example, the variation of capillary pressure with liquid saturation for one of the media used in the laboratory experiments described in Section 4. These large negative pressures are not caused by the familiar kind of surface tension forces, since the required capillary diameter would be only of molecular (or smaller) dimensions. Consequently, conceptual modeling is made even more difficult by the lack of an easily measured physical property that characterizes such large suction pressures.

Relative Permeability. In an unsaturated porous medium, the resistance to flow of a fluid component i is greater than the resistance for the same fluid in a saturated medium. This increase is a consequence of the fact that the flow channels are only partially full and thus have a larger wetted area per unit cross-sectional area and a greater viscous friction than full channels. The decreased permeability for a fluid component i in an unsaturated medium is specified by the relative permeability, $k_{rel,i}$, cited as a fraction of the (saturated) permeability. Relative permeability, like suction pressure, is a function of saturation. For media with a pore-size distribution comparable to tuffaceous rock, $k_{rel,i}$ decreases by many powers of ten when the saturation decreases only slightly. Figure 2-3, which shows the relative permeability for the media used in some CNWRA laboratory experiments, demonstrates this observation.

As a result of the dependence of permeability on saturation, flow in an unsaturated medium can exhibit various kinds of instabilities. For example, when water infiltrates at a boundary, the flow rate at a point depends on the saturation level at that point (because of the relative permeability), which in turn depends on the amount of water that has already infiltrated to that location. Thus, locations that receive slightly more than the average infiltration are more open to the flow and receive even more infiltration than other locations. Consequently, preferential flow, called fingering, can occur (Miller and Gardner, 1962; Glass et al., 1989a,b). It is also common that a flow distribution, for the same saturation level, is different when the saturation is increasing from when it is decreasing. This difference indicates that relative permeability can also exhibit a hysteresis effect.

Fracture-Matrix Interaction. For fractured media, the effects of saturation on suction pressures and relative permeability can dominate the flow and liquid distribution. Because the effective pore size of a fracture is much larger than that of the matrix, the suction pressures in the matrix are much greater than in the fractures. The matrix will tend to imbibe any mobile liquid out of the fractures (unless the matrix is nearly 100 percent saturated), and thus fractures remain dry. However, this liquid extraction takes time, thus liquid can flow in the fractures during transient events. In addition, mineral coatings on fracture surfaces can limit the imbibition into the matrix. Similarly, the relative permeability of the fractures for gas flow is much larger than that of the matrix. This phenomenon tends to make the gas flow preferentially through the fractures rather than through the matrix.

Figure 2-3. Variation of liquid suction pressure and relative permeability with liquid saturation level for the Apache Leap Test Site tuff used in laboratory cylinder experiment Test 11

Taken together, the large suction pressures in the matrix and the high gas relative permeability of the fractures can lead to a heat pipe effect when the fluid in a fractured, porous medium is heated locally to near the boiling point of the liquid. As sketched in Figure 2-4, vapor flows away from the heated region through the fractures, condenses in cooler regions, and flows back to the heated region through the matrix (Pruess, 1985; Lichtner and Walton, 1994). These kinds of heat pipes are capable of transporting large amounts of thermal energy away from the heat source and of maintaining, under some conditions, a relatively large volume of material near the heated region at a nearly constant temperature for extended periods of time.

Water Chemistry. When liquid water and vapor are both present in the pores of an unsaturated medium, water chemistry (e.g., solutes) will affect many heat and mass transfer processes. The study reported here did not investigate these mechanisms and, unless stated otherwise, they are assumed to be negligible.

Figure 2-4. Schematic diagram of heat and mass transfer in a porous-medium heat pipe

2.1.2 Conservation and Constitutive Equations for Flow

With the concepts just described, the mathematical model of heat and mass transport in an unsaturated, heated porous medium can be summarized as follows.

2.1.2.1 Mass Conservation for Liquid and Gas Components

As an example of the relevant conservation of mass requirements, the differential equation that describes the conservation of the vapor phase of the liquid component is presented. The mass of vapor contained in a small differential volume can change because of: (i) phase changes (evaporation, condensation), (ii) transport due to pressure and buoyancy gradients (Darcy's law), and (iii) diffusion caused by mass concentration gradients. This change in vapor mass is expressed mathematically as:

$$\frac{\partial}{\partial t} (\phi \rho_g S_g w_v) = - \nabla \cdot (w_v \bar{V}_g) - \nabla \cdot \bar{q}_v + \dot{m}_{\text{evap}} \quad (2-2)$$

where in addition to the parameters already defined, the new symbols are:

ϕ	=	porosity (-)
ρ_g	=	density of gas (kg/m ³)
S_g	=	saturation level of gas (-)
w_v	=	mass fraction of water vapor in the gas mixture (-)
$\vec{V}_g$	=	Darcy velocity (advection) of the gas (m/s)
$\vec{q}_v$	=	mass diffusion flux of the vapor through the gas mixture (kg/m ² -s)
$\dot{m}_{\text{evap}}$	=	rate at which liquid water is evaporated per unit volume, negative if vapor is condensed (kg/m ³ -s)
t	=	time (s)

The small effects due to diffusion of the gas through the liquid phase are neglected in this equation. The conservation of mass relations for the other components are similar in form to Eq. (2-2).

There are several equivalent ways of expressing Eq. (2-2) that involve other choices for the controlling variables. Furthermore, by combining Eq. (2-2) with the similar one for the liquid component, the mass transfer between the liquid and vapor phases (i.e., $\dot{m}_{\text{evap}}$) can be eliminated.

Inter-Phase Mass Transfer Rates. In general, an empirical transfer model is needed to evaluate the rate, $\dot{m}_{\text{evap}}$, at which liquid and vapor are transferred between the phases. For porous media flow, however, the need for this model is eliminated by assuming that the partial pressure of the vapor in the air-vapor mixture is equal to the saturation pressure; hence, the relative humidity of the gas is always 100 percent. This assumption, which is equivalent to an infinitely large mass transfer coefficient, is reasonable (even when non-condensibles are present or phenomena are resolved over short distances) because (i) the rates of change in porous media flow are slow compared to the mass transfer rate, and (ii) the liquid and gas phases always remain in intimate contact. There are cases of large suction pressures, as described in the following, when the assumption of 100-percent relative humidity must be modified. Even for these cases, the partial pressure of the vapor can be specified so a mass transfer model is not needed.

2.1.2.2 Energy Conservation

The media of interest are locally heated by a thermal energy source. The transport of thermal energy affects the flow of fluid through the media and, conversely, the fluid flow may affect the energy flow. These interactions are expressed mathematically as:

$$\frac{\partial}{\partial t} [\phi (\rho_l S_l u_l + \rho_g S_g u_g) + (1-\phi) \rho_s u_s] = - \nabla \cdot (\rho_l h_l \vec{V}_l + \rho_g h_g \vec{V}_g) - \nabla \cdot \kappa \nabla T + Q \quad (2-3)$$

in which the subscripts l , g , and s represent the liquid, gas, and solid matrix respectively. The new symbols are defined as:

- u = fluid internal energy per unit mass (J/kg)
- h = fluid enthalpy per unit mass (J/kg)
- κ = thermal conductivity of the gas-liquid-solid combination (W/m-K)
- T = temperature (K)
- Q = heat sink/source rate of energy addition per unit volume (W/m³)

An order-of-magnitude analysis of the terms in Eq. (2-3) shows that the temperature distribution is determined almost entirely by thermal conduction for media with small porosity, even when there is significant vaporization or condensation of water (Green, et al., 1993b). Thus, the terms involving liquid and vapor in Eq. (2-3) can usually be neglected in computations.

Equation (2-3) must be supplemented by constitutive relations that describe how to evaluate, for example, u or κ as a function of temperature and pressure of the pure components. These relations are described later. Note that in Eq. (2-3), the liquid, gas, and solid components are assumed to have the same temperature, which is justified by the slow rate of change of the system compared to the respective thermal diffusivities for the processes of interest.

2.1.2.3 Constitutive Relations

Three kinds of constitutive relations are needed to evaluate the terms in the differential equations listed above: (i) flux laws (actually, conservation of momentum relations specialized for specific kinds of transport), (ii) material relations, and (iii) basic definitions or closure relations.

Flux Laws. The mass transport of fluid component i by advection is given by Darcy's law:

$$\vec{V}_i = - \frac{k k_{rel,i}}{\mu_i} (\nabla p_i + \rho_i g \vec{e}_z) \quad (2-4)$$

where

$k_{rel,i}$ = is relative permeability (-)

The porous media considered in this study are heated locally, and thus the fluid flows are nonisothermal. Consequently, the change of fluid properties, such as viscosity in Eq. (2-4), with temperature can influence the flow. These changes are generally neglected for simplicity, and when numerical computations are made, the fluid properties are evaluated at an appropriate average temperature. The main exception to this neglect of temperature-dependent fluid properties is the change in fluid density, because, as is well known, it can produce a buoyancy-driven natural-convection flow. To account for these buoyancy effects in Eq. (2-4), the Boussinesq assumption is used to express the density in terms of a reference density and the temperature change from the reference condition, and the gravitational contribution to the pressure gradient is combined with the gravitational body force at the reference condition. The result is:

$$\vec{V}_i = - \frac{k k_{rel,i}}{\mu_i} (\nabla \tilde{p}_i - \rho_{io} \beta_i \Delta T g \vec{e}_z) \quad (2-5)$$

where the pressure $\tilde{p}_i$ is now the nonhydrostatic or dynamic component only and

$$\begin{aligned} \rho_{io} &= \text{reference density (kg/m}^3\text{)} \\ \beta_i &= \text{thermal expansion coefficient of the } i^{\text{th}} \text{ component (K}^{-1}\text{)} \\ \Delta T_0 &= \text{temperature change from the reference condition (K)} \end{aligned}$$

Equations (2-4) and (2-5) neglect interfacial drag between the fluid phases. This assumption is justified for flow in porous media because of the much larger drag, or viscous friction, between the fluid phases and the solid matrix modeled by Darcy's law.

The mass flux in the gas phase due to diffusion is given in terms of the gradient of the relevant mass fraction w_i by Fick's law (Lichtner and Walton, 1994):

$$\vec{q}_i = - \tau \phi S_i \rho_i D \nabla w_i \quad (2-6)$$

where the new symbols are defined as

$$\begin{aligned} \vec{q}_i &= \text{mass flux of the } i^{\text{th}} \text{ component (Kg/m}^2\text{-s)} \\ \tau &= \text{tortuosity or flow path length relative to a straight line (-)} \\ D &= \text{binary gas diffusion coefficient (m}^2\text{/s)} \end{aligned}$$

Fick's law is valid when the pore size is larger than the mean free path of the gas molecules (e.g., when the partial pressure of the fluid is not small).

Material relations. The thermal properties of the liquid and solid are reasonably assumed to depend only on temperature; the relations are not presented here, since they can be obtained easily from standard references (Hirschfelder et al., 1954; van Wylen and Sonntag, 1968). Similarly, the densities of the gas-phase components are assumed to be given adequately by the ideal gas laws in terms of their mixture partial pressures. Other physical properties, such as viscosity of the pure gas-phase components, can be a function of pressure and temperature, but these relations can also be obtained from standard references. The mixture of air and water vapor is also assumed to respond as an ideal gas composed of nonreacting pure components.

The internal energy and enthalpy of the liquid and air are assumed to be linear functions of temperature over the range of interest, with the proportionality constant being the specific heats at constant volume, c_v , and constant pressure, c_p ; the error induced by this assumption over a temperature range from 20 to 250 °C is less than ± 1 percent for saturated water and ± 1.5 percent for air. The internal energy and enthalpy of the water vapor differ from the internal energy and enthalpy of the liquid water by the respective latent heats of vaporization, u_{ig} and h_{ig} .

When the liquid suction pressure is large, the partial pressure of vapor in equilibrium with the liquid is reduced, in comparison to the thermodynamic saturation pressure for the liquid temperature, because of the need to maintain equality of the chemical potential for both fluid phases. This reduction is known as the Poynting effect (Hatsopoulos and Keenan, 1965), and is given by Kelvins' equation:

$$p_v = p_{sat} \exp\left(\frac{-p_c}{\rho_l R_v T}\right) \quad (2-7)$$

The new symbols are defined as:

p_v	=	partial pressure of the vapor (Pa)
p_{sat}	=	thermodynamic saturation pressure of the pure substance (Pa)
p_c	=	suction (capillary pressure), a positive value (Pa)
R_v	=	ideal gas constant for the pure substance (J/kg-K)

One important consequence of the vapor pressure lowering given by Eq. (2-7) is that a gas mixture in regions where the suction pressure is large will have a relative humidity of less than 100 percent, since the relative humidity is equal to the ratio p_v/p_{sat} , and this ratio is less than one. Stated another way, the mixture, if put in contact with liquid that did not have a large capillary pressure, could take up more vapor from the liquid before becoming saturated.

The thermal conductivity, κ , of the mixture of solid, liquid, and gas is a function of the saturation levels. There are several models in use to predict the thermal conductivity. A common model is (Somerton et al., 1973, 1974):

$$\kappa(S_l) = \kappa_d + \sqrt{S_l} (\kappa_w - \kappa_d) \quad (2-8)$$

where the subscripts d and w denote dry and wet, respectively. The utility of this relationship is evaluated during the characterization of test media (Section 3.4.3.4).

Models are also needed to predict the way capillary suction pressure and relative permeability vary as the saturation level changes. Again, a number of models are in use, but here the van Genuchten-Mualem soil property model (Mualem, 1976; van Genuchten, 1978) is adopted. This model relates the relative permeability of the liquid to the liquid saturation by:

$$k_{rel,l} = (S_{eff})^{\frac{1}{2}} \left[1 - \left(1 - S_{eff}^{\frac{-n}{1-n}} \right)^{\frac{n-1}{n}} \right]^2 \quad (2-9)$$

where

n	=	empirically determined parameter (-)
S_{eff}	=	effective liquid saturation level, $(S_l - S_r)/(1 - S_r)$ (-)
S_r	=	minimum saturation possible (residual saturation) (-)

The residual saturation is very small for most media. Therefore, unless it is stated otherwise, S_r is assumed to be zero here. For this condition, S_{eff} is the same as S_l . Typically, Eq. (2-9) predicts that $k_{\text{rel},l} < 1$ for any liquid saturation even slightly less than one. Equation (2-9) was used to compute the results shown in Figure 2-3.

There is no widely accepted comparable relation for the relative permeability of the gas phase. Here, it is assumed that:

$$k_{\text{rel},g} = 1 - k_{\text{rel},l} \quad (2-10)$$

Although Eq. (2-10) is in common use (Pruess, 1987; Nitao, 1990), its physical validity is questionable. Other relations have also been used (Rasmussen et al., 1993), but it is not evident that they are any more physically realistic. The main consequence of Eq. (2-10) for a specific medium is that $k_{\text{rel},g}$ is approximately one for any liquid saturation even slightly less than one.

The van Genuchten model is also used to relate the capillary pressure to liquid saturation:

$$p_c = \alpha^{-1} \left(S_{\text{eff}}^{-\frac{n}{n-1}} - 1 \right)^{\frac{1}{n}} \quad (2-11)$$

where α is an empirically determined constant (Pa^{-1}). Typically, $\alpha < 1$ and n is about 1.5 to 5 for most of the media of interest here, so Eq. (2-11) predicts that the capillary pressure will increase substantially as the liquid saturation decreases. Equation (2-11) was used for the computations of capillary pressure shown in Figure 2-3. Equations (2-9) and (2-11) were used in the numerical simulations described later in this report.

Basic definitions. The closure relations can be stated in simple terms. The capillary pressure is the difference between the gas and the liquid pressure:

$$p_c = p_g - p_l \quad (2-12)$$

The total gas pressure is the sum of the partial pressures of the vapor and the air:

$$p_g = p_v + p_a \quad (2-13)$$

The sum of the liquid and gas saturations is always unity:

$$S_l + S_g = 1 \quad (2-14)$$

and the sum of the mass fractions of the gas components in the gas mixture is also always unity:

$$w_v + w_a = 1 \quad (2-15)$$

2.1.2.4 Initial and Boundary Conditions

The response of a partially fractured porous medium to local heating can be dominated at early time by the initial conditions (saturation distribution, for example) existing at the start of heating, and at late time by conditions imposed at the boundaries (zero heat flux, for example) of the region of interest. For those reasons, the initial and boundary conditions imposed on theoretical and laboratory investigations must be chosen with the goal either of simulating the conditions in the YM repository or of eliminating the influence of the initial and boundary conditions on the investigated responses.

In the absence of detailed knowledge of the repository, reasonable assumptions for the initial state for these investigations are (i) isothermal conditions, and (ii) saturation distribution as a function of elevation equal to the equilibrium gravitational distribution. Alternatively, a linear temperature profile can be estimated using the geothermal gradient, whereas the initial saturation can be determined by solving the steady-flow equation.

Reasonable assumptions for boundary conditions depend on the problem to be investigated. Constant temperature (i.e., a heat sink or source) and constant saturation conditions (liquid sink or source) may be appropriate for some of the boundaries; for example, to simulate the water table below the heat sources in the repository. Other boundaries may be appropriately assumed to have zero heat flux (insulated) or zero fluid-flow conditions. In any case, it is important that either the boundary conditions used in laboratory and theoretical investigations simulate the physical situation of interest, or that the boundaries be so far removed from that region that conditions at the boundaries do not affect the region over the time scale of interest.

2.1.2.5 Closure

Equations (2-1) through (2-15) complete the basic mathematical description of two-component, two-phase flow in a fractured, locally heated porous medium. These equations must be supplemented by other assumptions or models in particular cases. For example, a model is needed to determine an average permeability for a volume of solid that contains fractures when only the permeability of the fractures and the porous matrix are known individually. In addition, some of the terms in the equations may be negligible for certain cases; these cases can be determined by a dimensional or similarity analysis of the terms or effects in conjunction with idealized conceptual models that highlight the effects. The following sections describe these kinds of similarity analyses.

2.2 SIMILARITY ANALYSIS OF THERMOHYDROLOGIC PERIODS

Scaling theories can be developed using the techniques of either dimensional analysis or similitude. Dimensional analysis is defined here as the procedure by which the variables are grouped together to form dimensionless terms by dimensional considerations alone. An implicit knowledge of all pertinent variables and parameters is required in dimensional analysis (Buckingham, 1914; Fox and McDonald, 1978; Corey, 1986). Similitude theory, conversely, is the procedure in which dimensionless parameters are developed by starting with the relevant mathematical equations and transforming these equations into dimensionless form. All aspects of the actual physical system and all the macroscopic phenomena need to be expressed in terms of the mathematical equations for similitude analysis to be used (Bear, 1972; Baker et al., 1973; Fox and McDonald, 1978; Miller, 1980; Corey, 1986). The scaling analyses described in the following sections were developed by similitude theory.

2.2.1 General Application of Similarity Analysis

A laboratory experiment conducted with a physical scale model of a larger system will simulate or represent the response of a larger system if the scale model is geometrically, kinematically, dynamically, and constitutively similar to the large system. The definitions of these types of similarity are (Baker et al., 1973):

- (i) Geometric Similarity—The model has the same shape and proportions as the large system for those parts of the system in which geometry affects the responses
- (ii) Kinematic Similarity—The velocity at each point in the model has the same direction as that in the large system, and the magnitude of the model velocities is a constant multiple of the larger system velocities
- (iii) Dynamic Similarity—The forces, torques, and accelerations at each point in the model have the same direction as those in the large system, and their magnitudes are a constant multiple of those in the large system
- (iv) Constitutive Similarity—The constitutive properties of the model materials (e.g., the relation between relative permeability and saturation) have the same functional relationship as the large system materials

When the conditions for all four similarities are fulfilled, the response of the model is identical to that of the large system, at homologous locations and homologous times. Similarity does not apply only to linear systems; nonlinear phenomena can also be duplicated.

All four kinds of similarity will be satisfied when a physical scale model and a larger system have the same numerical values for all the dimensionless groups resulting from the similarity analysis. In addition, the dimensionless groups can be used to define scaling factors, or ratios of similar effects of phenomena, such as a time scale factor defined as the time duration for an event to occur in the model to the time duration of the same event in the larger system. Various kinds of implementation difficulties generally become evident when the dimensionless groups for the model and large system are mathematically equated and the consequences of the equality examined. In some cases, two different scale factors are required for the same parameter. In other cases, a physical property must take on a value that is not realizable; for example, the surface tension of the model liquid must be larger than that of any known liquid, or the geometric size of some feature must be smaller than is practical or can be fabricated. However, even when not all the dimensionless groups for the model can be made equal to those of the larger system, the model can still be used to investigate some limited part of the general response of the larger system, but conceptual and mathematical models are then needed to help interpret the model responses.

The laboratory models used in this study to investigate moisture transport could only obtain partial equality with all the relevant dimensionless groups of the repository, because of the required small geometric scale factor (about 1 to 1,000) and the multiplicity of phenomena. In particular, it was impractical to construct laboratory models that would represent in a realistic way the interaction between a matrix and a system of fractures. This difficulty is also true for numerical models. To compensate for the laboratory model limitations, idealized mathematical models of several types of responses were

developed to aid in interpreting the model results. These conceptual models included the three different response periods discussed earlier.

- Heating period—A model was developed to determine the heating conditions for which large pressure gradients and velocities in the gas phase would be created (and the time duration for which such responses can be sustained)
- Cooling period—A model was developed to determine the re-wetting rate of a dried-out region after the heat load has decreased, and the time duration required for substantially complete re-wetting
- Transition period—The cooling period model was sufficiently general to include the transition between the heating and cooling periods, although this period was not investigated explicitly

In addition, an idealized model was developed to investigate large-scale, buoyancy-induced recirculation flows for low heat loads. This mathematical model was not, however, evaluated using a laboratory physical model.

2.2.2 Conceptual Model for the Heating Period

During the heating period, the rate at which heat is released has a dominant influence on thermohydrologic responses. Large heating rates can lead to a so-called hot or extended-dry repository, while smaller heating rates lead to a cool or moist repository. The DOE G-Tunnel heater tests (Zimmerman et al., 1986; Ramirez et al., 1991) and numerical simulations and laboratory tests conducted at the CNWRA indicate that one of the distinguishing features of the heating regime is whether large pressure gradients develop in the gas phase. If they do, the repository will tend to become the dry type, because the large gas flow produced by the pressure gradients transports significant amounts of water, in the form of vapor, away from the heated region. Since the source of this water is the liquid water initially in the porous matrix, the repository tends to dry out. Consequently, the focus of the conceptual model developed for the heating regime is the occurrence of significant gas-phase pressure gradients.

The conceptual model for the heating phase is a generalization of the similar case in which buoyancy is the only important force driving the flow. For that case, the gas-phase pressure gradients are of the same magnitude as buoyancy body forces, and an overall circulation of fluid is produced. For this kind of circulatory flow pattern, Darcy's law can be expressed in the following dimensionless form (Green et al., 1993b):

$$\hat{V}_g = -\hat{\nabla} \hat{p}_g + \theta \vec{e}_z \quad (2-16)$$

where the caret (^) indicates a dimensionless quantity, $\theta = \Delta T / \Delta T_0$ is the dimensionless temperature change, and ΔT_0 is a maximum or characteristic temperature increase of the heated region. The nonhydrostatic gas pressure has been made dimensionless by normalizing the pressure with respect to a characteristic nonhydrostatic pressure magnitude:

$$p \sim \rho_{go} g L \beta_g \Delta T_o \quad (2-17)$$

in which ρ_{go} is the characteristic, or representative, gas density of the flow, and L is the characteristic length scale of the flow.

Similarly, the gas flow velocity can be made dimensionless using the characteristic, representative velocity of the flow:

$$V_g \sim \frac{k k_{rel,g}}{\mu_g} (\rho_{go} g \beta_g \Delta T_o) \quad (2-18)$$

where the gas phase has been assumed to be continuous. All the dimensional quantities in Eq. (2-16) have a numerical range from zero to about one, that is, they are of order unity. The magnitude of the characteristic nonhydrostatic pressure and velocity, Eqs. (2-17) and (2-18), depends on the magnitude of the heating through the characteristic temperature increase ΔT_o . However, because of the small numerical value of β_g , the characteristic nonhydrostatic pressure is much less than the characteristic hydrostatic pressure, $\rho_{go} g L$. Hence, the buoyancy-induced circulation in a heated porous medium has a relatively small velocity. An application of this conceptual mathematical model for low heating rates is discussed in Section 2.2.5.

Pressure and velocity scale factors, which are needed to interpret or scale-up measurements made on a scale model to a larger system, can be derived from Eqs. (2-17) and (2-18). For example, the pressure scale factor is the ratio of the characteristic pressure of the model system to that of the larger system; as can be seen from Eq. (2-17), this scale factor will involve the ratio of characteristic lengths (i.e., the geometric scale factor) as well as the ratio of characteristic temperature increases and other parameters. The time scale factor of the flow can be computed as the ratio of the length scale factor to the velocity scale factor. For this case, the velocity is caused by the interaction of two generalized forces, namely buoyancy and viscous effects, and so only one characteristic velocity and one velocity scale factor can be defined. But when there are more than two generalized forces driving the flow, more than one velocity scale can be defined. For such cases, all the velocity scales must be made equal by imposing restrictions on the physical scale model, such as using a more viscous fluid in the model than in the larger system or imposing a larger temperature increase.

To determine when large pressure gradients occur in a heated porous medium, characteristic pressure, velocity, and time scales of a more general form than Eqs. (2-17) and (2-18) are needed. Just as for the buoyancy flow described above, the analysis starts from Darcy's law.

2.2.2.1 Control Volume Analysis of a Heated Partially Saturated Region

An imaginary control volume encompassing the region of high gas pressures, as shown in Figure 2-5, is used to develop the conceptual model. For this conceptual model, a 2D geometry (i.e., a line heat source) is considered but the same analysis would hold for area heaters and 3D geometries, except for some numerical factors of order unity. The spatial extent of the control volume is somewhat indeterminate, so it will be specified by a characteristic length, L , that can be the same as the control volume radius r_o .

Boundary of 2D
Control Volume

Figure 2-5. Sketch of control volume used for the conceptual model of pressure-driven gas flow during the heating phase

Gas Flow at the Control Volume Boundary. Considering first only the advective component of the gas flow out of the control volume driven by the pressure gradient, Darcy's law can be expressed as:

$$\dot{m}_{out} = -(2\pi r_o) \frac{k k_{rel,g}}{\mu_g} \left(\rho_g \frac{dp_g}{dr} \right)_{r_o} \quad (2-19)$$

where the pressure gradient is evaluated near the boundary of the control volume.

Ideal Gas Law in the Control Volume. The gas flow crossing the control volume boundary can be related to the change in mass of gas M_g contained in the control volume by the ideal gas law. By taking the derivative of the ideal gas law with respect to time, it is found that:

$$\bar{V}_g \left(\frac{dp_g}{dt} \right) + p_g \left(\frac{d\bar{V}_g}{dt} \right) = M_g R_g \frac{dT}{dt} + R_g T \frac{dM_g}{dt} \quad (2-20)$$

where $\bar{V}_g = \phi S_g \bar{V}$ is the volume of that part of the total control volume $\bar{V}$ containing gas, and p_g and T are characteristic or lumped averages of the control volume pressure and temperature. The pressure derivative on the left-hand side of Eq. (2-20) is much larger than the volume derivative (for cases when significant pressures are created) because the volume of gas within the control volume can change only when the gas saturation changes. Thus, in this idealized conceptual model, the volume derivative is neglected.

Conservation of Mass. The rate at which the mass of gas, M_g , in the control volume changes is also related to the rate of vapor generation, $\dot{m}_v$, and the gas outflow rate, $\dot{m}_{out}$:

$$\frac{dM_g}{dt} = \dot{m}_v - \dot{m}_{out} \quad (2-21)$$

Equations (2-20) and (2-21) are combined to give:

$$\dot{m}_{out} = \dot{m}_v + \frac{M_g}{T} \frac{dT}{dt} - \frac{M_g}{p_g} \frac{dp_g}{dt} \quad (2-22)$$

Vapor Generation Rate. The rate at which vapor is generated inside the control volume is computed by assuming, as discussed previously, that the relative humidity remains at 100 percent. Vapor pressure lowering may cause the relative humidity to be somewhat less than 100 percent, but this effect is neglected in the heating regime analysis (although not in the cooling regime analysis). Thus, from the ideal gas law for the vapor, it is found that:

$$\dot{m}_v = \frac{\bar{V}_v}{R_v T} \frac{dp_v}{dt} - \frac{M_v}{T} \frac{dT}{dt} \quad (2-23)$$

where M_v is the mass of vapor in the control volume and $\bar{V}_v$ is its partial volume. Since, for 100-percent relative humidity, the vapor pressure is the saturation pressure, p_v can be related to other thermodynamic variables by the Clapeyron equation. Thus, Eq. (2-23) can also be rewritten in the form:

$$\dot{m}_v = \frac{\bar{V}_v}{R_v T} \left(\frac{\rho_v h_{lg}}{T} \right) \frac{dT}{dt} - \frac{M_v}{T} \frac{dT}{dt} \quad (2-24)$$

Mass Flow Rate at Control Volume Boundary. Equations (2-22) and (2-24) are now combined to give an expression for the mass flow rate at the control volume boundary. This expression is:

$$\dot{m}_{\text{out}} = \frac{M_v}{T} \left(\frac{h_{lg}}{R_v T} \right) \frac{dT}{dt} + \left(\frac{M_g - M_v}{T} \right) \frac{dT}{dt} - \frac{M_g}{p_g} \frac{dp_g}{dt} \quad (2-25)$$

The factor $M_g - M_v$ is the mass of air M_{air} in the control volume. Now M_g , M_v , and M_{air} are of the same order of magnitude, as are the quantities $(dT/dt)/T$ and $(dp_g/dt)/p_g$. However, the quantity $h_{lg}/R_v T$ has a numerical magnitude of about 20. Thus, to a good approximation, Eq. (2-25) can be replaced by:

$$\dot{m}_{\text{out}} \approx \frac{M_v}{T} \left(\frac{h_{lg}}{R_v T} \right) \frac{dT}{dt} \quad (2-26)$$

This relation simply expresses the conclusion that most of the gas flow out of the control volume is composed of the vapor created by heating the initial mass of liquid in the matrix.

Characteristic Pressure Gradient. Equation (2-26) is substituted into Darcy's law, Eq. (2-19), to yield an expression for the nonhydrostatic pressure gradient at the control volume boundary:

$$\left(\rho_g \frac{dp_g}{dr} \right)_{r_o} = - \frac{\mu_g M_v}{2 \pi r_o k k_{\text{rel},g} T} \left(\frac{h_{lg}}{R_v T} \right) \frac{dT}{dt} = - \frac{\phi S_v \mu_g \rho_v r_o}{2 k k_{\text{rel},g} T} \left(\frac{h_{lg}}{R_v T} \right) \frac{dT}{dt} \quad (2-27)$$

where S_v is vapor saturation. This expression can be used to define a characteristic pressure gradient in terms of other representative quantities after a characteristic or maximum temperature change is determined from the heating rate.

By making the realistic assumption that the maximum temperature occurs before any substantial fraction of the energy addition rate Q (per unit length of the heater, i.e., W/m) is conducted to distant parts of the medium, the temperature increase in Eq. (2-27) can be approximated by an energy balance on the control volume:

$$\frac{dT}{dt} \approx \frac{Q}{\pi r_o^2 \rho_s C_s} \quad (2-28)$$

It has been assumed, for the reasons given after Eq. (2-3), that the temperature distribution is governed primarily by heat conduction (Green et al., 1993c) and that the thermal properties of the solid medium are representative of the properties of the solid-liquid-gas mixture. Alternatively, dT/dt can be expressed in terms of the characteristic temperature change ΔT_o and the time duration required to obtain this value, which is roughly the thermal diffusion time scale L^2/α_s , where α_s is the thermal diffusivity of the solid.

This alternative gives the estimate:

$$\frac{dT}{dt} \approx \frac{\alpha_s \Delta T_o}{L^2} \quad (2-29)$$

Equations (2-28) and (2-29) are order-of-magnitude equivalent and are connected by the temperature increase ΔT_o . The expression based on Q is more convenient to use to establish heating rates for laboratory and numerical investigations when the heating rate of the larger system is known. The expression involving ΔT_o is perhaps more convenient to use to interpret the results of these investigations. Both forms will be carried along in the subsequent discussions.

With these expressions for dT/dt , a characteristic pressure gradient can be defined:

$$\frac{dp_g}{dL} \sim \frac{\phi S_{vo} \mu_{go} \alpha_s Q}{k k_{rel,go} \kappa L T_{avg}} \left(\frac{\rho_{vo}}{\rho_{go}} \right) \left(\frac{h_{lg,o}}{R_v T_{avg}} \right) \approx \frac{\phi S_{vo} \mu_{go} \alpha_s \Delta T_o}{k k_{rel,go} L T_{avg}} \left(\frac{\rho_{vo}}{\rho_{go}} \right) \left(\frac{h_{lg,o}}{R_v T_{avg}} \right) \quad (2-30)$$

where S_{vo} is the characteristic vapor saturation and κ is the thermal conductivity of the solid material. The first form of dp_g/dL is derived from Eq. (2-28) and the second from Eq. (2-29).

Dimensionless Darcy's Law and Characteristic Gas Velocity. With this expression for a characteristic pressure, the full Darcy's law can be rewritten in dimensionless form as:

$$\hat{V}_g = - \left(\frac{\mu_{go}}{\mu_g} \right) \left(\frac{k_{rel,g}}{k_{rel,go}} \right) \left(\hat{\nabla} \hat{p}_g - \frac{(\beta_g/\beta_{go})\Theta}{Ad_g} \bar{e}_z \right) \quad (2-31)$$

The dimensionless group Ad_g , which is called the gas Advection Number, will be discussed below. The ratios of viscosity, relative permeability, and thermal expansion coefficient in Eq. (2-31) are all of order-of-magnitude unity and could be neglected if desired. The dimensionless pressure gradient and the dimensionless buoyancy are also of order unity. Consequently, the relative importance of pressure gradients and buoyancy with respect to vapor transport depends solely on the magnitude of the dimensionless number Ad_g in Eq. (2-31).

The gas velocity in Eq. (2-31) has been made dimensionless by normalizing to a characteristic velocity equal to:

$$V_g \sim \frac{\phi S_{vo} \alpha_s Q}{L \kappa T_{avg}} \left(\frac{\rho_{vo}}{\rho_{go}} \right) \left(\frac{h_{lg,o}}{R_v T_{avg}} \right) \approx \frac{\phi S_{vo} \alpha_s \Delta T_o}{L T_{avg}} \left(\frac{\rho_{vo}}{\rho_{go}} \right) \left(\frac{h_{lg,o}}{R_v T_{avg}} \right) \quad (2-32)$$

The first form is based on Eq. (2-28) and the second on Eq. (2-29).

2.2.2.2 Gas Advection Number

The dimensionless Darcy's law, Eq. (2-31) introduced a new dimensionless number, the gas Advection Number, Ad_g . The gas Advection Number is defined in terms of the relevant parameters by:

$$Ad_g = \frac{\phi S_{vo} \alpha_s \mu_{go} Q}{k k_{rel,go} L \rho_{go} g \beta_{go} \kappa \Delta T_o T_{avg}} \left(\frac{\rho_{vo}}{\rho_{go}} \right) \left(\frac{h_{lg,o}}{R_v T_{avg}} \right) \quad (2-33)$$

$$\approx \frac{\phi S_{vo} \alpha_s \mu_{go}}{k k_{rel,go} L \rho_{go} g \beta_{go} T_{avg}} \left(\frac{\rho_{vo}}{\rho_{go}} \right) \left(\frac{h_{lg,o}}{R_v T_{avg}} \right)$$

where the two alternative forms result from using either Eqs. (2-28) or (2-29) to evaluate the characteristic pressure. The first form of Ad_g is a combination of independent and dependent parameters, since ΔT_o depends on Q , and so is not a useful dimensionless group. The second form will therefore be used in the following discussions.

The gas Advection Number is physically the ratio of nonbuoyancy pressure gradient to buoyancy body-force gradient. Thus, a value of $Ad_g > 1$ implies that the gas flow is controlled by pressure gradients, and the advective component of gas velocity is much larger than the buoyancy-induced component. Conversely, when $Ad_g < 1$, gas flow is controlled by buoyancy. When $Ad_g = 1$, pressure gradients and buoyancy are comparable in their effects and Eq. (2-31) is then the same as Eq. (2-16). It should be noted, however, that for $Ad_g \leq 1$, the characteristic gas velocity is quite small.

Some of the more important factors that determine the magnitude of Ad_g are:

- Permeability k —smaller values (tighter porous media) lead to larger values of Ad_g
- Porosity ϕ —smaller values (media that can contain less gas) lead to smaller values of Ad_g
- Matrix thermal diffusivity α_s —larger values (equivalent to a more rapid increase in temperature) lead to larger values of Ad_g

As can be seen from the second form given for Ad_g in Eq. (2-33), neither the heating rate Q nor the temperature increase ΔT_o directly affects the magnitude of Ad_g (There is a secondary effect given by the average temperature T_{avg} and the change in fluid properties with temperature.) This lack of dependency on Q (or ΔT_o) is the result of the fact that Ad_g is the ratio of two effects, both of which are proportional to Q (or ΔT_o). Nonetheless, it is required that $Q > 0$ since otherwise there are no gas pressures or velocities to consider. It should be noted, also, that both the characteristic pressure, Eq. (2-30), and characteristic velocity, Eq. (2-32), increase in proportion to Q or ΔT_o ; hence, the flow and the rate of drying out do depend on Q .

2.2.2.3 Characteristic Gas Pressure Buildup Time Scale

According to the heating phase conceptual model, the time duration over which large pressure gradients will be created in the gas phase is roughly the same as the duration needed to obtain a steady-state temperature; that is, the time scale of this phenomenon is the thermal diffusivity characteristic time:

$$t \sim \frac{L^2}{\alpha_s} \quad (2-34)$$

This expression for the time scale assumes that the heating duration is at least equal to L^2/α_s . If it is of shorter duration, the maximum pressures will occur near the end of the heating period. The time scale given by Eq. (2-34) depends on both the geometric size L of the heated region and the thermal diffusivity, α_s , of the heated material.

After the gas pressure obtains its maximum value represented by the characteristic pressure, the pressure will slowly decay. The decay time cannot be predicted by this conceptual model, although, if the heating persists, it will be as least as long as the time L^2/α_s required for the pressure to increase to its maximum.

2.2.3 Transitional Period

Eventually, the temperature of the heated volume approaches a near steady-state and the gas pressure thereafter begins to decrease. The advective gas flow thus decreases in magnitude, although the gas flow is still away from the heat source. As the pressure continues to decrease, the capillary pressure gradient becomes larger than the gas pressure gradient and liquid water begins to flow back toward the heated region. The net flow of water (vapor away from the heated region, liquid toward the heated region) remains near zero for an extended period of time. When the vapor flow has decreased sufficiently, however, there is a net flow of water back toward the heated region. This point represents the initiation of the cooling period.

A separate conceptual model is not developed specifically for the transitional period. The model developed below for the cooling period is of a general form and could be adapted to the transitional period, if necessary.

2.2.4 Conceptual Model for the Cooling Period

In the cooling period, the heat generation rate is negligible compared to that during the heating period, and the temperature distribution gradually equalizes throughout the medium. As a result, the water thermally driven away from the vicinity of the heat source moves back toward this dried-out region as both liquid and vapor. The primary thermohydrologic concern for this phase is the time required to complete this rewetting as a function of the medium geometry, physical properties, and initial heating rate. Just as for the heating period, a conceptual model of the rewetting is desirable to (i) delineate the dominant phenomena, and (ii) ensure that laboratory and field experiments are designed and interpreted correctly with respect to repository behavior.

2.2.4.1 Rewetting by Liquid Transport

The liquid saturation level near the heating source decreases significantly during the heating period. The resulting saturation gradients in the medium lead to corresponding capillary pressure gradients directed toward the heating source. After the impressed gas pressure gradient caused by the heating diminishes sufficiently (i.e., after the heating rate has diminished sufficiently), these capillary gradients will produce a return transport of liquid water to the dried-out region. The first part in the development of an idealized conceptual model for the cooling period is thus to estimate the capillary pressure gradients.

Pressure Gradients. For the cooling phase conceptual model, the liquid pressure is expressed as the sum of the gas pressure impressed on the liquid and the pressure difference between the gas and the liquid:

$$P_l = P_g + P_{lg} \quad (2-35)$$

The pressure difference, P_{lg} , is the negative of the capillary pressure, p_c (where the negative sign is used so that P_{lg} itself is a positive value). Further, to ensure that only gradients that create motion are considered, p_c is written relative to the equilibrium pressure, p_{ce} , that balances the gravitational gradient. Hence:

$$P_{lg} = -P_c + P_{ce} + (\rho_{lg}gz - P_{ce}) - \rho_{lg}gz \quad (2-36)$$

The quantity in parentheses in Eq. (2-36) is equal to zero, and the sum of the first two terms is defined as $-\Delta p_c$, which is the nonhydrostatic component of capillary pressure.

The nonhydrostatic capillary pressure is a function of pore size d , liquid saturation S_l , and liquid surface tension σ (or some other surface property such as adhesion), and whether the liquid wets the medium. Since water wets the media of interest here, the gradient of nonhydrostatic pressure can be expressed in the general form:

$$\nabla (\Delta p_c) = \frac{\partial \Delta p_c}{\partial S_l} \nabla S_l + \frac{\partial \Delta p_c}{\partial d} \nabla d + \frac{\partial \Delta p_c}{\partial \sigma} \frac{d\sigma}{dT} \nabla T \quad (2-37)$$

where the gradient of σ has been written in a way to show explicitly its dependence on temperature T . For the conceptual model, an equivalent continuum model is adopted, so the variation of capillary pressure with respect to d is neglected. Further, although surface tension gradients may not be totally unimportant during rewetting, they are neglected here for simplicity. Thus, Eq. (2-37) is expressed here simply as:

$$\nabla (\Delta p_c) = \frac{d\Delta p_c}{dS_l} \nabla S_l \quad (2-38)$$

Since $d\Delta p_c/dS_l < 0$, Eq. (2-38) demonstrates that Δp_c increases in the direction in which the saturation decreases and roughly in proportion to it.

Characteristic Darcy's Law. With these definitions and simplifications, Darcy's law for liquid transport is expressed as:

$$\bar{V}_l = -\frac{kk_{rel,l}}{\mu_l} \left(\nabla p_g - \frac{d\Delta p_c}{dS_l} \nabla S_l - \rho_{lo} g \bar{e}_z + \rho_l g \bar{e}_z \right) \quad (2-39)$$

As explained in Section 2.1.2, the net gravitational gradient is expressed in terms of the temperature change ΔT from ambient and the liquid expansion coefficient β_l , with the result that:

$$\bar{V}_l = -\frac{kk_{rel,l}}{\mu_l} \left(\nabla p_g - \frac{d\Delta p_c}{dS_l} \nabla S_l - \rho_{lo} \beta_l g \Delta T \bar{e}_z \right) \quad (2-40)$$

For the general model, the capillary pressure Δp_c in Eq. (2-40) is made dimensionless by dividing it by the characteristic gas pressure of the heating period. This choice for the characteristic gas pressure recognizes the fact, that during the transition period, the gas pressure gradient and the capillary pressure gradient can be comparable in magnitude although opposite in sign. Consequently, the dimensionless Darcy's law for the general case is:

$$\hat{V}_l = -\frac{\mu_{lo} k_{rel,l}}{\mu_l k_{rel,lo}} \left[\hat{\nabla} \hat{p}_g - \frac{d\Delta \hat{p}_c}{dS_l} \nabla S_l - \frac{(\beta_l/\beta_{lo})\theta}{Ad_l} g \bar{e}_z \right] \quad (2-41)$$

and the corresponding characteristic liquid velocity is:

$$V_l = \left(\frac{\mu_{go}}{\mu_{lo}} \right) \left(\frac{k_{rel,lo}}{k_{rel,go}} \right) V_g \quad (2-42)$$

For this case, the dimensionless liquid Advection Number in Eq. (2-41) is defined as:

$$Ad_l = \left(\frac{\rho_{go}}{\rho_{lo}} \right) \left(\frac{\beta_{go}}{\beta_{lo}} \right) Ad_g \quad (2-43)$$

During the cooling period, the general transitional period model can be simplified because the capillary pressure gradient is no longer coupled to the heating period. Consequently, a more appropriate characteristic pressure for the cooling period is the capillary pressure, Δp_∞ , created by the characteristic decrease in liquid saturation, ΔS_{lo} , of the dried-out region. Hence, the characteristic liquid velocity of the cooling period is expressed as:

$$V_l \sim \left(\frac{k k_{rel,lo}}{\mu_{lo}} \right) \left(\frac{d\Delta p_{co}}{dS_l} \right) \left(\frac{\Delta S_{lo}}{L} \right) \quad (2-44)$$

Following a similar procedure again in Darcy's Law, it is found that the liquid Advection Number for the cooling phase is defined as:

$$Ad_l = \frac{\Delta p_{co} \Delta S_{lo}}{\rho_{lo} \beta_l L g \Delta T_o} \quad (2-45)$$

The interpretation of Ad_l is similar to Ad_g , namely, $Ad_l > 1$ implies that pressure gradients are much larger than buoyancy gradients.

2.2.4.2 Rewetting by Liquid Advection

The characteristic liquid velocity for the cooling phase model is used to estimate the time for the volume near the heating source to regain its original liquid saturation level when only liquid-phase transport is active. If the characteristic decrease in liquid saturation during the heating period is ΔS_l , the mass of liquid ΔM_l that must be replaced during rewetting is about $\bar{V} \phi \rho_{lo} \Delta S_l$, where $\bar{V}$ is the affected volume (roughly equivalent to the control volume introduced in Section 2.2.1) and ϕ is the medium porosity. The rewetting mass flow rate is roughly $A \rho_{lo} V_l$, where A is the area bounding the volume $\bar{V}$, and V_l is the characteristic liquid velocity given by Eq. (2-44). Thus, the time required to rewet the dried-out zone by liquid flow alone is:

$$\begin{aligned} t_l &= \left[\frac{(\mu_{lo}/\mu_{go})(k_{rel,go}/k_{rel,lo})(T_{avg}/\Delta T_o)}{S_{vo}(h_{lgo}/R_v T_{avg})(\rho_{vo}/\rho_{go})(\Delta \hat{p}_c/\Delta S_l)} \right] \left(\frac{L^2}{\alpha_s} \right) \\ &= \frac{\phi \mu_{lo} L^2}{k k_{rel,lo} (d\Delta p_{co}/dS_l)} \end{aligned} \quad (2-46)$$

The first form of the definition of the t_l given in Eq. (2-46) is derived from the general model (valid for both the transition and the cooling periods). This form demonstrates that the rewetting period is proportional to the time required to obtain the maximum gas pressure during the heating period; it is convenient when experimental values of this time and of the maximum gas pressure are available to evaluate L^2/α_s and $\Delta \hat{p}_c$. The second form of the definition of t_l in Eq. (2-46) is derived from the cooling period model; this form is convenient when a moisture release curve or model is available to evaluate $d\Delta p_{co}/dS_l$ but no other experimental data are available. Note that in both definitions the explicit

dependence on the characteristic saturation decrease ΔS_{lo} cancels out. However, ΔS_{lo} must be known or estimated to compute appropriate values for $k_{rel,lo}$ and Δp_{co} .

The saturation decrease ΔS_{lo} needed to estimate both $k_{rel,lo}$ and Δp_{co} can be estimated in principle by using the relations derived in Section 2.2.2 for the heating period. However, the estimate is likely to be fairly crude because the heating phase conceptual model is capable of making predictions only to within an order of magnitude, and the total range of ΔS_{lo} is typically only one order of magnitude. Thus, a more reasonable approach is to assume that ΔS_{lo} is about 0.5, which is the approach taken here.

Rewetting Time Similitude. Equation (2-46) represents the similarity relation that can be used to interpret or scale-up laboratory and field tests.

2.2.4.3 Rewetting by Vapor Diffusion

Diffusion of vapor into the dried-out region followed by condensation can also contribute to rewetting the dried-out region. The diffusion is driven by the vapor partial pressure gradient created by vapor pressure lowering in zones of low liquid saturation, as explained in Section 2.1. This kind of vapor pressure gradient has also been called a relative humidity gradient.

Vapor Mass Flux. For Fickian diffusion, the vapor flux is given by:

$$\vec{q}_v = \tau \phi S_v \rho_v D \nabla w_v \quad (2-47)$$

where D is the binary diffusion coefficient of air and water vapor, τ is the tortuosity of the porous medium, and w_v is the mass fraction of water vapor in the gas mixture. The mass fraction w_v can be determined in terms of the partial pressure p_v of the vapor as follows:

$$w_v = \frac{M_v}{M_g} = \frac{M_v}{M_v + M_a} = \frac{M_v}{M_v + 1.61 M_v (p_a/p_v)} = \frac{p_v}{p_g + 0.61 p_a} \quad (2-48)$$

where the ideal gas law has been used, and the numerical factor 1.61 is the ratio of the gas constants for water vapor and air, note that $p_g = p_a + p_v$.

During the rewetting period, the total gas pressure p_g remains approximately constant and equal to ambient throughout the region of interest. Thus, a vapor pressure gradient is accompanied by an approximately equal air partial pressure gradient in the opposite direction. Consequently, the gradient of vapor mass fraction can be found from Eq. (2-48) to be:

$$\nabla w_v = \left[\frac{p_g + 1.22 p_a}{(p_g + 0.61 p_a)^2} \right] \nabla p_v \approx \left(\frac{1}{2 p_v} \right) \nabla p_v \quad (2-49)$$

(The last approximation follows from the assumption that the partial pressures of air and vapor in the mixture are roughly the same).

Rewetting Times. The mass flow of vapor into the dried-out region is given by the product of the mass flux and the flow area. The time required for this flow to increase the liquid saturation by condensation to its initial saturation level is thus about:

$$t_g = \left(\frac{\rho_{lo}}{\rho_{wo}} \right) \left(\frac{\Delta S_{lo}}{\tau S_v} \right) \left(\frac{p_v}{\Delta p_v} \right) \frac{L^2}{D} \quad (2-50)$$

where Δp_v is the magnitude of the vapor pressure difference. This relation can be compared to the liquid-flow rewetting time estimate by noting that D has a value that is approximately 30 times larger than the thermal diffusion coefficient α_s . Thus:

$$t_g \approx 0.03 \left(\frac{\rho_{lo}}{\rho_{wo}} \right) \left(\frac{\Delta S_l}{\tau S_v} \right) \left(\frac{p_v}{\Delta p_v} \right) \frac{L^2}{\alpha_s} \quad (2-51)$$

This relationship will be used in Chapter 5 in a proposed scaling theory.

Rewetting Time Similitude. Although the contribution of vapor diffusion to rewetting is less important than liquid water flow in most cases, Eqs. (2-50) and (2-51) provide a similarity relation to interpret laboratory and field tests for those cases in which vapor mass diffusion should be considered.

2.2.5 Conceptual Model for Low Heating Rate, Large-Scale Buoyancy Recirculation

When the gas Advection Number Ad_g is of order one or less, the overall flow is a circulation governed by Eqs. (2-16)–(2-18). This conceptual model is valid for low heating rates. On a mountain scale, this flow is similar to a thermosyphon, which is defined as shown in Figure 2-6 by a set of streamtubes that (i) begins at the ground surface at a distance away from the repository, (ii) travels downward toward the water table below the repository, and then (iii) travels upward through the repository and exits at the ground surface above the repository. To develop a conceptual model of this buoyancy-driven flow, the repository is modeled as a disk-shaped heat source halfway between the ground surface and the water table, and the flow is assumed to be one dimensional (1D) (i.e., variation only in the streamtube direction).

Equation (2-18), which gives the characteristic gas velocity for a buoyancy-driven flow, is modified slightly to allow the vertical temperature gradient to be accounted for explicitly:

$$V_g = \frac{kg\beta_g}{4\nu_g L} \int \Delta T dz \quad (2-52)$$

where ν_g is the kinematic viscosity of the gas. It has also been assumed, for simplicity, that the relative permeability for gas flow is one. The total length of the thermosyphon stream tube is $4L$, where the characteristic length L is the distance from the repository to the surface.

Figure 2-6. Anticipated streamtubes for buoyancy-driven gas flow

2.2.5.1 Vapor Transfer.

If there were no buoyant flow, the vapor generated at the repository would be transported by molecular diffusion equally to the cooler regions above and below the repository. With the buoyant flow, however, it is possible that a larger fraction of the vapor will be transported to regions above the repository than to regions below it. To assess this effect, an expression is needed for the amount of vapor generated at the repository. The vapor generation rate per unit volume, $\dot{m}_{\text{evap}}$, is given by a water mass balance (in which the accumulation of water vapor is negligible) that considers the diffusive q_{wd} and advective fluxes q_{wa} of water vapor:

$$\dot{m}_{\text{evap}} = \frac{\partial}{\partial z} (q_{\text{wd}} + q_{\text{wa}}) \quad (2-53)$$

Each term on the right hand side of this expression can be defined further.

The advective flux is equal to the vapor density times the gas velocity. As explained in earlier sections, the vapor density can be evaluated as if the relative humidity is 100 percent when vapor pressure lowering is negligible and the maximum temperature does not exceed the boiling temperature. Thus:

$$\frac{\partial q_{wv}}{\partial z} = V_g \frac{d\rho_v}{dT} \frac{dT}{dz} = V_g \rho_v \left(\frac{h_{lg}}{R_v T^2} \right) \frac{dT}{dz} \quad (2-54)$$

where Clapeyron's equation has been used to evaluate the vapor density.

The diffusive flux is given by Fick's law:

$$\frac{\partial q_{wd}}{\partial z} = -\rho_v D \frac{\partial^2 \rho_v}{\partial z^2} = -\rho_v D \left(\frac{h_{lg}}{R_v T^2} \right) \left[\left(\frac{h_{lg}}{R_v T^2} \right) \left(\frac{dT}{dz} \right)^2 + \frac{d^2 T}{dz^2} \right] \quad (2-55)$$

where the diffusive coefficient has been assumed to be constant, and the tortuosity factor neglected.

The combined expression for $\dot{m}_{\text{evap}}$ is, thus:

$$\dot{m}_{\text{evap}} = -\rho_v \left(\frac{h_{lg}}{R_v T^2} \right) V_g \frac{dT}{dz} - D \left[\left(\frac{h_{lg}}{R_v T^2} \right) \left(\frac{dT}{dz} \right)^2 + \frac{d^2 T}{dz^2} \right] \quad (2-56)$$

This expression can be made dimensionless by introducing a new "pressure" number Vp which is defined as:

$$Vp = \left(\frac{h_{lg}}{R_v T^2} \right) \Delta T_o \quad (2-57)$$

It should be noted that Vp is proportional to the characteristic temperature increase caused by the heating. The dimensionless vapor generation rate is thus:

$$\dot{m}_{\text{evap}} = -\frac{\rho_v}{\rho_o} \left[\left(\frac{Pe}{Vp} \right) \left(\frac{d\theta}{dz} \right) - \left(\frac{d\theta}{dz} \right)^2 - \left(\frac{1}{Vp} \right) \frac{d^2 \theta}{dz^2} \right] \quad (2-58)$$

where Pe = Peclet Number, $V_g L/D$. For an approximately linear temperature gradient, $d\theta/dz$ is equal to +1 above the repository and -1 below it, so Eq. (2-58) can be simplified to give:

$$\dot{m}_{\text{evap}} = \begin{cases} \left(\frac{\rho_v}{\rho_o} \right) \left[1 + \left(\frac{Pe}{Vp} \right) \right] & \text{above repository} \\ \left(\frac{\rho_v}{\rho_o} \right) \left[1 - \left(\frac{Pe}{Vp} \right) \right] & \text{below repository} \end{cases} \quad (2-59)$$

This equation quantifies the conditions for which vapor will condense preferentially above the repository; that is when the ratio Pe/Vp has a magnitude of one or greater. For typical ranges of repository parameter values, it is found that $0.001 < Pe/Vp < 10$ (Manteufel, 1994). Hence, the overall large-scale buoyancy-induced circulation, according to this conceptual model, can in fact cause somewhat more vapor to condense above the repository than below it.

2.2.5.2 Ratio of Total Vapor Flux to Diffusive Flux

The above expressions establish when the advective flux must be considered in evaluating the total vapor flux. The ratio of the total flux to the diffusive flux can be expressed in dimensionless form as:

$$\frac{q_{va} + q_{vd}}{q_{vd}} = 1 + \left(\frac{Pe}{Vp} \right) \quad (2-60)$$

For typical values of the parameters for the repository, the ratio Pe/Vp is ten or less. Thus, as was anticipated for $Ad_g \leq 1$, the advective and buoyancy fluxes are comparable for this conceptual model.

2.2.5.3 Ratio of Total Heat Flux to Conductive Flux

It is also of interest to determine when the energy transported by the vapor must be considered to evaluate the temperature distribution created by the heating. The conduction flux is simply $\kappa(dT/dz)$, and the energy flux associated with the evaporation and condensation of vapor can be expressed as:

$$\text{mass transfer energy flux} = h_g \left(\rho_v V_g + D \frac{d\rho_v}{dz} \right) \quad (2-61)$$

Thus, after some algebraic manipulation, the ratio of the energy fluxes is:

$$\frac{\text{Total energy flux}}{\text{conduction flux}} = 1 + \frac{(h_g)^2 \rho_v D}{\kappa R_v T^2} \left(1 + \frac{Pe}{Vp} \right) \approx 1 + 10^{-2} \left(1 + \frac{Pe}{Vp} \right) \quad (2-62)$$

where the final approximation is based on typical values for the thermodynamic properties of water, air-vapor diffusion coefficient, and thermal conductivity of tuffaceous rock. Since $0.001 < Pe/Vp < 10$, it is concluded that the temperature distribution is determined primarily by heat conduction; this helps to justify the conduction assumption made in Section 2.1.2.2 to derive a general energy equation for flow in unsaturated porous media.

3 DESCRIPTION OF LABORATORY EXPERIMENTS

Laboratory-scale experiments were conducted to study thermally induced redistribution of moisture in porous media. For the purpose of identifying the various experiments, they are designated as Tests 1 through 11. Results from the laboratory-scale experiments are intended to be used in addressing basic technical concerns regarding thermohydrologic phenomena and in formulating scaling theories. This section provides information on the experimental groups, instrumentation and sensors, and the hydraulic and thermal characterization methods. Also included is a summary of the properties of the test media used in the laboratory experiments. Additional information on these topics can be found in: (i) the report by Green et al. (1993b) which describes Test 1 in great detail; (ii) Manteufel et al. (1992) and Manteufel and Green (1993), which summarize Tests 1 and 2; and (iii) semi-annual CNWRA progress reports (Dodge and Green, 1993a; Manteufel and Green, 1993; Green et al., 1993a,b; Manteufel and Green, 1993).

3.1 THERMOHYDROLOGIC ISSUES AND CONSIDERATIONS

Laboratory experiments have been performed in an attempt to replicate and characterize the three distinct thermal periods: heating, transitional, and cooling. To study thermohydrologic phenomena at the laboratory scale, the experiments were designed in a manner that would permit addressing the following four basic technical questions:

- What are the principal mechanisms controlling the redistribution of moisture?
- Under what thermohydrologic conditions and time frames do individual mechanisms predominate?
- What driving mechanism is associated with a particular hydrothermal regime?
- What are the temporal and spatial scales of each hydrothermal regime?

The data described here were used in the interpretation of the laboratory experiments and in evaluating scaling theories. The interpretations and evaluations are presented in Chapters 4 and 5.

3.2 DESCRIPTION OF EXPERIMENTAL GROUPS

The laboratory-scale experiments are categorized according to: (i) fluid phase that is the focus of the study, (ii) temperature regime, (iii) geometry, and (iv) test medium. Two groups of experiments were designed to address the four basic technical questions regarding coupled thermal and hydrologic flow processes and to provide the data necessary for testing various scaling theories proposed in Section 2. The first group, referred to as the liquid flow experiments, was designed to study the flow patterns in the liquid phase. The second group, designated as the gas flow experiments, focused on the dynamics of the gas phase and the buildup of gas pressure. The critical question addressed in both groups is how the fluid flow regimes are related to system variables: pressure, temperature, heat source, and media properties. Of particular interest are the rates and directions of liquid and vapor flow and their time histories during the heating and cooling periods. The primary features of the laboratory-scale experiment designs are summarized in Table 3-1.

Table 3-1. Summary of laboratory-scale thermohydrology experiments

Test Number	Group	Water Temperature Regime	Geometry	Medium
1	Liquid flow	Sub-boiling	1D rectangular	silica beads
2	Liquid flow	Sub-boiling	1D rectangular	$\leq 149 \mu\text{m}$ tabular alumina
3	Liquid flow	Sub-boiling	2D rectangular	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina
4	Liquid flow	Sub-boiling	2D rectangular	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina
5	Liquid flow	Boiling	2D rectangular	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina
6	Liquid flow	Boiling	2D rectangular	ceramic
7	Liquid flow	Boiling	2D rectangular	cement slurry (C3)
8	Gas flow	Boiling	1D cylindrical	$\leq 250 \mu\text{m}$ tabular alumina
9	Gas flow	Boiling	1D cylindrical	cement slurry (C4)
10	Gas flow	Boiling	1D cylindrical	cement slurry (C6)
11	Gas flow	Boiling	1D cylindrical	tuff

Both groups of laboratory experiments followed the basic strategy of beginning with test media designed to approximate homogeneity under simple hydrothermal conditions, and then progressing to more complex media and hydrothermal conditions that would better represent the repository setting. The absence of heterogeneous hydraulic characteristics in the initial experiments was desired to allow direct observation of thermohydrologic phenomena and to simplify interpretation of results. The knowledge gained in the idealized setting was helpful in designing and instrumenting the later, more complex experiments, as well as in interpreting those experimental results. This approach allowed each subsequent experiment to build upon the knowledge gained in previous experiments and to focus on specific experimental design modifications. Additionally, all experiments were pneumatically sealed to ensure an essentially constant mass balance, although one fitting was loosened to prevent gas pressure buildup. Moisture loss (or gain) through this loosened fitting was presumed to be insignificant.

3.2.1 First Group: Liquid Flow Redistribution Experiments

To investigate thermally driven moisture redistribution in partially saturated porous media, seven experiments were conducted. These tests can be divided into two subcategories according to geometry,

the first subcategory with Tests 1 and 2 and the second with Tests 3 through 7. The two subcategories had slightly different objectives.

The primary objective of the first subcategory was to observe the redistribution of moisture through partially saturated porous media in response to a 1D horizontal thermal gradient. The geometry of the two tests in this subcategory was intentionally simple and uniform media were used (with the exception of the simulated fracture in Test 1) to permit observation of heat and mass transfer in the absence of complex boundary conditions and heterogeneities. It is important to note that even though these tests were designed to be 1D, apparent 2D, or even 3D flow features were observed in the actual experiments. A similar statement can be made with regard to the 2D and 1D radial experiments. Nonetheless, the experiments are referred to as 1D because their primary design was limited to 1D.

Theoretical development conducted simultaneously with Tests 1 and 2 identified a need for experimental data to test the proposed scaling theories. Therefore, the second subcategory (Tests 3 through 7) had the objective of providing observable and quantifiable experimental results for evaluating heat and mass transfer mechanisms predicted for different geometries and possibly to assess the proposed scaling laws. The heat source in Tests 3 through 7 was designed to be a point source, rendering these tests into a 2D configuration. This change in the geometry of the experimental design was made to provide a database more appropriate for evaluating the scaling theories under development. It was anticipated that information on fluid flow derived from this category of tests would not only aid in evaluating the scaling relationships, but also contribute to the basic investigation of heat and mass transfer mechanisms. Further development of the proposed scaling theories eventually necessitated an additional change in the objective of the experiments. This change resulted in the gas pressure buildup experiments, which will be discussed in a later section.

The seven experiments in the liquid flow group differed somewhat in instrumentation, type of medium, and heat source; detailed descriptions of the configurations, design, and instrumentation are summarized in Table 3-2. In all the liquid flow redistribution tests, an upright rectangular cell filled with uniform porous media was heated to induce moisture redistribution. All seven rectangular test cells were of similar construction. The right and left vertical side boundaries were constructed of anodized aluminum through which water was circulated to maintain their respective temperatures constant. These constant-temperature boundaries also served as the heating source for Tests 1 and 2. The top, bottom, front, and back surfaces of the test cell were constructed of clear plexiglass to permit direct visual observation of fluid flow using injected dyes. Temperature and matric potential were measured directly with thermistors and tensiometers, respectively. Moisture content was measured indirectly with a horizontally oriented gamma-ray densitometer. Figure 3-1 illustrates the general configuration for Tests 1 and 2, and Figure 3-2 shows the general configuration for Tests 3 through 7.

The direction of liquid fluid flow in Tests 1 through 4 was determined visually by injecting dye to provide optical contrast and photographing the dye distribution as the experiment progressed. The dye was injected at two locations in Tests 1 and 2 (near the right and left sides of the test cell) and at five locations in Tests 3 and 4 (one above, below, right, and left of the heater and one located horizontal to the heater but near the left test cell boundary). No more than 0.1 ml of dye was used per injection to minimize any potential fluid movement resulting from a local increase in saturation. A red food color dye was used in all experiments. The dye injection tubes in all these tests extended through most of the test medium from the back of the test cell so that the dye could be introduced at a point very close to the front plexiglass wall. Two dye ports were also installed in the Test 7 cell through the front plexiglass wall of the cell into the cement slurry late in the duration of the experiment. However, this proved to be

Table 3-2. Summary of laboratory-scale experimental configuration, thermal design, and instrumentation

Test Number	Saturation	Test Geometry (cm)	Thermal Conditions	Instrumentation		Saturation Measurements (Densitometer Measurements)	Dye Injection
				Temperature Sensor	Pressure Sensor		
1	0.65	20.3×15.2× 5.7 fracture	right 60 °C for 98 days, left 20 °C	3 internal 2 external	2 tensiometers	4 rows of 6	2 ports
2	0.50	20.3×15.2× 5.7	right 90 °C for 80 days, left 20 °C	8 internal 2 external	6 tensiometers	4 rows of 6	2 ports
3	0.70	15.2×15.2×6.6	right & left 20 °C, internal heater at 60 °C for 89 days, 90 °C for 58 days	6 internal 2 external	6 tensiometers	8 rows of 12	5 ports
4	0.70	15.2×15.2×6.6 fracture	right & left 20 °C, internal heater at 60 °C for 90 days, 90 °C for 84 days	6 internal 2 external	6 tensiometers	8 rows of 12	5 ports
5	0.585	15.2×15.2×6.6	right & left 20 °C, internal heater ramped to 122 °C in 30 days, 30 days at 122 °C	2 external	none	8 rows of 12	none

Table 3-2 (Cont'd). Summary of laboratory-scale experimental configuration, thermal design, and instrumentation

Test Number	Saturation	Test Geometry (cm)	Thermal Conditions	Instrumentation		Saturation Measurements (Densitometer Measurements)	Dye Injection
				Temperature Sensor	Pressure Sensor		
6	0.80 and 0.50	15.2x15.2x5.5	right & left 20 °C, 8 days at 58 °C, 3 days at 90 °C, 7 days at 120 °C, 4 days at 20 °C, 5 days at 95 °C, 11 days at 124 °C, 4 days at 178 °C	2 external	none	4 rows of 12 6 rows of 11 7 rows of 17	none
7	0.50	15.2x15.2x6.6	right & left 20 °C, 25 days at 144-160 °C	2 external	None	4 rows of 12 6 rows of 11 7 rows of 17	2 ports added late
8	0.50	11.4 tall, 30.5 diameter cylinder	side wall at 20 °C 120 °C for 4 hr	1 at heater 1 at side wall	1 at heater 2 at side wall	none	none
9	0.47	11.4 tall, 30.5 diameter cylinder	side wall at 20 °C 8 days at 193 °C	1 at heater 1 at side wall	1 at heater 2 at side wall	2 radial lines of 34	none
10	0.50	11.4 tall, 30.5 diameter cylinder	side wall at 20 °C 7 days at 215-240 °C	1 at heater 1 at side wall	1 at heater 2 at side wall	1 radial line of 34	none
11	0.30	11.4 tall, 30.5 diameter cylinder	side wall at 20 °C, 7 days at 162 °C	1 at heater 1 at side wall	1 at heater 2 at side wall	1 radial line of 34	none

Figure 3-1. Experimental cell for Tests 1 and 2. Internal thermistors for Test 1 are denoted with a 1. All thermistors, except the internal thermistor along the midline, were used in Test 2. Tensiometers only at locations denoted with a 2 were used in Test 1. Tensiometers were used at all six locations in Test 2. The simulated fracture was incorporated into Test 1 but not Test 2.

Figure 3-2. Experimental cell for Tests 3 through 7. Thickness of Test 6 was 5.5 cm. Tensiometers are numbered 1 through 6 from left to right and top to bottom. All five dye injection ports were used only for Tests 3 and 4, and only the injection ports above and below the heater were used in Test 7. The simulated fractured was only incorporated into Test 4.

ineffective, possibly due to the low permeability of the cement; the dye became too faint for viewing prior to any flow movement becoming apparent.

The horizontally oriented densitometer used in the liquid flow redistribution tests, identified as the x-z densitometer, was configured to measure density contrasts in an x-z oriented plane. Density contrast measurements were acquired along several horizontally oriented traverses in each experiment, from which saturation levels were calculated by methods described below. The number of traverses and measurements per traverse varied with the tests. Evenly spaced measurements were collected in most traverses although more closely spaced densitometer measurements were collected in Tests 6 and 7 near the heater. The saturation values calculated from the densitometer measurements represented an average saturation through the short dimension of the rectangular enclosure at the point at which the densitometer measurement was recorded. Although variations in saturation along the short dimension were not detectable with this experimental configuration, the relatively short horizontal dimension (5.5 or 6.5 cm) of the test medium tended to minimize any importance this variation might have had. Therefore, either a vertically oriented 2D saturation distribution or a vertically or horizontally oriented 1D profile of saturation was constructed from the x-z densitometer measurements.

3.2.2 Second Group: Gas Pressure Buildup Experiments

Continued development and refinement of the scaling theories identified specific heat and mass transfer mechanisms for experimentation. In particular, identification of the buildup of gas pressure as a key indicator in the scaling analysis led to the design of the last set of laboratory-scale experiments. These experiments, identified as Tests 8 through 11, were designed to permit the observation of gas pressure buildup and the associated concurrent redistribution of moisture. The fundamental objective of the gas pressure buildup tests was to provide a database for evaluation of the proposed scaling relationships and to contribute to the continued investigation of heat and mass transfer mechanisms.

In the gas pressure buildup tests, an upright cylindrical configuration was used to provide a medium in which the buildup of gas pressure in an intact matrix could be monitored. The cylinders were 12 cm tall and had a diameter of 30.5 cm. Instrumentation in the gas pressure buildup tests included a thermocouple and pressure transducer incorporated into an axially centered, vertically oriented electric cartridge heater, and a thermocouple, pressure transducer, and manometer inserted into the outside wall of the test cell (Figure 3-3). Intrusive instrumentation was minimized in the gas pressure buildup tests to ensure that the test medium was intact and that new gas pathways were not inadvertently introduced via the instrumentation. Additionally, great care was exercised to prevent gas flow along the two horizontal ends of the cylinders by covering the consolidated test medium ends (of Tests 9 through 11) with silicon cement prior to enclosure within the plexiglass end plates. Descriptions of these tests are also summarized in Tables 3-1 and 3-2.

The vertically oriented densitometer used in the gas buildup tests, identified as the x-y densitometer, was configured to measure density contrasts in an x-y oriented plane. Density contrast measurements were acquired along two radially oriented traverses in each experiment, from which saturation levels were calculated. The calculated saturation values represented an average saturation for the vertical span of the cylinder at the point at which the densitometer measurement was recorded. Although vertical variations in saturation were not detectable with this experimental configuration, the relatively short vertical dimension (12 cm) and the cylindrical shape of the test medium tended to minimize any impact this variation might cause. The number of radial traverses and measurements per

Figure 3-3. Experimental cell for Tests 8 through 11

traverse varied with the tests. Traverses in two radial directions separated by 90° were measured in Test 9, but this configuration was reduced to a single radial traverse in Tests 10 and 11 to increase the frequency of the saturation profile measurements, since each profile required 1.5 to 2.0 hr of measurement to obtain the desired accuracy. Although some time-dependent saturation information may have been missed by the relatively long measurement times, no feasible alternative was possible. Media saturation was also measured at the end of Tests 9 and 11 by direct measurement of saturation of media samples collected from the dismantled cylinders.

Three different types of media were used in the gas pressure buildup tests; tabular alumina, cement slurry mixture, and tuff. The first two of these media were selected to provide a uniform test medium of sufficiently low permeability to accommodate the objectives of the gas pressure buildup tests. Tabular alumina was used in the first experiment in this group. This experiment, Test 8, was conducted as a scoping experiment to evaluate the feasibility of the gas pressure buildup experiments. However, the relatively high permeability of the alumina powder ($5.5 \times 10^{-14} \text{ m}^2$) rendered it inadequate for experiments in which gas pressure gradients were of interest. Tests 9 and 10 had cement slurry mixtures as their media material. The permeability of the cement slurries proved to be adequately low, and a sufficiently uniform cement slurry mixture was attained after several attempts; however, this medium also proved to be unsatisfactory. Although the cement slurry mixtures were allowed to cure at room temperature for a period in excess of 30 days, additional alteration of the cement slurry mixture was encountered throughout the course of the experiment. Unfortunately, a continued decrease in the permeability was also experienced with this alteration. This phenomenon was noted and measured during saturated hydraulic conductivity measurements of samples of the cement slurry mixtures. For the final gas pressure buildup test (Test 11), a stable medium of sufficiently low permeability was obtained through the use of an intact piece of tuff from the Apache Leap Test Site (ALTS); this choice of test medium however, provided less uniformity.

3.3 DESCRIPTION OF INSTRUMENTATION AND SENSORS

To monitor the laboratory-scale experiments, instrumentation was used to measure changes in: (i) temperature, (ii) moisture content, (iii) capillary pressure head, (iv) gas pressure, (v) tracer movement, and (vi) heater power. The specific instrumentation selections were based on a detailed review of various intrusive and nonintrusive sensing techniques; this review is documented in Green et al. (1993b). A description of the instrumentation and sensors used in the laboratory experiments is presented in the following sections.

3.3.1 Temperature Sensors

Thermistors were used to measure the temperature of the heater plates and the media in Tests 1 through 7. In order to reduce the effects of sensor intrusion on the flow field, small-diameter (1 mm) thermocouples were used in Tests 8 through 11. The specific temperature sensors used in the experiments are listed in Table 3-3.

3.3.2 Gas Pressure Sensors

Gas pressure sensors were used in Tests 8 through 11 to measure the gas pressure at the heater and in the media container. The pressure sensors were Model 142PC05D, manufactured by the Micro Switch Corporation. The sensor measurement range was from 0 to 5 psig (0 to 0.34 bar) with a measurement uncertainty of ± 1.0 percent of full-scale output. The locations of the pressure taps for these tests are shown in Figure 3-3.

Table 3-3. Temperature sensors used in experiments

Manufacturer	Model	Accuracy
YSI Incorporated	Thermistor: #031-46031-4RPM-120-ST	± 0.5 °C
YSI Incorporated	Thermistor: #030-44006-4RPM-120-ST	± 0.5 °C
OMEGA Engineering Co.	Thermocouple: TMTSS-020U-6	± 1.0 °C

3.3.3 Tensiometers

Tensiometers were used in Tests 1 through 5 to measure capillary pressure. A schematic of the tensiometer design is shown in Figure 3-4. The tensiometer consisted of a porous ceramic cup that was bonded to a plastic tube. The ceramic cup was inserted into the medium before the test medium was placed in the test cell. The tensiometer porous cups were 9.5 mm in diameter and 28 mm long. The Soil Moisture Equipment Corporation Model 652X07-B1M3 cups were used as 1-bar high-flow cups. The pressure sensors, manufactured by Micro Switch Corporation, were Model 140PC05G with a pressure range from 0 to -5 psi (0 to -3.5 m of water) with an accuracy of ± 1.0 percent of the full-scale output.

The tensiometers were filled with water prior to initiation of the experiment. After injection of the water, a pressure sensor was attached to the end of the tensiometer. Water would flow between the tensiometer and the medium (through the porous cup) until pressure in the tensiometer equaled the capillary pressure in the medium. When this equalization occurred, hydraulic equilibrium through the porous cup was assumed to exist. An intentionally loosened fitting in each of the tests prevented gas pressure buildup inside the test cell, thereby pressure corrections were not necessary. For Tests 7 and 8, temperature sensors were placed inside the tensiometers to provide additional temperature measurements without further disturbing the medium by introducing additional sensor intrusions into the medium.

3.3.4 Moisture Content Measurements

Moisture content of the test media was determined using several approaches: (i) gamma-ray densitometry, (ii) calculation by adding known quantities of water to media with known void volumes, and (iii) direct calculation of saturation on samples of the media. These methodologies were used either individually or combined to determine the moisture content of the test media. In particular, post-test measurement of saturation on samples extracted from the media used in Tests 9 and 11 was useful in calibrating saturation values made from densitometer measurements.

The gamma-ray densitometry methodology (Nichols and Heaviside, 1988, Gilboy, 1984) was selected to provide saturation measurements of the test medium because: (i) the technique is nonintrusive and does not disrupt the flow in the test medium, (ii) measurements can generally be conducted within an acceptable period of time, and (iii) the accuracy of the measurement technique is acceptable for most applications in this project. The standard method for calculating water saturation level from the

TENSIOMETER

Figure 3-4. Schematic of the tensiometer

densitometer reading requires detailed information about material and fluid properties in order to account for the attenuation of all components of the system (e.g., cell walls, dry medium, and water). Saturation is calculated from the total count rate using the exponential expression (Gardner, 1986):

$$I/I_o = e^{-[X(\mu_m \rho_m + \mu_w \rho_w \phi S) + 2 X' \mu_c \rho_c]} \quad (3-1)$$

where

I	=	gamma-ray intensity, detector (counts/s)
I_o	=	gamma-ray intensity, source (counts/s)
X	=	medium thickness (m)
X'	=	cell wall thickness (m)
μ_m	=	attenuation coefficient of medium (m^{-1})
μ_w	=	attenuation coefficient of water (m^{-1})
μ_c	=	attenuation coefficient of cell (m^{-1})
ρ_m	=	density of the medium (kg/m^3)
ρ_c	=	density of the cell (kg/m^3)
ϕ	=	porosity (-)
S	=	liquid saturation in media ($0 \leq S \leq 1$) (-)

In the thermohydrology experiments, ideally the only parameter in the attenuation expression that changed during an experiment was the local water content (equivalent to saturation for a given porosity). That is, if the container wall thickness and the medium thickness remain constant, changes in the measured count rate would be entirely attributed to a change in local saturation. Equation (3-1) could then be used to determine changes in the local saturation by recording changes in the gamma beam intensity. It was possible that the density of either the silica beads (Test 1) or the cement mixtures (Tests 7, 9, and 10) varied during the experiment. However, the consistency of densitometer measurements of the silica beads and, particularly, the cement mixture throughout the duration of each experiment, would suggest that matrix density remained constant, at least in terms of gamma-ray attenuation. In this case, measured changes in densitometer counts are wholly attributed to changes in saturation. However, densitometer measurements would not detect pore water that chemically bonded to the cement during additional curing of the mixture. In this circumstance, a reduction in available pore water would not be detectable with a densitometer. The amount of water chemically taken into the matrix, if any, was not independently quantified during testing. A listing of the equipment used in the densitometer measurements is given in Table 3-4.

Differences in the objectives of the experiment groups required the use of two differently oriented densitometers. Both of these densitometers were mounted on traversing systems that simultaneously moved the detector and radiation source to scan the test containers. The densitometers were constructed with traversing systems that moved in two orthogonal directions in accordance with an automated data acquisition system (DAS).

Tests 1 through 7 were vertically oriented 1D and 2D experiments. Flow and moisture redistribution in the x-z plane were of interest in these experiments and flow in the y-direction was neglected. A densitometer that measured attenuation over the x-z plane (by integrating attenuation in the y-direction) was used in these experiments. The radiation source was placed on one side of the test container, and the radiation detector was placed on the other side. This x-z densitometer used a 500 mCi ^{137}Cs radiation source equipped with a scintillation-type detector. The energy level of the ^{137}Cs source is 662 KeV.

Tests 8 through 11 had different objectives and a correspondingly different geometric configuration. The densitometer used in these experiments traversed in the x-y plane and integrated attenuation in the z-direction. The x-y (or x-r) densitometer was equipped with a 300 mCi ^{137}Cs radiation source and a pulse height analyzer. In practice, either a single or double radial traverse was measured in these experiments to take advantage of the radial symmetry and assumed matrix homogeneity of the experiment.

In conducting Tests 1 through 6 and Test 8, an adaptation of the standard method was used to calculate the water saturation levels. By taking densitometer readings for the fully saturated and completely dry test container, it was possible to eliminate the attenuation of the container and solid media. Thus, Eq. (3-1) results in the Beer-Lambert law (Moore, 1963):

Table 3-4. Gamma-ray densitometer components

Test Numbers	Gamma Source	Detector	Traverse Direction
1-7	500 mCi ^{137}Cs (662 keV) 3.2 mm dia. collimator	Ludlum Instruments Model 44-14 NaI Detector Model 2200-1 Scaler/Ratemeter	x and z
8-11	300 mCi ^{137}Cs (662 keV) 3.0 mm dia. collimator	Canberra Nuclear Products Model 802-3 NaI Detector Model 35+ Multichannel Analyzer	x and y

$$S = \frac{\ln \left(\frac{I_d}{I} \right)}{\ln \left(\frac{I_d}{I_w} \right)} \quad (3-2)$$

where

I_d = gamma beam intensity through container and dry media (counts/s)
 I_w = gamma beam intensity through container and saturated media (counts/s)
 I = gamma beam intensity at unknown saturation level (counts/s)

With this equation, the attenuation coefficients, media porosity, container thickness, and media thickness are eliminated, and a direct measure of the saturation level is obtained.

For Tests 7 and 9 through 11, another variation of the standard method was used to calculate saturation level. A densitometer measurement for a medium at a known saturation can provide sufficient information to determine the saturation change associated with a different densitometer reading at the same location, provided that saturation is the only property changed. Given this information, all other unknowns in the attenuation equation [Eq. (3-1)] can be summed and cumulatively determined. After this cumulative unknown has been determined, saturation can then be determined from densitometer measurements made at the identical location but at different saturation values. This technique was used to calculate saturation from densitometer measurements in tests in which the initial saturation was known but densitometer values at zero and full saturation were not. Initial saturation averaged for the entire test medium was known for all experiments; however, this saturation was vertically variable through test media with a relatively high permeability (i.e., silica beads, tabular alumina, and ceramic). Thus, saturation at each densitometer measurement point was not well known even though average saturation was known. Determination of saturation with this technique was better suited to test media with low permeability (i.e., Tests 7, 9, 10, and 11).

Attenuation measurements were made on aluminum standards prior to and subsequent to each traverse to normalize measurements made over a period of time. The aluminum standards were maintained constant throughout the course of the experiments; thus, attenuation of gamma rays through these standards was assumed to remain constant. Measurement of attenuation before and after each traverse allows normalization of the attenuation measurements to remove those transient effects that impact the measurements, both during each traverse and throughout the duration of the experiment. Normalizing each measurement to the aluminum standards allows quantitative comparison of attenuation measurements that reflect changes in test container density (from which saturation can be calculated or inferred) rather than transient effects not related to the objective of an experiment. All densitometer data were normalized to the aluminum standards prior to use in these analyses.

Gamma-ray production from a radioactive source is not constant with time but instead follows a Poisson distribution. Consequently, there will be fluctuation in the count rate measured at the detector. An average count rate with mean N will have a standard deviation of $\sqrt{N}$. As an example, the typical count for Test 11 was about 200,000 counts (over a 1 min count period); hence, the standard deviation due to the random emission nature of the gamma source was $\sqrt{200,000}$ or about 450 counts. In accordance with the second saturation determination method discussed above, a 1-percent decrease in saturation corresponded to an increase of about 585 counts. Therefore, the accuracy limit for the saturation calculations was about 1 percent in Test 11. Similar calculations for the other tests with similar total counts also indicate an accuracy in saturation calculations of about 1 percent.

3.3.5 Liquid Flow Measurements

In order to study the relationship between thermohydrologic phenomena and solute transport in partially saturated media, various methods of monitoring the liquid flow patterns were reviewed (Green et al., 1993b). Based on this review, a dye tracer method was selected. This method of tracking the liquid movement was used in Tests 1, 2, 3, 4, and 7. In conducting the tracer test, a very small amount of liquid dye (i.e., <0.1 ml) was injected into the test media, which was enclosed in transparent walls. Photographs were taken periodically to capture the dye patterns representing the flow features. The time-lapse photographs provided a flow visualization that captured the general flow directions and solute-spreading patterns.

3.3.6 Heater Control and Measurement

All experimental tests incorporated heating of the porous media to create a range of hydrothermal conditions. For Tests 1 through 4, heat was supplied by circulating water from a constant-temperature bath (Neslabs EX-251HT and Neslabs Model EN-850 cooler) through a bayonet heater placed in contact with the porous media. The heat source was changed to electric resistance heaters for Tests 5 through 11 to provide temperatures in excess of 100 °C and to allow for measurement of heater power. The heater power was set using a Variac, and was measured using an Ohio Semitronics Model GW5-001X5 watt meter.

3.4 HYDRAULIC AND THERMAL CHARACTERIZATION OF TEST MEDIA

In conducting the sequence of thermohydrology experiments, both unconsolidated and consolidated media were used. The unconsolidated media consisted of silica and tabular alumina, while the consolidated media consisted of an industrial ceramic, cement mixtures, and tuff. In the early series

of laboratory-scale experiments, unconsolidated media were used because of their uniform properties. This series of experiments was followed by experiments with consolidated media, which were progressively more representative of the geologic media at the proposed repository site.

Silica beads were used as the initial test medium in the first laboratory experiment, which was designated as Test 1. Next, experiments referred to as Tests 2 through 5, and Test 8, were conducted with tabular alumina. These experiments were followed by Tests 7, 9, and 10, which used cement slurries as the test medium. The final experiment, Test 11, used a tuff rock sample from the ALTS in Arizona.

Physical, thermal, and hydraulic properties of the test media, for the most part, were obtained through direct laboratory measurement. In some cases, estimates of these properties for certain test media were obtained from the literature. Measurements were performed at CNWRA laboratories for (i) bulk density, (ii) effective porosity, (iii) saturated liquid permeability, and (iv) water retention and relative permeability curves. Thermal conductivity measurements for consolidated media samples were obtained with the assistance of the Southern Methodist University (SMU). Thermal conductivity values for the unconsolidated media and other property values of media samples, for which no other measurement values were available, were taken from the literature or estimated using analytical methods. This section provides a detailed description of the test media used, the characterization methodologies, and summaries of the characterization data compiled for the test media.

3.4.1 Description of Test Media

The silica-glass coated beads used in Test 1 were obtained from FERRO Corp., Cataphote Division. The beads are Class IV, annealed unispheres of soda-lime glass with manufacturer's specifications of ≤ 15 percent irregular shaped particles. Two separate fractions of factory-sieved beads (one from 28 to 53 μm and the other from 74 to 105 μm) were combined to create the bead mixture used in Test 1. The resulting 50/50-percent by volume bead mixture had a bimodal size distribution.

The tabular alumina samples used in Tests 2 through 5 (and later Test 8) were manufactured by ALCOA, Inc., and are described as massive sintered alumina, thoroughly shrunk and consisting of coarse well-developed alpha alumina crystals (ALCOA Chemical, 1969). Chemical analysis indicates that the tabular alumina contains 99.7 percent Al_2O_3 , 0.16 percent Na_2O , 0.06 percent Fe_2O_3 , and 0.04 percent of SiO_2 and CaO . Three different sieve fractions of tabular alumina were used in the experiments. Mesh size for the tabular alumina used in the experiments included 60, 100, and 325, which translate to grain sizes of ≤ 250 , ≤ 149 , and ≤ 44 μm , respectively. The 100-mesh tabular alumina was used in Test 2. Tests 3, 4, and 5 also used 100-mesh tabular alumina, however, only after the alumina was wet-sieved with a 325 mesh to eliminate the fines. The 60-mesh tabular alumina was used in Test 8, a scoping experiment for the gas-flow experiments.

An industrial ceramic from Refractron Technologies was used in Test 6. The ceramic consisted of 90 percent Al_2O_3 and 10 percent aluminum silicate. Cement slurry mixtures were used in Test 7 (cement slurry C4), Test 9 (cement slurry C3), and Test 10 (cement slurry C6). Cement slurry C3 consisted of cement and water. C4 and C6 were of similar composition and contained additives in addition to water and cement. The mixture used in these two tests consisted of type 1 Portland cement, barite powder, bentonite powder, water, Draceon, Vynsol resin (for air entrainment), and ivory soap. The Test 10 sample differed in preparation from Test 7 in that it was vibrated as it was poured into the test enclosure. All cement slurry mixtures were cured at room temperature for a minimum of 30 days prior to use in the experiments. The chemical effects of the concrete cylinder on liquid or vapor transport were recognized but not considered in the analyses.

The cylindrically shaped tuff sample, that was used in Test 11 was prepared from a larger 0.46-m-diameter core sample. This tuff sample was collected from an abandoned road tunnel located approximately 2 km west of the ALTS (Hsiung et al., 1994). The 0.12-m-tall 0.30-m-diameter cylinder used in Test 11 was cored and cut from the larger core sample extracted from the road tunnel. The tuff at the road tunnel is more densely welded than the tuff at the ALTS; therefore, media properties for the Test 11 sample were measured and not taken from Rasmussen et al. (1990) who had initially characterized the ALTS tuff.

3.4.2 Characterization Methodologies

Laboratory characterization methodologies for soils were directly applicable to the silica bead and tabular alumina media. Characterization methodologies for consolidated media, which are typically adapted from soil characterization procedures, were used to measure the ceramic, cement slurry mixtures, and the ALTS tuff. A brief description of the characterization methodologies is summarized in this section. A more detailed description of the characterization methodologies is presented in Green et al. (1994), with the exception of the thermal conductivity measurement methodology. The thermal conductivity measurement methodology used for the consolidated media is described in Blackwell and Spafford (1987). A description of estimation techniques used to determine thermal conductivity for unconsolidated media from published values is contained here.

Standard testing procedures were used to determine the material properties, namely bulk density, effective porosity, and thermal conductivity. Bulk density of the unconsolidated and consolidated media was measured using a standard testing procedure described in Rasmussen et al. (1990), in which bulk density is defined as the dry mass (g) of a sample divided by the sample volume (cm^3). Two methods were used to determine the effective porosity: (i) the gravimetric method, and (ii) the pycnometric method. The gravimetric method is described in Rasmussen et al. (1990) and the pycnometric method was adapted from that described in Gardner (1986). Saturated and dry thermal conductivities of the consolidated test media were measured using the divided bar method (Blackwell and Spafford, 1987). Thermal conductivities of the unconsolidated tabular alumina and the silica beads were taken from the manufacturer's data sheets and calculated using analytical methods (Woodside and Messmer, 1961).

Saturated permeability was measured for both unconsolidated and consolidated media using a constant-head permeameter following the procedure described in American Society for Testing and Materials (ASTM) 5084-90. Moisture retention data were obtained using three different methodologies, each for a different range of matric potentials. Saturation/matric potential data at low matric potentials (i.e., up to 15 bar), or relatively wet conditions, were measured with a porous plate extractor following ASTM D3152-72 and ASTM D2325-68 procedures. Retention curve data for samples with matric potentials from about 2 to 15 bar were measured with the centrifuge methodology adapted from Flint and Flint (1990). Samples at the dry end of the drying curve, with matric potentials as low as 10 bar to greater than 1,000 bar, were measured using an Aqualab CX-2 water activity meter (Gee et al., 1992). In all three methods, the percent saturation was determined gravimetrically. All retention curve data were collected during drying. The measured matric potential/saturation relationship for each test medium was used to identify a moisture retention curve for that medium. Relative permeability curves were estimated using the van Genuchten-Mualem theory (van Genuchten, 1978). All hydraulic characterization measurements were conducted at room temperature.

3.4.3 Summary of Test Media Properties

Measurements of the material, thermal, and hydraulic properties of the unconsolidated and consolidated test media are summarized and discussed in the following sections.

3.4.3.1 Bulk Density

Bulk density measurements for the unconsolidated test media were conducted on samples collected from the same supply as the test media. In the case of the consolidated media, such as the cement slurry, additional samples of the medium were prepared at the same time the test medium was constructed, then retained for property characterization. Problems encountered in obtaining accurate bulk density measurements for the unconsolidated media are attributed to inconsistency in packing, which resulted in variations of bulk density as large as 18 percent. Bulk density measurement of the silica beads was also affected by bead degradation, that is, dissolution and precipitation of silica.

Difficulties with packing were not encountered during bulk density measurement of the consolidated media, although the bulk density of the cement slurry mixtures may have been changed by the continued alteration they experienced during testing. Bulk density measurement of the cement slurry mixtures was conducted on pre-test samples prior to any alteration that might have resulted from the conduct of the experiments. The effect of continued alteration on bulk density measurements was not further evaluated. Bulk density measurements listed in Table 3-5 for all test media were taken for pre-experiment media samples. Also included in Table 3-5 are the mean, maximum, and minimum bulk density values.

3.4.3.2 Effective Porosity

Porosity data for the test media were obtained using standard measurement methods. Sample preparation for effective porosity measurements was similar to that for the bulk density measurements. As in bulk density measurements, problems were encountered with maintaining packing consistency of the unconsolidated media, degradation of the silica beads, and continued alteration of the cement slurry mixtures. Packing inconsistencies in the unconsolidated media resulted in porosity measurements that varied by about 20 percent. Effective porosity measurements of the test media are summarized in Table 3-6. The mean, maximum, and minimum effective porosity values are also given in the table.

3.4.3.3 Saturated Liquid Permeability

Saturated permeability was measured for each test medium using a standard constant-head permeability test. Permeability measurements for the tabular alumina, ceramic, and the tuff were successful, and the permeability appeared to remain constant throughout the duration of their respective measurements. However, some problems were encountered in performing the measurements for the silica beads and cement slurries. For example, the permeability of silica beads varied during the conduct of the experiments. Scanning electron microscope (SEM) photographs of the silica beads taken after the execution of Test 1 indicated degradation of the medium and apparent changes in the permeability value. Water flow through the cement slurry mixture samples was not constant during the constant-head permeability test. This transient effect, in addition to growth of calcite minerals on the end plates of the permeability testing apparatus, indicated that the cement may not have been fully cured and that mineralogical alteration occurred during testing.

Table 3-5. Bulk density measurements of the test media

Bulk Density (g/cm ³)					
Test Number	Test Medium	Mean	Maximum	Minimum	No. of Samples
1	silica beads	1.53	1.59	1.45	8
2	≤149 μm tabular alumina	2.35	2.48	2.15	17
3	≥44 μm and ≤149 μm tabular alumina	2.00	2.09	1.93	8
4	≥44 μm and ≤149 μm tabular alumina	2.00	2.09	1.93	8
5	≥44 μm and ≤149 μm tabular alumina	2.00	2.09	1.93	8
6	ceramic	1.68	1.73	1.64	5
7	cement slurry (C3)	1.60	1.63	1.56	10
8	≤250 μm tabular alumina	2.29	2.55	2.14	10
9	cement slurry (C4)	1.57	1.67	1.49	17
10	cement slurry (C6)	1.82	n/a	n/a	1
11	tuff	2.44	2.49	2.42	6

Consequently, the saturated permeability data presented here are for the test media prior to actual conduct of the laboratory experiment. Whether these pre-test values are sufficiently representative of the actual test medium permeability, under the conditions of the experiments, is uncertain. Saturated permeabilities measured on pre-test samples are summarized in Table 3-7.

3.4.3.4 Thermal Conductivity

Although the thermal conductivities of different geologic media are, in general, relatively similar, they can vary significantly with water saturation level. Media exposed to heat sources will experience wide variability in saturation levels. This dependence on saturation level appears to be greater for high-porosity earth materials than for low-porosity materials (Woodside and Messmer, 1961). In the case of low-porosity tuff, for example, the ratio of wet to dry thermal conductivity has been found to be no greater than 2 (Ashworth, 1992) and often much less, while high-porosity sands have a ratio of about 10 (Woodside and Messmer, 1961).

Thermal conductivity values for the test media used in this study were compiled through a combination of: (i) direct measurements, (ii) analytical methods, and (iii) published values. Thermal

Table 3-6. Effective porosity measurements of the test media

Test Number	Porosity				No. of Samples
	Test Medium	Mean	Maximum	Minimum	
1	silica beads	0.38	0.43	0.34	8
2	≤149 μm tabular alumina	0.37	0.39	0.34	9
3	≥44 μm and ≤149 μm tabular alumina	0.45	0.48	0.42	8
4	≥44 μm and ≤149 μm tabular alumina	0.45	0.48	0.42	8
5	≥44 μm and ≤149 μm tabular alumina	0.45	0.48	0.42	8
6	ceramic	0.42	0.44	0.41	5
7	cement slurry (C3)	0.50	0.52	0.48	10
8	≤250 μm tabular alumina	0.31	0.31	0.30	8
9	cement slurry (C4)	0.36	0.39	0.30	17
10	cement slurry (C6)	0.45	n/a	n/a	1
11	tuff	0.06	0.07	0.05	6

conductivity values for unconsolidated media (silica beads and tabular alumina) were determined using published values, and values for the consolidated media (ceramic, cement slurry, and tuff) were determined by direct measurement. Where available, published thermal conductivity values for the test media were compared with the calculated or measured values.

For the silica beads, thermal conductivity values were taken from Woodside and Messmer (1961). These values are assumed to represent the pre-test silica beads, and the effect of bead degradation on thermal conductivity was not measured. Similarly, the thermal conductivity of the tabular alumina was not measured; they were assigned dry thermal conductivity values obtained from the manufacturer's specification sheet. The thermal conductivity value of 2.6 W/m-K for the tabular alumina corresponded to a porosity of 26 percent, a porosity similar to the 27-percent porosity for the un-sieved tabular alumina used in Test 2, but less than the 37-percent porosity of the sieved tabular alumina used in Tests 3, 4, and 5.

For three different sand samples, Woodside and Messmer (1961) report wet to dry thermal conductivity ratios of about 10. Similarly, for glass beads, they report a ratio of about 4. The porosity of the sands was 19 to 59 percent, and the glass beads 38 percent in their study. Based on these observations,

Table 3-7. Saturated liquid permeability measurements of the test media

Saturated Liquid Permeability			
Test Number	Test Medium	Permeability (m^2)	No. of Samples
1	silica beads	6.23×10^{-13}	6
2	$\leq 149 \mu\text{m}$ tabular alumina	2.95×10^{-14}	10
3	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina	8.04×10^{-13}	10
4	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina	8.04×10^{-13}	10
5	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina	8.04×10^{-13}	10
6	ceramic	3.75×10^{-13}	5
7	cement slurry (C3)	n/a	—
8	$\leq 250 \mu\text{m}$ tabular alumina	5.5×10^{-14}	1
9	cement slurry (C4)	2.06×10^{-18}	4
10	cement slurry (C6)	n/a	—
11	tuff	5.0×10^{-17}	1

the thermal conductivity for wet tabular alumina was estimated to range from about 3 to 5 W/m-K. Although these values are high, they are significantly less than the measured thermal conductivity of 18 W/m-K for a consolidated alumina (99.5-percent Al_2O_3 ceramic) with porosity less than 1 percent (ALCOA Chemicals, 1969). The relatively lower wet thermal conductivity for the tabular alumina was estimated to account for the measured porosity of 27 to 37 percent.

Dry and wet thermal conductivity values for the consolidated samples [ceramic, cement (C3), cement (C4), and tuff] were measured at the SMU Geothermal Laboratory using the divided bar thermal conductivity technique (Blackwell and Spafford, 1987). Cement (C6) was assigned the same values as cement (C4), since both cement slurry mixtures had the same composition. Thermal conductivity values for the test media are summarized in Table 3-8.

A number of candidate relationships exist for calculating thermal conductivity as a function of water saturation. First, however, an appropriate relationship relating solid- and liquid-phase fractions to an effective thermal conductivity must be considered. For a parallel model of the matrix and fluid-filled pore space of the medium, Domenico and Schwartz (1990) give a linear relationship between the matrix and fluid components, namely:

Table 3-8. Summary of dry and wet thermal conductivities for test media

Thermal Conductivity					
Test Number	Medium	Porosity	Thermal Conductivity-Dry (W/m-K)	Thermal Conductivity-Wet (W/m-K)	No. of Samples
1	silica beads	0.38	0.2	0.9	—
2	≤149 μm tabular alumina	0.31	2.6	3-5	—
3	≥44 μm and ≤149 μm tabular alumina	0.41	2.6	3-5	—
4	≥44 μm and ≤149 μm tabular alumina	0.41	2.6	3-5	—
5	≥44 μm and ≤149 μm tabular alumina	0.41	2.6	3-5	—
6	ceramic	0.42	2.194	3.4091	5
7	cement slurry (C3)	0.50	0.502	1.0207	1
8	≤250 μm tabular alumina	0.32	2.6	3-5	—
9	cement slurry (C4)	0.36	0.728	0.9746	2
10	cement slurry (C6)	0.45	0.728	0.9746	—
11	tuff	0.06	1.744	1.9091	5

$$\kappa_e = \phi \kappa_f + (1 - \phi) \kappa_s \quad (3-3)$$

where κ is thermal conductivity, ϕ is porosity, and the subscripts e , f , and s denote effective, fluid, and solid, respectively. Likewise, Woodside and Messmer (1961) propose a series model

$$\kappa_e = \frac{\kappa_s \kappa_f}{\phi \kappa_s + (1 - \phi) \kappa_f} \quad (3-4)$$

A tortuosity term can be added to Eq. (3-3) to accommodate the parallel model for the nonparallel structure encountered in porous media (Slattery, 1972). This added term yields

$$\kappa_e = \phi \kappa_f + (1 - \phi) \kappa_s - \kappa_s \kappa^* \quad (3-5)$$

where κ^* represents a reduction in free transport because of the tortuosity of porous media.

These three relationships can be used to calculate fully saturated (wet) and fully unsaturated (dry) thermal conductivity values by assigning either water or air values, respectively, as the fluid thermal conductivities. However, these expressions do not define variations in thermal conductivity values as a function of saturation. The heat and mass transfer simulator V-TOUGH (Pruess, 1987; Nitao, 1990) provides two models that represent the thermal conductivity/saturation relationship—either a linear model or a relationship weighted by the square root of saturation (Somerton et al., 1973, 1974). The linear model is:

$$\kappa(S_l) = \kappa_d + S_l(\kappa_w - \kappa_d) \quad (3-6)$$

and the weighted model is

$$\kappa(S_l) = \kappa_d + \sqrt{S_l} (\kappa_w - \kappa_d) \quad (3-7)$$

where the subscripts d and w denote dry and wet, respectively. Dry or wet thermal conductivities calculated with either Eqs. (3-3), (3-4), or (3-5) could be incorporated into Eqs. (3-6) or (3-7).

Thermal conductivity measurements by Woodside and Messmer (1961) indicate that a linear relationship may not be appropriate for selected geologic porous media (e.g., various sand samples). Selection of the appropriate thermal conductivity/saturation relationship for unconsolidated media is difficult. There is not an extensive database of thermal conductivity/saturation measurements for the unconsolidated media used in this investigation. Thus, the presence of significant nonlinear features may go undetected. Also, thermal conductivity in unconsolidated media is sensitive to packing. Methods and degree of packing can have a profound effect on grain-to-grain connectivity and, consequently, on the funicularity of water and the resultant thermal conductivity of unconsolidated sample. Nonetheless, a linear thermal conductivity/saturation model was assumed for the unconsolidated media due to the lack of detailed saturation dependent thermal conductivity measurements.

Data reported by Ashworth (1992) for tuff samples from the ALTS indicated a plateau/jump feature in thermal conductivity near mid-saturation. Several alternative models were proposed by Ashworth to explain this departure from linearity. However, since this departure from a linear thermal conductivity/saturation relationship is not significant and there is no evidence to support a weighted model, the assumption of a linear thermal conductivity model for the tuff samples has been made in these analyses.

3.4.3.5 Water Retention and Relative Permeability Curves

Unsaturated hydraulic properties consisting of the water retention and relative permeability curves were determined for each test media. Water retention curves have been determined for all test media using

saturation and matric potential data measured with porous plate extractors, centrifuge, and a water activity meter. All measurements were made at room temperature. No attempt was made to evaluate the effect of changes in temperature on the saturation-matric relationship exhibited by the media. Each set of saturation-matric potential data was fitted using the RETC computer code (van Genuchten, et al, 1991) which calculates the fitting parameters for the van Genuchten (1978) soil properties models. The curves produced with these soil property models are shown in Figures 3-5a through 3-5g. The water retention curves are plotted with their respective data set. Values for the van Genuchten fitting parameters, α , n , and S_r , are summarized in Table 3-9 for each test medium. The relative permeability curves were estimated using the Mualem theory (Mualem, 1976). The van Genuchten retention curve relationship and the relationship of $m=1-1/n$ have been assumed in these calculations. Goodness of fit between the measured retention curve data and the fitted retention curve was determined by visual observation. The highly nonlinear saturation-matric potential relationships of media with narrow pore-size distributions resulted in less than desirable curve fitting. This lack of agreement was particularly noticeable at low saturation with the $\leq 149 \mu\text{m}$ tabular alumina (Figure 3-5b). The source for this particular discrepancy has not been discerned. However, these representative models were the best possible and were used in subsequent analyses.

(a)

(b)

Figure 3-5. Water retention curves for test media: (a) silica beads (b) $\leq 149 \mu\text{m}$ tabular alumina

(c)

(d)

Figure 3-5 (Cont'd). Water retention curves for test media: (c) $\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina, and (d) ceramic

(e)

(f)

Figure 3-5 (Cont'd). Water retention curves for test media: (e) cement slurry (C3), and (f) $\leq 249 \mu\text{m}$ tabular alumina

(g)

Figure 3-5 (Cont'd). Water retention curves for test media: (g) ALTS tuff

Table 3-9. van Genuchten α and n parameter values for the test media

Unsaturated Hydraulic Parameters				
Test Number	Test Medium	van Genuchten α ($\times 10^5 \text{ Pa}^{-1}$)	van Genuchten n	Residual Saturation
1	silica beads	7.19	6.81	0.08
2	$\leq 149 \mu\text{m}$ tabular alumina	3.58	2.70	0.02
3	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina	13.10	5.00	0.08
4	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina	13.10	5.00	0.08
5	$\geq 44 \mu\text{m}$ and $\leq 149 \mu\text{m}$ tabular alumina	13.10	5.00	0.08
6	ceramic	2.42	8.23	0.02
7	cement slurry (C3)	0.0636	1.373	0.05
8	$\leq 250 \mu\text{m}$ tabular alumina	—	—	—
9	cement slurry (C4)	—	—	—
10	cement slurry (C6)	—	—	—
11	tuff	0.0144	1.575	0.02

4 HEAT AND MASS TRANSFER MECHANISMS ANALYSES

This chapter summarizes the analyses of heat and transfer mechanisms using the results of the laboratory-scale experiments conducted in this study. These results provided the necessary information to investigate fluid flow formation near a heat source, particularly in the region of vaporization and condensation.

Of the 11 experiments conducted in this study, the first 7 provided the physical basis for evaluating the heat and mass transfer mechanisms affecting redistribution of thermally driven moisture through partially saturated porous media. The other four, Tests 8 through 11, provided information for evaluating the proposed scaling laws; in addition, these gas pressure buildup tests also contributed to the evaluation of heat and mass transfer mechanisms. The soundness of the interpretation of the heat and mass transfer mechanisms was further tested by conducting numerical analyses of the laboratory-scale experiments.

Analyses were performed using experiments and numerical simulations designed to isolate specific heat and mass transfer mechanisms identified as important in earlier theoretical studies and reviews of previous laboratory- and field-scale experiments. Numerical analyses were conducted using either V-TOUGH (Pruess, 1987; Nitao, 1990) or a modified version of V-TOUGH, referred to as C-TOUGH. Modifications to V-TOUGH that resulted in C-TOUGH include new pre- and post-processors and a new iterative solver. Comparisons between results from V-TOUGH and C-TOUGH indicate that both codes generate practically identical numerical predictions. C-TOUGH was used in most numerical analyses reported in this document because of the added ease provided by the modified pre- and post-processors, and because of the increased numerical efficiency.

Results from the laboratory-scale experiments, field-scale heater tests, and numerical analyses contribute to the understanding of heat and mass transfer mechanisms instrumental in thermally driven moisture redistribution in partially saturated porous media. The first issue addressed in these analyses is the identification of the driving mechanisms responsible for moisture redistribution at a geologic HLW repository. Results of experiments conducted under both sub-boiling ($T < 100^{\circ}\text{C}$) and boiling conditions ($T > 100^{\circ}\text{C}$) were used to identify the contribution of water transport as both vapor and liquid to moisture redistribution observed in laboratory- and field-scale experiments. Some unresolved questions, however, were identified. These questions include (i) the contribution of each phase to heat and mass transfer, (ii) the duration of their respective contributions, and (iii) the spatial scale at which each phase of transport operates. Practical limitations were encountered in attempting to resolve these issues. For example, liquid flow could be directly monitored using dyes injected into the flow field of some experiments; however, vapor phase flowlines could only be inferred. Similar difficulties were encountered when attempting to measure the quantity of water transported as vapor or as liquid. Again, liquid quantities at least could be estimated using measured values for saturation, permeability, and pressure gradients; however, vapor transport quantities only could be inferred. The indirect inference for vapor transport is a source of uncertainty.

The nature of the fluid flow fields is primarily dependent on the hydraulic properties and thermal conductivity of the medium, strength of the heat source, and saturation level of the medium. These properties, as well as other factors, were monitored and controlled during each experiment. The sensitivity of the flow fields to these properties was assessed by varying their values in both laboratory and numerical experiments. Numerical simulations of experiments were also conducted in this evaluation to assess the

sensitivity of flow fields to changes in these property values. The effect of enhanced vapor diffusion was not considered in these analyses, although results by Lichtner and Walton (1994) indicated this effect could be significant for some conditions.

4.1 LIQUID FLOW REDISTRIBUTION EXPERIMENT RESULTS

Liquid flow redistribution was the focus of experiments conducted under sub-boiling conditions in four experiments (Tests 1 through 4), and under boiling conditions in three experiments (Tests 5 through 7). As discussed in Chapter 3, the type of test medium, boundary conditions, and heat source were among the factors varied in these experiments. In the sub-boiling tests, experiments designed to examine liquid flow regimes caused by a heat source were studied for both 1D (Tests 1 and 2) and 2D (Tests 3 and 4) geometries. The boiling tests (Tests 5 through 7) were designed to examine mass and heat transfer in 2D geometries. For both of the 1D tests and some of the 2D tests, the direction of liquid flow in the test cells was monitored by observing the movement of dyes injected at strategic locations. The state of the liquid phase was monitored using temperature, densitometer, and matric pressure measurements. An analysis and discussion of results from the 1D and 2D liquid flow redistribution experiments are presented in the following subsections.

4.1.1 Tests 1 and 2: One-Dimensional Experiments

Two experiments (Tests 1 and 2) were conducted in a 1D geometry as part of the liquid flow redistribution experiments. The design and objectives of these experiments built on the results of an earlier series of separate effects and scoping experiments conducted as part of the Thermohydrology Research Project that are summarized in Green et al. (1993b). Preliminary results of Test 1 are contained in this earlier report. (Note: The test numbering system was revised after the earlier work. Test 1 in the present report was identified as Test 6 in the earlier work.) Test 2 was designed and conducted to address uncertainties raised in Test 1 results. These uncertainties may have resulted from the inclusion of the artificial fracture in Test 1. Preliminary results and discussions of Test 1 and 2 have been published previously in Manteufel et al. (1992) and Manteufel and Green (1993).

The objective of Tests 1 and 2 was two-fold: (i) to understand basic mechanisms of heat and mass transfer in a 1D geometry, and (ii) to help guide the design of more realistic and insightful experiments. To accomplish this goal, the 1D experiments were designed to avoid complications arising from media heterogeneities and complex boundary conditions. Some complications, but not all, were successfully avoided in the execution of these experiments. Nonetheless, lessons learned from Tests 1 and 2 contributed to the design of subsequent experiments whose results responded more directly to issues of thermally driven moisture redistribution through naturally occurring porous media.

The experimental designs of Tests 1 and 2 were similar, with the exceptions that different media were used, Test 1 contained a simulated fracture, and Test 2 included a higher degree of instrumentation. The silica bead test medium used in Test 1 and in the earlier scoping experiments was not used in subsequent experiments because it exhibited significant degradation during the conduct of the experiment. The SEM photograph shown as Figure 4-1 illustrates the dissolution and precipitation of silica observed after Test 1. The degradation has been attributed to the aggressive effect of the slightly acidic (pH-5) deionized water used in the experiment. Because of the degradation, the silica bead retention curve reported in Section 3.4 did not represent the saturation/matrix potential relationship of the silica beads over the entire duration of Test 1. Measurement of a representative value for permeability of the silica beads was not possible. Although difficulties were encountered with the media in Test 1, quantitative assessments of the tests have been made and are reported here.

Figure 4-1. Scanning electron microscope photograph of the post-test silica beads used in Test 1

Several distinct manifestations of moisture redistribution were observed near the heated boundary in these experiments. The best defined and most pertinent of these manifestations was the way in which thermally driven water redistributed in the porous media. It was observed that liquid can accumulate in a narrow zone near the heat source (Test 1) or lead to a gradual saturation gradient in the media (Test 2). In both tests, a dryout zone was observed near the heat source. Vaporization, vapor diffusion, condensation, and liquid advection were observed to be the primary driving mechanisms which, when coupled with hydraulic properties of the media, dictate the liquid redistribution.

The formation of the dryout zone/moisture buildup zone has potentially important implications. Moisture that remains close to the heat source rather than moving to a greater distance before condensing would have a greater hydraulic potential and shorter distance back to the heat source than moisture uniformly condensed at a greater distance. Therefore, the source mechanism(s) for this dryout zone/moisture buildup zone should be identified. This moisture redistribution mechanism is evaluated by analyzing Test 1, which exhibited a defined, narrow moisture buildup zone, and Test 2, which exhibited liquid redistribution over a broad area. Physical properties of Test 1 that differed from Test 2 are potential candidates for causing the formation of a prominent dryout/moisture buildup zone in Test 1. Included are differences in media properties (i.e., thermal conductivity, permeability, matric pressure/saturation

relationship, etc.) between the silica beads and the tabular alumina, and the increased temperature gradient in Test 2. The tabular alumina also had higher suction pressures which resulted in a higher capability to advect liquid that dissipated the condensate buildup. As mentioned, additional complications were encountered when attempting to interpret the results because of the degradation of the silica beads used in Test 1.

4.1.1.1 Experimental Results

A combination of experimentally measured and observed results was used in the analysis of the 1D series of experiments. Test variables measured in the 1D liquid flow redistribution experiments that were used in the analyses included:

- Temperature distributions measured using internal and external thermistors
- Liquid flow pathlines measured using injected dyes
- Liquid saturation determined using a gamma-ray densitometer
- Matric potential measured using internal tensiometers

Temperature Profiles. Horizontal temperature profiles for Test 1 (from 20 °C on the left to 60 °C on the right) and for Test 2 (from 20 °C on the left to 90 °C on the right) are illustrated in Figure 4-2. The temperature gradient was higher near the right heated side in both tests, indicating some heat loss through the uninsulated plexiglass front and back walls or thermal conductivity variation. Although approximately steady-state temperature regimes were established soon after initiation of heating in both Tests 1 and 2, the temperature distributions varied slightly throughout the duration of the experiments as illustrated in Figure 4-3. The time-varying behavior became more pronounced by the end of the experiment. An explanation for this time-varying temperature is that the thermal conductivity was moisture-dependent and the saturation profile changed during the test. As illustrated in Table 3-8, the thermal conductivities of the silica beads and the tabular alumina vary from dry (0.2 W/m-K for the silica beads and 2.6 W/m-K for the tabular alumina) to wet (0.9 W/m-K for the silica beads and 3.5 W/m-K for the tabular alumina). The potential of these two candidate physical mechanisms to cause a nonlinear temperature gradient was numerically evaluated.

Liquid Movement. Movement of liquid through the test media in Tests 1 and 2 was examined by injecting neutrally buoyant inert dye into the test container at two locations about a third of the distance up from the bottom boundary, one near the heated boundary and the other near the cool boundary. Figure 4-4 photographically illustrates the dye movement over a duration of 6 days for Test 1, and Figure 4-5 shows the dye movement for Test 2 over an 8-hr period. The dye flow patterns in each test exhibited similarities and differences. In both tests, dye injected at the left injection port (near the cool boundary) exhibited mostly diffusion-driven flow, except for some downward late-time movement as shown in the photographic sequence for Test 1. The lateral rate of diffusion was more than twice as large for Test 2, being about 8×10^{-8} m/s compared to the 3×10^{-8} m/s measured for Test 1. Since the same dye was used in both tests and the saturation was not greatly different, the different rates of diffusion are attributed to the different media types.

The major difference in the dye flow patterns of the two tests was exhibited at the injection port near the heated boundary. For Test 1, the dye injected in Test 1 moved downward and, eventually, away

Figure 4-2. Horizontal temperature profiles for Tests 1 (60 °C) and 2 (90 °C)

Figure 4-3. Transient temperature variations for Test 2

Figure 4-4. Series of photographs over a 6-day period for Test 1 using injected dye to help illustrate the dryout zone/moisture buildup zone phenomenon

Figure 4-5. Series of photographs over an 8-hr period for Test 2 using injected dye to help illustrate the movement of liquid

from the heated boundary. The expansion of a dryout zone in the lower portion of the test container was well defined by the dye. The dryout zone expanded to a distance of 3.5 cm at the bottom of the test container at a rate of almost 3×10^{-8} m/s. For Test 2, there was less dye movement near the heated boundary than for Test 1. Additionally, the dryout zone was less extensive than the dryout zone in Test 1, even though the temperature of the heated boundary was greater. One final important observation is that the movement of dye from the right injection port was directly toward the heated boundary, while in Test 1, the movement of dye was obliquely away from the boundary. The advection-driven flow was downward at a rate of 2×10^{-7} m/s in Test 1 and laterally at 1×10^{-6} m/s in Test 2. Similar to the measured rates of diffusion-driven dye movement, the advection-driven flow in Test 2 near the heated boundary was a factor of two to five times more rapid than advection-driven flow in Test 1.

Potential reasons for higher flow rates in Test 2 than in Test 1 include differences in the permeability of the test media and the higher boundary temperature in Test 2, even though the pre-test silica bead matrix actually had a higher measured permeability than the tabular alumina. However, degradation of the silica beads undoubtedly altered the hydraulic properties of the test medium in Test 1. Inspection of the SEM photograph of the silica beads in Figure 4-1 suggests that a significant portion of the inter-bead pore space was filled with precipitate by the end of the experiment. The permeability of the silica beads evidently changed, although the permeability during or after the test was not measured.

Saturation Profiles. Evidence of actual moisture redistribution was provided by gamma-ray densitometer measurements periodically recorded throughout Tests 1 and 2, as explained in Section 3. Figure 4-6 shows saturation profiles for Test 1 at four different distances from the top of the test cell at three different times (days 75, 99, and 113). The heater was turned on at day 6 and off at day 105. The plotted results are for densitometer measurements that were averaged over a full day to increase accuracy. Although the number of calculated saturation values in both tests is sparse due to the relatively few number of densitometer measurement locations (four rows of six measurements), trends are observed in the saturation plots. For example, the graphs for the three times illustrate the growing size of the dryout zone next to the heater at the base of the test container. Although the saturation measurements do not clearly define this dryout zone, except at the base of the container ($y = 0.1651$ m), because of the lack of measurements close to the heated boundary, the formation of a band of high saturation located immediately to the cool side of the dryout zone is well illustrated. These trends indicate that most of the water that vaporized near the heated boundary condensed in a narrow band nearly parallel to the heater. These data provide the best evidence of the formation of a dryout/moisture buildup zone during Test 1.

For Test 2, Figure 4-7 illustrates the saturation profiles measured at the three lower horizontal transects measured at day 60. A greater density of data was collected in Test 2 than in Test 1 to better define the possible formation of a dryout/moisture buildup zone. A narrow zone of moisture buildup was detected 2 to 3 cm from the heated boundary. The 0.02 to 0.04 increase in saturation next to the dryout zone was significantly smaller than the more prominent but less well-defined 0.10 to 0.20 saturation buildup in Test 1. An additional important observation is that the average saturation along the left side of the test medium in Test 2 uniformly increased above the pre-test saturation of 0.50 to about 0.60 – 0.65. The area of greatest saturation increase in Test 2 occurred near the cool boundary, not next to the dryout zone as in Test 1.

Matric Pressure. For Test 1, matric pressure measured using tensiometers provided an independent means to verify densitometer-determined saturations; these pressure measurements are presented in Figure 4-8. The matric pressures for the tensiometer closest to the heated boundary increased from pre-heat pressures of about 8 kPa to pressures of 13 kPa after 80 days of heating. Matric pressure near the cool boundary

Figure 4-6. Horizontal densitometer-determined saturation profiles for Test 1 at (a) day 75. The dimension y is measured downward from the top of the test container.

Figure 4-6 (Cont'd). Horizontal densitometer-determined saturation profiles for Test 1 at (b) day 99. The dimension y is measured downward from the top of the test container.

Figure 4-6 (Cont'd). Horizontal densitometer-determined saturation profiles for Test 1 at (c) day 113. The dimension y is measured downward from the top of the test container.

Figure 4-7. Horizontal densitometer-determined saturation in Test 2 located at (a) 8.9 cm, (b) 11.4 cm, and (c) 16.5 cm from top of container

Figure 4-8. Tensiometer measurements from Test 1

Figure 4-9. Tensiometer measurements from near the cool boundary in Test 2

remained constant for the duration of the test. For Test 2, matric pressure measurements were less conclusive because of problems encountered by frequent dryout of the tensiometers, but measurements at one location near the cool boundary are presented in Figure 4-9.

The measured matric pressure/saturation relationship for the pre-test silica beads used in Test 1 is illustrated in Figure 3-5a. According to this relationship, matric pressures of 8 and 13 kPa are both equivalent to a saturation of about 0.04. This tensiometer-determined value for saturation is not in agreement with the densitometer-determined saturation. Two uncertainties were encountered in the calculation of saturations from the retention curve. First, the measured retention curve is representative of the pre-test silica beads and, therefore, does not reflect any changes that occurred during the test because of bead degradation. Second, because of the relatively narrow pore-size distribution of the beads, the retention curve is highly nonlinear, and thus minor changes in matric pressure result in large changes in saturation. Therefore, there is not a high level of accuracy in the saturation values calculated from matric pressure measurements. Nonetheless, matric pressure evidence of drying at the location of the right tensiometer is conclusive, corroborating the densitometer-calculated saturations.

The tensiometer measurements from Test 2 (located near the container base at the cool boundary) indicated matric pressures were about 12 kPa until day 56, at which time the matric pressure decreased to zero. At 80 days, the heater was turned off and the matric pressure returned to about 12 to 14 kPa. The rapid increase in matric pressure at day 96 occurred during drying of the test medium. Saturation was determined from the tabular alumina retention curve in Figure 3-5b to be about 0.05 to 0.10 for a matric pressure of 12 to 14 kPa and near full saturation when matric pressure approached zero. This indicates that water condensed near the cool boundary and away from the dryout zone during heating, then decreased back to pre-heat saturations soon after heating ceased. This observation confirms conclusions regarding moisture condensation drawn from densitometer measurements.

4.1.1.2 Numerical Analysis

Thermally driven redistribution of moisture in Tests 1 and 2 was numerically simulated using V-TOUGH. The prime objective of the numerical analysis was to ascertain the mechanism for the dryout/moisture buildup phenomenon well defined in Test 1 and weakly defined in Test 2. A secondary objective was to assess the ability of V-TOUGH to replicate the thermally driven moisture redistribution exhibited in the 1D group of experiments. Rigorous analysis of Test 1 results using numerical simulations was hampered by the apparent alteration in the hydraulic properties of the silica beads throughout the conduct of the experiment.

Assessment of the 1D group of experiments identified four media parameters that are potentially responsible for the formation of the dryout/moisture buildup zone. The four media properties are:

- Spatial and moisture-dependent variations in thermal conductivity
- van Genuchten α parameter (inverse of air-entry value)
- Liquid permeability
- Chemical effects associated with silica degradation

The potential for chemical degradation of the silica beads to lead to the formation of a dryout/moisture buildup zone was not directly evaluated. However, degradation was indirectly evaluated in terms of how the degradation potentially affected permeability and the van Genuchten α parameter.

Since the geometric configuration and the heat and mass transfer mechanisms for both Tests 1 and 2 were designed to be essentially 1D, a 1D numerical model was configured to span the horizontal distance from the cool to the hot boundaries. The basecase models for Tests 1 and 2 were assigned the property values presented in Section 3.4 and summarized in Table 4-1. The silica beads in the basecase were assigned the pre-test permeability of $6.23 \times 10^{-13} \text{ m}^2$. Several numerical grids were assessed in this analysis. The element size was decreased until no difference in numerical results was observed. These basecase simulations were used to evaluate the appropriateness of the numerical model and assigned parameter values. The effect of the fracture in Test 1 was not considered in this analysis. Preliminary attempts to simulate the effect of the fracture in Test 1 can be found in Green et al. (1993b).

Basecase Results. Temperature and saturation profiles numerically predicted using the basecase model properties are illustrated in Figures 4-10 and 4-11 for Tests 1 and 2. These temperature and saturation profiles are not in qualitative agreement with the observed results for either Test 1 or Test 2. Hence, three model input parameters were varied either separately or together in a set of sensitivity analyses to resolve the differences between the model and experimental results (permeability, the van Genuchten α parameter, and thermal conductivity). Thermal conductivity was first varied to attain agreement in the temperature regime. After the temperature was adequately replicated, agreement in saturation was attempted by variation of the two hydraulic parameters.

Thermal Conductivity. The thermal conductivity values of the test media used in Tests 1 and 2 exhibit relatively large variations between zero and full saturation. Values for the dry and wet thermal conductivity for the silica beads changed by a factor of 4.5. The tabular alumina had values that varied by as much as a factor of 2. In the V-TOUGH simulations, thermal conductivity varied linearly with saturation. The effect of a moisture-dependent thermal conductivity was not apparent in the basecase simulations because saturation varied by less than 0.02 in Test 1 and by 0.12 in Test 2. The thermal conductivity change would be expected to be more prominent in models that predicted large variations in saturation.

Thermal conductivity was adjusted to be spatially variable in the numerical simulation in addition to being moisture-dependent. Spatially variable thermal conductivity was incorporated into the simulation as a means to accommodate 3D heat loss through the plexiglass front and back sidewalls. A piece-wise linear thermal conductivity model was used for both the dry and wet conductivities. Thermal conductivities assigned to the three segments of each piece-wise approximation were normalized relative to the segment closest to the cool boundary. The lengths of the three segments were 7.5, 5.2, and 2.5 cm from left to right. The assigned thermal conductivity values are summarized in Table 4-2.

With the linear piece-wise approximation for thermal conductivity, the simulated temperature profiles for both Tests 1 and 2 were reasonably replicated, as shown in Figures 4-12(a) and 4-13(a). However, only a minor variation was introduced into the simulated saturation values and, as shown in Figures 4-12(b) and 4-13(b), the predicted saturation profiles did not adequately replicate any of the basic features of the experimentally observed saturation profiles.

Table 4-1. Summary of numerical parameters used in one dimensional numerical analyses for Tests 1 and 2

Parameter	Test 1	Test 2
Bulk Density (g/cm^3)	1.53	2.35
Permeability (m^2)	6.23×10^{-13}	2.95×10^{-14}
Porosity	0.38	0.41
Saturation	0.65	0.50
van Genuchten n	2.70	5.00
van Genuchten α (Pa^{-1})	7.19×10^{-5}	3.58×10^{-5}
Thermal Conductivity - Dry (W/m-K)	0.2	2.6
Thermal Conductivity - Wet (W/m-K)	0.9	3-5

Permeability. The permeability of each of the simulation models was next adjusted to attain better model/experiment agreement. For the Test 1 simulation, the permeability of the silica beads was reduced in the calculation by three orders of magnitude to $6.23 \times 10^{-16} \text{ m}^2$, which is justified by the degradation experienced by the silica beads. For Test 2, the assigned permeability of the tabular alumina was reduced by a factor of 10 to $2.95 \times 10^{-15} \text{ m}^2$, using the rationale that packing inconsistency in the tabular alumina caused changes in the permeability. These final assigned values for permeability for the Tests 1 and 2 media are now in relative agreement with the measured flow velocities which indicated a higher permeability for the tabular alumina than for the silica beads. Temperature and saturation profiles for these adjusted models are illustrated in Figures 4-14 and 4-15. Both the temperature and saturation profiles for this Test 2 model are reasonably close to the experimental results. The Test 1 predictions of saturation buildup (<0.04), however, do not replicate the observed significant (i.e., 0.10 to 0.20) moisture buildup.

van Genuchten α Parameter. As a final modification from the basecase values in the Test 1 model, the van Genuchten α parameter was increased by a factor of 10 to $7.19 \times 10^{-4} \text{ Pa}^{-1}$. Reasonable agreement between the model and experimental results was attained with this modification. The magnitude of the moisture buildup feature grew to 0.10 to 0.20, values similar to those observed near the base of the Test 1 container (Figure 4-16). Modification of the simulation model by decreasing the permeability and increasing the α parameter from the pre-test property measurements was justified by changes in pore structure resulting from silica bead degradation. Although a decrease in permeability is typically associated with a decrease in α (Wang, 1992), simulations of Test 1, in which α was decreased, provided predictions that did not agree with the experimental results. Thus, agreement between the numerical/experimental results was achieved by altering α in a manner contrary to standard practice, but justified by the significant changes experienced by the medium during the test.

(a)

(b)

Figure 4-10. Profile for the basecase properties for Test 1 (a) horizontal temperature for observed (dash) and predicted at 120 days (solid), and (b) saturation

(a)

(b)

Figure 4-11. Profile for the basecase properties for Test 2 (a) horizontal temperature for observed (dash) and predicted at 120 days (solid), and (b) saturation

Table 4-2. Spatially variable thermal conductivity used in one dimensional numerical analyses for Tests 1 and 2 where the cool boundary is at $x=0$ cm and the hot boundary is at $x=15.2$ cm

	Segment, cm	Test 1	Test 2
Thermal Conductivity – Dry (W/m-K)	$0 < x < 7.5$	0.20	2.60
	$7.5 < x < 13.7$	0.15	1.98
	$12.7 < x < 15.2$	0.11	0.88
Thermal Conductivity – Wet (W/m-K)	$0 < x < 7.5$	0.90	4.00
	$7.5 < x < 13.7$	0.68	3.00
	$12.7 < x < 15.2$	0.31	1.36

4.1.1.3 Conclusions from One Dimensional Tests and Simulations

Results from the 1D liquid flow moisture redistribution experiment and analyses are summarized as follows:

- Laboratory-scale experiments exhibited two distinct vaporization and condensation models for thermally driven moisture redistribution:
 - (i) Model 1—condensate buildup over a narrow zone proximal to a heat source (Test 1) observed in media with low permeability (i.e., less than about $1 \times 10^{-13} \text{ m}^2$) and a large van Genuchten α parameter (i.e., greater than about $5 \times 10^{-5} \text{ Pa}^{-1}$)
 - (ii) Model 2—condensate buildup over a broad area at some distance from a heat source (Test 2) observed in media with a low permeability (i.e., less than about $1 \times 10^{-13} \text{ m}^2$) and a small van Genuchten α parameter (i.e., less than about $5 \times 10^{-5} \text{ Pa}^{-1}$)
- A third condensation model was identified using numerical analyses:
 - (iii) Model 3—condensate redistributes near the heat source resulting in no significant liquid gradient. Numerical analyses indicate that permeabilities less than about 1×10^{-13} to $1 \times 10^{-14} \text{ m}^2$ are required before prominent saturation gradients can be developed, otherwise the returning liquid flow exceeds the outward vapor flow
- Incorporation of saturation-dependent thermal conductivity into the numerical model adequately matched temperature measurements recorded in the experiments

(a)

(b)

Figure 4-12. Profile for the basecase properties but with spatially variable thermal conductivity for Test 1 (a) horizontal temperature for observed (short dash), predicted at 0.5 day (long dash), and predicted at 120 days (solid); and (b) saturation

(a)

(b)

Figure 4-13. Profile for the basecase properties but with spatially variable thermal conductivity for Test 2 (a) horizontal temperature for observed (dash) and predicted at 120 days (solid), and (b) saturation

(a)

(b)

Figure 4-14. Profile for the basecase properties but with spatially variable thermal conductivity and lower permeability for Test 1 (a) horizontal temperature for observed (long dash), predicted at 0.5 day (dot-dash), predicted at 20 days (dot), and predicted at 120 days (solid); and (b) saturation

(a)

(b)

Figure 4-15. Profile for the basecase properties but with spatially variable thermal conductivity and lower permeability for Test 2 (a) horizontal temperature for observed (dash) and predicted at 120 days (solid), and (b) saturation

Figure 4-16. Profile for the basecase properties but with spatially variable thermal conductivity, lower permeability, and larger van Genuchten α parameter for Test 1 saturation at 0.5, 1.0, 2.0, 5.0, 20.0, 50.0, and 120.0 days

- Agreement between numerical/experimental results was achieved by decreasing the permeability in both 1D models, and increasing the van Genuchten α parameter for Test 1
- Test results indicated that the 1D group of experiments were not wholly 1D as evidenced by the oblique movement of dye in Test 1

Results from the 1D group of experiments and analyses provided the following conclusions that contribute to understanding the fundamental basis of thermally driven moisture redistribution through partially saturated porous media. Two fundamentally different condensation models have been identified:

- Media with low permeability and a large van Genuchten α parameter (small air-entry value) will be more likely to experience a relatively narrow moisture buildup zone on the cool side of the dryout zone
- Media with a low permeability and a small van Genuchten α parameter (large air-entry value) will tend to exhibit condensation over a broad area beyond the zone of dryout
- Media with a high permeability will not tend to exhibit a liquid gradient or dryout zone near a heat source.

Although supported by limited experimentation and analysis, the importance of these three condensation models is that moisture that condenses in a narrow zone near the dryout zone will have a larger hydraulic gradient and a shorter travel path back to the heater after temperatures have decreased than moisture that condenses over a broad area at a distance from the heat source. Further analysis is required to ascertain if these condensation models are also exhibited in natural rock.

4.1.2 Tests 3 Through 7: Two-Dimensional Experiments

Results from five related experiments (Test 3 through 7) were used to examine mechanisms of heat and mass transfer in a 2D geometry. Tests 3 and 4 were conducted for sub-boiling conditions, and Tests 5 through 7 were conducted for boiling conditions. The results used to evaluate heat and mass transfer mechanisms were drawn from several different experiments because no single experiment provided all the necessary information for the analysis. The evolution in experimental design over the duration of these tests provided different types of results. For example, early tests were equipped with ports for injected dyes to illustrate flow patterns and contained internal instrumentation for measurement of temperature and suction pressure. As the understanding of heat and mass transfer mechanisms and of the physical state of the flow field improved based on the results of these earlier tests, the introduction of dyes into the flow field and the use of intrusive instrumentation became less necessary. Hence, later tests contained less internal instrumentation and used consolidated media with lower permeabilities which more closely resembled natural rock.

4.1.2.1 Experimental Results and Analysis

Several distinctive features indicative of heat and mass transfer mechanisms were observed in the liquid flow fields of the 2D experiments. Prominent among these features was the downward movement of liquid toward the heater from above, a zone of rapid upward liquid movement toward the heater from below, and a dryout or capture zone along the sides of the heater.

A combination of experimental results was used to identify, describe, and examine these features. A key observation was that the moisture redistribution features were consistent throughout all five related experiments, even though there were differences among the experiments with respect to material properties and thermal conditions. The principal components used in evaluation of the moisture redistribution features were:

- Dye patterns observed in Test 3
- Densitometer-determined saturation measurements from Test 3
- Comparison of experimental and numerical simulation results for Test 3
- Densitometer-determined saturation measurements from Tests 6 and 7

Results from Test 3 were selected for emphasis in the analysis of the 2D experiments since these results provided the strongest and best documented evidence of the 2D experiments. Results from Tests 6 and 7 were also used in the analysis since these tests were conducted under boiling conditions in consolidated media; however, detailed analysis of the heat and mass transfer mechanisms under boiling conditions was prevented by the complex two-phase flow phenomena observed near the heater. Results from Test 4 results were not used in the analysis due to the uncertain effect the simulated fracture may have had on thermally driven moisture redistribution. Interpretation of Test 5 results did not substantively contribute to the analysis.

Liquid Movement. The formation of the moisture redistribution features near the heater was best illustrated by the movement of dye in Test 3. At several different times during this test a neutrally buoyant inert dye was introduced into the medium within 5 mm of the front face of the test cell through different combinations of all five ports shown in Figure 3-2. Movement of the dye was easily observed through the clear plexiglass front face of the test enclosures. Two sequences of photographs illustrate essentially all flow components of moisture redistribution observed in the experiments. One sequence was taken when the heat source was set at 60 °C, and the second sequence was taken with the heater at 90 °C. The first sequence contains five photographs from Test 3 over a period of 4 days starting 26 days after the initiation of heating at 60 °C (Figure 4-17). The second series of photographs was taken over a 4-day interval, 120 days after the start of heating, and 23 days after the heater temperature was increased from 60 to 90 °C (Figure 4-18).

Figure 4-16 illustrates the coupled stagnation/rapid flow and dryout/capture zone formation. Dye injected at the port located 3 cm directly below the heater tended to move relatively quickly upward toward the heater at a rate measured from the photographs to be 1×10^{-6} m/s. Dye injected at the port located 3 cm above the heater, however, tended to spread uniformly away from the point of injection at a relatively slow speed, which appeared to be diffusion-driven at a rate measured to be 7×10^{-8} m/s, or more than an order of magnitude slower than the advective flow observed for the part below the heater. The lateral component of the diffusion-driven dye was measured to avoid possible buoyancy effects from affecting the measurement. Because of the apparent lack of advective movement, the area located more than 2 cm above the heater is believed to be a stagnation zone. Downward movement of dye below the stagnation region was observed in Test 3 at both 60 and 90 °C after the dye had diffused to a point closer to the heater (unfortunately this is not well illustrated in the photographs). Upon reaching a point sufficiently below the point of injection (within about 1.5 cm of the heater), the dye exhibited a downward rate of movement that was in excess of that due to diffusion alone.

Day 26

Day 27

Day 28

Day 29

Day 30

Figure 4-17. Sequence of photographs Test 3 illustrating movement of dye injected at day 26 as viewed through plexiglass side wall with a heater temperature of 60 °C. The 4-day sequence was taken at days 26 to 30 of the experiment. Heater location is indicated by the black dot at days 27, 28, and 29.

Figure 4-18. Sequence of photographs Test 3 illustrating movement of dye injected at day 120 as viewed through plexiglass side wall 23 days after the heater temperature was increased to 90 °C. The 4-day sequence was taken at days 120 to 123 of the experiment. Heater location is illustrated by faint dot in last four photographs.

Away from the heater, the only flow feature observed was a relatively slow downward movement of dye at the far left injection port. This flow consisted of both diffusion and advection. The measured flow velocity of the dye was 1×10^{-7} m/s, a rate slightly greater than that measured for lateral diffusion alone and an order of magnitude less than advection-driven flow near the heater.

Figure 4-18 shows dye movement after the heater temperature was increased to 90 °C. Dye movement at the right and left of the heater indicated inconsistent flow features. Initially, dye injected at both the right and left of the heater moved toward the left by a combination of advection and diffusion (7.3 hr after injection, photograph 3 in Figure 4-18). Dye from the right injection port appeared to actually reach the heater. This particular flow feature was not generally observed during the experiments. An excessive volume of injected dye is one possible cause for dye from the right injection port reaching the heater. The most common behavior of flow in this region is illustrated in photographs 4 through 7 in Figure 4-17. These photographs show the formation of either a dryout or capture zone extending about 1.5 cm to the right and left of the heater.

An additional feature in the flow field of Test 3 was noted on several occasions when dye was injected at either the top and bottom, or the right and left pairs of injection ports. After the injected dye had migrated away from the points of injection (by either advection or diffusion), two additional small, yet distinct, plumes of dye appeared at the upper left and the upper right edges of the heater. These secondary plumes extended less than 0.5 cm from the heater and were very distinct, suggesting that the dye had concentrated at these two points. The small secondary plumes resulting from dye injected at the side ports are illustrated in the photographs in Figure 4-18. Several candidate pathways for the source of the secondary plumes are identified. The dye could have moved directly toward the heater from the different points of injection before concentrating near the heater, the dye may have traveled through the interior of the medium possibly indicating a 3D flow mechanism, or the dye may be an indication of the formation of secondary circulation cells near the heater. Unfortunately, the actual pathway was not discernable during testing.

Additional evidence of a possible 3D flow mechanism was illustrated by the arrival of dye at the back plexiglass wall near the bottom edge of the heater cartridge in Test 3. This was observed 1 day after the heater temperature was increased to 90 °C. The possibility of 3D flow is suggested because this dye had originally been introduced within 5 mm of the front plexiglass wall. After arriving at the bottom edge of the heater near the back wall, the dye moved downward toward the base of the test cell. The movement of dye upward at the front of the cell, coupled with downward movement at the back of the cell, suggested that liquid circulation may have formed in the region below the heater. One caveat in this interpretation is that dye arrival at the back of the test cell was intermittent and not observed in all tests. It is not known if 3D circulatory flow was present below the heater throughout the experiment nor if it was simply a spurious anomaly at the time the heater temperature was increased. This limited evidence appears to be inadequate to suggest that any 3D flow components were of a sufficient magnitude to preclude consideration of the experimental results as 2D.

Flow features observed near the heater in experiments under both sub-boiling and boiling conditions may have been different at microscopic levels; however, the major flow features deduced from saturation measurements under both sets of conditions were similar. The major flow features in the 2D experiments, as indicated by dye movement observed in Test 3, are illustrated in the drawing in Figure 4-19. The major flow components in this summary illustration are:

Figure 4-19. Graphical illustration of the major near-heater flow features in the two dimensional experiments determined using dye movement from Test 3. Heater is indicated by slanted pattern, primary dye plumes by cross-hatch pattern, secondary plumes by solid pattern, and dye injection ports by open circles.

- Relatively rapid upward flow from below the heater.
- A stagnation zone more than 1.5 to 2.0 cm above the heater.
- Downward flow below the stagnation zone above the heater.
- Stagnation zones to the far (i.e., more than about 1.5 cm) right and left of the heater.
- Two secondary, small (less than 0.5 cm) plumes located at the upper right and left edges of the heater.
- Capture or dryout zones located between the right and left stagnation zones and the heater (referred to here as the lateral capture/dryout zones).
- Possible inactive or dead zones separating the major plumes to right, left, top, and bottom of the heater. These zones may be either no-flow areas separating zones of inward and outward flow on opposing sides or areas of flow not observed due to an absence of dye.

The fluid redistribution mechanisms associated with the last three of these features are not well understood. Two hypotheses, A and B, are proposed to explain these near-heater flow features. The

capture/dryout zone acts as a dryout zone in Hypothesis A and as a capture zone in Hypothesis B. Sketches of these hypotheses are illustrated in Figures 4-20 and 4-21.

For Hypothesis A, the dryout zone is analogous to the dryout zone phenomenon observed and documented in the 1D experiments. In this interpretation, fluid flows toward the heater and is vaporized. The vapor is then transported away as vapor from the heat source to a point where it condenses at lower temperatures. Water vapor could condense in a narrow band immediately outside the dryout zone (i.e., similar to Test 1) or more evenly over a wider region beyond the dryout zone (i.e., similar to Test 2). In this hypothesis, dye injected to the right and left of the heater is the probable source of the secondary dye plumes because the dye is injected at points near the outer limits of the dryout zone. Minimal dye from above and below the heater reaches the heater because of the greater distance traveled and the vaporization of liquid as it approaches the heat source.

For Hypothesis B, water is circulated as liquid within the capture zone near the heater. Liquid flow to the heater from above and below continues as liquid away from the heater in the lateral directions. Dye injected at the top and bottom ports is the probable source of the secondary dye plumes in this hypothesis. Liquid flow in the capture zone at the locations of the secondary plumes of dye is outward; however, liquid flow away from the heater is limited at the furthest outward extent of the secondary dye plumes.

Saturation Profiles. The direction of flow, in either the lateral dryout/capture zone or the dead zones separating the four major plumes, is not easily discerned from observing the dye movement. Hence, to help interpret the flow features, saturation profiles and contour plots were calculated from densitometer readings measured in experiments for four cases: tabular alumina (Test 3 for heater temperatures of 60 and 90 °C); the relatively highly permeable ceramic (Test 6); and the low-permeability cement slurry mixture (Test 7). Saturations were calculated for each case study for two horizontal profiles (one 0.6 cm above the center of the heater and one 0.6 cm below the center of the heater), one vertical profile through the center of the heater, and for a height versus width saturation contour plot. All plots represent saturations thought to be at steady-state. These saturation plots are illustrated as Figures 4-22, 4-23, and 4-24 for Test 3 at 60 °C; Figures 4-25, 4-26, and 4-27 for Test 3 at 90 °C; Figures 4-28, 4-29, and 4-30 for Test 6; and Figures 4-31, 4-32, and 4-33 for Test 7; saturation for Test 7 is also shown at six different times during the test. The dotted lines included in saturation profiles for Test 3 are from numerically simulated saturations and are discussed in Section 4.1.2.2.

For the two Test 3 tabular alumina cases, the saturation profiles (Figures 4-22, 4-23, 4-25, and 4-26) and contour plots (Figures 4-24 and 4-27) exhibit significantly less resolution than those for the ceramic in Test 6 (Figures 4-28, 4-29, and 4-30) and the cement slurry mixture in Test 7 (Figures 4-31, 4-32, and 4-33). Lack of resolution in the Test 3 data is attributed to difficulties associated with packing, preparing a uniform test medium, and a spatial density of densitometer data. The horizontal and vertical saturation profiles for Test 3 reflect the general trend of lower saturation near the heater but do not provide adequate detail for analysis. No identifiable trends in moisture redistribution are exhibited in the saturation contour plots for Test 3 at 60 and 90 °C. Implied decreases in saturation, such as the 0.60 to 0.65 valley in the upper central portion of the Test 3 contour plot (Figure 4-24), are attributed to a decrease in density resulting from an inconsistency in packing of the granular material.

Saturation plots for the ceramic (Test 6) and the cement slurry mixture (Test 7) provided significantly better accuracy than those for the tabular alumina. This improved accuracy is attributed to the uniformity of the media. In addition, the boiling temperatures of Tests 6 and 7 created larger density

Figure 4-20. Hypothesis A. Lateral capture/dryout zones result from inward movement and vaporization of liquid water. Dye injected at right and left is the source of the secondary dye plumes. Heater is indicated by slanted pattern, primary dye plumes by cross-hatch pattern, secondary plumes by solid pattern, and dye injection ports by open circles.

Figure 4-21. Hypothesis B. Lateral capture/dryout zones result from outward movement of liquid water. Dye injected at top and bottom is the source of the secondary dye plumes. Heater is indicated by slanted pattern, primary dye plumes by cross-hatch pattern, secondary plumes by solid pattern, and dye injection ports by open circles.

(a)

(b)

Figure 4-22. Solid line is saturation calculated for Test 3 at 60 °C from densitometer measurements along a horizontal profile located (a) 0.6 cm above the center of the heater, and (b) 0.6 cm below the center of the heater. Dotted line is the numerically predicted saturation.

Figure 4-23. Solid line is saturation calculated from densitometer measurements along a vertical profile through the center of the heater for Test 3 at 60 °C. Dotted line is the numerically predicted saturation.

Figure 4-24. Saturation contours calculated from densitometer measurements for Test 3 at 60 °C

(a)

(b)

Figure 4-25. Solid line is saturation calculated for Test 3 at 90 °C from densitometer measurements along a horizontal profile located (a) 0.6 cm above the center of the heater, and (b) 0.6 cm below the center of the heater. Dotted line is the numerically predicted saturation.

Figure 4-26. Solid line is saturation calculated from densitometer measurements along a vertical profile through the center of the heater for Test 3 at 90 °C. Dotted line is the numerically predicted saturation.

Figure 4-27. Saturation contours calculated from densitometer measurements for Test 3 at 90 °C

(a)

(b)

Figure 4-28. Saturation calculated from densitometer measurements in Test 6 along a horizontal profile located (a) 0.6 cm above the center of the heater for the ceramic, and (b) 0.6 cm below the center of the heater

Figure 4-29. Saturation calculated from densitometer measurements along a vertical profile through the center of the heater for the ceramic in Test 6

Figure 4-30. Saturation contours calculated from densitometer measurements for the ceramic in Test 6

(a)

(b)

Figure 4-31. Saturation calculated from densitometer measurements for Test 7 at six times along a horizontal profile located (a) 0.6 cm above the center of the heater for the cement slurry mixture, and (b) 0.6 cm below the center of the heater. Heater was turned on after day 13 measurement and turned off after day 39 measurement.

Figure 4-32. Saturation calculated from densitometer measurements at six times along a vertical profile through the center of the heater for the cement slurry mixture in Test 7. Heater was turned on after day 13 measurement and turned off after day 39 measurement. Top of container is at the left.

Figure 4-33. Saturation contours calculated from densitometer measurements for the cement slurry mixture in Test 7

contrasts, which provided larger saturation differences that were easier to discern. A distinct desaturation anomaly is visible in the saturation contour plots for Test 6 (Figure 4-30) and Test 7 (Figure 4-33). The relatively highly permeable ceramic in Test 6 was desaturated only to a minimum of 0.65 from an initial saturation of 0.80, as compared to the low-permeability cement in Test 7, which was completely desaturated near the heater. Also plotted are saturation contours for the ceramic with an initial saturation of 55 percent and heated to over 170 °C (Figure 4-34). Return flow of liquid in the ceramic toward the heater was sufficiently rapid to keep the heater from complete dryout (at least at the locations of measurement) even though the heater temperature exceeded 170 °C.

The horizontal saturation profiles of these four tests indicate the same basic trend of desaturation near the heater. There is no compelling evidence in either the saturation profiles or the contour plots of a moisture buildup zone at the edge of the dryout zone. It appears that moisture vaporized at the heater did not condense in a narrow band immediately outside of the dryout zone, but instead was transported away from the heater before condensing uniformly over the total area between the dryout zone and the test container edges. Although minor anomalies in the saturation profiles could arguably be interpreted as evidence of the presence of a moisture buildup zone (i.e., the best example is to the right of the heater in Test 7), there was no evidence of a prominent dryout/moisture buildup zone in any of the 2D experiments.

Figure 4-34. Saturation contours calculated from densitometer measurements for ceramic in Test 6 at 170 °C

Suction Pressures. Suction pressures measured at five tensiometers for Test 3 are presented in Figures 4-35 and 4-36. All five tensiometers indicate an increase in matric pressure throughout the experiment although matric pressure may have approached steady-state in the last days of heating at 60 °C. The matric pressures of tensiometers 1, 3, 4, 5 and 6 were 6,080, 5,900, 5,720, 5,440 and 5,440 Pa and 6,980, 6,080, 6,000, 5,600 and 5,560 Pa at the end of heating at 60 °C (97 days) and 90 °C (155 days), respectively. Moisture redistribution within the test cell does not appear to adequately explain the observed increase in matric pressure at all measurement points. In particular, saturation distributions determined from densitometer measurements indicate a net increase in saturation in the lower left corner of the test cell. The greatest relative level of dryout, as indicated by the largest matric pressures, occurred at tensiometers 1 and 4, the two tensiometers closest to the cool boundary. This observation is contrary to the supposition that the greatest matric pressure, and the greatest level of desaturation, would occur closer to the heat source. It is important to note that the temperature in Test 3 was set at 60 °C from day 8 until day 97, then increased to 90 °C until day 155. The effect of temperature change on the matric pressure/saturation relationship in the retention curve was not examined. It is possible that the retention curve determined at 20 °C for tabular alumina is not valid at higher temperatures. The full implications of discrepancies in tensiometer values are not clear.

Liquid Resaturation. The rates and times for resaturation of the Test 7 medium after the cessation of heating were estimated using saturation measurements made at different times. Time durations required

Figure 4-35. Test 3 tensiometer matric pressure measurements at locations 1 and 3. Temperature of Test 3 was 60 °C from days 8 to 97 and 90 °C from days 97 to 155 (see Figure 3-2 for tensiometer locations).

Figure 4-36. Test 3 tensiometer matric pressure measurements at locations 4, 5, and 6. Temperature of Test 3 was 60 °C from days 8 to 97 and 90 °C from days 97 to 155 (see Figure 3-2 for tensiometer locations).

for resaturation were estimated from the two horizontal profiles and the one vertical profile by calculating the rate of resaturation from saturation measurements soon after the heater was turned off and from saturation measurements at the end of the experiment. The estimated time durations for resaturation calculated from the upper horizontal, lower horizontal, and vertical profiles were 250, 100, and 80 days. The rates of resaturation (defined as the rate at which a particular level of saturation moves) were calculated to be 1×10^{-9} to 1×10^{-8} m/s in the horizontal direction, 1×10^{-8} m/s in the downward direction, and negligible resaturation from below the heater.

4.1.2.2 Numerical Simulations

The computer code V-TOUGH was used to simulate liquid redistribution resulting from the point heat source in the 2D liquid flow experiments. The numerical analyses were conducted to: (i) identify whether Hypothesis A or B is most likely to represent the transport mechanisms for moisture redistribution in the near-heater region, and (ii) evaluate the ability of V-TOUGH to replicate the liquid flow regimes observed in the 2D experiments. No attempt was made to replicate the secondary flow features observed near the heater, since numerical simulation of flow features similar to these have been shown to be unstable; hence these secondary features are not suitable to modeling (Bonano and Davis, 1980). Model results are only used to assess the primary flow features observed in the experiments. Additional analysis of grid resolution could aid in interpreting the secondary features.

The numerical model was constructed to replicate Test 3, with the experimental properties and thermal conditions measured for Test 3 used in the numerical simulations. The vertical and horizontal dimensions of the numerical model are the same as for Test 3, and the boundary conditions for the numerical simulations approximate those of the laboratory-scale experiments. The vertical and horizontal boundaries are prescribed as having no fluid flow. The assigned values for experimental parameters are taken from Tables 3-2 and 3-5 through 3-9. A porosity of 0.41 and a permeability of 8.04×10^{-13} m² were assigned to the tabular alumina. The van Genuchten values of the fitted retention curve were 1.31×10^{-4} Pa⁻¹ for α and 5.00 for n . Saturation was originally measured to be 0.70, however, densitometer measurements and review of the laboratory procedure indicated that the actual saturation for Test 3 was probably closer to 0.75. Therefore, a saturation of 0.75 was used in the simulation.

The right and left vertical boundaries of the numerical model were maintained at 20 °C. The top and bottom boundaries were adiabatic. The heat source was modeled as an impermeable 0.75x0.75 cm square. The power input into the water-circulating bayonet heater of Test 3 could not be measured and was not known. The numerical model values for heat load for the two heater temperatures of Test 3 were adjusted to achieve an acceptable comparison between the experimentally observed and numerically predicted temperature at the heater; the final heat rates assigned to the heaters were 13.2 W for the 60 °C and 22.8 W for the 90 °C cases. This calibration process was used to accommodate, at least in part, the 3D heat loss experienced through the plexiglass side walls during the tests.

Differences between predicted and experimental temperatures (measured at the heat source and at other locations) at steady-state are a function of the property values assigned to the medium, particularly thermal conductivity, in addition to the strength of the heat source. The transient formation of the temperature regime depends on the specific heat of the medium. However, since the thermal regime was established relatively quickly in these tests, the experimental results are relatively insensitive to minor variations in the values of the specific heat. Therefore, specific heat was not examined in detail. Values assigned to thermal conductivity, however, can significantly affect the outcome of model predictions.

Difficulty in directly measuring the thermal conductivity of tabular alumina was due to variations in packing and the nonuniform distribution of moisture in tested samples. Therefore, published thermal conductivity values for tabular alumina were assigned to the Test 3 medium in the numerical simulations. The assigned dry and wet thermal conductivities were 2.6 and 4.0 W/m, respectively, for tabular alumina (ALCOA Chemicals, 1969).

Temperature Distribution. The cumulative effect of the values assigned to the heat source load and the thermal properties of the medium can be estimated by comparing the measured temperature distribution with that predicted in the simulation. The simulated steady-state temperature distributions for Test 3 with the heater set at 60 and 90 °C are illustrated in Figures 4-37 and 4-38, respectively. Also presented in these figures are the temperatures recorded by the six internal thermistors. As illustrated in these figures, the numerical model was successful in replicating the temperatures observed during Test 3 at 60 °C. The temperature distribution predicted for the 90 °C heater agreed with four of the six internal thermistors (i.e., the difference between measured and predicted temperatures were within ± 1 °C). However, the temperature recorded at the two thermistors located midway on the horizontal scale differed by as much as 4 °C from the predicted values. This difference is attributed to possible inappropriate property values assigned to the medium or to heat loss through the plexiglass side walls. Higher temperatures near the heat source are indications of actual thermal conductivities higher than those assigned to the numerical model. A nonlinear thermal conductivity-saturation model that predicted higher thermal conductivities at lower saturations could resolve this discrepancy. Regardless of the source of the difference in the temperature regimes, the differences suggest that temperatures in the test enclosures may not be as well replicated at higher temperatures as at the lower temperatures. Nonetheless, predicted temperature distributions for Test 3 at 60 °C and for most measurement locations at 90 °C were sufficiently similar to observed temperatures that no adjustment in assigned thermal conductivity values was required.

Matric Pressures. Simulated capillary pressure distributions were compared with measured matric pressure values for Test 3 at 60 and 90 °C. The predicted matric pressures for the 60 and 90 °C simulations are illustrated in Figures 4-39 and 4-40, respectively, along with the measured pressures. Tensiometer 2, which was apparently rendered inoperable during installation, did not provide results. The measured matric pressures were taken from Figures 4-35 and 4-36 at day 97 for the 60 °C heating and at day 155 for the 90 °C heating. The simulated matric pressure contour plots are essentially smooth, except for a small variation near the heater. Except for tensiometer 4 at 90 °C, all measured matric pressures were less than those predicted in the simulation. This would suggest that the container media had a higher liquid saturation than presumed. The matric pressure/saturation relationships for the tabular alumina used in Test 3 (Figure 3-5c) indicates saturations of greater than 0.99 for matric pressures in the range of 5,500 to 6,500 Pa. The retention curve for the tabular alumina illustrated in Figure 3-5c is apparently not representative of the tabular alumina used in Test 3. This inconsistency is attributed possible thermal variations affecting the matric pressure/saturation relationship or to packing variations between the tabular alumina used in water retention measurements and that used in Test 3.

Saturation Profiles. The densitometer-determined saturation distribution in Test 3 was compared with liquid saturation predictions made with the numerical model. Comparisons of numerically predicted saturation along horizontal transects located 0.6 cm above and below the heat source are illustrated with the measured data at 60 °C in Figure 4-22 and at 90 °C in Figure 4-25. Vertical transects through the heater comparing measured and predicted saturation are illustrated in Figures 4-23 and 4-26. Predicted contour plots in Figures 4-41 and 4-42 can be compared with the measured saturation distributions in Figure 4-24 and 4-27. As illustrated in the horizontal profiles, there is general agreement in the trend of desaturation near the heater although the lack of resolution in the observed data for Test 3 limits in-depth

Figure 4-37. Temperature distribution for Test 3 with a 60 °C heat source. Contour lines are from the numerical simulation and point measurements are from the laboratory experiment.

Figure 4-38. Temperature distribution for Test 3 with a 90 °C heat source. Contour lines are from numerical simulation and point measurements are from the laboratory experiment.

Figure 4-39. Numerically predicted capillary pressure distribution compared with measured matric pressures for Test 3 with a 60 °C heat source

Figure 4-40. Numerically predicted capillary pressure distribution compared with measured matric pressures for Test 3 with a 90 °C heat source

Figure 4-41. Predicted saturation contour plot for Test 3 at 60 °C

Figure 4-42. Predicted saturation contour plot for Test 3 at 90 °C

analysis. A marked increase in saturation below the heater horizon is noted in both the predicted and measured data, but the predicted saturation increase above the heater was not observed in Test 3 data.

It is believed that the lack of a vertical saturation gradient in the contour plots constructed from measured data (Figures 4-24, 4-27, 4-30, and 4-33) is a result of the assumption of a uniform saturation throughout the test medium that was made in the densitometer data reduction method. This assumption eliminated from all remaining measurements any vertical saturation gradient (due to gravity-driven equilibration) present at the time when the baseline densitometer measurements were made. For relatively high permeability media, such as the tabular alumina and ceramic, this data reduction technique might have removed evidence of vertical saturation gradients because the gravity-driven equilibration was relatively rapid and probably occurred prior to densitometer measurements. For low permeability media such as cement slurries, the gravity-driven moisture redistribution required a longer time, thus densitometer measurements prior to equilibrium would have observed the vertical gradient. Nonetheless, a vertical saturation gradient cannot be discerned in the Test 7 profile (Figure 4-33) which used a cement slurry.

Flow Patterns. To make an additional comparison of the flow regime observed in the experiments and the numerically predicted flow regime, streaklines were introduced into liquid flow velocity plots simulated for Test 3 at 60 °C (Figure 4-43) and at 90 °C (Figure 4-44) at the approximate locations of the four dye injection ports located near the heater. It should be noted that the streaklines injected into a flow field are assumed to be steady as compared to streamlines, which are injected into flow fields as the flow field evolves. Although the streaklines do not incorporate diffusion flow mechanisms, they do indicate the pathway of liquid flow in the simulations.

The numerically simulated flow fields indicate two major features, the formation of a clockwise circulation cell located to the right of the heater, a counter-clockwise rotating circulation cell to the left of the heater, and several smaller features near the heater. Within each circulation cell is a well-defined zone of stagnation. Stagnation in these zones is indicated by the relatively short velocity vectors. Streaklines introduced into the simulated flow fields at the approximate locations of the right and left dye injection ports are sufficiently within these cells that their trajectories remain, for the most part, within the cells and their respective stagnation zones.

Streaklines were also introduced into the simulated flow field at the dye injection points located above and below the heater. A streakline originating at the location of the injection port below the heater moved directly upward in both the 60 and 90 °C simulations. This same upward flow feature was observed in the experiments using the injected dye (Figures 4-17, 4-18, and 4-19). The downward movement of dye in the region immediately above the heater was also captured by the streaklines in the numerical model, but only for the 90 °C case. For the 60 °C case, the streaklines originating at locations above and below the heater are in the upward direction. Even for the 90 °C numerical simulation, the zone of downward movement above the heater extended upward to a distance of 0.5 cm, and this does not compare well with the observed results for Test 3 at both 60 and 90 °C that show this zone extending to as much as 1.5 to 2.0 cm above the heater.

4.1.2.3 Conclusions of Two Dimensional Experimental Result and Analyses

Conclusions drawn from analyses of the 2D experiments can be summarized as follow:

- Formation of a dryout/moisture buildup zone was not observed in any of the 2D experiments. Thermally driven water vapor tended to condense uniformly throughout the test containers and not near the dryout zone. All test media used in the 2D experiments had van Genuchten α

Figure 4-43. Streaklines introduced into the simulated liquid flow velocity field at 60 °C at the dye injection ports located right, left, above, and below the heater

Figure 4-44. Streaklines introduced into the simulated liquid flow velocity field at 90 °C at the dye injection ports located right, left, above, and below the heater

parameter values of less than $1.5 \times 10^{-4} \text{ Pa}^{-1}$. By comparison, Test 1, which exhibited a moisture buildup zone, had an adjusted van Genuchten value of $7 \times 10^{-4} \text{ Pa}^{-1}$.

- The permeability of the test media significantly influences the level of saturation near a heat source at temperatures exceeding boiling. Complete dryout was not detected in media with permeability greater than $1 \times 10^{-13} \text{ m}^2$ even at temperatures in excess of 170°C .
- The conceptual and numerical models were successful in predicting the major flow features, but not all the detailed moisture redistribution phenomena, observed in the series of 2D experiments.
- Flow features near the heater in Test 3 were not predicted well by the numerical model. This discrepancy may be attributed to an inadequate conceptual model of near-heater heat and mass transfer mechanisms since the precise nature of several secondary flow features could not be determined.
- Experimental evidence and numerical analyses were insufficient to resolve which of two differing hypotheses describe fluid flow patterns near the heater.
- Temperature-sensitive matric pressure/saturation relationships may affect local saturation which, in turn, influences fluid flow regimes.
- The cement in Test 7 had estimated resaturation times of 80 to 250 days and resaturation rates of 1×10^{-8} to $1 \times 10^{-9} \text{ m/s}$ after termination of heating. These resaturation rates during the cooling period were at least 10 times slower than the advection flow rates (i.e., $1 \times 10^{-7} \text{ m/s}$) measured during the heating period.

These results from the 2D group of experiments and analyses provided the following conclusions that contributed to resolving the fundamental basis of thermally driven moisture redistribution through partially saturated porous media.

- Temperatures as high as 170°C were apparently not sufficient to completely dry out media with permeabilities greater than $1 \times 10^{-13} \text{ m}^2$. This permeability/temperature relationship may be size dependent. A similar limitation may also be present at the canister scale, but with a different quantitative value.
- Fluid flow fields near a heat source may be more complex than indicated by numerical simulation. This may be attributed to an inadequate conceptual model of near-heater heat and mass transfer mechanisms since the precise nature of several flow features could not be determined experimentally. In particular, the physically observed downward movement of liquid from above the heat source was not well replicated in the numerical model. If present at the canister or repository scales, this downward flow of water could provide a source of water at the canister during the heating period of the repository. Coupling this matrix phenomenon with gravity-driven refluxing down fractures could lead to a potentially adverse scenario.

- Condensation buildup in a narrow zone next to the heat source induced dryout zone was not observed in media with a van Genuchten α parameter less than $1.5 \times 10^{-4} \text{ Pa}^{-1}$. This quantitative value may be size dependent.
- Resaturation rates measured during the cooling period were at least 10 times slower than drying rates measured during the heating period for media tested.

4.2 GAS PRESSURE BUILDUP EXPERIMENT RESULTS

A series of four related experiments (Tests 8 through 11) was designed and conducted to monitor the buildup of gas pressure and the redistribution of moisture in a porous medium in a controlled laboratory environment. This series of tests is referred to as the gas pressure buildup tests. One of the primary objectives of this research project was to formulate and investigate scaling laws that would allow a complete examination of heat and mass transfer mechanisms operating at a variety of scales—from the laboratory (10^{-1} to 10^0 m), to the field (10^0 to 10^1 m), to the repository (up to 10^2 m). These experiments were designed and conducted to provide the requisite data for testing the proposed scaling laws. Results from these experiments are also useful in the investigation of those mechanisms that contribute to thermally driven moisture redistribution in partially saturated porous media. The use of the gas pressure buildup test results for this latter purpose is discussed in this subsection.

The design of the experiments and instrumentation remained essentially constant in all four of the gas pressure buildup experiments. Only the test medium was changed in order to evaluate and to select a test medium in which a gas pressure gradient could be created and that was suitable for meaningful measurement of the test variables. Tabular alumina was used as the medium in Test 8, the first experiment of this group; however, a significant gas pressure gradient was not attained due to the relatively high permeability of this test medium. The next two experiments, Tests 9 and 10, were conducted using cement slurry mixtures as the test media. A gas pressure gradient measurable within the confines of the test container was successfully attained in Test 9, but Test 10 failed due to fracturing of the consolidated block within the first 20 min of heating the cylinder. Test 11 used tuff from the ALTS as the test medium; and a significant gas pressure gradient was successfully attained in this experiment. Because only Tests 9 and 11 successfully provided a medium with a measurable gas pressure gradient, only the results of these two experiments will be discussed here. Of these two experiments, results from Test 11 are discussed in greater detail because the test medium of this experiment was more relevant to the objectives of the investigation and because the experiment was the last and best controlled experiment of the series.

4.2.1 Experimental Results

The gas pressure buildup experiments were conducted in cylindrically shaped containers. Because of the cylindrical geometry of the test cell and the uniform boundary conditions at the cylinder wall, these experiments are considered to be essentially 1D in the radial dimension even though some 2D flow behavior was not avoidable. Descriptions of the experiments are included in Section 3.2, and a schematic of the test container is shown in Figure 3-3. In addition to the difference in media for Tests 9 and 11, there was a difference in heater emplacement methods. For Test 9, the cement slurry was poured around the cartridge heater. For Test 11, a hole was bored in the tuff cylinder and the heater inserted in the hole; consequently, the heater stem extended along the entire length of the borehole. This method of heater emplacement for Test 11 caused a significant energy loss due to the small air gap between the cartridge heater and the borehole wall and to conduction of heat through the heater stem to the test container, which

prevented the full heater power from being conducted to the test container. It was not possible to insert a heat conducting material (i.e., films, gels, etc.) in the borehole-heater air gap to reduce energy losses because the gas pressure was measured in the air gap. As will be discussed later, the unknown magnitude of the energy losses for Test 11 led to some uncertainty in the numerical simulation of the test.

Test variables measured in the gas pressure buildup experiments and used in the analyses included:

- Heater power (recorded intermittently during the experiments).
- Temperature measured at the heater and at the outer edge of the test medium.
- Pressure measured at the heater using a pressure transducer and at the outer edge of the test medium using both a pressure transducer and a water manometer.
- Saturation profile calculated from densitometer measurements in the radial direction from the center to the edge of the cylinder.

Figure 4-45 shows the temporal evolution of heater power measured as input into the electrical cartridge heater for both Tests 9 and 11; Figure 4-46 shows the temperature at the heater, and Figure 4-47 shows the gas pressure difference between the pressure recorded at the heater and the gas pressure measured at the outside edge of the cylinder. Although Test 9 ran for 32 days and Test 11 for 76 days, only measurements for days 10 to 21 for Test 9 and for days 4 to 12 for Test 11 are presented in these figures. After this juncture in the experiments, the heater power was turned off, and the temperature and pressure at the heater quickly (i.e., within several hours) returned to pretest ambient conditions.

Heater power was ramped up more gradually in Test 11 than in Test 9 (Figure 4-45). This allowed easier characterization of the power input during analysis, particularly mathematical modeling. As expected, the heater temperature rise in Test 11 was not as abrupt as in Test 9.

4.2.1.1 Gas Pressure Observations

The gas pressure differences measured during Test 9 exhibited a monotonic rise to about 20 kPa over an 8.5-hr period. This rise was then followed by a rapid decrease to about 5 kPa, probably because the initial gas pressure rise was sufficiently high to force an open gas pathway from the heater to the cylinder edge through previously saturated pores. After the pressure returned to ambient, only one other gas pressure increase was observed during Test 9, although other gas pressure increases may have been missed during an absence in continuous data recovery from days 12 to 18 in the test. It is believed that a gas pathway was opened that allowed gas flow from the heat source to the outer boundary for the last three days of the heating period of Test 9.

During Test 11 the gas pressure difference increased monotonically to about 17 kPa within a 4.5-hr period of time. Then there was rapid pressure difference decrease that reduced the pressure difference to about 5 kPa, after which the gas pressure difference exhibited a series of increases and decreases until the heater was turned off after 7 days of heating. In this case, it seems that after the gas pressure difference initially decreased, the largest pores in the gas pathway refilled with water, thereby closing off that gas pathway and allowing gas pressures to increase. On two occasions the gas pressure difference rapidly decreased to approximately zero followed by fairly rapid increases to 5 kPa and 7 kPa.

Figure 4-45. Heater power as input to the electric cartridge heaters of the cement slurry mixture cylinder in Test 9 (dashed line) and the Apache Leap Test Site tuff cylinder in Test 11 (solid line)

Figure 4-46. Temperature (°C) measured at the electric cartridge heaters in the cement slurry mixture cylinder in Test 9 (dotted line) and the Apache Leap Test Site tuff cylinder in Test 11 (solid line)

Figure 4-47. Gas pressure difference (Pa) measured between the electric cartridge heaters and the outside edge of the cement slurry mixture cylinder in Test 9 (dotted line) and the Apache Leap Test Site tuff cylinder in Test 11 (solid line)

However, no discernable periodicity in the gas pressure difference buildup and decrease phenomenon was detected during the heating periods of Tests 9 and 11.

The level to which the buildup of thermally induced gas pressure can be expected to achieve is a function of the nature of the gas pathway. The mechanistic response of the gas pathway is believed to be a function of the pore structure and size, degree of saturation, and rate of heating. Stated simply, the rate of heating has to be sufficiently rapid and the gas pathways must be sufficiently restricted for gas pressure to build up. Additionally, the length of the gas pathway affects the time over which pressure builds up and decreases. For a small-scale system, such as the cylinder test, the size of the pores available for gas flow has greater influence on when gas discharge occurs than the relatively short length of the pathway. Gas pressure could conceivably increase until the air-entry pressure of the minimum equivalent pore diameter of the initial gas pathway is exceeded. The initial gas pathway is that pathway which has the largest minimum equivalent pore diameter and will be the first continuous gas pathway to connect the pressurized area at the heater with the constant pressure boundary. The pathway forms when segmented or entrained air coalesces into a continuous pathway. The air-entry pressure, p_c , is defined as

$$p_c = \frac{2 \sigma}{r} \quad (4-1)$$

where σ is surface tension of the liquid (0.072 n/m for water at 25 °C) and r is the radius of the pore. If the gas pressure differences at the time of gas discharge (20 kPa in the cement slurry mixture of Test 9 and 17 kPa in the ALTS tuff of Test 11) are assumed to be the air-entry values of the media, then the corresponding equivalent pore radii were 7 and 8 μm , respectively. The pore-size distribution of the cement slurry mixture is not known but published values for the pore-size distribution (Rasmussen et al., 1990) indicate that the largest equivalent pore radii measured in tuff samples from ALTS are about 10–20 μm . The air-entry pressures for this range of equivalent pore radii are about 15 to 7 kPa. Therefore, the discharge pressure measured in Test 11 met or exceeded the air-entry pressure of the ALTS tuff. Additional gas pathways, perhaps longer and more tortuous but with larger minimum equivalent pore diameters, may have developed subsequent to the initial gas discharge. This would allow gas to discharge at lower gas pressure differences after the initial gas pathway was opened. The subsequent gas discharge events observed in Test 11 occurred at equivalent pore-size radii of 20 to 30 μm , somewhat larger than the minimum equivalent pore radius of the initial gas pathway.

The intermittent gas discharge phenomenon observed in Tests 9 and 11 has also been observed at the field scale. For example, a field-scale heater experiment conducted by Lawrence Livermore National Laboratory (LLNL) at the G-Tunnel facility detected similar gas pressure buildup responses at all three locations at which gas pressure was monitored (Ramirez, 1991). The three gas measurement locations, identified as P1, P2, and P3, were located in fractured welded tuff at distances of 0.8, 2.0, and 1.0 m from the center of a 3,300 W-heater. Gas pressures at the three measurement locations during the 9-month G-Tunnel experiment have been reproduced from Ramirez (1991) in Figure 4-48 for comparison with gas pressures measured during Tests 9 and 11. Although the pressure responses at each of the three locations exhibited distinctively different characteristics, features of gas pressure responses measured in the CNWRA laboratory-scale experiments exhibited remarkable similarity to those observed in the field-scale G-tunnel experiment. In particular, a rapid increase in gas pressure was observed after the onset of heating at P1. The absence of the gas pressure spike at P2 and possibly P3 was attributed to mechanical failure in the instrumentation. Intermittent pressure relief at P2 was observed for about 37 days into the test, after which the recorded pressure remained close to the pre-test ambient pressure of 11.7 psia (about 80 kPa absolute).

Figure 4-48. Gas pressure measurement from Lawrence Livermore National Laboratory G-tunnel heater experiment for (a) P1, (b) P2 (after Ramirez, 1991)

(c)

Figure 4-48 (Cont'd). Gas pressure measurement from Lawrence Livermore National Laboratory G-tunnel experiment for (c) P3 (after Ramirez, 1991)

The return to ambient pressure after 37 days at P2 is also exhibited in pressure responses recorded during Tests 9 and 11. All three responses are indications that a gas pathway remained open allowing gas pressure to be discharged for the remainder of their respective tests. Behavior analogous to the long gradual gas pressure buildup past the duration of the heating period at P3 and subsequent to the initial pressure spike at P1 was not observed in the relatively short-term laboratory experiments.

Intermittent pressure discharge analogous to that observed in Test 11 were also reported by Persoff et al. (1992) and Ransohoff and Radke (1988) and analyzed by Thunvik and Braester (1990). A significant difference among the case studies is that the discharge events observed in Test 11 occurred in porous media whereas in the previous studies the discharge phenomenon applied to fractures.

4.2.1.2 Saturation Observations

To avoid introduction of unintentional gas pathways caused by intrusive instrumentation, densitometer measurements were the only means used to determine saturation in the gas pressure buildup experiments. Such measurements require a baseline measurement at a known saturation to compute saturation changes during the tests. For Test 9, baseline saturation measurements were established using several samples acquired from the test cylinder at the conclusion of the experiment test. The saturation, which was visibly discolored by moisture movement, was 0.66 for a cement sample taken near the heater, 0.89 to 0.92 for samples midway between the heater and the cylinder edge; and 0.96 to 0.97 for samples at the outer edge of the cylinder. The average pre-test saturation was thus calculated to be 0.90, and this value was used for reducing the densitometer measurements. The value of 0.90 is about twice the pre-test

saturation value of 0.47 measured on a separate sample made from the same cement slurry. However, this separate sample may have lost moisture after preparation and prior to measurements and, furthermore, the slurry mixture used in Test 9 may have experienced additional chemical alteration effects due to heating that were not experienced by the separate sample.

For Test 11, the low permeability of the tuff prevented complete saturation and drying of the medium to make baseline densitometer measurements. The measured saturation of a rock sample taken from the same oversized rock core as the Test 11 cylinder was 0.30. Similar to the cement slurry cylinder in Test 9, the turf cylinder in Test 11 was dismantled after the experiment to determine post-experiment saturation. Saturation was measured on twelve rock subsamples extracted from different locations within the cylinder using a hammer and chisel to insure that saturations were not altered by either heat or water-cooling during cutting or coring. As determined in these twelve saturation measurements, a pre-experiment saturation of about 0.34 appears to have been appropriate. The densitometer measurements were converted to saturation values using the pre-experiment measurements taken at the assigned 0.34 uniform saturation values. And although considerable effort was expended to insure that the tuff cylinder was prepared uniformly (e.g., evenly cut with a ground surface), heterogeneities within the rock were apparent as indicated in the densitometer readings.

Figures 4-49 and 4-50 show the saturation values calculated from the densitometer measurements along two radial profiles separated by 90 °C at several times during the period from day 8 to day 31 of Test 9. The two radial directions are identified as r_1 and r_2 . The heater was turned on at day 10 and off at day 21. Most notable is the uniformity in saturation values provided by the cement slurry mixture. The uniformity in values demonstrates that the high level of heterogeneity observed in the unconsolidated media in the 1D and 2D experiments was successfully avoided through the use of a synthetic consolidated medium in Test 9. An inspection of the reduced data suggests that densitometer readings at the exact location of the heater and beyond the outside edge of the test medium exceeded the limit of possible saturations (i.e., greater than 1.0 or less than 0.0). Since these unrealistic values occur outside the regions of interest, they were dismissed and have not been included in these figures. Regardless of these errant values, the good agreement between the directly measured saturation values and the calculated values for Test 9 indicate the baseline saturation estimate was reasonable.

Several features in the moisture redistribution of the Test 9 test cylinder are noticeable in the saturation plots shown in Figures 4-49 and 4-50. First, the maximum effect of dryout extended to a distance of about 5 cm beyond the edge of the heater. Although it is difficult to ascertain with certainty, it appears that the medium was completely desaturated next to the heater. Second, a relatively uniform increase in saturation was noticed from the outer edge of the dryout zone to the outer boundary of the test cell. This observation is in agreement with most of the 2D experimental results and analyses discussed in Subsection 4.1.2 that indicated condensation over a relatively wide area, as opposed to in a narrow zone immediately on the cool side of the dryout zone observed in Test 1. The occurrence of a dryout zone was substantiated by the appearance of a narrow zone of discoloration that was visibly observed when the cement cylinder was dismantled to obtain samples for saturation measurement. Third, resaturation at a distance of 3 cm from the heater was observed at the end of Test 9. The observed rate of resaturation in the r_1 -direction profile exceeded that in the r_2 -direction profile. Resaturation along the r_1 profile was measured to be about 0.01 per day in the region that had been totally desaturated during heating, and at about 0.005 per day in the region that had been desaturated to about 0.40 to 0.50. The rate of movement of the resaturation front was measured at 3×10^{-7} m/s. Therefore, if the rate of resaturation remained constant, complete resaturation would have been expected to occur in approximately 100 days.

Figure 4-49. Radial saturation profile in the r_1 direction for the cement slurry mixture cylinder in Test 9 at days 8, 11, 18, 23, and 31. Heat was initiated on day 10 and turned off on day 21.

Figure 4-50. Radial saturation profile in the r_2 direction for the cement slurry mixture cylinder in Test 9 at days 8, 11, 18, 23, and 31. Heat was initiated on day 10 and turned off on day 21.

Resaturation in the r_2 -direction profile was measured at 0.0025 per day in an area with 0.40 to 0.50 saturation. Full saturation would be attained in 200 days if resaturation continued at this same rate. The rate of movement of the saturation front along the r_2 -direction profile varied from negligible to about 3×10^{-7} m/s.

For Test 11, Figure 4-51 shows the total densitometer counts at 30 different locations separated by 0.5 cm along a radial profile for several times during the test. Figure 4-52 shows the change in densitometer counts from the start of the experiment for the same radial locations and times. The densitometer count changes are indicative of saturation changes. For the reasons discussed earlier, only changes corresponding to densitometer counts in excess of 250 (the standard deviation for total counts in the range of 60,000) are considered to be significant. Consequently, as can be seen in Figure 4-52, only densitometer measurement changes within 3 to 4 cm of the center of the cylinder are sufficiently above background noise to be considered significant. This change in counts near the heater is the most prominent feature of the saturation distribution.

An approximation to the resaturation behavior of Test 11 was calculated from the relative changes in densitometer counts measured at three times during the experiment: (i) baseline counts prior to initiation of heating; (ii) at a time soon after heating was terminated (day 13); and (iii) at the end of the experiment (day 74). Resaturation rates were estimated at the four densitometer measurement points closest to the heater since the measurements at these locations were above the calculated background noise level (i.e., 250 counts). During the 61 days following shutoff of the heater, resaturation at four locations in the near-heater or dryout zone during this 61-day period was 0.13, 0.76, 0.87, and 0.59, calculated from the measurement locations closest to the heater to the farthest. This is equivalent to total resaturation times of 470, 80, 70, and 103 days, which are similar with the results from Test 9.

4.2.2 Numerical Simulation

The thermally driven redistribution of moisture in Test 11 was simulated using the C-TOUGH code. The tuff cylinder was modeled in cylindrical coordinates with dimensions similar to those of the test cylinder. All boundaries in the model were specified as no-fluid-flow boundaries. The heater was characterized as a 5-cm-long, 1-cm-radius test cylinder set in the interval of 4 and 3 cm from the top and bottom of the cylinder, respectively (Figure 3-3). The outer cylinder boundary was maintained at 22 °C, and the upper and lower boundaries were assigned thermal conductivities of 0.4 W/m-K to allow for heat loss through the plexiglass base and top. The boundary layer thermal conductivities were adjusted to allow boundary temperatures at a point above the heater to rise to about 40 to 50 °C, the same temperature as estimated for Test 11. As illustrated in Figure 4-45, the heater power was ramped up to about 64 W over a period of about 4.5 hr. Preliminary numerical simulations identified a discrepancy between the amount of power registered at the Variac in the experiment and the temperatures in the medium predicted by the simulation. A significant amount of energy was apparently lost from the test cell because for an assigned heater power of 64 W the simulated temperatures exceeded 300 °C, much greater than the 165 °C measured at the heater during Test 11. As discussed earlier, the heater mounting method for Test 11 did not ensure that all the energy from the heater entered the test cell. For the simulation, the effective heater power input into the tuff was therefore determined by adjusting the heater power in the simulation until the predicted temperature matched the observed (165 °C). No attempt was made to incorporate the heat transfer mechanisms associated with air gap located between the heater and the rock medium. The predicted and observed temperatures were both taken at the location of the heater. Temperatures of the rock medium closest to the heater were not measured but are believed to be significantly less than at the

Figure 4-51. Radial profile of total densitometer counts for Apache Leap Test Site tuff cylinder in Test 11. Data presented are for days 3, 6, 10, 13, 41, and 74. Heat was initiated on day 5 and turned off on day 12.

Figure 4-52. Radial profile of change in densitometer counts from initiation of experiment for Apache Leap Test Site tuff cylinder in Test 11. Data presented are for days 6, 10, 13, 25, 41, and 74. Heat was initiated on day 5 and turned off on day 12.

heater. The adjusted heat load was thereby determined to be approximately 36 W. This back-calculation of heater power was deemed appropriate because the dry and wet thermal conductivity values of the test medium were accurately measured.

All property values assigned to the model were taken from laboratory measurements. The heat load was the only input parameter adjusted during computation of the basecase numerical model. The values for porosity, permeability, saturation, and thermal conductivity used in the simulation were measured on samples taken from the same oversized rock core as the Test 11 cylinder. These measured values were porosity of 0.07, permeability of $5 \times 10^{-17} \text{ m}^2$, and saturation of 0.34. Dry and wet thermal conductivities were measured as 1.74 and 1.90 W/m-K, respectively, and the van Genuchten parameters α at $1.44 \times 10^{-7} \text{ Pa}^{-1}$ and n at 1.575. Property values assigned to the Test 11 simulation are summarized in Table 4.3

In summary, the numerical model configured for the basecase of Test 11 had well established values for permeability, porosity, saturation, the van Genuchten α and n parameters, and thermal conductivity. Values assigned to boundary thermal conductivity and heater power were less well known but still had a reasonable sense of appropriateness.

4.2.2.1 Simulation Predictions

Agreement between the predicted results from the numerical model and the experimental results was examined with respect to: (i) the time at which the gas pressure difference attained a maximum value, (ii) the maximum gas pressure attained, and (iii) the temperature recorded at the heater. Because the heater power was adjusted to ensure that the simulated heater temperature was the same as the measured heater temperature of 165 °C, the numerical model was judged based on the first two criteria—the time and amplitude of the gas pressure peak. The experimental measured time and amplitude of the maximum gas pressure peak in Test 11 were 4.5 hr and 17 kPa, respectively. As shown in Figure 4-53, the resulting basecase numerical model for Test 11 predicted a Δp_g of 86 kPa which occurred after 7 hr of heating. The pressure pulse of 15 kPa predicted at 1 hr is a computational artifact of the rapid power increase that occurred at 0.8 hr. This cause/effect relationship is graphically illustrated in Figure 4-54, in which pressure and power are jointly presented. As illustrated, the simulated Δp_g response using the basecase property values occurred at the same approximate time as the observed peak Δp_g . The predicted magnitude of the maximum gas pressure, however, was greater and occurred later than the observed peak Δp_g . The prominent decrease in Δp_g , observed soon after the peak Δp_g was attained, was not predicted in the basecase simulation.

4.2.2.2 Sensitivity Analyses

The specific cause for the discrepancy between the observed and predicted Δp_g is not readily apparent. To determine which parameters have the most effect on the predictions and to determine if the pressure increase prediction could be made to agree better with the measured value, the sensitivity of the numerical model to changes in several input parameters was evaluated. These analyses were accomplished by modifying one parameter value at a time, while maintaining all other input parameters at the basecase values. Parameters modified in this exercise included heater power, permeability, porosity, initial saturation, and the van Genuchten α and n parameters. The basecase parameter values used in the

Figure 4-53. Numerically predicted gas pressure difference for Test 11 cylinder using basecase properties (solid line) compared to observed gas pressure difference (dashed line)

Figure 4-54. Gas pressure difference (solid line), Δp_g , and heater power (dashed line) (relative to heater power at initiation of experiment) plotted versus time

sensitivity analysis are listed in Table 4-3. The impact of changing the parameter values is evaluated relative to the peak Δp_g of 17 kPa and the maximum temperature of 165 °C at 4.5 hr as measured in Test 11. The effect of modifying each of these values on the predicted time and amplitude of the maximum Δp_g is discussed in the following paragraphs.

When the heater power was increased to 64 W (i.e., no heat inefficiency), the temperature increased to about 300 °C and pressure increased to 228 kPa. The Δp_g occurred sooner than the peak temperature, indicating that the modeled system was not dynamically similar to Test 11, for which the maximum temperature and pressure occurred simultaneously. This calculation further supports the premise that there was an approximately 45 percent heat loss. A decrease of heater power to 20 W resulted in a peak Δp_g of about 22 kPa, similar to the observed peak Δp_g and a maximum temperature of 65 °C. This predicted performance is illustrated in Figure 4-55.

An increase in permeability by a factor of 100 from 5.0×10^{-17} to 5.0×10^{-15} m² decreased the peak Δp_g to about 3 kPa and the temperature to 146 °C. The time at which these peaks occur was increased to 7.2 hr (Figure 4-56). A decrease in permeability to 1×10^{-18} m² increased the peak Δp_g to 413 kPa at a time of about 5 hr. As illustrated in Figure 4-55, a permeability of about 5×10^{-16} m² would provide better agreement between the simulated and observed responses than either of the test simulations, although no adjustment of permeability results in the distinct pressure decrease observed after the peak Δp_g was attained.

Porosity was modified to 0.03 and 0.15 from the basecase value of 0.07. Decreasing porosity to 0.03 decreased the simulated peak Δp_g to about 55 kPa (Figure 4-57). The peak Δp_g was increased to 117 kPa when porosity was increased to 0.15. A greater decrease in the Δp_g was observed after the peak Δp_g was attained for those simulations when porosity was increased compared to the basecase simulation, which exhibited minimal decrease in pressure after the peak Δp_g was attained.

The direct response to Δp_g that occurred because of changes in heater power, permeability, and porosity was not observed when initial saturation was increased. As illustrated in Figure 4-58, the peak Δp_g increased when the initial saturation was increased to 0.50 from the basecase saturation of 0.34. However, a decrease in peak Δp_g was observed when the initial saturation was either further increased to 0.80 or decreased to 0.20 from the basecase value. In all cases in which saturation was varied, the time at which the peak Δp_g occurred was invariant.

The value of the van Genuchten α parameter was measured as 1.44×10^{-7} Pa⁻¹ in the basecase for Test 11. The measurement of 1.44×10^{-7} Pa⁻¹ was both increased and decreased by an order of magnitude in the sensitivity analysis. The maximum Δp_g predicted for these modified values of α are illustrated with the baseline case in Figure 4-59. Increasing the value to 1.44×10^{-6} Pa⁻¹ resulted in a predicted peak Δp_g of 86 kPa. This predicted Δp_g was about five times higher than the measured value of 17 kPa (Figure 4-58). When the value of α was reduced to 1.44×10^{-8} Pa⁻¹, the corresponding predicted Δp_g was 16 kPa. Although this latter value is close to the measured Δp_g reducing α by an order of magnitude is difficult to justify. This adjustment is illustrated in Figure 4-60 where retention

Table 4-3. Summary of Test 11 basecase parameter values used in sensitivity analysis

Parameter	Value
Heater Power (W)	36
Permeability (m^2)	5.0×10^{-17}
Saturation	0.34
van Genuchten α (Pa^{-1})	1.44×10^{-7}
van Genuchten n (-)	1.575
Tuff Thermal Conductivity-Dry (W/m-K)	1.74
Tuff Thermal Conductivity-Wet (W/m-K)	1.90
Boundary Thermal Conductivity-Dry (W/m-K)	0.4
Boundary Thermal Conductivity-Wet (W/m-K)	0.4

curves with varying values for α are plotted with the measured retention curve data. Furthermore, a predicted decrease in Δp_g in response to a decrease in α , which is the inverse of the air-entry value, is counter intuitive. A partially saturated medium that has smaller equivalent pore sizes would be expected to impede the movement of gas, thus resulting in increased pressures rather than decreased pressures predicted by the numerical model. Of added interest in Figure 4-59 is that a rapid decrease in Δp_g was observed after the peak Δp_g for the larger α value of $1.44 \times 10^{-6} \text{ Pa}^{-1}$ but not for smaller values of Δp_g .

The van Genuchten n parameter was decreased to 1.29 and 1.26 from the basecase value of 1.575. Since increases in n only resulted in a greater differences between predicted and observed Δp_g , they are not reported here. The effect of decreasing n on the peak Δp_g is illustrated in Figure 4-61. As illustrated, agreement between the predicted and observed Δp_g was attained for an n value of 1.29. This value for n also exhibited a decrease in Δp_g after the peak was attained, although the predicted decrease was less than that observed. A further decrease in n to 1.26 exhibited an additional decline in Δp_g . Although assigning a value of 1.29 to n provides good agreement with the observed Δp_g , as illustrated in the matric pressure/saturation plot in Figure 4-62, an n value of 1.29 is not realistically representative of the ALTS tuff sample used in Test 11.

A reduction in heater power from 36 to 20 W was equivalent to a reduction in α from 1.44×10^{-7} to $1.44 \times 10^{-8} \text{ Pa}^{-1}$, or in n from 1.575 to 1.29. All resulted in approximate agreement between the observed and predicted peak Δp_g . Similarly, an increase in permeability by a factor of 10 from the basecase value of $5 \times 10^{-17} \text{ m}^2$ resulted in a peak Δp_g of about 17 kPa. Neither reductions nor increases in the basecase values of porosity or initial saturation resulted in agreement of the peak Δp_g . Although agreement between the numerical model and observed results is possible by varying heater power, α , n ,

Figure 4-55. Variation in predicted gas pressure difference, Δp_g , in response to heater power increase to 65 W (short dash) or decrease to 20 W (long dash)

Figure 4-56. Variation in predicted gas pressure difference, Δp_g , in response to permeability decrease to $1 \times 10^{-18} \text{ m}^2$ (short dash) or increase to $5.0 \times 10^{-15} \text{ m}^2$ (long dash)

Figure 4-57. Variation in predicted gas pressure difference, Δp_g , in response to porosity increase to 0.15 (long dash) or decrease to 0.03 (short dash)

Figure 4-58. Variation in predicted gas pressure difference, Δp_g , in response to initial saturation increase to 0.50 (dotted line) and 0.80 (long dash) and to decrease to 0.20 (short dash)

Figure 4-59. Variation in predicted gas pressure difference, Δp_g , in response to the van Genuchten α parameters increase to $1.44 \times 10^{-6} \text{ Pa}^{-1}$ (short dash) or decrease to $1.44 \times 10^{-8} \text{ Pa}^{-1}$ (long dash)

Figure 4-60. Variation in predicted retention curve for the Apache Leap Test Site tuff sample in response to a 10-fold increase (long dash) or a 10-fold decrease (short dash) in the van Genuchten α parameter (Pa^{-1}). Measured data are represented with dots.

Figure 4-61. Variation in predicted gas pressure difference, Δp_g , in response to the van Genuchten n parameter decreased to either 1.29 (long dash) or 1.26 (short dash)

Figure 4-62. Variation in predicted retention curve for the Apache Leap Test site tuff sample in response to decreases in the van Genuchten n parameter. Measured data are represent with dots.

or permeability, none of these adjustments are justifiable. The source of the discrepancy between the predicted and observed peak Δp_g is not fully resolved.

A possible source for the inconsistency between predicted and observed Δp_g is the way gas permeability is calculated in the code used in these simulations. The relative permeabilities of gas and liquid are summed to 1.0 in the V-TOUGH and C-TOUGH codes. These values may not be appropriate for all media. Air and water permeability measurements on the ALTS tuff reported by Rasmussen et al. (1993) indicated that the measured relative permeabilities do not sum to a constant. Inappropriate characterization of gas flow permeabilities could have also been a source for the discrepancy between predicted and measured peak Δp_g .

Another potential source for the discrepancy between predicted and observed Δp_g are the values assigned to the binary diffusion term in the numerical code. Lichtner and Walton (1994) have identified the assignment of values to binary diffusion as important when simulating heat and mass transfer.

4.2.3 Conclusions of Gas Pressure Buildup Experiments and Analyses

Conclusions from the gas pressure buildup experiment results are summarized as the following:

- Gas pressure buildup experiments were successfully conducted and monitored in two media types, a cement slurry mixture and a tuff sample from the ALTS. Gas pressure differences of 22 kPa and 17 kPa were measured.
- Low permeability rock was desaturated close to the heater during heating. Vapor generated at the heater condensed relatively uniformly in the rock matrix between the dryout zone and the outer boundary.
- After the initial gas pressure buildup was released, intermittent gas pressure releases were observed.
- Times and rates of resaturation were measured in both cylinder experiments, Tests 9 and 11. Resaturation times of 100–200 days for the cement and 70–470 days for the tuff were measured. A resaturation rate of 3×10^{-7} m/s was measured for the cement. The resaturation rate could not be measured in the tuff.
- The maximum temperature and the time at which the maximum temperature and peak gas pressure occurred were predicted using C-TOUGH with measured property values. The maximum gas pressure difference was reproduced within a factor of about five of the numerical model. The predicted time at which the peak gas pressure difference occurred was similar to the observed time.
- Sensitivity analyses evaluated the effect of changes in model parameter values assigned to heater power, permeability, porosity, initial saturation, thermal conductivity and the van Genuchten parameters α and n . Adjustment of input values for heater power, permeability, α , and n provided better agreement between numerical and experimental results. However, no justification to make these adjustments was identified.

Results from the gas pressure buildup experiments provided the following conclusions that contribute to understanding the fundamental basis of thermally driven moisture redistribution through partially saturated porous media.

- Moisture vaporized at the heat source condensed relatively evenly through the low permeability tuff matrix with a small van Genuchten α parameter (i.e., large air-entry value) between the dryout zone and the constant temperature outer boundary. The formation of a moisture buildup zone immediately past the dryout zone was not observed.
- The gas pressure buildup experiments support the conceptual model for thermally driven moisture redistribution through partially saturated porous media which states that water is transported primarily as vapor during the heating period and as liquid during the cooling period.
- Gas pressure buildup and release were observed at the heat source. This mechanism can potentially transport large amounts of water as vapor relatively long distances from the heat source.

5 ASSESSMENT OF SCALING LAWS

The scaling laws for the conceptual models developed in Section 2.2 to describe moisture transport in a locally heated, partially saturated porous medium were assessed by comparing predictions of time durations and pressure magnitudes estimated from the scaling laws against: (i) experimental results at the laboratory scale; and (ii) numerical simulation predictions at the laboratory, field, and mountain scales. The assessments were used to establish the range of validity over which the idealized conceptual models and scaling laws can be used to design field-scale experiments and to interpret such experiments in terms of mountain-scale responses.

Analyses of the results from the laboratory-scale experiments were strengthened by using results from previous field-scale experiments to gain a better understanding of thermally driven moisture redistribution. These field-scale heater tests are described by Patrick (1986), Zimmerman et al. (1986), and Ramirez (1991). The soundness of the interpretation of the proposed scaling laws was further tested by conducting finite-difference mathematical analyses of the laboratory-scale experiments, field-scale heater tests, and the repository system. Tests 8 through 11 provided laboratory-scale information for evaluating the proposed scaling laws.

5.1 THERMAL EVOLUTION MODEL

As discussed in Chapter 2, the scaling laws are predicated on a thermal evolution model of the proposed geologic HLW repository that is characterized by three distinct periods: (i) an early heating period, (ii) an intermediate transitional period, and (iii) a late cooling period. One set of scaling laws was developed for the heating period and a separate set for the cooling period. This generalization of thermal periods and of the transport mechanisms during each period is based on the assumption that the strength of the repository heat source is sufficient to cause significant vaporization near the heat source; a smaller heat generation rate would not necessarily result in the formation of the three distinct thermal periods. The scaling laws, in fact, can be used to help determine whether the heating rate is sufficient to cause significant vaporization and a consequent large buildup of gas pressure. After a discussion of the database used in these evaluations, the heating and cooling periods scaling laws assessments are presented.

5.2 LABORATORY EXPERIMENTS AND NUMERICAL SIMULATIONS USED IN THE SCALING LAW ASSESSMENTS

5.2.1 Experiment Database

The primary experimental data available for assessing both sets of scaling laws were the results of the gas pressure buildup tests. Four experiments (Tests 8 through 11) were conducted in this group of tests. Results of only Tests 9 and 11, however, were suitable for analysis of the scaling laws. These two experiments were similar in geometry and heating, but a different medium was used for each: a cement slurry for Test 9 and a sample of tuff from the ALTS for Test 11. The other cylinder tests also had the objective of investigating gas pressure buildup and moisture transport; however, media difficulties or failures were encountered during these tests. In one case, the permeability of the medium was too large to allow for a significant gas pressure buildup (Test 8); in the other, the integrity of the medium was compromised when the consolidated medium cracked soon after heating was initiated (Test 10). Thus, data from these other tests did not qualify for use in assessing the scaling laws.

5.2.2 Numerical Simulations

Finite-difference mathematical simulations were conducted to evaluate the proposed scaling laws over a wider range of parameters and geometric sizes than are covered by the experimental results. Three general length scales were addressed in the evaluation: laboratory, field, and mountain. The approximate spatial dimensions of these three simulations are 0.1, 1, and 100 m; thus a spatial scale of three orders of magnitude was addressed. The test cases for each of the three scales were Test 11, the Large Block Test (LBT) at Fran Ridge near YM (Buscheck et al., 1993; Lin et al., 1994), and the proposed HLW repository at YM, respectively. The test case for the laboratory scale was also simulated to gain confidence that the heat and mass transfer mechanisms were appropriately represented in the mathematical modeling approach. Five simulations representing the three spatial scales were conducted in this part of the analysis: the basecase for Test 11, the LBT at heat rates of 1,500 and 3,000 W, and YM at heat loads of 57 and 114 kW/acre. All the analyses used either V-TOUGH or C-TOUGH. Only portions of a sixth case, Test 9, were considered in these analyses.

5.2.2.1 Laboratory Scale Simulation

Test 11, a 1D radial gas pressure buildup experiment, was numerically simulated by a 2D model to accommodate heat lost through the top and bottom boundaries and other 2D features. This mathematical model was the same as the one used for the investigation of heat and mass transfer mechanisms and is discussed in Section 4.2.2.

5.2.2.2 Field Scale Simulation

The LBT at Fran Ridge was numerically modeled as a vertically oriented 2D domain. Because of the axisymmetry of the system, only a vertical half section was modeled. A schematic of the LBT numerical model is presented in Figure 5-1. The actual block has cross-sectional dimensions of 3 m in both the x- and y-directions and a total height of 4.5 m above the excavated surface of the bedrock. The numerical model has a vertical dimension of 6 m (thus, extending an additional 1.5 m below ground surface in an attempt to diminish adverse boundary effects) and a horizontal dimension of 1.5 m, which takes advantage of the symmetry of the experiment. The vertical boundary above the excavated surface was specified as no-fluid flow and adiabatic. This characterization was justified by the planned placement of an impervious layer and guard heaters on this surface. The top boundary, which is to remain open to the atmosphere, was assigned a high permeability ($4.0 \times 10^{-2} \text{ m}^2$), low thermal conductivity (0.2 W/m-K), and large elemental volumes to allow moisture movement and heat loss across the top of the model. The bottom boundary of the model and that part of the vertical boundary below the actual ground surface were assigned the same permeability as the block, low thermal conductivity (0.2 W/m-K), very low specific heat, and very large elemental volumes to allow for fluid flow and heat loss through the base of the model. The heat source was simulated as five horizontal cylinders (two and one-half in the half plane) perpendicular to the plane of the model. These heat sources were placed 1.5 m above the excavated surface (3 m above the base of the model), similar to the design of the LBT. Each heater was capable of providing 300 W for a total heat rate of 1,500 W to the block. A second model of the LBT was simulated with the heat rate assigned to each of the five heaters doubled to 600 W, giving a total heat rate of 3,000 W. The second simulation was conducted to assess the effect of higher temperatures on fluid flow and gas pressure buildup.

Fran Ridge Large Block Test

Figure 5-1. Schematic of the Lawrence Livermore National Laboratory large block test numerical model

The LBT medium was assumed to be a homogeneous composite block of fractures and rock matrix and was treated as an equivalent continuum (Wang and Narasimhan, 1986; Klavetter and Peters, 1986; Nitao, 1988). The relative permeability for the equivalent continuum is expressed as a volume average of the fracture and matrix relative permeabilities and the hydraulic conductivities K :

$$k_{rel,B} = \frac{[K_f k_{rel,f} \phi_f + K_m k_{rel,m} (1 - \phi_f)]}{K_B} \quad (5-1)$$

where the subscript B denotes bulk properties. The saturated bulk liquid hydraulic conductivity, K_B , is defined in this model by the relation:

$$K_B = \phi_f K_f + K_m (1 - \phi_f) \quad (5-2)$$

The property values for LBT were taken from Klavetter and Peters (1986). According to the formulation given in Eq. (5-2), the LBT medium with a matrix porosity of 0.10, fracture porosity of 0.00183, matrix permeability of $1.9 \times 10^{-18} \text{ m}^2$, and fracture permeability of $1.0 \times 10^{-11} \text{ m}^2$ has a composite permeability of $1.8 \times 10^{-14} \text{ m}^2$.

5.2.2.3 Mountain-Scale Simulation

A vertically oriented 1D numerical model was used to simulate mass and heat transfer in the YM repository-scale model. A 1D model was selected over a more representative geometric model to provide greater vertical resolution in the region closest to the heater horizon. The numerical model extended from ground surface, which had an assigned saturation of 0.5 and temperature of 15 °C, to full saturation and a temperature of 30 °C at a depth of 600 m. The upper and lower boundaries were characterized as no-fluid flow and constant-temperature boundaries. The medium was assumed to be a uniform composite medium with the same properties as those assigned to the LBT model. Two cases representing different heat loads were simulated. In the first, a nominal maximum heat load of 57 kW/acre was imposed at the repository horizon depth of 375 m. The heated repository horizon is modeled as an infinite horizontal plane at a depth of 375 m in the 1D numerical model. For the second case, the heat load was increased to 114 kW/acre to represent an extended-dry repository scenario. In both cases, the heat load was decreased over time (Brandshaug, 1991).

The intrinsic and hydraulic properties of the media in the experiments and simulations are summarized in Table 5-1. For Tests 9 and 11, many of these properties were measured directly (when such measurements were feasible). In the simulations, some of the properties were varied about the measured values to examine the sensitivity of the predictions to changes in the property values (Section 4.2). For Test 9, the properties changed with time during the test, so the values listed in the table are considered to be best estimates rather than exact measurements.

5.3 ASSESSMENT OF THE CONCEPTUAL MODEL SCALING LAWS FOR THE HEATING PERIOD

5.3.1 Criteria for Similarity During the Heating Period

To compare systems of different geometric scales requires that the systems are sufficiently similar. According to the similarity relations developed in Section 2.2, the magnitude and time duration

Table 5-1. Summary of property values assigned to the laboratory-scale cylinder model, the field-scale large block test model, and the mountain-scale Yucca Mountain repository model

Parameter	Test 9 and Test 11 (Laboratory Scale)	Fran Ridge LBT (Field Scale)	YM Repository (Mountain Scale)
liquid saturation S_l	0.90 (Test 9) 0.50 (Test 11)	0.70	0.68
matrix porosity ϕ	0.32 (Test 9) 0.07 (Test 11)	0.10	0.10
matrix permeability k (m^2)	2.0×10^{-18} (Test 9) 5.0×10^{-17} (Test 11)	1.9×10^{-18}	1.9×10^{-18}
matrix value of van Genuchten n	1.323 (Test 9) 1.575 (Test 11)	1.798	1.798
matrix value of van Genuchten α (Pa^{-1})	6.36×10^{-7} (Test 9) 1.44×10^{-7} (Test 11)	5.8×10^{-7}	5.8×10^{-7}
fracture porosity ϕ	—	0.00183	0.00183
fracture permeability k (m^2)	—	1.0×10^{-11}	1.0×10^{-11}
composite permeability k (m^2)	—	1.8×10^{-14}	1.8×10^{-14}
fracture value of van Genuchten n	—	4.23	4.23
fracture value of van Genuchten α (Pa^{-1})	—	1.315×10^{-7}	1.315×10^{-4}

of the gas pressure buildup and the advective- and buoyancy-induced gas velocities will be the same at homologous locations and homologous elapsed time durations for porous media of different geometric sizes and hydrologic properties if the gas Advection Number has a similar magnitude. This gas Advection Number, as defined previously by Eq. (2.33), is:

$$Ad_g \approx \frac{\phi S_{vo} \alpha_s \mu_{go}}{k k_{rel,go} L \rho_{go} g \beta_{go} T_{avg}} \left(\frac{\rho_{vo}}{\rho_{go}} \right) \left(\frac{h_{fg,o}}{R_v T_{avg}} \right) \quad (5-3)$$

Thus, systems at different scales are similar with respect to gas pressure buildup and vapor transport during heating if their Ad_g values have a similar magnitude.

The strength of the heat source, Q , directly affects the magnitude of T_{avg} in Eq. (5-3) and the characteristic fluid properties. There is considerable interest in designating the best value of Q for the repository and in understanding the impact of the choice of Q on the response of the repository. Selection of the repository design will determine if the repository follows the Site Characterization Plan (SCP) design with relatively low areal thermal loading (and consequently, relatively low temperatures) or if an extended-dry repository design concept (with relatively high temperatures) is selected (Ramspott, 1991; Nitao et al., 1992; Wilder, 1993; Buscheck and Nitao, 1992, 1993, 1994). As will be demonstrated, differences in the thermal loading can affect the nature of the fluid flow regimes to be expected at both the LBT and the proposed YM repository. An indication of which flow regimes are to be expected is indicated by the magnitude of Ad_g , as discussed in Section 2.2. When $Ad_g > 1$, large pressure gradients and advective gas flows will be created, and the heated region will tend to be of the extended-dry type.

To evaluate Ad_g for the various systems, representative values must be chosen for all the parameters, including those such as vapor density, which may vary with time and location in the system. As an example of this selection, vapor saturation can vary from approximately zero near the heat source to approximately full saturation in zones of condensation; hence, a representative average is $S_{vo} = 0.5$, and this value is used in Eq. (5-3) in all the computations to assess the validity of the scaling laws. It was also necessary to estimate ΔT_o and T_{avg} and the characteristic length, L , for each system. The temperatures ΔT_o and T_{avg} for a given heating rate can be estimated by combining Eqs. (2-28) and (2-29) or from a separate heat conduction analysis. But here, for simplicity, results of the numerical simulations were used to calculate these temperatures. Numerically predicted values for ΔT_o for the six test cases are listed in Table 5-2.

The characteristic lengths of the laboratory experiments and LBT were reasonably assumed to be the size of the respective models. The L value of the repository simulation was not so evident. A heat conduction analysis could be used to estimate the size of the repository's affected volume, but here the numerical simulation results were again used for simplicity. In addition, the heating rate for the YM repository model was specified in terms of power released per unit area, rather than in terms of per unit heater length, which is the form assumed in the definition of Ad_g . A characteristic area of $L \times 1 \text{ m}^2$ was assumed in the areal specification of Q in Ad_g . (As explained in Section 2.2.2.1, a change in geometry of the idealized conceptual model from 2D to 1D or 3D will introduce different numerical factors in the

Table 5-2. Summary of characteristic parameters assigned to scaling law model for test cases assessed

Experiment	L (m)	Q	ΔT_0 (°C)	k (m ²)	Ad_g
Test 9	0.145	35 W	170	2.0×10^{-18}	1.1×10^6
Test 11	0.145	35 W	145	5.0×10^{-17}	9,500
LBT	1.6	1,500 W	134	1.8×10^{-14}	8
LBT	1.6	1,500 W	134	1.9×10^{-18}	35,700
LBT	1.6	3,000 W	180	1.8×10^{-14}	6
LBT	1.6	3,000 W	180	1.9×10^{-18}	33,000
YM	100	57 kW/acre	80	1.8×10^{-14}	0.1
YM	100	57 kW/acre	80	1.9×10^{-18}	500
YM	200	114 kW/acre	157	1.8×10^{-14}	0.1
YM	200	114 kW/acre	157	1.9×10^{-18}	450

model results but will not affect the parameters that make up the dimensionless groups. All numerical factors are ignored in the model). The results of the Ad_g calculations for the six test cases are summarized in the, following section. As illustrated in Table 5-2, Ad_g has been calculated at two candidate values for permeability for the field- and mountain-scale test cases. As will be discussed, there is some discretion in the choice of assigned permeability for the field and repository scales.

5.3.1.1 Laboratory Scale

A characteristic length of 0.145 m was assigned to the laboratory experiments. The maximum ΔT_0 was measured to be 170 °C in Test 9 and 145 °C in Test 11. The computed value of Ad_g was thus about 10^6 for Test 9 and about 9.5×10^3 for Test 11, both at a heating rate of 35 W. Since $Ad_g > 1$ for each case, both of these tests were conducted for conditions that represent strongly pressure-driven advective gas flow. Incidentally, if the heating rate is increased, the value of Ad_g for these tests decreases slightly because of the change in the representative thermodynamic properties with temperature.

5.3.1.2 Field Scale

A characteristic length of 1.6 m was used in the LBT scaling law computations, to agree with the LBT numerical simulation. For a heat release rate of 1,500 W, ΔT_o was predicted to be 134 °C, while ΔT_o was 180 °C for a heat release rate of 3,000 W. The value of Ad_g depends on the permeability. If the composite block permeability ($1.8 \times 10^{-14} \text{ m}^2$) is used, to agree with the mathematical simulations, the compiled values of Ad_g are about 8.0 for a heat release rate of 1,500 W and about 6.0 for a heat release rate of 3,000 W. With this characterization, the gas flow regime is predicted by the idealized conceptual model to be pressure driven, but not strongly so. However, if the permeability of the matrix ($1.9 \times 10^{-18} \text{ m}^2$) is assigned to the model medium for reasons discussed below, the values of Ad_g are increased substantially to 35,700 and 33,000, respectively, for the two heat loads and the gas flow regime is predicted to be strongly pressure-driven.

For the actual LBT experiment, there is compelling evidence from previous similar field-scale experiments that a significant gas pressure will occur during the heating period; if so, then apparently the matrix permeability is the relevant permeability to use in assessing similarity requirements during heating. This previous evidence is from the LLNL G-Tunnel heater test, in which gas pressure buildups as great as 330, 20, and 22 kPa were measured at distances of 0.8, 2.0, and 1.0 m, respectively, from the middle of the heater (Ramirez et al., 1991). In fact, gas pressure buildup was observed at all three locations in which gas pressure was recorded during this test. The G-Tunnel heater experiment was conducted in the Grouse Canyon tuff, a fractured, welded tuff with properties believed to be similar to the proposed repository horizon at YM (Zimmerman and Finley, 1986) and Fran Ridge, the site of the LBT. Although the medium at the site of the G-Tunnel field test is fractured, pressures were obviously measured at locations not directly connected by an open gas pathway to the heat source. Apparently, the fracture component to the medium did not actively participate in the dissipation of gas pressure from the heater to the points of gas pressure measurement.

5.3.1.3 Mountain Scale

For YM at a 57 kW/acre heating load, the characteristic length was inferred from the extent of noticeable thermal impact in the numerical simulation to be 100 m, and the maximum ΔT_o was predicted to be 80 °C. For the 114 kW/acre heating load, the corresponding quantities were 200 m and 157 °C. If the composite block permeability ($1.8 \times 10^{-15} \text{ m}^2$) is used to evaluate Ad_g , the predicted value of Ad_g is about 0.1 for both heat loads. These low values of Ad_g indicate that the gas flow regime would be dominated by buoyancy or diffusion effects rather than by pressure gradients. If the matrix permeability ($1.9 \times 10^{-18} \text{ m}^2$) is used, the values of Ad_g are 500 and 450, respectively, thus suggesting that the gas flow would be pressure driven.

As demonstrated at the field scale in the G-Tunnel heater experiment, if the connectivity of fractures is not sufficient to dissipate gas pressures, the composite permeability model may be inappropriate. This observation raises an important question of the representative elemental volume (REV) relevant to this scaling exercise (Bear, 1979), namely, will fractures contribute to gas flow at the repository or mountain scale even though fractures did not contribute to gas flow at the field scale? Additional site characterization may be required to address this question.

The characteristic Ad_g values for these different representations at the three geometric scales are summarized in Table 5-2. The values of Ad_g indicate that, if the medium is assigned the permeability of the matrix, the laboratory-, field-, and mountain-scale systems are all similar (i.e., $Ad_g > 1$) with respect to heating period responses.

5.3.2 Similarity Criteria Values for Different Scales

The validity of the proposed heating period scaling laws as a method to correlate thermal responses of the various systems was first assessed by comparing the idealized heating-period model to the experimental results for Tests 9 and 11 and to the numerical simulation of Test 11. After this assessment of the validity of the heating-period scaling laws, the idealized model is then compared to the numerical simulations of heat and mass transfer for the LBT and the YM repository. The key indicators for the heating period assessment were the magnitude of the gas pressure increase, Δp_g , and its time of occurrence.

5.3.2.1 Laboratory Scale

The relevant experimental results from Tests 9 and 11 are summarized as follows: Test 9, a peak Δp_g of 20 kPa after 8.5 hr of heating; Test 11, a peak Δp_g of 17 kPa after 4.5 hr of heating. The relevant predictions of the numerical simulation of Test 11 are: a peak Δp_g of 86 kPa after 7 hr of heating. As illustrated in Figure 4-53, the numerical simulation of Test 11 using basecase properties is in close agreement with the time of occurrence of the peak Δp_g , however, the simulated Δp_g is a factor of five greater than the observed Δp_g . Whether the source of this discrepancy is an improper assignment of property values or an inadequacy of the numerical model is not known. The effect of variation of several key physical parameter values is assessed in Section 4.2.2.2. Although prediction of the peak Δp_g differs from the observed peak Δp_g by a factor of five, good agreement between the predicted and observed times of the peak Δp_g support the use of the numerical simulation in these order-of-magnitude calculations.

For the idealized conceptual model, the predictions of Δp_g and the heating duration required to obtain the peak Δp_g are given by Eqs. (2-29) and (2-30) respectively. These relations are based on representative values of the gas and vapor properties appropriate for the average temperature, as explained earlier. The characteristic values assigned to the laboratory scaling model are summarized in Table 5-2. The conceptual model predictions for the experiments are as follows: Test 9, a peak Δp_g of 430 kPa and time of 11.7 hr to obtain this peak; Test 11, a peak Δp_g of 12 kPa, and time of 11.7 hr to obtain this peak. The results are summarized with the observed values and numerically simulated predictions for the laboratory-scale experiments in Table 5-3.

For Test 11, the conceptual model predicts the experimental results well within the accuracy expected of an order-of-magnitude model. The medium properties for Test 11 were well defined by measurements, so the close agreement is not unexpected. For Test 9, there was considerable doubt about the medium properties, particularly the permeability. Hence, the considerable difference between the conceptual model predictions and the experiment results are not thought to invalidate the conceptual

Table 5-3. Summary of measured, numerically predicted, and scaling law predicted gas pressure peaks and time at which the peak occurred

Experiment	Observed Δp_g Peak (kPa)	Observed Time of Δp_g Peak (hr)	Numerical Δp_g Peak (kPa)	Numerical Time of Δp_g Peak (hr)	Scaling Law of Δp_g Peak (kPa)	Scaling Law Time Δp_g Peak (hr)
Test 9	20	8.5	n/a	n/a	430	11.7
Test 11	17	4.5	86	7	12	11.7

model. Furthermore, the conceptual model predictions from Test 11 also compare well with the simulation of Test 11. It is therefore concluded that the conceptual model for the heating period is validated for laboratory-scale systems when the assumptions made in the model development (as discussed below) are met in the experiments. Consequently, scaling laws derived from the conceptual model are a valid method of interpreting and scaling-up results from laboratory-scale experiments.

5.3.2.2 Field Scale

The predictions of the numerical simulation for the LBT at a heating rate of 1,500 W are summarized as: ΔT_o of 132 °C, peak Δp_g of 20 kPa, after a heating duration of 115 days. For a heating rate of 3,000 W, the simulation predictions are: ΔT_o of 180 °C; peak Δp_g of 35.5 kPa, after a heating duration of 50 days. Figures 5-2 and 5-3 show the detailed time histories of the gas pressure predicted by the simulations. These predictions are based on the use of a composite block permeability.

The conceptual model predictions of the peak Δp_g are of the order of 100 Pa for both heating rates when the composite block permeability is used in the computations. These predictions are only about 2 to 5 percent of the numerical simulation predictions. But these small values of Δp_g correspond to the expected results for media such as the composite block that have relatively small values of Ad_g . When the matrix permeability is assigned to the test medium in the calculations, the conceptual model predicts a peak Δp_g of 250 kPa after a heating period of 42 days for a heating rate of 1,500 W, and a peak Δp_g of 280 kPa, again after a heating period of 42 days, for a heating rate of 3,000 W. Although the predicted conceptual model heating periods required to obtain the peak Δp_g agree well with the numerical simulations, the conceptual model peak Δp_g values are about a factor of ten larger. However, the conceptual model peak Δp_g predictions are reasonable when compared to the measured values of 100 kPa to 300 kPa in the G-tunnel heater test (which had a comparable L , matrix k , and ΔT_o relative to the LBT). It is therefore concluded, on the basis of the G-tunnel experiment results, that the conceptual model for the heating period is validated for field-scale systems when the assumptions made in the model development are met in the experiments. Scaling laws derived from the conceptual model are thus a valid method of interpreting and scaling up results from laboratory-scale experiments to at least the field scale.

Figure 5-2. Numerically predicted maximum gas pressure differences for the large block test at 1,500 W

Figure 5-3. Numerically predicted maximum gas pressure differences for the large block test at 3,000 W

5.3.2.3 Mountain Scale

The predictions of the finite-difference mathematical simulation for the YM model are summarized as follows: ΔT_0 of 157 °C and peak Δp_g of 42 kPa after about 160 yr, for a heat load of 114 kW/acre; ΔT_0 of 80 °C, and peak Δp_g of 5.5 kPa after about 63 yr, for a heat load of 57 kW/acre. Figures 5-4 and 5-5 show the detailed time histories of the gas pressures predicted by the simulations, which are based on the composite block permeability.

The conceptual model predictions of the peak Δp_g are of the order of only 50 Pa for both heat loads, when the composite block permeability is assigned to the medium in the computations. When the matrix permeability is assigned to the medium, the model predicts a peak Δp_g of 160 kPa after a heating period of 264 yr for the 57 kW/acre heat load, and a peak Δp_g of 210 kPa after a heating period of 1,050 yr for the 114 kW/acre heat load. Just as for the LBT case, these peak Δp_g values are about a factor of ten larger than the numerical simulations. There are no measurements of peak Δp_g available from a mountain-scale experiment. Thus, the validity of the conceptual model cannot be assessed with certainty. Nonetheless, the model validation provided by laboratory- and field-scale experimental measurements allows the conclusion to be drawn that the conceptual model, and scaling laws derived from it, will give satisfactory results for mountain-scale systems when the model assumptions are met. Table 5-4. summarizes the various experimental, simulations, and conceptual model results for the heating period.

5.3.3 Summary of Heating Period Scaling Law Assessment

The conceptual model predictions of peak Δp_g and the heating time duration required to obtain this peak agreed well (i.e., within a factor of five) with laboratory- and field-scale experimental results when the properties of the experiment porous media (particularly permeability) were well defined. These comparisons indicate that scaling laws for peak pressure and heating duration required to obtain the peak Δp_g derived from the conceptual model represent a valid method to design, interpret, and scale-up heating period experiments.

Conversely, the conceptual model under-predicted by a factor of ten to a hundred the results of the numerical simulation of the LBT and the YM repository when the media permeability was assumed to be that of a composite block composed of a matrix and fractures. The heating duration required to obtain the peak Δp_g was, however, predicted satisfactorily. The conceptual model over-predicted, again by a factor of ten to a hundred, the results of the simulations when the media permeability used in the conceptual model was assumed to be that of the matrix alone. But these predictions for the LBT agreed well with the gas pressures measured in the G-tunnel heater tests, which had a similar L matrix k and ΔT_0 as the LBT.

The reason for these inconsistent predictions of Δp_g compared to the numerical simulations is the assumption made in the conceptual model that the gas pressure buildup is caused primarily by the combination of vapor generation at the heater and media confinement. The model is therefore not likely to represent accurately the gas pressure buildup in a medium that has little confinement (i.e., a relatively large permeability) but that is heated to temperatures significantly above the boiling point of the vapor; for this case, the pressure buildup is caused primarily by the high partial pressure of the vapor, and the

Figure 5-4. Maximum gas pressure differences for the Yucca Mountain repository at 57 kW/acre

Figure 5-5. Maximum gas pressure differences for the Yucca Mountain repository at 114 kW/acre

Table 5-4. Comparison of numerical and heating period scaling law predictions of magnitude and time of peak gas pressure difference

Experiment	Q	Numerical Prediction			Scaling Law Prediction		
		ΔT_o (°C)	Time of Δp_g Peak	Δp_g (kPa)	ΔT_o (°C)	Time of Δp_g Peak	Δp_g (kPa)
Test 11	35 W	145	7 hr	87	145	11.7 hr	12
LBT	1,500 W	132*	115 days	22	134	42 days	250
LBT	3,000 W	209*	50 days	35	209	42 days	280
YM	57 kW/acre	80	63 yr	5	80	264 yr	160
YM	114 kW/acre	157	160 yr	42	157	1,050 yr	210

* Denotes temperature at time of maximum gas pressure

confinement of the medium is of little importance. Both the LBT and the YM simulations represent these kinds of conditions. Hence, it is concluded that the conceptual model is not valid when both (i) $Ad_g < 10$ to 100, and (ii) $\Delta T_o > 125$ °C. The conceptual model can be modified to treat such cases but the modification is not thought to be necessary for the following reason. Actual fractured but otherwise tight porous media (which have a relatively large composite block permeability) are likely to exhibit high gas pressures caused primarily by matrix confinement, rather than by high vapor partial pressures, as demonstrated by the G-tunnel heater tests. This lack of connectivity among fractures has also been observed during gas flow tests at the ALTS (Bassett et al., 1994). Hence, the conceptual model is likely to be a valid representation of the pressure buildup and gas flow dynamics in most geologic applications.

As a further confirmation of the validity of the conceptual model for the heating period, when a numerical simulation of the LBT (again using a composite block permeability) was conducted for a heating rate of 750 W, the predicted peak pressure was about 1.5 kPa and ΔT_o was 105 °C (Dodge and Green, 1994b). The conceptual model (using a composite block permeability) agrees reasonably well with this peak pressure. Furthermore, the value of Ad_g is 11, which indicates that the gas flow should exhibit a noticeable buoyancy-driven component. Figure 5-6 demonstrates this conclusion; the gas flow for the 750 W heating rate shows a marked upward buoyancy component, while the gas flow for the 1,500 W heating case is primarily directed away from the heater, about equally upward and downward. This kind of buoyancy-driven gas flow pattern is also supported by the conceptual model for low heating rates described in Section 2.2.5 (Manteufel, 1994).

The presence of high gas pressures at three measurement locations near the G-Tunnel heater raised important questions regarding the connectivity of fractures. At a minimum, it can be stated that the

Distance from Center of Block (m)

Distance from Center of Block (m)

Figure 5-6. Numerically simulated gas flow velocity vectors of the Fran Ridge Large Block Test at 92.5 days at: (a) 50-percent heating rate (750 W), and (b) 100-percent heating rate (1,500 W)

high gas pressures were an indication that the fractures were not adequately connected to dissipate gas pressure buildup at a field scale of 1 to 2 m. Additional questions raised by this observation are: (i) do the high gas pressures imply that this lack of fracture connectivity will also inhibit the flow of liquid through the same rock, and (ii) are the mechanisms that inhibit fluid flow through connected fractures at the field scale expected to occur at the mountain scale. Although neither question is easily answered, mountain-scale measurements of both gas and liquid flow are prohibitively difficult. Future field-scale experiments similar to the G-Tunnel heater test that are conducted to closely monitor redistribution of moisture can contribute to resolving the question of fracture connectivity at least at the field scale.

5.4 ASSESSMENT OF THE CONCEPTUAL MODEL SCALING LAWS FOR THE COOLING PERIOD

Repository performance, in terms of maintaining HLW isolation, will be strongly affected by rewetting and the time when rewetting occurs. Hence, the critical response during the cooling period of the repository's thermal evolution is the time required to rewet the previously dried media near the heat source. Rewetting, as described by the conceptual model developed in Section 2, can be caused by both liquid flow and vapor mass diffusion followed by condensation. The conceptual model does not, however, address gravity driven refluxing down fractures. Although the refluxing is an important mechanism for rewetting the canister environment, neglecting the refluxing does not significantly limit the relevance of the conceptual model because vaporization and condensation activity will decrease substantially after the heating period. Hence, the prospect of liquid draining through vertically oriented fractures to rewet the dryout zone at the heater, which could be prevalent during the heating period, is much reduced during the cooling period. The rewetting liquid flows through the matrix because capillary pressure gradients exist primarily in the matrix. Predictions of rewetting during the cooling period should therefore be based on matrix properties rather than on composite block properties, even for fractured media. As a result of this dominant influence of the matrix permeability on liquid rewetting, the rewetting conceptual model should be valid even for systems for which the heating conceptual model is not (i.e., media highly permeated with open fractures and high heating rates).

In the following sections, predictions from the idealized conceptual model of the cooling period are compared to measured rewetting times from the laboratory experiments and to results extrapolated from the numerical simulations of the experiments and of LBT and YM. It should be noted that the effects of hysteresis, which could be significant, are not considered in these analyses.

5.4.1 Criteria for Similarity During the Cooling Period

Similarity during the cooling period for systems of different geometric scales depends on the liquid Advection Number Ad_l , defined in Section 2.2.4 by Eq. (2-44). To evaluate Ad_l for the laboratory experiments and the LBT and YM simulations, representative values of the saturation decrease, ΔS_l , during heating and the corresponding capillary pressure increase, Δp_{∞} , are needed for each case. The appropriate choices for these quantities will be discussed in detail in Section 5.4.2, and only a summary is given here. For Test 9: $\Delta S_l = 0.45$ and $\Delta p_{\infty} = 1.2 \times 10^4$ kPa; for Test 11: $\Delta S_l = 0.25$ and $\Delta p_{\infty} = 2.5 \times 10^5$ kPa; for LBT: $\Delta S_l = 0.35$ and $\Delta p_{\infty} = 4.0 \times 10^3$ kPa; and for YM: $\Delta S_l = 0.35$ and $\Delta p_{\infty} = 4.0 \times 10^3$ kPa. Based on these characteristic quantities, the computed values of Ad_l for the various systems are presented in Table 5-5. Since all the values of $Ad_l > 1$, the rewetting dynamics will be similar

Table 5-5. Gas and liquid advection numbers for different scales at different heat loads

Experiment	Q	$k \text{ (m}^2\text{)}$	Ad_g	Ad_l
Test 9	35 W	2×10^{-18}	170,000	110
Test 11	35 W	5×10^{-17}	10,000	7
LBT	1,500 W	1.9×10^{-18}	200,000	14
LBT	3,000 W	1.9×10^{-18}	180,000	13
YM	57 kW/acre	1.9×10^{-18}	2,500	2
YM	114 kW/acre	1.9×10^{-18}	4,000	5

for all the systems during the cooling period; that is, the results measured or predicted for one system can be scaled to the other systems. There is, however, a tendency of Ad_l to decrease as the geometric size increases. Consequently, buoyancy effects will be slightly more significant for the YM repository than for the other systems.

5.4.2 Similarity Criteria Values for Different Scales

5.4.2.1 Laboratory Scale

The duration of both Tests 9 and 11 was sufficiently extended after the end of heating that estimates of rewetting rates and durations were made during the cooling period. The estimates were made from the relative measurements of saturation shown previously in Figures 4-49 and 4-52. For both tests, there was a transition period of about 2 days after the heater was turned off before rewetting measurements were initiated.

For Test 9, all the rewetting measurements were made in the dryout region within 5 cm of the heater. The rewetting rate varied somewhat with measurement location within this region. At a location near the heater where the saturation was practically zero at the end of the 11-day heating period, the saturation increased by a little less than 1 percent of the initial saturation (about 0.85) per day during the cooling period. By linearly extrapolating this rate, it was estimated that complete rewetting would require 120 days. At a location about 3 cm away from the heater, where the saturation had decreased to only 0.5, the rewetting rate was a little slower, but because of the higher saturation at the start of cooling, the rewetting duration was estimated to be 85 days, or a little less than for the location near the heater. A representative average duration for complete rewetting was thus estimated to be 100 days. It should be noted that these estimates are based on linear extrapolations of rewetting rates for saturation levels less than the final saturation. Since, as shown by Eq. (2-11), the capillary pressure that drives the liquid flow is a nonlinear function of saturation, the rewetting rate will tend to decrease as the saturation increases. Consequently, the actual rewetting duration may be slightly longer than these estimates.

Estimates for rewetting of the ALTS tuff sample used in Test 11 were calculated by the same procedure used for Test 9. The slower water flux rates during the 7-day heating period for Test 11 yielded saturation changes that extended only to a region within about 3 cm of the heater. For locations 1 to 2 cm from the heater, the linearly extrapolated rewetting duration was estimated to vary from 70 to 450 days, depending on the location. A representative average time for complete rewetting of the tuff was estimated to be 150 days. Even though the heating period was shorter for Test 11 than for Test 9 and the dried out zone smaller, the slower flux rates in tuff as compared to cement produced a longer rewetting period during the cooling period.

Rewetting was also estimated by the numerical model for Test 11. The rewetting predictions are illustrated in Figure 5-7. Complete rewetting was predicted to occur within 10 days, thus underpredicting the experimental estimates by a factor of ten. For that reason, numerical simulations of the laboratory experiment rewetting estimates were not used for the conceptual model assessment. However, numerical simulations performed using C-TOUGH were used to evaluate the conceptual model predictions at the field and mountain scale because no other independent assessment was available. The numerical simulation is believed to be adequate for this order of magnitude analysis.

The conceptual model recognizes two mechanisms for rewetting during the cooling period: rewetting either as liquid or as water vapor (which subsequently condenses). Rewetting as liquid is driven by capillary pressure gradients while rewetting by water vapor is driven by mass diffusion. Each of these mechanisms is evaluated below for the laboratory experiments.

According to Eq. (2-46), the time required to rewet dried media solely by liquid flow is:

$$t_l = \left[\frac{(\mu_{lo}/\mu_{go})(k_{rel,go}/k_{rel,lo})(T_{avg}/\Delta T_o)}{S_{wo}(h_{lg,o}/R_v T_{avg})(\rho_{wo}/\rho_{go})(\Delta \hat{p}_c/\Delta S_l)} \right] \left(\frac{L^2}{\alpha_s} \right) \quad (5-4)$$

$$= \frac{\phi \mu_{lo} L^2}{k k_{rel,lo} (d\hat{p}_c/dS_l)}$$

As was discussed in Section 2.2.4.1, the first form of t_l in Eq. (5-4) (referred to as Scaling Law A) is convenient to use when experimental estimates of the maximum gas pressure and of the time duration required to obtain the maximum are available. The second form (referred to as Scaling Law B) is convenient for more general cases. For both forms, representative values of $k_{rel,lo}$ and the capillary pressure derivative $d\hat{p}_c/dS_l$ have to be computed from relations such as Eqs. (2-9) and (2-11). Both $k_{rel,lo}$ and $d\hat{p}_c/dS_l$ depend on saturation, so a representative value of saturation during rewetting must be estimated first. For Test 9 (cement slurry), the initial saturation was 0.8 to 0.9, so a representative value is 0.4. For Test 11 (tuff sample), the initial saturation was 0.35, so a representative value is 0.2. With these values of saturation and the assigned values of the van Genuchten parameters (Table 4-4), the relevant computations for Test 9 are: $k_{rel,lo} = 1.45 \times 10^{-4}$ and $d\hat{p}_c/dS_l = 2.2 \times 10^5$ kPa. The computations for Test 11 are: $k_{rel,lo} = 3.1 \times 10^{-8}$ and $d\hat{p}_c/dS_l = 1.4 \times 10^7$ kPa. For Scaling Law A, the dimensionless capillary gradient $\Delta \hat{p}_c/\Delta S_l$ is 3,300 for Test 9 and 11.7×10^6 for Test 11.

With these estimates of the quantities in Eq. (5-4), the rewetting times predicted by the idealized conceptual model are summarized as: Test 9, rewetting time = 170 days; Test 11, rewetting time = 110

Figure 5-7. Numerically predicted rewetting of Test 11 at 0, 3, and 8 days after heating was discontinued

days. Both of these predictions compare well with the experimental estimates, although just as for the heating period assessment the uncertainty in the Test 9 media properties has caused a larger error for the Test 9 predictions. [Both forms of Eq. (5-4) are equivalent for these predictions, since the conceptual model was used to compute all the quantities in Eq. (5-4)].

The time required to rewet the dried out media by vapor diffusion alone (followed by condensation) is given by Eq. (2-50):

$$t_i \approx 0.03 \left(\frac{\rho_{ls}}{\rho_w} \right) \left(\frac{\Delta S_l}{\tau S_v} \right) \left(\frac{p_v}{\Delta p_v} \right) \frac{L^2}{\alpha_s} \quad (5-5)$$

To use this expression, a representative value of the vapor partial pressure difference Δp_v caused by vapor pressure lowering is needed. Here, Δp_v is estimated to be about 0.2 times the average vapor pressure p_v over the heated region. The predicted rewetting time from Eq. (5-5) due solely to mass diffusion is hence about $48/\tau$ days for both Test 9 and Test 11. A representative value of the tortuosity τ for these media is not known. Lichtner and Walton (1994) state that values for tuff range from about 0.01 to about 0.05 when the porosity is 0.1. Assuming, then, an average value of 0.017 for τ , the predicted rewetting time by mass diffusion for Test 11 is in excess of 2,500 days, or about 20 times longer than that predicted by liquid flow. It is expected that the tortuosity for the cement slurry used in Test 9 is as least as small as that for the tuff used in Test 11, so the predicted rewetting time by mass diffusion for Test 9 is also much longer than the rewetting time by liquid flow. Rewetting driven by vapor diffusion as a result of relative humidity gradients can therefore be neglected for these media. Experimental measurements experiments, however, cannot verify this conclusion since the contributions of liquid transport and vapor diffusion to rewetting could not be separated in the experimental rewetting estimates.

Considering the close comparison of the conceptual model predictions to the experimental measurements, it is concluded that the conceptual model for the cooling period is validated for laboratory-scale systems. Consequently, scaling laws derived from the conceptual model are a valid method of interpreting and scaling-up results from laboratory-scale systems.

5.4.2.2 Field Scale

For reasons discussed earlier, the medium in the numerical simulations of rewetting in the LBT and YM models was characterized as uniform with matrix properties. The LBT and YM rewetting models were otherwise the same as the models used for the heating period analysis.

For the LBT, numerically predicted saturation values showing rewetting during the cooling period are illustrated in Figure 5-8 for the 1,500 W heating rate case and in Figure 5-9 for the 3,000 W heating rate case. The figures show the saturation at various times along a vertical line through the middle of the LBT from the heater horizon to the top of the block. From these plots, the rewetting time for both heating rates was estimated to be 190 yr for complete resaturation at the heater horizon. The calculations were based on linear extrapolation of the rewetting rate at 20 yr. Although the block was desaturated to a much greater degree for the higher heating rate, the rewetting rates were very similar. This similarity is attributed to the observations that temperatures in the block returned to ambient relatively quickly in both cases and that the source of water for most of the rewetting duration originated from below the heater horizon.

The initial saturation for the LBT simulation was 0.7. Thus, the representative average saturation assumed for the conceptual model was 0.35. Just as for the laboratory-scale assessment, this value of

Figure 5-8. Numerically predicted rewetting at the large block test for a heat load of 1,500 W. Curves are, from right to left, at 270, 365, 1,459, 3,650, and 7,300 days after start of heating. Heat was linearly ramped to zero from 300 to 365 days.

Figure 5-9. Numerically predicted rewetting at the large block test for a heat load of 3,000 W. Curves are, from right to left, at 365, 547, 1,459, 3,650, and 7,300 days after start of heating. Heat was linearly ramped to zero from 300 to 365 days.

saturation was used in Eqs. (2-9) and (2-11) to compute representative values of $k_{rel,0}$ and dp_c/dS_i . Since the numerical simulation provided estimates of the peak Δp_g during the heating period and the time required to obtain this peak, it was possible in the case of the LBT to compute rewetting times by both forms of t_i in Eq. (5-4) independently. For Scaling Law A, the conceptual model predicts that the rewetting duration is $324 L^2/\alpha_s$ when the heating rate is 1,500 W; assuming that L^2/α_s is equal to the required heating time given by the simulation, the conceptual model predicts that the rewetting duration is 102 yr. For Scaling Law B the conceptual model predicts that the rewetting duration is 38 yr. For a heating rate of 3,000 W, the two conceptual estimates are 70 yr and 38 yr, respectively. These estimates compare well with the numerical simulation value of 190 yr for both heating rates.

Considering the close agreement of the conceptual model predictions to the numerical simulation, it is concluded that the conceptual model for the cooling period is validated for field-scale systems. Consequently, scaling laws derived from the conceptual model are a valid method of interpreting and scaling-up results from field-scale systems.

5.4.2.3 Mountain Scale

The rewetting simulations of the YM repository were conducted with the same models used for the heating period analyses. Figure 5-10 shows the saturation contour predictions for the 57 kW/acre heat load case as a function of time along a 1D profile from ground surface to the water table 600 m below the heater horizon, for times of 285, 635, 1,585, and 100,000 yr. Rewetting to the preheated ambient saturation was completed between the simulation times of 1,585 yr and 100,000 yr. The rate of rewetting inferred from these data gives a time to complete rewetting of 4,750 yr. Figure 5-11 shows the saturation contour predictions for the 114 kW/acre heat load case, for times of 1,585, 2,220, 63,400, and 98,300 yr. Because the medium dried out to a much greater extent than for the smaller heat load, the rewetting duration was much longer for this case. Linear extrapolation from the rate of rewetting at 98,300 yr gave a time for complete rewetting of about 127,000 yr.

The initial saturation for the YM simulation was 0.7, just as for the LBT simulation. Thus, the representative average saturation assumed for the YM conceptual model was also 0.35, so the values of $k_{rel,0}$ and dp_c/dS_i were the same as for the LBT. Likewise, the numerical simulation provided estimates of the peak Δp_g during the heating period and the time required to obtain this peak, so it was again possible to compute the rewetting times by both forms of t_i in Eq. (5-4) independently. For Scaling Law A, the conceptual model predicts that the rewetting duration is $232 L^2/\alpha_s$ when the heat load is 57 kW/acre; assuming that L^2/α_s is equal to the required heating time given by the simulation, the conceptual model predicts that the rewetting duration is 14,000 yr. For Scaling Law B, the conceptual model predicts that the rewetting duration is 28,000 yr. Although both estimates are somewhat larger than the simulation prediction of 4,750 yr, they are within the accuracy that can be expected of an order-of-magnitude conceptual model.

For a heat load of 114 kW/acre, the two conceptual model estimates are 36,000 yr and 236,000 yr, respectively. Both estimates compare well with the simulation value of 127,000 yr.

Figure 5-10. Numerically predicted rewetting at the Yucca Mountain repository for 57 kW/acre. Curves are, from left to right horizon (220 m), 285, 634, 1,585, and 100,000 yr after start of heating.

Considering the close comparison of the conceptual model predictions to the numerical simulation, it is concluded that the conceptual model for the cooling period is validated for mountain-scale systems. Consequently, scaling laws derived from the conceptual model will give satisfactory results for mountain-scale systems.

These predictions of rewetting times from the numerical simulations and from the conceptual model are summarized in Table 5-6.

5.5 CONCLUSIONS OF THE SCALING LAWS ASSESSMENT

Comparisons of the conceptual models to the laboratory experiments and the LBT and YM simulations for both the heating and cooling periods have demonstrated the usefulness and the range of validity of the model. Conclusions from the heating period scaling law assessment can be summarized as follows.

- Gas pressure buildup observed in the laboratory-scale cylinder test and the field-scale G-Tunnel heater experiment raised questions about the connectivity of fractures in partially saturated fractured porous media. Gas pressure buildup during the heating period at the G-Tunnel experiment indicates that a high density of fractures does not necessarily ensure fracture connectivity.
- The heating period conceptual model is a valid representation of systems that have

$Ad_g \approx 1$ and $\Delta T_o < 100$ °C (open media, low heating rates), and

$Ad_g > 1$ for all values of ΔT_o (tight media, low/high heating rates)

- It is not a valid representation for systems that have

$Ad_g \leq 10$ and $\Delta T_o > 125$ °C (open media, high heating rates)

- For all systems, the heating period conceptual model is an adequate representation of the duration over which large gas pressures can be anticipated. However, this is merely a consequence of the fact that the duration of gas pressure buildup is established by thermal conduction, not the confining effect of the media.

For the cooling period, a set of scaling laws has been formulated that can be used to interpret the rewetting time observed or predicted for one geometric scale to systems of larger geometric scales. Conclusions from the assessment of these cooling period scaling laws can be summarized as follows:

- The relative importance of rewetting by vapor diffusion and rewetting by liquid flow has been assessed. For the particular systems evaluated here, rewetting is dominated by liquid flow, and rewetting by vapor diffusion from relative humidity gradients can be neglected.
- Rewetting times predicted with the cooling period scaling laws were in agreement with rewetting times of two laboratory-scale experiments. The rewetting time predicted by the numerical simulation did not, however, agree with either the cooling period scaling law prediction or the laboratory results.

Table 5-6. Comparison of rewetting times predicted by the numerical simulating predicted by the conceptual model based on the predicted peak gas pressure and required heating duration (Scaling Law A), and predicted by the conceptual model based on represented capillary pressures (Scaling Law B).

Systems	Numerical Prediction (yr)	Scaling Law A (yr)	Scaling Law B (yr)
LBT at 1,500 W	190	102	38
LBT at 3,000 W	190	70	38
YM at 57 kW/acre	4,750	14,000	28,000
YM at 114 kW/acre	127,000	36,000	236,000

- Rewetting times for the LBT and the YM repository were predicted from the cooling period conceptual model by (i) a method based on the peak gas pressure and the heating duration required to obtain it, using capillary gradients and relative permeability predicted by the numerical simulations; and (ii) a method based on a representative capillary pressure gradient. Both methods were in reasonable agreement and compared well with rewetting times predicted by the numerical simulations.
- Rewetting times for the LBT are predicted to range from 38 to 190 yr for the LBT with a heating rate of either 1,500 or 3,000 W. Rewetting times for YM are predicted to range from 4,750 to 28,000 yr for a heat load of 57 kW/acre and from 36,000 to 236,000 yr for a heat load of 114 kW/acre. Rewetting exceeds the initial drying times by a factor of about 10^2 for both the LBT and YM at any of the heating rates or loads.

Results from the analyses conducted with a set of scaling laws for the cooling period of the thermal evolution of the HLW repository have contributed to resolving the fundamental basis of moisture redistribution through partially saturated porous media.

To the extent that the comparisons discussed in this section validate the conceptual models of the response of a porous medium during heating and cooling periods, the conceptual models can be used to design laboratory or field experiments to achieve specified objectives. In particular, the gas Advection Number, Ad_g , provides a dimensionless parameter that allows an experiment to be designed to investigate either pressure-driven gas flow during heating and to ensure that pressure-driven gas flow does not occur. In general, pressure-driven gas flow would tend to dry out a heated region much more extensively and rapidly than flows induced by buoyancy or vapor diffusion.

The conceptual model of the cooling period of the system's response makes evident the parameters that control the time duration required for rewetting of the previously dried out region. This model, for example, could be used to design an experiment that would allow rewetting to be investigated in the laboratory or field for a time duration of practical length.

The conceptual models can also be used to make predictions of the response of larger systems from the measured responses obtained in experiments of smaller systems. The various pressure, velocity, and time duration expressions of the model are, in effect, the recommended methods of scaling up the smaller system responses.

Figure 5-11. Numerically predicted rewetting at the YM repository for 114 kW/acre. Curves are, from left to right at repository horizon (220 m), at 1,585, 2,220, 63,420, and 98,300 yr after start of heating.

6 CONCLUSIONS AND RECOMMENDATIONS

The central objective of the Thermohydrology Research Project was to develop a technical understanding of thermally driven redistribution of moisture in partially saturated porous media, as it applies to a geologic repository. A series of laboratory-scale thermohydrology experiments were conducted to provide data to help identify and evaluate individual driving forces that control water (liquid and vapor phases) movement from and to a heat source. Scaling theories were derived from similarity analyses to relate the thermohydrologic phenomena observed at the laboratory scale to that of field and full repository scale. Computer simulations of two-phase flow were performed to provide a basis for evaluating the scaling theories.

The Thermohydrology Research Project began with the intent of addressing a broad spectrum of generic questions regarding thermohydrologic phenomena. While some of these questions were answered in the conduct of the study, other new and challenging ones were encountered. Initial progress made in addressing those technical questions was documented in an interim progress report (Green et al., 1993b). Subsequent to that report, the laboratory-scale experiments were designed to address four fundamental questions regarding thermohydrologic phenomena:

- (i) What are the principal mechanisms controlling the redistribution of moisture?
- (ii) Under what hydrothermal conditions and time frames do individual mechanisms predominate?
- (iii) What hydrothermal regimes are associated with each driving mechanism?
- (iv) What is the temporal and spatial scale of each hydrothermal regime?

In essence, these questions identify the need to understand the factors, conditions, and processes that control the rates of dryout and rewetting of the repository. The findings and mathematical theories developed to address these questions are summarized below. Technical recommendations for a field-scale thermohydrology experiment are also presented.

6.1 FINDINGS OF LABORATORY-SCALE EXPERIMENTS

Eleven laboratory-scale thermohydrology experiments were conducted which are categorized according to: (i) the fluid phase (i.e., liquid or gas) considered, (ii) hydrothermal regime (i.e., boiling or sub-boiling), (iii) test cell geometry (i.e., rectangular or cylindrical), and (iv) test medium (i.e., consolidated or unconsolidated). Two groups of experiments were designed to address the four basic technical questions regarding two-phase flow processes. In addition, they were designed to provide the data necessary for testing various scaling theories proposed in Section 2. The first group, referred to as the liquid flow experiments, was designed to study the flow patterns in the liquid phase. The second group, designated as the gas flow experiments, focused on the dynamics of the gas phase and the buildup of gas pressure. The analysis of experimental results attempted to relate the fluid-flow regimes to system variables. Of particular interest are the rates and directions of liquid and vapor flow and their time histories during the heating and cooling periods.

The results of the laboratory-scale experiments were interpreted and extended using numerical simulations of two-phase flow. The major observations, inferences, and conclusions drawn from the experimental results and computer modeling are:

- Three condensation models have been identified: (i) media with low permeability and small air-entry pressure will be more likely to experience a relatively narrow moisture buildup zone on the cool side of a dryout zone near a heat source; (ii) media with a low permeability and large air-entry pressure will tend to exhibit condensation over a broad area beyond the zone of dryout; and (iii) media with a high permeability allow a sufficiently large return flow of water so that minimal or no dryout occurs near the heat source and no significant hydraulic gradient is formed.
- Temperatures much above boiling may not be sufficient to completely dry out media with relatively high permeability (for example, temperatures greater than 170 °C did not appear to completely dry out ceramic with a permeability of $1 \times 10^{-13} \text{ m}^2$).
- Fluid flow patterns near a heat source may be more complex than predicted by numerical simulation. In particular, complex flow of liquid near the heat source in a laboratory-scale experiment, including the downward flow of water from above the heat source, was not well replicated in the numerical model.
- Experimental measurements confirmed the occurrence of gas pressure buildup and subsequent pressure-driven vapor flow in media with low saturated liquid permeability.
- Intermittent gas pressure buildup and release near the heat source can potentially transport large amounts of liquid and vapor relatively long distances from the heat source.
- Measured rewetting rates were one to two orders of magnitude smaller than the drying rates.

Based on these observations, it is inferred that the extent of the repository dryout zone will be a strong function of the bulk liquid permeability of the matrix. Media with lower permeabilities will dry out more slowly, but will also rewet at significantly lower rates than high permeability media. The nature of condensation, that is, will moisture condense near the dryout zone or at a distance from the heat source, is also dependent on the hydraulic properties of the medium.

6.2 FINDINGS OF SIMILARITY ANALYSIS

Using similarity theory, scaling laws were formulated for use in predicting the rates of dry out and rewetting at the field and mountain scales using results from laboratory-scale models. Because the driving mechanisms were different for the heating and cooling periods, a separate set of scaling laws was developed for each period. The conceptual models associated with each set of scaling laws are based on the general mathematical theory of two-component, two-phase flow in heated, partially saturated porous medium. The scaling laws were specialized and simplified to apply to: (i) the buildup of gas pressure during the initial period of large heating rates, and the attendant drying out of the media; and (ii) the rewetting of the dried-out region during the later cooling phase. The two conceptual models were characterized in terms of dimensionless parameters.

Heating Period Model. The conceptual model of the heating period demonstrated that the requirements for similarity among systems of various geometric sizes and thermohydrologic properties are summarized in a new dimensionless number called the gas Advection Number, Ad_g . Like other dimensionless numbers, Ad_g is the ratio of two physical effects, in this case the ratio of gas pressure gradients created by the confining effect of the medium to buoyancy-induced body forces. Ad_g is formally expressed in terms of thermohydrologic parameters such as permeability and porosity, fluid parameters such as density, viscosity, and coefficient of thermal expansion, and heating rate parameters such as the temperature increase of the media near the heater.

For cases where $Ad_g > 1$, the heating is sufficient to cause the creation of large pressure gradients and high advective gas flows. Under these conditions, the region near the heat source is likely to experience a significant degree of drying. The model also predicts the magnitude of the peak gas pressure gradient that will be produced. The time at which the peak gas pressure occurs is predicted to be the same as the characteristic thermal diffusion time. For cases where $Ad_g \leq 1$, heating is expected to produce only small gas flows away from the heat source and buoyancy has a dominant role in setting the characteristics of fluid flow. For these conditions, less drying of the repository is expected.

The heating period model was compared to the results and numerical simulations of laboratory-scale experiments and to numerical simulations of the LBT and of the YM repository. The value of Ad_g for the laboratory-scale tests was computed to be 10^4 or greater, and so the model predicted that large pressure gradients and a significant degree of drying should be observed in the experiments. This assessment was, in fact, confirmed by the results of the experiments. Conceptual model predictions of the magnitude of the peak pressure and the time required to obtain the peak also compared well with experimental results. A similarly close comparison was found for the numerical simulation of the laboratory-scale experiments although the numerically predicted peak Δp_g was a factor of five greater than that observed.

Evaluations of these inferences and trends were made using computer model representations of the LBT scale and YM scale systems. Uncertainty in the LBT and YM conceptual models was associated with assignment of media permeability. Two approaches for designating the medium permeability were used: (i) a model with a permeability equivalent to the matrix, and (ii) a model with a composite matrix/fracture permeability. The permeability of the matrix was about four orders of magnitude less than that for the composite model. For the composite model, the computed value of Ad_g for LBT was of order 10 and that for YM was of order 0.1. Hence, the composite permeability conceptual model predicted that little gas pressure buildup should occur.

Values of Ad_g for the LBT and YM based on a matrix permeability assumption were relatively large (i.e., 10^2 to 10^5) thereby predicting high gas pressure buildup and velocities. The numerical simulations predicted that the peak pressure for both cases was at least 10 kPa, thus substantiating the matrix permeability model. Further supporting the assignment of matrix permeability to the conceptual model, high gas pressures (i.e., 300 kPa) observed during a heater test conducted in highly fractured tuff at G-Tunnel (Ramirez, 1991) indicated that high gas pressures will occur even in highly fractured tuff. Thus, the matrix permeability model is more appropriate than the composite permeability for use in the conceptual scaling model. Thus, conceptual scaling models predicted on a medium with a matrix permeability were in agreement with numerical models with a composite permeability.

Cooling Period Model. The most important aspect of moisture redistribution during the cooling period is the time required to rewet the region dried out during the heating period. Rewetting time is important because it is a measure of when water comes back into contact with the canister environment after it has been dried out. This rewetting aspect of the cooling period was investigated using the conceptual model. Analogous to the heating period, a liquid Advection Number Ad_l was developed. The rewetting response of various systems is expected to be similar when the values of Ad_l are of a similar order of magnitude for the systems. The values of Ad_l for the laboratory scales and for the LBT model were all of order 10 or larger, thus indicating that both systems are good analogues of each other for the cooling period. The values of Ad_l for the YM repository model were of order 1; hence, liquid buoyancy effects are predicted to be a little more prominent for this system than for the two smaller-scale systems, but the smaller systems should still be satisfactory analogues of the YM repository system.

The conceptual model considered rewetting both by liquid transport and by vapor phase diffusion. In all cases studied, the conceptual model predicted that rewetting due to vapor diffusion was negligibly small. Liquid transport rewetting always occurs in the matrix even for fractured media, because of the large capillary pressure gradients created in the matrix by the drying during the heating phase. Hence, the conceptual model of the cooling period should apply equally to fractured or nonfractured media.

The cooling period conceptual model scaling predictions were compared to laboratory-scale experiments and numerical simulations. For the reasons given for the heating period, the conceptual model simulations of rewetting were based on the permeability of the matrix rather than that of the composite media. The times predicted by the conceptual model for liquid transport rewetting compared very well to the measured values for the laboratory-scale experiments (100 to 150 days) and to the simulated rewetting times for the LBT (190 yr) and YM (127,000 yr). The comparisons of the conceptual model predictions to laboratory test data and to numerical simulations show that the model is capable of determining and assessing the hydrologic and heating rate conditions required for drying out and rewetting of heated, partially saturated porous media. Measured times for rewetting exceeded the time for drying at the laboratory scale by a factor of 10^1 to 10^2 . The times to rewet the LBT and YM predicted numerically and substantiated with the conceptual models exceeded the dryout times by a factor of about 10^2 .

Scaling Implications of the Conceptual Model. The scaling law conceptual models can be used with confidence to evaluate laboratory- and field-scale experiments as analogues of repository responses to heating. The pressure, velocity, and time scaling laws that arise in the conceptual model can also be used to interpret, or scale-up, the responses measured in laboratory- and field-scale experiments in terms of repository responses, when the thermohydrologic and heating rate conditions of the experiments are considered to be sufficiently similar to the repository. Likewise, the conceptual model can be used to guide numerical simulations of these responses. However, similarity approaches have limited use for the canister scale because flow in individual discrete features such as fractures cannot be appropriately scaled.

6.3 RECOMMENDATIONS

The overall results of this project suggest that similarity analyses can provide reasonable predictions of the spatial and temporal scales of heat and mass transfer mechanisms active at a repository scale. However, they do not appear to be a viable analytical tool to assess canister-scale moisture redistribution mechanisms where the physics of flow many depend on discrete features of the geologic

media. Understanding and predicting moisture redistribution in fractured rock near a heat-generating canister is of critical importance since the performance of a HLW repository is dependent on the rate at which the canister environment dries out during the heating period, stays dry, and eventually rewets during the cooling period. Few field-scale experiments have been conducted to answer this information need. The G-Tunnel heater experiment (Ramirez, 1991; Buscheck et al., 1991) and the spent fuel test at Climax (Patrick, 1986) did fulfill, in part, the requirements of such tests. Only one field-scale experiment is currently active that would provide information toward these information needs, the Fran Ridge LBT (Lin et al., 1994; Buscheck et al., 1993). The scales (characteristic lengths) of these three field-scale experiments are all about 1 to 3 m. Not all information needs were met or will be met by these field-scale experiments.

An additional field-scale experiment is proposed that would contribute to the investigation of thermally driven moisture redistribution in partially saturated fractured, porous media. The scale of the proposed field-scale experiment is 8 to 10 m and the medium is a fractured, welded tuff. The proposed field-scale experiment would be conducted at the Peña Blanca Natural Analog site near Chihuahua, Mexico (Pearcy, 1994; Green et al., 1994; Green and Rice, 1995). The Peña Blanca Natural Analog field site currently offers a physical setting highly conducive to the conduct of a field-scale heater experiment. Peña Blanca, as a natural analog of YM, offers unique opportunities to measure the hydraulic properties and observe thermally driven moisture redistribution at a field scale that is large enough to permit investigation of the composite effect of fractures and matrix, but sufficiently limited that scales of time and distance are not prohibitively large that measurements cannot be made in reasonable times and at reasonable distances. The physical and geometric attributes providing surface and subsurface exposure of the site are not known to be available at any other site.

The analog site exhibits a high degree of exposure provided through the removal of a large amount of the overlying host rock and debris conducted as part of prior activities associated with a uranium mine that operated at the site. The deposit has been exposed through the excavation of the mine. Enhancing the accessibility of the site is the presence of 80 m of horizontal adits located 8 to 10 m below the most extensive level surface of exposed rock and a series of 10-m-deep vertical boreholes located near the adit. The proposed heater test would actually consist of a number of separate heater tests throughout the adit in which individual heaters would be emplaced 1 to 3 m above the top of the adit. Because the adit transects a wide range of permeabilities and differing fracture sets, each heater test would be conducted under widely differing hydrogeologic conditions. A vertical cross-sectional schematic of the proposed heater test is illustrated in Figure 6-1.

Results gained from the field-scale heater tests would be compared to moisture redistribution predicted using conceptual and mathematical models to assess their ability to predict flow and transport for a field-scale application. The models would be constructed using information gained in the laboratory-scale experiments and field characterization measurements, but not using the actual field-scale test results. Controlled blind comparison of model predictions based on site-specific property values and observed field-scale thermally driven moisture redistribution experiments would provide independent assessment of conceptual and mathematical models.

Figure 6-1. Schematic of proposed Peña Blanca field-scale heater test

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11. ABSTRACT (200 words or less)

Experimental and theoretical studies have been conducted to develop a quantitative understanding of the thermohydrologic phenomena induced by emplacement of high-level radioactive waste (HLW) in an unsaturated fractured porous media. A series of laboratory experiments was conducted in a variety of media to study the physics of thermally driven moisture redistribution through porous media. Principles of similarity theory were applied to develop dimensionless parameters to be used to predict thermohydrologic behavior at the field and repository scales from information gained from the laboratory and field scales. Results from the dimensional analyses indicated that dimensionless parameters are useful to design field-scale experiments so as to maximize the information gained from the experiment and to predict heat and mass transfer of larger scale porous media systems. Dimensional analysis did not prove to be useful in scaling systems containing discrete features such as faults or fractures. A major conclusion of this report is that conduct of a heater test at field scale is crucial to investigate and understand heat and mass transfer through partially saturated fractured, porous media at the scale of a geologic repository.

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