Data Collection and Field Experiments at the Apache Leap Research Site

May 1995 - 1996

Manuscript Completed: July 1997
Date Published: August 1997

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U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001
NRC Job Code W6387

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ABSTRACT

This report documents the research performed during the period May 1995-May 1996 for a project of the U.S. Nuclear Regulatory Commission (sponsored contract NRC-04-090-051) by the University of Arizona. The project manager for this research is Thomas J. Nicholson, Office of Nuclear Regulatory Research. The objectives of this research were to examine hypotheses and test alternative conceptual models concerning unsaturated flow and transport through fractured rock, and to design and execute confirmatory field and laboratory experiments to test these hypotheses and conceptual models at the Apache Leap Research Site near Superior, Arizona.

Each chapter in this report summarizes research related to a specific set of objectives and can be read and interpreted as a separate entity. Topics include: crosshole pneumatic and gaseous tracer field and modeling experiments designed to help validate the applicability of continuum geostatistical and stochastic concepts, theories, models, and scaling relations relevant to unsaturated flow and transport in fractured porous tuffs; use of geochemistry and aquifer testing to evaluate fracture flow and perching mechanisms; investigations of $^{234}\text{U}/^{238}\text{U}$ fractionation to evaluate leaching selectivity; and transport and modeling of both conservative and non-conservative tracers.

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EXECUTIVE SUMMARY

This report documents the research performed during the period May 1995-May 1996 for a project of the U.S. Nuclear Regulatory Commission (sponsored contract NRC-04-090-051) by the University of Arizona. The project manager for this research is Thomas J. Nicholson, Office of Nuclear Regulatory Research. The objectives of this research were to examine hypotheses and test alternative conceptual models concerning unsaturated flow and transport through fractured rock, and to design and execute confirmatory field and laboratory experiments to test these hypotheses and conceptual models at the Apache Leap Research Site near Superior, Arizona.

Each chapter in this report summarizes research related to a specific set of objectives and can be read and interpreted as a separate entity. Chapter 3 describes crosshole pneumatic and gaseous tracer experiments designed to help validate the applicability of continuum geostatistical and stochastic concepts, theories, models, and scaling relations relevant to unsaturated flow and transport in fractured porous tuffs. In Chapter 4, infiltration tests in the fractured rock are modeled. Geochemical evaluation of fracture flow discussed in Chapter 5 indicates that fractures are the primary pathways by which water is transferred to the perched aquifer at Apache Leap. Investigations of $^{234}\text{U}/^{238}\text{U}$ fractionation in Chapter 6 showed that leaching selectivity is probably significantly greater than the observed mobile phase activity ratio, and that within the likely range of effective partitioning behavior, the contribution from direct recoil to observed activity ratios is minor. In Chapter 7, the transport of both conservative and non-conservative tracers was tested; methods and techniques for monitoring and sample collection were evaluated; and modeling approaches were compared. Finally, in Chapter 8, mechanisms for the formation of perched water bodies were evaluated, and hydrologic parameters of the perched aquifer were measured and shown to be indicative of a fracture-flow dominated system.

FOREWORD

This technical report, NUREG/CR-6497, was prepared by The University of Arizona under their research project for the Waste Management Branch, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission (JOB CODE W6387). The report documents research results from field experiments designed to investigate a range of conceptual flow and transport models; pneumatic and infiltration testing in fractured porous tuff, geochemical evaluations of fracture flow, tracer tests and transport modeling in fractures, and effects on formation and recharge of perched-water zones. Data summaries, analyses and significant conclusions for the experiments are described in detail within each chapter. The research results are relevant to site characterization and data analysis issues encountered in the review and confirmation of flow and transport data and models in support of high-level radioactive waste disposal in unsaturated, fractured tuff.

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1. INTRODUCTION AND REGULATORY BACKGROUND

The material in this section has been taken from the UA Contract (US NRC RS-RES-95-041), and the UA Experimental Plan (1995) for explanatory purposes.

Yucca Mountain (YM) was originally selected as a candidate repository site because: (i) it is situated in a remote location, (ii) the general area is characterized by a low population density, and (iii) it is characterized by a thick (several hundred meters) unsaturated zone (U.S. Department of Energy, 1986). The last condition led scientists to presume that high fluxes of water would not readily reach the repository, thus rendering unlikely the occurrence of corrosion and spent fuel dissolution problems. The complex hydrologic regimes associated with highly heterogeneous rocks, nonisothermal flow, and conductive fracture and fault zones, however, have stressed the need for further research regarding the suitability of the site for High Level Waste (HLW) disposal.

Research requirements dealing with such site characteristics as groundwater travel time (GWTT), favorable conditions (FACs), and potentially adverse conditions (PACs) relate to support of the US Nuclear Regulatory Commission (NRC) staff's License Application Review Plan (LARP) (Nuclear Regulatory Commission, 1994a). For example, understanding the subregional (site) and regional hydrogeology is required in order to determine the GWTT in the unsaturated and saturated zones. Other processes and phenomena of importance include, but are not limited to, the potential for flooding of the repository as a consequence of water table rise from meteorological or climatic changes, volcanism, or faulting. Furthermore, it will be necessary to assess the inherent variability and distribution of hydrogeologic and transport properties, initial and boundary conditions, hydro-geostratigraphic unit interfaces, and coupled effects modeling strategies used by the U.S. Department of Energy (DOE) to support its estimation of GWTT and moisture fluxes.

In the NRC LARP (Nuclear Regulatory Commission, 1994a), these research requirements are expressed in the context of several Key Technical Uncertainties (KTUs) that are influenced, or pertain to, various subregional hydrogeologic flow and transport processes. These are: (i) developing a conceptual groundwater flow model that is representative of the YM site groundwater flow system, (ii) developing a mathematical groundwater flow model that is representative of the YM site groundwater flow system, (iii) determining the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment, (iv) uncertainties associated with determining characterization parameters, (v) uncertainty in modeling the formation of perched zones, (vi) conceptual model representations of the natural and engineered systems, (vii) variability (temporal, spatial, etc.) in model parametric values, (viii) appropriateness of assumptions and simplifications in mathematical models, and (ix) validation of mathematical models. In the case of the YM site, these issues are complicated by the highly heterogeneous and nonlinear nature of the subsurface flow processes. It will be useful to describe briefly some aspects of the hydrogeologic conditions prevailing at the site before formulating the specific objectives of this research.

First, the proposed repository is intended to be situated deep in relatively dry, unsaturated

tuffs, about 300 m below land surface and 250 m above the water table (U.S. Department of Energy, 1988). Second, in addition to the presence of markedly distinct geologic units and tectonic faults, the geologic units are also variably fractured. For example, the Topopah Spring welded unit, where the proposed repository is to be located, is a low-porosity welded tuff believed to be densely fractured, while the underlying Calico Hills, nonwelded-vitric or zeolitized unit is a higher porosity, nonwelded tuff with seemingly much lower fracture density (U.S. Department of Energy, 1988). Finally, the net annual infiltration from rainfall and surface water over YM has not been determined yet, but may vary from -1.0 to 5.0 mm/yr, from a mean annual rainfall of about 150 mm/yr. These mean values do not take into account the more extreme rainfall rates that may occur due to inter-annual fluctuations, inter-seasonal fluctuations, and individual storms. In addition, these values only reflect contemporary rainfall and infiltration conditions.

Under ambient conditions, it is likely that radionuclides released from the repository zone will be transported predominantly in the unsaturated flow regime. However, locally saturated flow conditions may also occur in the vadose zone, possibly due to short and intense rainfalls, or to extremes in climatic fluctuations on larger time scales, or to elevated temperatures. The potential for existing or future perched-water bodies of this nature is identified in 10 CFR 60.122(c)(23) as a PAC for the storage of HLW in a geologic repository. This is of concern, due to the possibility of either flooding portions of the repository or providing a faster pathway for groundwater traveling from the repository to the accessible environment. Perched-water bodies tend to be transient features that are formed where there is a contrast in hydrologic properties (Freeze and Cherry, 1979). Contrasts may result from differences between stratigraphic units. For example, matrix hydraulic conductivity at YM tends to decrease with increased welding of the tuff units. Contrasts may also occur due to the juxtaposition of low-conductivity strata adjacent to more permeable and conductive strata along a structural feature such as a fault or any other form of identifiable (e.g., through geophysical testing) persistent geological discontinuity. The rotation of these blocks may create a structural trap to permit accumulation of infiltrating water, allowing a perched-water body to form. This will also depend on whether the fault/fracture acts as a barrier to fluid flow or a conduit. Preliminary analyses of the role of fault zones have been presented by Bagtzoglou and Muller (1994) who indicated that, depending on the properties of the surrounding material, fault zones can interchangeably act as both barriers and conduits to flow. Mineralogical changes within or between strata may also cause a change in permeability due to changes in volume during mineral formation. One example is the formation of relatively impermeable layers in response to alteration of primary phases such as feldspar to secondary clays such as kaolinite and smectite. It should be noted, however, that there exist many different processes capable of altering permeability, even without changes in volume, such as cementation of flow paths in the saturated zone due to geochemical processes.

Perched water is typically identified by encountering water flow at elevations above the regional water table. Perched water flows from seeps in the zeolitized Tunnel Beds of the Indian Trail Tuff in the U12n tunnel at Rainier Mesa, approximately 50 km to the northwest of YM (Thordarson, 1965; Russell et al., 1987; Wang et al., 1993). Many of the volcanic units are similar at both locations, but precipitation is approximately twice as great at the higher elevations of Rainier Mesa. Hydrochemistry and mineral chemistry provide a means of distinguishing different

water bodies in geologic systems. Hydrochemical evidence indicates that seep waters from the Indian Trail Tuff are chemically similar to pore waters from the unsaturated zone below the Indian Trail Tuff, but are more dilute and chemically distinct from the pore waters in stratigraphically higher units (Wang et al., 1993). Stable isotope (δD and $\delta^{18}O$) evidence indicates that the waters in the perched-zone are similar to the modern meteoric water at Rainier Mesa (Russell et al., 1987). This similarity suggests that recharge is relatively quick and predominantly from winter storms.

Evidence for perched water may also have been encountered at YM (U.S. Department of Energy, 1992) in drill holes USW UZ-1 and USW H-1 where flowing water was observed. There is still some question, however, whether this water occurred naturally or resulted from drilling fluids used in completing these and other nearby wells. Recent drilling has also encountered perched water at depths of about 400 m in the northern part of YM (U.S. Department of Energy, 1994; Nuclear Regulatory Commission, 1994b), although no data on the hydrochemistry of these samples have been published. Perched water has also been encountered at the Apache Leap Research Site (ALRS), one of the NRC-sponsored hydrology research sites. More specifically, a perched-water table has been identified within the tuff section at the Deep Slant Borehole (DSB) site at the ALRS (Bassett et al., 1991, 1994b).

One method of evaluating the possible formation of future perched-water zones is to use water and mineral chemistry to identify where these zones might have occurred in the geologic past, possibly under different climate conditions. Hydrochemical facies (Hem, 1985) have been used to establish relationships between bodies of water. Environmental tracers such as the stable isotopes of oxygen, carbon, hydrogen, and sulfur have long been used to distinguish between water bodies (such as waters in the unsaturated and the saturated zones), to estimate temperatures, and to identify potential flow paths, recharge areas, and fluid sources (e.g., Welhan, 1987; U.S. Department of Energy, 1988; National Academy of Sciences, 1992; Conrad, 1993; Mazor, 1991). Radiometric age dates can be determined for groundwaters using isotopes such as ^{14}C , ^{36}Cl , tritium, and uranium-series disequilibrium. If the length of the flow path is known or can be determined, these ages can be used to provide estimates of rates of fluid flow, and timing of changes in the paleohydrology of the site.

Finally, high-intensity rainfall events, occurring episodically, may drastically modify the subsurface flow regime from that which would be inferred using an average infiltration rate model. Perhaps the shortest significant time scale of climatic inputs to the system may be taken to be storm duration, typically on the order of hours or even less. This short term period is indeed much smaller than the time scale of interest for contaminant migration, say on the order of 10^3 to 10^4 yr or more. The problem to be investigated is the evaluation of various approaches for estimating subregional-scale infiltration and groundwater recharge fluxes. This problem involves assessment of the transient nature of infiltration, groundwater recharge and vapor migration coupled to surface (e.g., evapotranspiration, precipitation, snowmelt, and surface drainage features), and subsurface (e.g., focused recharge due to alluvial channels and vertically extensive discontinuities) processes and conditions. The amount and location of water infiltration are controlling factors in the movement of water through the subsurface. In fractured, unsaturated rock, such as that found at the YM site, the occurrence of sporadic high-intensity rainfall events

may drastically modify the subsurface flow regime from that calculated (or predicted) from an average infiltration rate model. The DOE has concluded that the spatial and temporal distribution and magnitude of infiltration into the system may be the most important independent parameters influencing flow path development (U.S. Department of Energy, 1992). Typically, groundwater flow assessments are made using simplistic, average infiltration rate models. This methodology may not be satisfactory for compliance demonstrations. The NRC needs to be cognizant of alternative infiltration models that could be applicable to the YM site.

Data derived from field testing may be used to test flow and transport modeling concepts and/or codes developed by the University of Arizona (UA) and others prior to their application at the YM site and region. The UA studies at the ALRS have produced databases for evaluating pneumatic, geochemical, hydrologic and transport processes on a site scale. Information is available for assessing fracture versus matrix flow conditions for unsaturated fractured tuff over a range of scales. Inclined boreholes at the 10-m scale have been used to evaluate pneumatic testing methods. A deep inclined borehole penetrating perched-water zones with associated core and water samples, is available to test site-characterization methods and strategies for determining effective field properties. The geochemical data allow for independent confirmation of groundwater mixing and residence times for fracture-dominated, as opposed to matrix-dominated, flow systems. The ALRS is located in fractured tuff with climatic and topographic conditions very similar to that of the region around YM, Nevada. It is, therefore, a very good, small-scale analog of the YM site. More importantly, however, it provides the unique opportunity to independently study flow, transport, and travel time issues in fractured unsaturated tuff.

UA researchers have designed field experiments to collect field data in order to develop data sets that will allow for testing various modeling approaches. The project team has made the necessary field visits and coordination meetings as determined by the NRC project manager in order to accomplish the studies at the ALRS.

The field studies being pursued relate to: (i) infiltration and recharge processes, (ii) perched-water zone formation, and (iii) groundwater flow and transport assessments. Research that will be pursued at the ALRS includes field-scale experiments at: (i) the Covered-Borehole site (CBS), (ii) the small watershed study at the DBS site, and (iii) the Never Sweat Tunnel/Queen Creek (NST/QC) site. These studies are discussed in detail in Section 2.

2. DATA NEEDS

The material in this section has been taken from the UA Contract (US NRC RS-RES-95-041), and the UA Experimental Plan (1995) for explanatory purposes.

2.1 Infiltration and Recharge Processes

In general, assessment of the transient behavior and spatial variability of infiltration, groundwater recharge, and vapor migration requires the use of mathematical models incorporating an abstraction of the active processes. The effects of various assumptions in the mathematical models are being explored, with the intention of identifying critical parameters and data requirements for each model.

Recharge of deep zones is affected by processes active in the near-surface zone, including evaporation, transpiration, liquid water flow, and vapor flow. Each of these processes is governed by several factors. For example, precipitation has been found to vary substantially over the YM region, both spatially and temporally, and winter storms are, in general, more uniform and severe than summer storms (Hevesi et al., 1992a,b; 1994). Similarly, evaporation from the ground surface is affected by air temperature, atmospheric vapor pressure, wind speed profile, incident solar radiation, surface soil and rock texture, plant activity, surficial temperature, and surficial moisture content. As key factors influencing groundwater recharge are identified, the location of potential high-recharge factors can be identified. It is anticipated that significant factors governing infiltration will include depth and character of the alluvial/colluvial cover, geologic layer underlying the alluvial cover, surface slope and orientation, fracture characteristics, and vegetative distribution.

Alternative conceptual models of infiltration include 1D, 2D, and 3D representations of a system. In order to explicitly incorporate the effects of evaporation, transpiration, and vapor-phase transport, various mathematical representations of the active processes can be made. An extremely detailed model would consider the flow of liquid water and water vapor, including nonisothermal effects and possibly air-phase movement. In addition, vegetation can strongly affect the movement of water: directly, by extracting water for transpiration within a root zone and, indirectly, by shading the ground surface and attenuating winds near the ground surface. Thus, a detailed model would incorporate such effects. Finally, a detailed model would require appropriate surficial boundary conditions. Typical models that might be used for ground-surface boundary conditions require estimates of some or all of the following: wind speed profile, atmospheric vapor density, atmospheric temperature, atmospheric pressure, solar radiation, precipitation, and cloud cover (Richardson and Wright, 1984).

An excellent method for assessing the predictions of alternative infiltration models is to test the predictions against field observations. Not only is the numerical coding of the mathematical model stressed, but the conceptual model itself is tested against ground truth. A discussion on the issue of validation of flow and transport models for unsaturated soils is presented by Nicholson et al. (1989). A number of field studies have been performed at the ALRS, and facilities are in place or can easily be established to help support infiltration studies on

a small watershed and subwatershed scale, including a meteorological metering station, runoff weirs, neutron probes, time-domain reflectometer (TDR) probes, solution samplers, and tensiometers. Ideally, these facilities will help to test models that range from simple 1D recharge models, through hillslope transect models, all the way through full watershed models.

One of the areas of uncertainty at the YM site is the potential for focused recharge due to runoff into the washes, cropping out of different geologic units and possible preferential pathways arising from fracture exposures. In order to address the focused recharge issue, a series of detailed simulations will be performed incorporating variability representative of the ALRS. Data gathered and mapped by the UA research team will be used to provide input on the spatial variability of factors pertinent to recharge. Based on these data, a number of survey simulations will be performed in order to assess extreme behavior expected for the site. Finally, a representative number of simulations will be used to estimate the magnitude of focused recharge across the site, both in space and in time. These simulations will be conducted for various topographic locations, such as the Covered Borehole Site and the Queen Creek/Haulage Tunnel.

2.2 Perched-Water Zone Formation

The objective here is to identify and study, if possible, areas where perched-water zones may have formed in the geologic past under different hydrologic conditions or might form in the future. The problem to be investigated is an assessment of the causative mechanisms and conditions that either have created perched-water zones or exhibit a potential for creating future perched-water zones. A perched-water zone is a locally saturated groundwater system separated from the deeper regional water table by an unsaturated zone. The focus shall be on evaluating strategies and information needed to model perched-water development at the scale of the YM site. In the unsaturated zone, there is the potential for saturation levels to reach 100 percent in isolated zones above the regional water table. The potential for existing or future perched-water bodies of this nature is identified in 10 CFR 60.122(c)(23) as a PAC for the storage of HLW in a geologic repository. This is of concern due to the possibilities of flooding portions of the repository and providing faster groundwater pathways from the repository to the accessible environment. Identification of perched-water zones in the present or in the past can help to constrain conceptual and mathematical models used to predict future hydrologic conditions.

As part of the DOE Site Characterization effort at YM, hydrochemical data will be obtained for the unsaturated zone at YM under Study Plan 8.3.1.2.2.7 Hydrochemical Characterization of the Unsaturated Zone (U.S. Department of Energy, 1988). The USGS has already obtained a large amount of data on water chemistry in the unsaturated zone (Yang et al., 1988, 1993), mineralogy (Levy, 1991), and mineral chemistry (e.g., National Academy of Sciences, 1992; Whelan and Stuckless, 1992; Peterman et al., 1992; Paces et al., 1993; Marshall et al., 1993; Whelan et al., 1994). Many of these data, particularly those on secondary calcite from the unsaturated zone, may provide information on interconnections between different water bodies and their sources. Age dating can be used to relate these data to known changes in the paleoclimate and paleohydrology.

It may be possible to provide a first-level screening for those areas that have a good

potential for the development of perched-water zones based on the hydrologic properties of the units at YM and the geologic structure. For example, those areas where faulting has juxtaposed units of contrasting hydraulic conductivity may be identified as areas favorable for perched-water zone formation. First-level screening criteria will be developed and used to the extent possible to identify possible areas for perched-water zones. The availability of geochemical data is likely to be one of the limiting factors in selecting those areas for more detailed examination.

Perched water has been reported in volcanic tuffs under semi-arid to arid conditions at Rainier Mesa (Russell et al., 1987), and at the UA ALRS (Bassett et al., 1991, 1994b). The ALRS can be used as an analog site in an effort to define those chemical parameters that are sensitive to the presence (or absence) of perched-water zones. Sensitive parameters may include water chemistry, water ages, and mineral chemistry. A focused effort may find the mechanisms responsible for perched-water development in one or more of these locations. Much of the data will be site specific and not necessarily representative of conditions at YM. Nevertheless, this type of information might be useful to constrain and test flow models, providing additional confidence in the modeling results.

A detailed description of the petrology and mineralogy of the tuffs immediately above, below, and within the perched-water body would be useful to document changes in mineralogy around a perched zone. Mineralogy, petrologic relationships, and mineral chemistries are all important to interpret potential relationships to flow and transport in a comprehensive manner. As noted in the "Project Plan for Field Studies at the Apache Leap Research Site" submitted by the UA to NRC (Bassett et al., 1995b), changes in mineralogy may affect stratigraphic permeability. Reductions in permeability due to alteration minerals such as clays or silica precipitation in fractures could result in hydraulic conductivity contrasts sufficient to result in the formation of perched water. Because there is still uncertainty regarding flow and transport in fractured, unsaturated tuffs, both fracture and matrix mineralogy and mineral chemistries should be documented at the ALRS to the extent possible.

Correlations between mineralogy and perched water at the ALRS would be compared to mineralogical and petrological information available from site characterization activities (e.g., Levy, 1991) at YM to evaluate the potential for similar hydrologic conditions at the proposed repository site. This may provide some insight into identifying areas that are likely to be favorable for the formation of future perched water at YM due to mineralogical and petrological changes. Mineral chemistries and petrology around the perched water at the ALRS may also serve as a means to fingerprint where perched water may have existed in the geologic past at YM. Once site characterization data become available on the mineralogies associated with known or suspected occurrences of perched water at YM (e.g., UZ-14), similarities may be noted, increasing confidence in the use of mineralogical indicators of perched zones.

For the purposes of modeling flow through the unsaturated zone and around a perched-water zone, hydraulic properties are clearly a critical need. Values for hydrologic properties such as hydraulic conductivities, characteristic curves, porosity, and permeability, determined through laboratory and field experiments, are necessary to provide the boundary and initial conditions of flow models used to evaluate the potential formation of perched water.

Neuman (1995) outlined the types of measurements that can be made at the DSB site. These include fracture characterization, single-hole pneumatic testing, and infiltration and tracer experiments using additional shallow boreholes. Laboratory experiments with drill core can be used to provide saturated conductivities and characteristic curves of unsaturated hydraulic conductivity. These data will be used to constrain conceptual models of flow through the unsaturated zone and boundary and initial conditions for flow and transport models.

Water and mineral chemistry can be used to identify where perched water zones might have occurred in the past and to provide boundary conditions for flow and transport models. Hydrochemical facies (Hem, 1985) can be used to establish relationships between bodies of water. Tracers such as stable isotopes have long been used to distinguish water bodies (e.g., unsaturated and saturated zones), and also to identify potential flow paths, recharge areas, and fluid sources (e.g., Welhan, 1987; National Academy of Sciences, 1992; Conrad, 1993). Age dates determined for groundwaters using isotopes such as ^{14}C , tritium, and ^{36}Cl can be used to provide estimates of rates of fluid flow, and timing of changes in paleohydrology.

Water chemistry data including major and trace elements will be compiled on the perched zone and on end-member fluids such as the saturated zone, surface runoff, precipitation, and unsaturated zone pore waters where possible. Isotopic signatures for these waters, both for stable isotopes and radiogenic isotopes will also be gathered. Chemical and isotopic definition of the perched water and the potential sources for these waters is a critical step in identifying and modeling water-rock interactions. Radiogenic age dates of waters using ^{14}C , ^{36}Cl , and tritium will also be useful in calibrating flow models. Some of these data have already been published (Bassett et al., 1994a; Davidson, 1995), and will be augmented by additional stable isotope data for elements such as sulfur, carbon and boron similar to that discussed by Bassett et al. (1995a).

Geochemical data obtained on the chemistry and ages of waters at the ALRS have been used by NRC staff in cooperation with University of Arizona researchers to develop conceptual models for perched-water formation in fractured tuffs in an arid environment. Insight gained at the ALRS are providing guidance as to what data are important and how to interpret available data at YM.

2.3 Groundwater Flow and Transport Assessments

The SUFLAT methodology and suite of codes (Bagtzoglou and Muller, 1994) will be evaluated in year two of the contract by the CNWRA regarding its capability to simulate the subregional-scale groundwater flow and transport conditions considered plausible at the YM site. Other conceptual and mathematical models (see Neuman, 1995) will be evaluated by the UA. Analysis of field data from the ALRS, collected in conjunction with the UA researchers, will facilitate a critical investigation of differences between various alternative models. Based on this analysis, modifications or enhancements to the SUFLAT methodology, and to UA models, will be made as deemed necessary.

At the CBS site, one research venture will select a small area containing several large fractures, over which gas tracers may be applied at a controlled rate. Through careful

instrumentation of the area with neutron probe access tubes, TDR probes, tensiometers, and gas detectors, the advancing gas tracer fronts can be monitored. Field results can then be compared with selected model predictions. Inclined boreholes at the 10-m scale have been used at the CBS site to evaluate pneumatic testing methods and to characterize rock permeability. As a consequence, the CBS is a very well-characterized site. Other types of information, such as geophysical logs, will also be very useful to identify the location and extent of geological features that exhibit very long correlation structures (i.e., significant spatial continuity). Features with these characteristics are often called persistent discontinuities and could enhance preferential flow and transport processes. These data will enable researchers to perform pilot flow and transport modeling activities.

In addition to the CBS, the NST/QC site provides a unique opportunity to investigate matrix-fracture interactions. Two potential field-scale experiments are under consideration: (i) burial of a tracer at a shallow depth below the QC bed, directly above the NST, so that rainy-season flow in the creek will provide a pulse of water and tracer that can be monitored in the underlying NST; and (ii) damming off a 30 to 40 m section of QC during the dry season, so that ponded water (containing some tracer) will infiltrate downward and, similarly, provide an advancing water and tracer front to be monitored in the underlying NST. In either case, data on experimental tracer (e.g., K-Br) tests will be useful in evaluating hydrologic properties such as matrix imbibition and fracture flow in partially saturated porous media. The Magma Mine Company has developed detailed geological maps, which can be used to infer fracture pattern characteristics and other pertinent information. These maps, if available for distribution, could prove very useful for the NST/QC site efforts.

One additional use for mineralogical and petrological information is to provide boundary and initial conditions for reactive transport models that incorporate precipitation/dissolution reactions. Predicting the stability of minerals such as clays in response to HLW thermal loading is one aspect of the flow and transport calculations. Using mineralogical information from the ALRS can be an important part of building confidence in these models. Reactive transport simulations for the ALRS will be conducted, accounting for geochemical interactions such as aqueous speciation, sorption, and mineral precipitation/dissolution reactions. 1D simulations of flow in the Queen Creek fracture network have been done by UA using DCM3D (Fitzmaurice, 1994; Updegraff and Lee, 1991) and will be coupled to the NEFTRANII solute transport code (Olague et al., 1991). As a comparison, UA recently modified the multicomponent speciation and solute transport code HYDROGEOCHEM (Yeh, 1992b) for use in the proposed tracer tests.

Data on environmental isotope profiles and other chemical indicators of mineral alteration during weathering are useful in reactive transport modeling. Especially useful are data on mineral alteration products produced during weathering of the tuff at the ALRS. These data will be useful for understanding the possible alteration of tuff at YM and testing numerical models of reactive transport in partially saturated porous media. Moreover, observed amount of calcium sulfate precipitated as a function of depth from the surface at the ALRS will aid in understanding the evaporation process in the subsurface and the amount of water infiltrating into the tuff rock. It will also be useful in testing models involving reactive transport in the partially saturated zone.

2.4 Statement of Work

Specific research needs identified by NMSS and NRS management include the following:

- (1) Test and confirm methods for characterizing the spatial distribution of infiltration and recharge and its effect on the development of perched systems.
This is being addressed as part of Subtasks 1.1, 1.2, 3.1, and 3.2 as discussed in Chapters 3, 4, and 8.
- (2) Investigate, test, and confirm the methods used in determining the role of fractures and fracture zones in unsaturated flow in the region above the water table.
This is being addressed as part of Subtasks 1.2, 2.1, 2.2, and 3.2 as discussed in Chapter 4, 5, 6, and 7.
- (3) Evaluate the conditions necessary to initiate episodic fracture flow and establish methods to estimate the location and duration of such events.
This is being addressed as part of Subtask 2.2, as discussed in Chapter 7.
- (4) Identify and test alternative conceptual models of flow and transport in fractured rock at the site scale, with emphasis on processes that may cause mixing and overall dilution or concentration of contaminants.
This is being addressed as part of Subtasks 1.1 and 2.2, as discussed in Chapters 3 and 7.

2.4.1 Contract Objectives

The objectives of the research are to:

- (1) Investigate continuum scales for predicting gas and liquid flow in matrix-fracture systems;
- (2) Determine the relationship between relative permeability of air and water in unsaturated fractured tuff;
- (3) Investigate field methods and instrumentation for developing data sets which facilitate the use of effective hydraulic, pneumatic, and transport properties to predict transport;
- (4) Investigate the use of isotope and geochemical modeling studies to determine the rate and pathway of solute flux in an unsaturated fractured tuff;

- (5) Investigate the role of fractures and fracture zones in unsaturated flow and transport in a region above the water table and subject to perched-water development; and
- (6) Investigate the mechanisms and conditions which affect groundwater flow and transport in unsaturated fractured tuff (e.g., fracture versus matrix-dominated flow, focused versus distributed recharge, and perched-water development due to persistent discontinuities or relic high-recharge events).

2.4.2 Relationship to Other Projects

The work outlined in this contract is to provide direct support to the following two projects:

- (1) UA studies under RES-95-038 on testing and evaluation of groundwater flow and transport models; and
- (2) the CNWRA studies under NRC-02-93-005 on Subregional Groundwater Flow and Transport Studies (Bassett et al., 1995c).

A related research project is:

- (3) the CNWRA studies under NRC-02-93-005 on Regional Hydrologic Processes (Bassett et al., 1995c).

A related technical assistance project for NMSS is:

- (4) the CNWRA studies under the "Performance Assessment and Hydrologic Transport Element" in the HLW Operations Plan (IPA Phase III).

The earlier UA studies at the Apache Leap Research Site (ALRS) produced databases for evaluating pneumatic, geochemical, hydrologic, and transport processes on a site scale. Information is available for assessing fracture versus matrix flow conditions for unsaturated fractured tuff over a range of scales. Inclined boreholes at the 10-meter scale have been used to test pneumatic testing methods. A deep inclined borehole to the local perched-water table and associated core and water samples are available to test site characterization methods and modeling strategies for determining effective field properties. The geochemical data allow for independent confirmation of groundwater mixing and residence times for fracture-dominated, as opposed to matrix-dominated, flow systems. The work in this contract builds on these accomplishments and should provide new opportunities for data collection in support of the first two cited related projects (see above), particularly the UA theoretical study (RES-95-038).

3. PNEUMATIC TESTING OF FRACTURED POROUS TUFFS AT THE ALRS (Subtask 1.1)

by W. A. Illman, D.L. Thompson, G. Chen, and S.P. Neuman

3.1 Introduction

The objective of Task 3 is to plan, conduct and interpret pneumatic and tracer field tests that will provide data, on scales of 1 - 100 m, to help validate the applicability of continuum geostatistical and stochastic concepts, theories, models, and scaling relations relevant to unsaturated flow and transport in fractured porous tuffs. To satisfy this objective, two field experiments, crosshole pneumatic and gaseous tracer experiments at the CBS, and pneumatic characterization of tuffs around the perched zone at the DSB, have been proposed. Crosshole tests are currently being conducted: 1) to obtain pneumatic properties of fractured tuffs on the 10 m scale, 2) to investigate the existence of dominant, pneumatic flow paths between selected injection and monitoring intervals, 3) to associate pneumatic parameters such as porosity and directional permeability with those flow paths, 4) to help verify heterogeneity patterns determined from single-hole test results, and 5) to employ the results in corroboration with the planned tracer test to obtain transport parameters of unsaturated fractured tuffs. During this phase, three-dimensional hydraulic and pneumatic property distributions at the CBS are being analyzed and modeled using geostatistical techniques based on available data. These distributions are being used to predict hydraulic and pneumatic connections between boreholes as controlled by both the rock matrix and fractures. The equipment for crosshole flow tests has been assembled and leak tested both in the laboratory and in the field. Systematic crosshole tests are being conducted at the CBS. Preliminary results support geostatistical continuum estimates of heterogeneity based on earlier data, suggesting that a continuum stochastic approach to flow and transport in fractured rocks at the site may be feasible. The main purpose of this progress report is to review the current status of the crosshole testing program.

Transient data from single hole pneumatic tests on the 1-m scale are also being analyzed to facilitate the understanding of unsaturated flow mechanisms in fractured tuffs and to aid the crosshole testing program by providing preliminary estimates of permeability near the injection point. Video images taken by COLOG (1993) of all the X,Y and Z-series boreholes have also been examined to help visualizing the spatial distribution of fractures.

The first phase of the crosshole pneumatic tests commenced on November 1995 and a framework for the gaseous tracer experiment has been formulated. The injection of dry air into borehole Y2 and monitoring the response in neighboring boreholes has shown the extensive interconnection of fractures that propagate throughout the fractured tuffs. The injection of dry air and monitoring of pneumatic pressure were conducted along the entire length of each borehole. From this initial test, we found that pneumatic pressures are more-or-less linearly related to injection mass flow rate (Fig. 3.1). This linear dependence of pneumatic pressures on injection mass flow rate suggests that an equivalent porous medium type curve analysis of these tests may be feasible.

Experience from the initial phase of the crosshole testing program taught us of the need to pack off all boreholes, including the more recently drilled G-series boreholes, so as to minimize

Figure 3.1. Plot shows the linear relationship of observed pneumatic pressures when the injection test is conducted at two mass flow rates ($Q = 50$ and 100 slpm). Note that the regression line ($R^2 = 0.893$) is forced through the origin.

air leakage into the atmosphere. Boreholes left open to the atmosphere act as infinitely conductive pathways which allow pressure to equilibrate almost instantaneously.

3.2 Site Characterization

Single hole air permeability tests have been conducted at 0.5, 1.0, 2.0, and 3.0 meter scales in borehole Y2, at 1.0 and 2.0 meter scales in borehole X2, and at 1.0 meter scale in boreholes V2, W2a, Y3, and Z2 (a schematic layout of the boreholes is shown in Fig. 3.2). These tests have resulted in 184 one-meter scale data sets relating to air permeability along six boreholes in a 35,000 m³ unsaturated porous fractured tuff block. The data have been organized to facilitate future use, sorted according to borehole, and backed-up for storage. A brief discussion of geostatistical analyses of the same data is found in section 4.2. Most available information concerns borehole series X, Y, and Z. It includes rock matrix parameters such as bulk and skeletal density, porosity, pore size distribution, and pore surface area. Information on fracture location, density, and spacing is also available, as well as matrix pneumatic permeabilities (Rasmussen et al., 1990). Neutron probes have been employed to monitor water content in all boreholes. These data supply initial conditions for our preliminary estimate of site conditions between the boreholes where data are lacking.

3.3 Preliminary Estimates

Prior to crosshole testing, we have analyzed geostatistically the spatial structure and distribution of available hydraulic and pneumatic data. Figure 3.3 shows the estimated distribution of natural log (ln) permeability to air, under near-ambient conditions, in a plane containing boreholes X2 and Y2. The distribution suggests that X2 and Y2 are connected by a high-permeability zone at a depth of about 15 m. More insight into the spatial extent of this zone is obtained from the additional planar sections in Figs. 3.4-3.7. These show that the zone is limited in its spatial extent, has more or less an elliptical shape, and is internally heterogeneous. Based on an earlier recording of fractures in boreholes at the CBS by Rasmussen et al. (1990), we suspect that it is associated with a local cluster of highly conducting subhorizontal fractures. Most of these fractures do not correlate from one borehole to another, nor do their occurrence and density correlate well with in situ measurements of permeability. We were generally not able to differentiate between the hydraulic and pneumatic properties of individual fractures and those of their neighbors or the nearby rock matrix. The high-permeability zone spans boreholes Y2, V3, V2, X2, W2, and W2a at a depth of about 15 m.

3.4. Crosshole Pneumatic Injection Experiments

3.4.1 Current Status

The second phase of our crosshole testing campaign has been set back for a few months due to severe wind damage to the covered site in January 1996. Repair work included disentangling the packer lines left in boreholes from previous tests, unrolling and repositioning the damaged plastic cover, welding and securing the damaged sections of the plastic cover, and

Figure 3.2. Plan view of borehole locations at the Covered Borehole Site.

Figure 3.3. Kriged estimate of $\ln$ permeability on section x_2 - y_2 .

Figure 3.4. Kriged estimate of $\ln$ permeability at $y = 5.2$ m.

Figure 3.5. Kriged estimate of $\ln$ permeability at $y = 6.9$ m.

Figure 3.6. Kriged estimate of ln permeability at y = 10 m.

Figure 3.7. Kriged estimate of ln permeability in a plane spanning three test intervals with largest measured permeability.

placing numerous sandbags on the perimeter of the plastic cover to prevent further wind damage. As of March 1996, the site is fully repaired and ready for testing.

The months of January through March 1996 were further devoted to preparatory work and minor improvements to the injection system. The basic configurations of the injection and monitoring systems remain unchanged. Minor improvements have been made to achieve greater efficiency in data collection and more accurate results. Fig. 3.8 is a scheme of the injection system presently installed in our field laboratory. The mass flow meter has a wider range (0 - 100 slpm) than that used previously during single-hole tests. Filters are included to remove moisture and entrained particles from the air stream before it enters a borehole. Measurements of pressure and discharge are made and relative humidity is recorded to ensure that the injected air stream is dry. All pressure transducers intended for crosshole testing have been calibrated and all corresponding electrical connections have been established. The large number of pressure transducers employed in this testing required the concatenation of two multiplexers to the datalogger. The data collection system has been upgraded to accommodate up to 34 pressure transducers of diverse types. The electronic system has been tested thoroughly for defects and the computer program which controls the data logger has been optimized for maximum efficiency. A removable, large capacity disk drive will soon be added to the personal computer located at our field laboratory to accommodate the large data sets we expect to obtain from long-duration tests.

Figure 3.9 is a schematic diagram of the air injection system used for single-hole testing at the CBS. It consists of a straddle packer assembly made of two rubber bladders, a set of flow meters and flow controllers, pressure regulators and valves, and an electronic monitoring system to collect field data in real time. The distance between bladders can be adjusted to make possible the testing of variable length intervals. Pressure (P), temperature (T), and relative humidity (RH) are measured in the injection interval. A series of flow controllers and flow meters on the soil surface supply a constant injection flow rate (Q) that can be adjusted between 10 and 20,000 standard cm^3/min (sccm).

Figure 3.10 depicts the modular components that have been used to construct the new injection and detection packer strings. The new interval design reduces significantly the volume of the injection interval, thereby reducing borehole storage effects. Fig. 3.11 is a schematic diagram of the main cross-hole injection packer string. The main benefit of a modular design is rapid replacement of failed components, which in turn results in less down time. Figure 3.12 illustrates the pneumatic/tracer detection packer string. The number of packers and detection intervals in each string are adjustable.

Packers employed in the study consist of two types; the F and G series. The F-series packer, a variation originally designed by earlier workers, is relatively more expensive and is employed in all of the boreholes that we expect to respond. The G-series packer is less expensive due to its simpler construction and has been placed in the outlying boreholes. There are no real technical differences between the two types. They are both intended for packing the boreholes and are thoroughly tested for leakage.

The F-series packers are designed as part of a modular design where the interval body,

Figure 3.8. Schematic diagram of improved cross-hole injection system currently installed at the Covered Borehole Site.

Figure 3.9. Schematic diagram of air injection system for single-hole testing at the Covered Borehole Site.

Figure 3.10. Components of the modular packer string.

Figure 3.11. Schematic diagram of injection packer string for cross-hole testing.

Figure 3.12. Schematic diagram of typical detection string.

upper and lower packers, guard intervals and guard packers are all interchangeable. This is accomplished by means of a 1.5 inch schedule 80 screw coupling placed on each subassembly (see Fig. 3.13).

During the initial field trials in November 1995, it was decided that all boreholes should be packed-off and monitored. The G-series packers were designed to be used for sealing boreholes near the surface with a single, pressure monitoring access port. Substantial cost savings was accomplished by using a closed-end PVC cap fitted with a brass, quarter-inch, pass-through hose fitting instead of a more expensive modular coupling design. Assembled almost entirely in the field with hand tools, these packers with a 15 Psig pressure transducer have cost substantially less than the F-series. In addition, the G-series packers are more robust and reliable with an almost zero leakage failure rate. The main disadvantage of the G-series is that they are stand-alone packers and cannot be utilized in a straddle assembly or as part of the modular F-series. However, the G-series packers were designed so that they can be converted to a more versatile F-series by fitting them with a one-half inch screw coupling.

3.4.2 Zero Permeability Test

An essential part of our testing methodology is a strict quality assurance program. As part of this program, a procedure to check the integrity of the packer assembly has been developed. This so-called "zero permeability" test is conducted in an impermeable PVC pipe having an inside diameter equal to that of a test borehole. The test involves placing the packer string (Fig. 3.10) inside the PVC pipe, inflating a packer to 80 psi to isolate the otherwise sealed PVC pipe below it from the atmosphere, injecting air below the packer until pressure reaches 20 psi, then shutting the injection valve and recording pressure and temperature below the packer as well as barometric pressure. If there is no leakage from the test interval to the atmosphere, pressure within it remains more or less constant. Otherwise, the rate at which air leaks from the interval is calculated as:

$$Q(\text{sccm}) = \frac{P_1 T_1 - P_2 T_2}{T_1 T_2} \frac{V T_{sc}}{P_{sc} \Delta t} \quad (3.1)$$

where:

- V = volume of test interval (cm³),
- P₁ = absolute pressure at reference time t₁ (cm Hg),
- P₂ = absolute pressure at reference time t₂ (cm Hg),
- P_{sc} = absolute pressure under standard conditions (76.0 cm Hg),
- T₁ = absolute temperature at time t₁ (K° = C°+273°),
- T₂ = absolute temperature at time t₂ (K° = C°+273°),
- T_{sc} = absolute temperature under standard conditions (293° K)
- Δt = t₂ - t₁.

If the leakage rate exceeds 5 sccm during any time interval, the leak is identified, an

G-Series Packer

inexpensive, simple, stand-alone version
employed to pack-off boreholes

F-series Packer

modular design allowing
straddle-packer assembly

For both packer types:

O.D. = 8 cm

I.D. = 5 cm

Figure 3.13. Comparison of G- and F-Series packer systems.

attempt is made to seal it, and the test is repeated. Of all twelve packers tested thus far, eleven have eventually passed the test while one continued to leak.

3.5 Preliminary Field Cross-Hole Tests

The first stage of cross-hole testing started on Nov. 1, 1995, and ended on Nov. 10, 1995. Its purpose was to test the equipment and our geostatistical estimation of the presence, and extent, of a high-permeability/fracture zone at a depth of 15 m. Based on this estimate, we placed one packer at a depth of 10 m in borehole Y2 and injected air into the entire borehole beneath it. Nine surrounding boreholes (X2, X3, Y1, Z2, V2, V3, W1, W2, and W2a shown in Fig. 3.2) were packed off at a depth of 3 m (to isolate them from the atmosphere) while all other boreholes remained open (for lack of packers; this will be remedied in future tests). Air was injected by means of the system illustrated in Fig. 3.9. Flow rate was kept constant by means of a mass flow meter at 50 slpm while continuously recording pressure and temperature in all packed intervals as well as relative humidity in the injection interval. After nearly 24 hours, injection ceased and pressures in all boreholes were allowed to recover while data recording continued. The test was then repeated by doubling the injection rate to 100 slpm.

Figures 3.14 and 3.15 show arithmetic plots of recorded flow rate, relative humidity and pressure during the two injection and recovery periods, respectively. Relative humidity in the injection interval is seen to drop rapidly at the start of injection and to recover very fast when injection stops. The injection pressure in the injection interval within borehole Y2 is seen to decline slowly with time. The same has been observed during single hole testing of many intervals and is attributed by us to the displacement of water by air in the immediate vicinity of the injection interval. Whereas in monitoring boreholes V3, V2, W2a, W2, X2, and W1 pressures increased and stabilized rapidly, in Y1 the pressure rose slowly and never stabilized, while in Z2 and X3 it showed no significant increase during either test. It appears that air flow from Y2 into Y1, Z2, and X3 is more restricted than that from Y2 to V3, V2, W2a, W2, X2, and W1, suggesting that the latter are interconnected through a more permeable zone. Though the shortest distance from boreholes V2, V3 to borehole Y2 is 2.6 m (at depths of 16 m and 17 m, respectively), the latter responded much more rapidly than did the former. This is consistent with the geostatistical image in Fig. 3.7 according to which (a) V2 lies farther from Y2 than does V3 in the plane of the previously identified high permeability zone, and (b) this zone is limited in areal extent and heterogeneous so that its permeability is smaller where it is intersected by V2 than where it is intersected by V3. Heterogeneity is also reflected in the fact that although the distance between W2a and Y2 is the same as that between W2 and Y2, and is larger than that between V2 and Y2, pressure response in W2a is much more pronounced than that in W2 and V2. Pressure responses in V2 and W2 are virtually identical because the two boreholes intersect.

Figures 3.16 through 3.20 include logarithmic plots of pressure data recorded in the injection interval and in all packed off monitoring intervals at an injection rate of 50 slpm. All the plots show a break caused by inadvertently shutting off the flow meter for a brief period during the test. Pressure in Y2 showed a very rapid increase at the start of the test and reached a near steady value of approximately 95,000 Pa after 2000 seconds. We find it of interest that wellbore storage effects are not immediately visible on this plot. In contrast, logarithmic plots of pressure

Figure 3.14. Cross-hole test with flow rate of 50 slpm.

Figure 3.15. Cross-hole test with flow rate of 100 slpm.

Figure 9a:

Figure 3.16. Observation borehole (Q = 50 slpm); logarithmic plot of data from (a) V2 and (b) V3.

Figure 10a:

Figure 3.17. Observation borehole (Q = 50 slpm); logarithmic plot of data from (a) W1, (b) W2, and (c) W2A (following page).

(c)

(Figure 3.17, continued)

Figure 11a:

Figure 3.18. Observation borehole (Q = 50 slpm); logarithmic plot of data from (a) X2 and (b) X3.

Figure 12a:

Figure 3.19. Observation borehole (Q = 50 slpm); logarithmic plot of data from (a) Y2 and (b) Y1.

Figure 3.20. Observation borehole (Q = 50 slpm); logarithmic plot of data from Z2.

in the monitoring intervals show a more gradual increase. Type curve matching will be attempted in the near future.

Figures 3.21 through 3.25 include logarithmic plots of pressure data recorded in the injection interval and in all packed off monitoring intervals at an injection rate of 100 slpm. Pressure responses in the monitoring intervals are almost twice as large as during the first injection test. This suggests that the system is responding linearly to injection into Y2. Contrary to the first test, there was now a measurable response in boreholes Z2 and X3. It is clear that, in the future, there will be a need to pack off all boreholes at the CBS to prevent leakage into the atmosphere through open holes during the crosshole tests.

3.6 Work Plan

Crosshole testing is being conducted in three phases. Phase 1 has been completed and described in the previous section. In phase 2 about to commence, air will be injected into a selected borehole interval isolated by two packers. Fig. 3.26 is a simplified scheme of the injection system currently placed within borehole Y2. The injection interval is isolated by an upper and lower guard packer, with a monitoring interval located above and below the guard packers. These monitoring intervals are required to detect possible short-circuiting of injection packers during a pneumatic crosshole test. A surface guard packer is placed at the top of the borehole to prevent loss of pressure into the atmosphere. Pneumatic injection will begin in Y2. A total of five pre-selected injection points are scheduled for this second phase and injection at each interval will be conducted at two mass flow rates. The breakdown of the five selected injection points are the following: 1) injection into a low permeability zone at the 26.6m level ($k=9.05 \times 10^{-17} \text{ m}^2$), 2) injection into three different, intermediate permeability zones starting at 10m ($k=1.92 \times 10^{-15} \text{ m}^2$), 19.7m ($k=1.91 \times 10^{-15} \text{ m}^2$), and 22.7m ($k=1.16 \times 10^{-15} \text{ m}^2$) and 3) injection into the high permeability zone located at 16m ($k=4.5 \times 10^{-14} \text{ m}^2$) measured from the top of the Y2 borehole. Additional intervals may be tested as we proceed with the second phase of the cross-hole testing program. The injection interval is currently placed at the 10 m level, measured from the lower lip of the casing on the ground surface to the center of the injection interval. Pneumatic injection will also be attempted in other boreholes, such as Y3 and Z1, if time and resources permit.

During the third phase of the crosshole testing program, we intend to isolate intervals not only within the injection borehole, but also within the monitored boreholes. Intervals will be selected for isolation based on the information gained from the first two phases of the testing program, previously conducted borehole television surveys, pneumatic permeability values previously obtained from single hole tests, and three-dimensional permeability distributions generated by means of geostatistical estimation and/or simulation. Hsieh and Neuman (1985) show that a minimum of six point measurements are required for each crosshole test to determine the three dimensional permeability tensor of a uniform medium. Since we are dealing with a strongly heterogeneous medium, many more tests may be required to meaningfully characterize the site. Pneumatic pressure responses are expected to vary considerably among successive tests. Injection directly into the high permeability zone, which is known to span the covered site (at approximately 15 - 16m from the top of casing) will cause a near instantaneous responses in some boreholes, which may propagate rapidly across the site. Injection into intermediate and low

Figure 14a:

Figure 3.21. Observation borehole (Q = 100 slpm); logarithmic plot of data from (a) V2 and (b) V3.

Figure 15a:

Figure 3.22. Observation borehole (Q = 100 slpm); logarithmic plot of data from (a) W1, (b) W2, and (c) W2A (following page).

(c)

(Figure 3.22, continued)

Figure 16a:

Figure 3.23. Observation borehole (Q = 100 slpm); logarithmic plot of data from (a) X2 and (b) X3.

Figure 17a:

Figure 3.24. Observation borehole (Q = 100 slpm); logarithmic plot of data from (a) Y2 and (b) Y1.

Figure 3.25. Observation borehole (Q = 100 slpm); logarithmic plot of data from Z2.

Figure 3.26. Schematic diagram of injection system currently installed in borehole Y2.

permeability zones may cause an appreciable pressure increase around proximal boreholes, but not likely in the distal boreholes (unless injection is conducted over long time).

Progress is also being made in redesigning the injection device so as to incorporate a water content measuring device such as a neutron or a moisture-density probe. The device will be employed to monitor local changes in water content during a pneumatic crosshole test. In a previous report (Bassett et al., 1995), we proposed to scan the injection interval before and after each pneumatic crosshole test. This, however, has the disadvantage of providing no information about changes in water content during a crosshole test. It may also be difficult to lower a standard neutron probe device into a hole while the injection system is being readied for use. The continuous collection of water content and pressure during a test (so we hope) allow us to obtain a moisture-pressure characteristic curve for the fractured rock, in situ.

Much thought has gone into deciding where to inject and monitor based mainly on the results of single hole packer tests, borehole video surveys completed several years ago, and geostatistical maps created from the single hole test results. We expect the response to vary considerably from test to test.

3.7 Transient Analysis of Single Hole Pneumatic Data

At the Apache Leap Research Site (ALRS), single-hole pneumatic tests have previously been conducted in selected boreholes by injecting air into a packed-off interval with a straddle-packer assembly. Steady-state analyses of late data from these tests have been conducted by Guzman et al. (1995). One objective of our current work is to analyze the transient records of selected single-hole tests at the ALRS by means of corresponding type curves developed for single-phase air flow. Our analyses of transient data have so far been based on linearized forms of radial and spherical, single-phase gas flow equations that are similar to those for liquid flow (p-based model). We are presently developing type curves based on other methods of linearization to see how sensitive is the analysis to these methods.

The equations that describe gas flow in partially saturated porous media are nonlinear due to the compressible nature of gas and displacement of water in both the matrix and fractures by gas. To properly simulate gas flow, therefore, requires considering both phases simultaneously. We are presently preparing for such simulations by means of two numerical computer codes, TOUGH (Pruess, 1987) and FEHM (Zyvoloski et al., 1995). The purpose of these simulations will be to supplement our analysis of the crosshole tests by type curves.

Type Curves Analyses

Type curve analyses have been performed on selected, single-step, pneumatic injection tests conducted at the Apache Leap Research Site (ALRS). We used type curves developed via numerical inversion of solutions in Laplace space given in Joseph and Koederitz (1985) and Raghavan (1993). The radial (2D) and spherical (3D) solutions given by these authors include wellbore storage and skin effects. Numerical inversion was carried out by a computer program modified slightly after Xu and Brusseau (1995) based on an algorithm due to De Hoog et al.

(1982). The algorithm accelerates the convergence of Fourier series obtained during inversion by means of the trapezoidal rule.

The characteristics of the radial and spherical flow models that include wellbore storage and skin effects are evident in Figs. 3.27a and 3.27b. Early time solutions for both the radial and spherical models show a characteristic unit slope on logarithmic paper. During this period, wellbore storage effects due to air compressibility dominate the pressure buildup. The effect of wellbore storage dissipates gradually as the injected air enters the fractured tuffs. At late time the radial flow system reaches a pseudosteady state, where pressure varies linearly with time. The derivative of the dimensionless pressure with respect to the logarithm of dimensionless time reaches a constant value of 0.5. In contrast, the spherical flow system tends asymptotically to a steady-state with a derivative of dimensionless pressure with respect to the logarithm of dimensionless time that vanishes at large time. The mathematics behind these two sets of type curves will be presented in a subsequent report.

Figs. 3.27 and 3.28 show pressure and pressure derivative matches of data from pneumatic injection tests JNA0713 (Y2 - 26.59m) and JJA0616 (Y2 - 17.77m) with radial and spherical type curves. The data from JNA0713 fit the spherical but not the radial type curves. Over 90% of the 30 type curve matches attempted thus far fit the spherical model, but there are a few exceptions. As one can clearly see in Fig. 3.28, the data from pneumatic test JJA0616 appear to fit the radial flow model more closely than the spherical flow model except at very late time. This late time deviation may be due to two-phase flow effects which manifest themselves as a time-varying skin effect. It should also be noted that skin values obtained from type curve matches with the spherical model are small (0 - 5). Some single-hole test data show a half slope on logarithmic paper at early time. Fig. 3.29 shows an attempted fit of one such set of pressure data (YAA0301 - 2.55 m) to a horizontal fracture model developed by Gringarten and Ramey (1974).

Air permeability values obtained from type curve matches to both the radial and spherical models are summarized in Table 2. It has been shown by Guzman and Neuman (see Rasmussen et al., 1996) that 1 m scale single-hole air permeabilities at ALRS are virtually the same whether one employs a radial or (prolate) spheroidal model. On the other hand, transient interpretations yield different permeabilities when based on radial and spherical flow models. Fig. 3.30 shows that permeabilities obtained by means of the spherical transient model generally compare more favorably with their steady-state counterparts than those obtained by means of the radial model. This is another indication (in addition to the improved type curve matches) that transient air flow around most 1 m single-hole test intervals at ALRS is closer to spherical than to radial.

3.8 Tracer Tests

3.8.1 Objectives and Data Needs

Field tracer tests are being planned to confirm the pneumatic injection tests, to yield transport related parameters such as kinematic (effective) porosity, matrix diffusion coefficient, and dispersivity, and to help validate transport theories and models as applied to fractured porous tuffs. The field tracer tests will start at the conclusion of the flow tests. The locations of injection

Figure 3.27. Pressure and pressure derivative match of data from pneumatic injection test (a) JNA0713, radial flow, and (b) JNA0713, $C_D = 10^4$.

Figure 3.28. Pressure and pressure derivative match of data from pneumatic injection test (a) JJA0616, radial flow, and (b) JJA0616, $C_D = 10^1$.

Figure 3.29. Type curve match of data from YAA0301 using the horizontal fracture model developed by Gringarten et al. (1974).

Figure 3.30. Comparison of permeability values obtained from transient and steady state analyses:
(a) spherical flow, (b) radial flow.

and monitoring intervals will be based on the results of the latter tests. We are considering the use of helium as a tracer due to the fact that it is nonreactive and relatively easy to detect. Consideration is also being given to additional compounds such as bromated fluorocarbons, SF_6 and tritiated methane.

There is a need to collect concentration data of injected and monitored tracers at multiple points on a real-time basis. Sampling should be done quickly and accurately, since injected tracers are expected to travel rapidly through some fractures. Figure 3.31 is a scheme of the proposed field apparatus of the gaseous tracer experiment. Multiple peaks of tracer breakthrough can be expected at our site due to multiple pathways that are usually present in fractured rocks. In order to detect multiple peaks, one may have to use a tracer which has a low detection limit (such as SF_6) and monitor the boreholes for a very long time.

3.8.2 Injection System

The injection system is based on the preexisting equipment setup for the crosshole testing program. We will first inject air as in crosshole tests until a steady value of pressure is reached in observation boreholes. Once steady-state is reached, a known volume of a gaseous tracer such as He, Ar, Ne and/or SF_6 will be injected into the borehole. Tracer tests will be conducted initially with one gas until the system is free of defects. The employment of multiple tracers may become desirable in the future once the integrity of the system is ensured. Currently, helium is our choice of tracer due to its nonreactive nature, low cost, ease of detection and safety.

Samples will be collected and analyzed periodically to record the concentration of tracer entering the borehole and into the medium. Potential problems associated with the injection system include determining the amount of tracer that should be injected without excessively raising the background level of helium at the site, and leakage of tracers into the atmosphere along its path (through vertical fractures and/or through leaky equipment).

3.8.3 Extraction System

The extraction system will be designed so that samples are collected periodically from the monitoring boreholes (min. 6 - max. 16). We will begin the tracer experiment by monitoring only one borehole to test our proposed setup. Once we are able to design a working system, we will increase the number of monitored boreholes. The minimum number of boreholes that need to be monitored is six, in order to characterize the hydraulic anisotropy of the fractured tuff. Sampling should be conducted in a manner which preserves the pressure conditions inside the borehole. Ideally, sampling and analysis should be conducted inside the borehole, but due to size and budgetary constraints, this sampling scheme is currently deemed not possible. An alternative to the in situ monitoring of gases is to extract a sample of gas from the interval and to analyze it on the surface. The proposed apparatus involves a continuous loop of gas, which circulates from the borehole into a sampling device and is sent back into the borehole without measurably perturbing pressure in the borehole. A small sample of gas will be taken to ensure a near constant value of pressure in the system. The sample will be discarded into the atmosphere after analysis. The biggest problem associated with the extraction system is to sample individual boreholes in an

Figure 3.31. Proposed setup of gaseous tracer experiment.

expeditious and synchronized manner without perturbing the pressure around the borehole.

We have determined that sampling and analysis from each borehole will take approximately two minutes employing (personal communication with technician from VARIAN corp., 1996) a multi-port sampler and a gas chromatograph (GC). Our challenge is to devise an apparatus which allows rapid and accurate sampling so as not to miss early breakthroughs of tracers.

Assuming that we can accurately and quickly obtain gaseous samples in the monitoring boreholes, we need to look for a device which analyzes the tracer concentration breakthrough. Our current preference is a thermal conductivity detector (TCD) attached to a gas chromatograph (GC). In fact, the TCD seems to be the only choice when concentration of noble gases is to be determined. TCD is a stable detector with moderate sensitivity and employs a nondestructive method of analyzing samples. The main disadvantage of TCD is that the instrument does not identify a specific compound. According to (Zemel, 1995), compounds are identified in the order that they are eluted from the gas chromatograph.

3.9 Future Field Work

In the coming six months, we plan to conduct the following field work:

1. Pneumatic crosshole tests by packing off all boreholes near the top and injecting air into various intervals within Y2 at two flow rates (point to line tests)
2. Pneumatic crosshole tests with monitoring of pressure differential at specific intervals in some boreholes (point to point tests).
3. One or more helium tracer tests(s).
4. Additional pneumatic and/or gaseous tracer test(s) as time and resources permit.

4. INFILTRATION TESTS IN FRACTURED POROUS TUFFS
AT THE ALRS (Subtasks 1.2 and 3.2)
by G. Chen, S.P. Neuman, and P.J. Wierenga

4.1 Introduction

The objective of Task 3 is to plan, conduct and interpret hydraulic and tracer infiltration tests to help validate the applicability of continuum geostatistical and stochastic concepts, theories, models, and scaling relations relevant to unsaturated flow and transport in fractured tuffs. To satisfy this objective, two field experiments, 3-D hydraulic and tracer infiltration experiments at the CBS, and single fracture infiltration experiments above the perched zone at the DSB, are being contemplated. Currently, we are executing phase one of the 3-D hydraulic and tracer infiltration experiments. During this preliminary phase, the three-dimensional spatial distribution of pneumatic and hydraulic parameters at the CBS is being analyzed and estimated geostatistically based on available laboratory and field data. Conditions similar to those anticipated during the infiltration experiments are being simulated on the computer. Simulations are being conducted in two ways: (1) by using the best available geostatistical estimates of how the relevant parameters are distributed in space, and (2) by using more realistic but less smooth random realizations of these parameters about their respective estimates. These results suggest that the infiltration front would descend only a few meters in three months. It must however be recognized that these predictions are probably on the low side and that actual infiltration may in fact be much faster than predicted. This is so because, in our simulations to date, we have treated the available pneumatic permeabilities as if they represented intrinsic permeabilities to air in the absence of water; since actual water saturation is quite high, the intrinsic permeabilities are probably much higher. Furthermore, we have ascribed the available matrix porosities to the fractured porous tuff; in reality, the effective flow porosity of the tuff may well be controlled by fractures and thus be much smaller than assumed. Increasing intrinsic permeability and reducing porosity would result in increased infiltration rates. Actual field experiments are scheduled for the second year, following completion of the pneumatic injection and gaseous tracer experiments at the site.

4.2 Site Characterization

The CBS has been extensively characterized in the past (Rasmussen et al., 1990; Bassett et al., 1994b). A considerable amount of laboratory and field information about the site is available from inclined and vertical boreholes, shown in Fig. 4.1. Available data that are most directly relevant to our planned infiltration tests include steady state pneumatic permeability values in 184 1-m sections of boreholes X2, Y2, Y3, Z2, V2, and W2a (Rasmussen et al., 1995), 105 laboratory values of rock matrix density, porosity, and moisture retention curves from the X, Y, and Z-series holes (Rasmussen et al., 1990), and 8 in situ neutron probe measurements of water content during May 1990 - April 1991 at each of 159 locations within all boreholes of the X-, Y-, Z- and W- series except W1. In the future we expect to incorporate information from pneumatic injection and gaseous tracer experiments into this site characterization data base.

Plan View of Covered Site Boreholes

Figure 4.1. Spatial location of boreholes at the CBS, a) plan view, b) 3D view.

All currently available data vary erratically in space, most notably air permeability (k), matrix porosity, the α parameter which defines matrix moisture retention capabilities of laboratory samples based on the van Genuchten model, and in situ water content. All of these data are being subjected to geostatistical analysis. Since geostatistical analysis is optimal when applied to variables that are distributed normally, we work with a natural logarithmic ($\ln$) transformation of air permeability, porosity, and α instead of the original data.

Figure 4.2 shows an omni-directional sample semivariogram of $\ln k$. The variogram exhibits nonstationarity and was analyzed by means of two different models: a model which views the data as belonging to a random fractal field that has a power-law semivariogram, and a more traditional model which views the data as belonging to a statistically homogeneous random field about a linear or quadratic spatial drift. To select the best among these conceptual models, we used formal model discrimination criteria based on the Maximum Likelihood Cross Validation (MLCV) approach of Samper and Neuman (1989a,b), coupled with the generalized least squares drift removal approach of Neuman and Jacobson (1984). MLCV estimates semivariogram parameters by maximizing the likelihood of kriging (geostatistical interpolation) cross validation errors. As MLCV assumes that the semivariogram model is known, it leads to optimum parameters for a given model structure without regard to the question how well this model represents the real system. Fortunately, a number of model identification criteria have been developed in the context of maximum likelihood estimation. Earlier work by Carrera and Neuman (1986a, b) and Samper and Neuman (1989a,b) have compared four such criteria: AIC (Akaike, 1974), MAIC (Akaike, 1977), HIC (Hannan, 1980), KIC (Kashyap, 1982), and concluded that the one which comes closest to satisfying these requirements is that due to Kashyap (1982). Kashyap's criterion favors the model which, among all alternatives considered, is least probable (in an average sense) of being incorrect. Stated otherwise, the criterion minimizes the average probability of selecting the wrong model among a set of alternatives. It supports the principle of parsimony in that, everything else being equal, the model with the smallest number of parameters is favored. While this means favoring the simpler model, the criterion nevertheless allows considering models of growing complexity as the data base improves in quantity and quality. The criterion recognizes that when the data base is limited and/or of poor quality, one has little justification for selecting an elaborate model with numerous parameters. Instead, one should prefer a simpler model with fewer parameters which nevertheless reflects adequately the underlying structure of the rock, and the corresponding flow and transport regime. The cited works by Carrera and Neuman, and Samper and Neuman, clearly indicate that an inadequate model structure is far more detrimental to its predictive ability than is noise in the data used to calibrate the model.

We have extended MLCV to render it applicable to non-stationary (statistically nonhomogeneous) models such as a random fractal characterized by a power-law semivariogram (while the random fractal field represented by such a semivariogram is statistically nonhomogeneous, it does possess statistically homogeneous spatial increments). Figure 4.2 shows the power model fitted to the original sample semivariogram, and an exponential model fitted to a sample semivariogram of residuals after removal of a second-order polynomial drift function. The power model represents a nonhomogeneous field which possesses neither a finite variance nor a finite spatial correlation scale. The exponential model represents a homogeneous

Figure 4.2. Semi-variogram of ln permeability.

field with finite variance and spatial correlation scale. Which of these models represents the data more accurately? An answer is found in Table 4.1 which shows that, whereas the exponential semivariogram model with a quadratic drift fits the data best (as measured and implied by the smallest negative log likelihood model fit criterion, NLL), all four model discrimination criteria (AIC, MAIC, HIC, KIC) consistently rank the power model as best and the former model as least acceptable among the three considered. The reason is that whereas all three models fit the data almost equally well, the power model is most parsimonious with only two parameters, and the exponential semivariogram model with second-order drift is least parsimonious with twelve parameters. As shown in Fig. 4.3a-b, both models yield very similar kriged (estimated) images of $\ln k$, but rather different measures of the associated estimation uncertainty.

Table 4.1 Variogram structure of $\ln$ permeability with and without de-trending

Trend Model	Original Data	1st Order De-trend	2nd Order De-trend
NLL	665.801	665.080	655.849
Variogram Model of Residual	Power	Exponential	Exponential
Number of Parameter	2	6	12
Variance (Scaling Coeff. For Power Model)	1.4396	3.0788	2.6248
Integral Scale (Power for Power Model)	0.4475	1.6650	1.2602
AIC	669.801	677.08	679.849
Rank	1	2	3
MAIC	677.231	696.37	718.428
Rank	1	2	3
HIC	672.407	684.898	695.486
Rank	1	2	3
KIC	680.016	690.088	700.907
Rank	1	2	3

Figure 4.3a. Kriged estimate and variance of $\ln k$ at $y = 6.9$ m using power model.

Figure 4.3b. Kriged estimate and variance of $\ln k$ at $y=6.9$ m with 2nd order de-trending.

A similar analysis has been performed on in situ water content data. Figure 4.4 shows original and residual sample semivariograms together with the best fit spherical model fitted to the latter. A power model does not seem to fit the data well. It is clear from Table 4.2 that all four model discrimination criteria (AIC, MAIC, HIC, KIC) consistently rank the spherical model with quadratic drift as better than an exponential model without drift. This is so despite the fact that the chosen spherical model with drift has twelve parameters, and is therefore less parsimonious than the exponential model without drift, which has only two parameters.

Table 4.2 Variogram structure of initial water content with and without de-trending

Trend Model	Original Data	2nd Order De-trend
NLL	398.105	319.180
Variogram Model of Residual	Exponential	Spherical
Number of Parameter	2	12
Variance	1.349	0.5609
Integral Scale (Range for Spherical model)	6.550	6.290
AIC	402.105	343.180
Rank	2	1
MAIC	397.913	375.028
Rank	2	1
HIC	394.307	356.085
Rank	2	1
KIC	402.116	364.712
Rank	2	1

Figures 4.5 and 4.6 show semivariograms for natural ln porosity and the α parameter together with their best fit exponential models without drift. No drift is indicated by the data in either case. The corresponding model parameters are listed in Tables 4.3 and 4.4, respectively. Three models are considered in these tables: exponential, exponential with a nugget (white noise at zero lag), and spherical. The second model yields a best fit for both ln porosity and α , yet is not always favored as best by model discrimination criteria due to the fact that it contains three

Figure 4.4. Semivariogram of water content.

Figure 4.5. Semivariogram of ln porosity.

Figure 4.6. Semi-variogram of $\ln \alpha$.

Table 4.3. Identification of variogram structure of ln porosity measured at the Apache Leap Covered Site

Model	Exponential	Exponential With Nugget	Spherical
NLL	-170.740	-178.84	-175.456
Number of Parameters	2	3	2
Nugget	0.0	5.369×10^{-4}	0.0
Variance	0.0167	0.0156	0.01617
Integral Scale (Range for Spherical model)	3.010	3.011	5.510
AIC	-174.740	-172.849	-171.456
Rank	1	2	3
MAIC	-169.432	-164.882	-166.148
Rank	1	3	2
HIC	-172.513	-169.628	-169.303
Rank	1	2	3
KIC	-158.734	-145.775	-153.703
Rank	1	3	2

parameters while the other two models contain only two. In general, the exponential model appears to be favored over the spherical model.

We see clearly that all data are amenable to continuum geostatistical analysis, and exhibit distinct spatial correlation structures, which suggests that they can be viewed as representative of a continuum. This is so despite the fact that the rock is fractured and therefore mechanically discontinuous. This finding may be contrary to geologic intuition, but it is supported strongly by similar findings in many other fractured rock terrains including crystalline rocks at Oracle, Arizona (Neuman and Depner, 1988); Stripa, Sweden (SKB Annual Report, 1993); and Fanay-Augeres, France (Kostner, 1993; Ando, 1995). It strongly supports the application of continuum flow and transport theories and models to fractured porous tuffs.

Based on the most favored semivariogram model(s) identified in the above manner for each data set, we have estimated the spatial distributions of ln permeability, ln porosity, ln α , and water content at the CBS by kriging each of them independently of all others in three dimensions. Figure 4.7 shows kriged images of ln permeability, porosity, α , and water content in a vertical plane corresponding to $y = 6.9$ m. These kriged estimates were used as input into numerical

Figure 4.7. Kriged images of $\ln$ permeability, porosity, α , and water content at $y = 6.9$ m.

Table 4.4. Identification of variogram structure of $\ln \alpha$ measured at Apache Leap Covered Site

Model	Exponential	Exponential With Nugget	Spherical
NLL	61.471	56.679	67.965
Number of Parameters	2	3	2
Nugget	0.0	0.0549	0.0
Variance	- 0.118	0.0645	0.1247
Integral Scale (Range for Spherical model)	2.253	5.5402	5.133
AIC	65.471	62.679	71.965
Rank	2	1	3
MAIC	70.775	70.642	77.265
Rank	1	2	3
HIC	67.613	65.898	74.111
Rank	2	1	3
KIC	77.634	79.065	87.050
Rank	1	2	3

simulations of infiltration. Since kriged distributions are much smoother than is the case in the field, we have also superimposed random fluctuations on the kriged results via conditional simulation to generate more realistic (less smooth) spatial distributions of the available data. The conditional random fields of $\ln$ permeability, $\ln$ porosity, $\ln \alpha$, and water content have been generated independently in three dimensions using GCOSIM3D, a sequential Gaussian simulation code developed at Stanford University (Gomez-Hernandez and Cassiraga, 1994). The algorithm requires that the simulated variables be Gaussian. Of the four variables we have simulated, only $\ln$ porosity deviates slightly from Gaussianity in that it failed to pass the Kolmogorfo-Smirnoff test at the 95% confidence level. Figure 4.8 shows conditionally simulated images of $\ln$ permeability, porosity, α , and water content in a vertical plane corresponding to $y = 6.9$ m. Note that these images are less smooth than their kriged counterparts but are otherwise quite similar.

4.3 Preliminary Predictions of Infiltration

Prior to finalizing the infiltration test design, we have simulated these tests in kriged parameter fields as well as in selected parameter fields obtained by conditional simulation. The purpose was to help select the most favorable method and area of water application; to anticipate the depth and spatial distribution of the infiltrating water, as well as the time and volume of water

Figure 4.8. Conditionally simulated images of $\ln$ permeability, porosity, α , and water content at $y = 6.9$ m.

required to reach a given depth; and to help select the exact location, number, and type of monitoring instruments. Currently, we are simulating the infiltration of water applied to the shaded 10 m x 10 m area in Fig. 4.1. The particular location was selected because the surface there is relatively flat, and it overlies a volume of rock spanned by enough boreholes to provide characterization data and allow the installation of monitoring instruments. Both the size and location of the infiltration area may change depending on the results of pneumatic cross-hole tests at the CBS and preliminary simulations of the infiltration tests. Special emphasis will be placed on the identification of shallow features (fractures) that may enhance infiltration rates.

In the simulations, the infiltration area of 10 m x 10 m (Fig. 4.1) is covered with 10 cm water and maintained so for the duration of the infiltration period. A larger area of 30 m x 30 m surrounds the infiltration domain for simulation purposes. No flow is allowed to take place along any boundary except that across which infiltration is taking place. For three-dimensional simulations we have constructed a grid of 30 x 30 x 20 blocks of size 1 m x 1 m x 1 m. Water contents measured in situ between May 1990 and April 1991, which varied very slowly in time, were taken to represent initial conditions for this preliminary simulation. Permeability, porosity, α , and initial water content for each block were obtained directly from kriged estimates or from conditionally generated distributions. The density values measured in the laboratory vary so slowly in space that it is reasonable to treat them as constant (Rasmussen et al., 1990). Unsaturated moisture retention and permeability were taken to follow the van Genuchten formulae

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{[1 + (\alpha h)^n]^m} \quad (4.1)$$

$$k_{uns} = k S_e^{1/2} \left[1 - \left(1 - S_e^{1/m} \right)^m \right]^2, \quad (4.2)$$

where θ , θ_r , and θ_s are volumetric water content, residual water content, and saturated water content, respectively; α , n , and $m=1-1/n$ are parameters that affect the shape of the retention curve; h is tension, k is saturated permeability, and k_{uns} is unsaturated permeability. The water retention curves of rocks at the ALRS have been measured in the laboratory by Rasmussen et al. (1990). They also used these data to estimate the van Genuchten parameters assuming a constant value of n and m for all samples, no residual saturation, and saturated water content as porosity. The procedure yielded the best fitting for $n = 1.26$ and α values that varied spatially as described earlier. In our simulations to date, we have equated k with measured, estimated, or conditionally generated pneumatic permeabilities. Since the latter represent conditions of partial saturation to air, we expect them to be much smaller than actual saturated k values. Furthermore, we have ascribed the available matrix porosities to the fractured porous tuff; in reality, the effective flow porosity of the tuff may well be controlled by fractures and thus be much smaller than assumed. The net effect is that our predicted infiltration rates may be on the low side as compared to those that may actually occur during the infiltration tests.

To date we have performed a number of two dimensional simulations in the vertical planes of $y = 6.9$; three-dimensional simulation is planned for the near future. The simulations were performed by means of a code developed by Hills et al. (1994). We have compared this code with VTOUGH, a code developed at Lawrence Berkeley Laboratory, with favorable results. Figure 4.9 illustrates simulated changes in water content after 30 days, and after 90 days, of infiltration in the plane of $y = 6.9$ m based on the kriged images in Fig. 4.7. The simulation results suggest that water infiltrates about 2 m in the first 30 days, and 3 m in the first 90 days. However, we consider it very possible that actual infiltration rates could be higher due to reasons mentioned in the preceding paragraph.

Figure 4.10 shows simulated changes in water content in the plane of $y = 6.9$ m based on one realization of the flow parameters generated by conditional simulation in Fig. 4.8. The depths of infiltration after 30 and 90 days are comparable with those obtained based on kriging. However, some preferential flow is now evident. Again, the computed infiltration rates are most probably on the low side. Additional details will be given in our next semiannual report.

4.4 Field Experimentation

The infiltration tests will require a source of water which is not presently available at the CBS. Preliminary simulation results (which may well underestimate infiltration rates, for reasons mentioned previously) suggest that about 2.5 m^3 of water may infiltrate into the rock during the first day, 11.5 m^3 during the first 30 days, and 15.0 m^3 during the first 90 days. The 1.16 m^3 water tank which is presently available to us at the site would not suffice for this purpose. We therefore are designing a water storage pool north of the CBS (where space and elevation are favorable) with a capacity of $10 - 30 \text{ m}^3$.

We are considering two possible methods of water application at the surface. In the first method, the area would be covered with water to a given elevation and maintained so for the duration of the infiltration period. As the surface is not entirely flat, the applied pressure head would vary from point to point across the surface. Another possibility is to maintain a more uniform pressure head across the site by constructing stainless steel sheet piles along topographic contours and maintaining different water levels on the two sides of each sheet pile so that the corresponding pressure heads remain more or less equal. At present we favor the first option due to its simplicity and lesser cost. Both options should allow accurate modeling of the surface boundary condition.

4.5 Future work

In the next six months we plan to conduct the following work:

1. Numerical simulation of infiltration in three-dimensions at different locations and over different size areas at the CBS. We will consider both kriged and multiple conditionally generated parameter fields using geostatistical models which treat log permeability either as statistically homogeneous with drift, or as statistically nonhomogeneous with power-law (fractal) behavior.

Figure 4.9. Changes in water content at $y = 6.9$ m after infiltration based on kriged estimates of rock properties.

Figure 4.10. Changes in water content at $y = 6.9$ m after infiltration based on conditional simulations of rock properties.

2. Analyze the sensitivity of infiltration to the effective porosity and saturated permeability by performing systematic numerical simulations. Analyze crosshole test results as soon as they are available to obtain more information on the effective porosity and saturated permeability, and update the simulation of infiltration.
3. Design infiltration tests based on these simulations (considering that they may underestimate infiltration rates) and start assembling the required instrumentation.

5. GEOCHEMICAL EVALUATION OF FRACTURE FLOW AT THE ALRS (Subtask 2.1)

by G.R. Davidson, R.L. Bassett, E.L. Hardin and D.L. Thompson

The occurrence and significance of fracture flow at the ALRS was investigated by drilling a deep slant borehole (DSB) in January of 1993 (Fig. 5.1). The DSB was positioned to intersect a series of nearly vertical fractures dipping in the opposite direction of the borehole (Fig. 5.2). Fractures potentially carrying water were identified using a suite of geophysical logs and a video log. Figure 5.3 shows sharp drops in density coincident with decreases in resistivity and increases in neutron absorption at multiple depths. The density drops are typical responses to fractures, while decreasing resistivity and increasing neutron capture can be caused by increased water content adjacent to the fractures. Increased water content associated with select fractures was confirmed by direct measurement of core samples from the DSB (Fig. 5.4).

If the downward migration of water is limited to percolation through the matrix, a plot of ^{14}C measurements from pore waters should demonstrate a relatively monotonic decrease in ^{14}C activity with depth. If fractures provide a fast pathway for some fraction of the water, partial imbibition should result in localized increases in the ^{14}C activity of pore water adjacent to these fractures. Figure 5.5 provides a plot of the ^{14}C activity of pore waters with depth. Increases in ^{14}C activity are observed at multiple depths, including the depths where fractured intervals were specifically targeted. The most significant increase occurs near the perched water table at 130 m where post-bomb ^{14}C activity was measured.

Advective transport of surface air through fractures can also produce elevated ^{14}C activity in adjacent pore waters, but the evidence suggests that water is the source of the increased ^{14}C activity: (1) water is known to travel through fractures intersected by the DSB; water was directly observed entering the borehole through a fracture at 72 m, and elevated water contents were measured at this depth and at other depths associated with fractures, (2) elevated matrix water content near fractures, and high saturation of the matrix in general, will serve to limit the efficiency of an advective driving force such as barometric pumping, (3) topographically driven convection, which causes elevated ^{14}C activity deep in some boreholes at Yucca Mountain, is not observed in the DSB, and (4) a comparison of the geochemistry of waters sampled from the surface, from matrix pores within the unsaturated zone, and from the perched aquifer indicate that most of the water in the perched aquifer must have bypassed the matrix pores by traveling through fractures.

Table 5.1 lists the average measured concentrations of dissolved species in surface runoff, pore waters squeezed from the upper 21 m of the DSB core, and perched water pumped from the saturated zone. It is clear from a comparison of the total dissolved solid (TDS) concentrations, that a significant portion of the perched water must have come from a source more dilute than pore water. No pore water samples were obtainable deeper than 21 m, but there is no reason to suspect that pore waters deeper than 21 m would be less concentrated than those above.

Figure 5.1 Location map of the Apache Leap Research Site (ALRS). Elevations are in feet. (CBS = Covered Borehole Site; AWS = Automated Weather Station; DSB = Deep Slant Borehole - drainage basin shown outlined)

Figure 5.2 Cross-section of the Deep Slant Borehole (DSB).

Figure 5.3 Neutron, density, and resistivity logs of the DSB. Highlighted bands are shown at depths where ephemeral water-bearing fracture zones were suspected based on video and geophysical logs. Additional zones bound by the two dashed lines were not specifically targeted, but their influence is also observed in the isotope data. The two locations where the borehole narrows are marked as *bn* (geophysical data from E. Hardin, 1994, written communication).

Figure 5.4 Water content of DSB core measured by gravimetric analysis (open circles, Geddis; 1995) and by vacuum distillation (filled circles; Davidson, 1995).

Figure 5.5 Carbon-14 activity of all samples measured from the DSB. Highlighted and dashed bands identify the suspected water-bearing fractures from Fig. 5.3. The broken line connecting the lowest formation air intervals signifies possible contamination at these depths. Analytical precision (1σ) is roughly the size of the data points.

A comparison of specific dissolved species further indicates that the perched water is not a result of simple dilution or of mixing between surface runoff and pore waters. Reaction with CO₂ and mineral phases must also be considered to account for the chemical composition of the perched water.

Table 5.1 Average aqueous chemistry of surface runoff, pore water from the upper 21 m of the DSB core, and perched water pumped from the DSB. Concentrations are in mg/L.

	Surface Runoff	Pore Water	Perched Water
HCO ₃	2.8	84.1	120.9
SO ₄	18.0	40.5	1.9
NO ₃	< 0.25	8.6	1.1
PO ₄	< 0.25	3.6	< 0.25
Cl	2.3	35.9	4.2
Na	3.7	53.3	21.9
K	1.3	2.9	0.9
Ca	5.0	24.6	20.2
Mg	1.4	5.4	3.7
SiO ₂	32.3	55.4	53.0
TDS	67	314	228

Mineral or anthropogenic sources have been identified for all the dissolved species in Table 5.1 with the exception of chloride. Increases in chloride must result from evaporative concentration, or mixing with high chloride waters. This places a constraint on the proportion of the perched aquifer that can be accounted for by contributions from unsaturated-zone pore water. Using the chloride values in Table 5.1, the total contribution of pore water to the perched zone cannot exceed 6% by volume. Using minimum pore-water and maximum surface-runoff chloride values from individual measurements (reported in Davidson, 1995), pore water contributions are limited to less than 13%. Geochemical reaction-pathway models considering possible dissolution of CO₂ and primary silicates (plagioclase, biotite, and hornblende), and possible precipitation of secondary silicates (smectite, illite, kaolinite, chlorite, and SiO₂) verify that it is possible to generate the chemical composition of the perched aquifer by allowing surface runoff to mix with small portions of pore water and react with aquifer minerals. In each simulation using the geochemical code NETPATH (Plummer et al., 1991), perched water composition could be modeled only by limiting the contribution from pore waters to less than 10% (Davidson, 1995).

Additional evidence of aqueous transport through fractures is provided by the discrepancy between the ¹⁴C activities of water pumped from the perched aquifer and water extracted from saturated-zone core (Fig. 5.5). The pore water samples represent water taken from a well defined location directly beneath the ephemeral stream where the borehole intersects the perched aquifer.

The pumped samples represent water drawn an unknown distance from the borehole and from the stream bed. The pore waters contain elevated ^{14}C activities and measurable tritium ($\sim 0.15\text{ T}$), while the pumped waters have lower ^{14}C activity and no measurable tritium. The most likely explanation is that recharge to the perched aquifer is focused through fractures beneath the ephemeral stream. The pore water samples came from beneath the stream bed close to a point source of recharge, while the pumped samples tapped into an older supply of water some distance removed from this source.

The similarity between the ^{14}C activity of the dissolved organic carbon (DOC) sample, and the dissolved inorganic carbon (DIC) samples (Fig. 5.5) is consistent with a system dominated by recharge through fractures. If water is transported from the surface to the perched aquifer rapidly through fractures, DOC may not experience significant retardation relative to DIC. If transport occurs primarily through the matrix, however, the slower flow rate, increased exposure to matrix surfaces, and smaller, restrictive pathways should result in significant retardation of DOC that is not observed in the data from the DSB.

Fractures appear to be the primary pathway by which water is transferred to the perched aquifer near the DSB. Post-bomb ^{14}C activities near the water table suggest that flow through at least some of these fractures is rapid. The total volume transferred annually may be small, however, based on the fact that no tritium is observed in perched water samples pumped from the DSB. Annual recharge at other locations at the ALRS may be higher based on tritium, SO_4/Cl ratios and $\delta^{34}\text{S}$ values. Dry fall from a nearby copper smelting operation is dissolved by runoff waters resulting in elevated levels of dissolved sulfate with a $\delta^{34}\text{S}$ value distinct from rainwater. This source of sulfate serves as a useful tracer for identifying contributions of modern water to the perched aquifer. The values in Table 5.2 for perched water seeping into the east end of the mine haulage tunnel (Fig. 5.1) are intermediate between rainwater and perched water from the DSB, indicating that recharge through fractures is more substantial at this site than near the DSB. Although tritium is also high at the Oak Flat borehole, the relative contribution of modern water at this site is less certain because the SO_4/Cl ratios and $\delta^{34}\text{S}$ values are nearly the same as found at the DSB.

Table 5.2 Comparison of isotope and geochemical data from surface runoff, perched water from the DSB, perched water from the Oak Flat borehole, and perched water seeping into Magma Mine's haulage tunnel (Fig. 5.1). (Tunnel, Oak Flat, and $\delta^{34}\text{S}$ data from Bassett et al., 1994a.)

	Runoff	DSB	Tunnel	Oak Flat
^{14}C (pmc)	118	67	69	69
^3H (TU)	6	< 0.1	1.2	1.9
$\delta^{34}\text{S}$ (‰)	-4 to +1	6 - 7	2 - 4	7
SO_4/Cl	6 - 10	0.4 - 0.5	1.1 - 2.5	0.4 - 0.8

6. $^{234}\text{U}/^{238}\text{U}$ FRACTIONATION IN VADOSE ZONE POREWATERS OF THE APACHE LEAP TUFF
by *E.L. Hardin and R.L. Bassett* (University of Arizona)
and *M.T. Murrell* (Los Alamos National Laboratory)

6.1 Abstract

Decay of U-238 in the natural environment leads to production of U-234 ($t_{1/2} = 2.46 \times 10^5$ yr). In a closed system of sufficient age the U-234/U-238 activity ratio (AR) approaches unity, but is > 1 in typical groundwater. The isotopes exhibit equivalent kinetic behavior in natural chemical reactions, so fractionation must result from the energy released by alpha-decay. The AR was analyzed in surface waters, near-surface fracture waters, perched waters, and vadose zone pore waters from the Apache Leap Tuff. This tuff has features that are similar to Yucca Mountain tuffs and amenable to investigation. Novel methods were used for sampling vadose zone pore waters from preserved drill cores. The AR for all surface, fracture, and near-surface pore water samples was in the range 1.4 to 2.1. A deeper transition in pore water AR from 2 to 5 correlated with trends in saturated matrix hydraulic conductivity and magnetic susceptibility, delimiting the penetration of oxidative weathering into the vadose zone. From C-14 apparent ages (Davidson, 1995) it is evident that this multiple transition does not reflect the former high stand of a perched water table. A lumped parameter model was used to evaluate the relative contributions from selective leaching and direct recoil mechanisms to perched water fractionation at Apache Leap, integrating mass balance, radioactive decay, sorption, isotopic exchange, and direct recoil effects. The strategy was to identify a set of model parameters describing the total U concentration and AR for perched waters from different sampling locations without direct recoil, then recompute the ratios with direct recoil. The results showed that leaching selectivity is probably significantly greater than the observed mobile phase AR, and that within the likely range of effective partitioning behavior the contribution from direct recoil to observed activity ratios is minor.

6.2. Introduction

This study was motivated by the observation of elevated U-234 activity in perched waters in tuffs at Yucca Mountain, Apache Leap, and elsewhere. The general objectives were to investigate the spatial distribution of pore water fractionation, evaluate alternative conceptual models for fractionation, and identify implications for transport of natural U. Methods were developed to sample vadose zone pore waters for U isotopes, and applied at the Apache Leap Research Site (ALRS) to investigate U-234 fractionation throughout the vadose zone.

Davidson (1995) described sampling pore waters from preserved tuff cores by core squeezing using the method and the equipment of Peters et al. (1992). In the Apache Leap Tuff welding increases with depth, and this method was effectively limited to the uppermost 30 m of the section because of low pore water yield. Using the chemical separation and isotopic analysis methods described by Goldstein et al. (1989) the U concentration and U-234/U-238 activity ratio (AR) of squeezed pore waters were compared with other waters from Apache Leap including surface waters, fracture waters from shallow borings, and perched waters (Table 6.1, Figure 6.1). A mixing plot shows that U leaching near the surface is different from the process that produces

Table 1. Uranium concentration and U-234/U-238 activity ratio in surface, near surface, vadose zone, and perched waters at the ALRS and vicinity.

Sample	Vertical Depth (m)	U _{tot.} (ppt)	Mass U (ng) ³	4/8 AR ¹
Watershed runoff (AQ-M; DSB ⁵ creek; 1/18/92)	0	23±2 ⁽⁴⁾ (N=3)		
Watershed runoff (AQ-M; DSB creek; 8/26/93)	0	40±7 ⁽⁴⁾ (N=3)		
Watershed runoff (DSB creek; 8/31/94)	0	28±1 ⁽⁴⁾ (N=2)	>40	1.43 ±0.0073
Fracture #6 (shallow boring; 8/31/94)	2	117 ⁽²⁾	155	1.94 ±0.0097
Fracture #20 (shallow boring; 8/31/94)	2	138 ⁽²⁾	195	2.09 ±0.010
Perched Water (DSB ⁵ , purged, 6/11/93)	~147	241 ⁽⁴⁾		
Perched Water (DSB, purged, 7/18/93)	~147	212±1 ⁽⁴⁾ (N=2)	>40	6.292 ±0.031
Analysis duplicate of above.			>40	6.294 ±0.031
Perched Water (DSB, purged, 11/2/93)	~147	232 ⁽⁴⁾		
Perched Water (mine tunnel, CP-4, 9/14/90)	~200	602 ⁽⁴⁾		
Perched Water (mine tunnel, 7920', 9/14/90)	~200	740 ⁽⁴⁾		
Perched Water (mine tunnel, CP-1, 7/29/93)	~200	672 ⁽⁴⁾	>100	5.350 ±0.027
Analysis duplicate of above.			>100	5.377 ±0.027
Perched Water (Oak Flat borehole, 4/4/90)	~100	737 ⁽²⁾	34.5	6.56 ±0.037

Notes: ¹Analyzed by TIMS. Estimated 0.5% internal precision, except as noted.²Analyzed by TIMS with isotope dilution. ³Est. mass for isotopic analysis.⁴Analyzed by ICP/MS. ⁵ Deep slant borehole. ⁶Estimated from flushed U mass, divided by pore volume. ⁷Weak signal, error estimate 5% of value.

Table 1. (cont.) Uranium concentration and U-234/U-238 activity ratio in surface, near surface, vadose zone, and perched waters at the ALRS and vicinity.

Sample	Vertical Depth (m)	U _{tot.} (ppt)	Mass U (ng) ³	4/8 AR ¹
Squeezed Pore Water (DSB ⁵ core from 6 m)	4	45 ⁽²⁾	1.0	1.93 ±0.049
Squeezed Pore Water (DSB core from 13 m)	9	389 ⁽²⁾	23.7	2.15 ±0.012
Squeezed Pore Water (DSB core from 14 m)	10	166 ⁽²⁾	7.5	2.04 ±0.010
Squeezed Pore Water (DSB core from 22 m)	15	198 ⁽²⁾	10.6	2.08 ±0.015
Squeezed Pore Water (DSB core from 22 m)	15	137 ⁽²⁾	6.7	2.06 ±0.017
MQ Leached Pore Water (DSB ⁵ core from 8 m)	6	8 ^(1,6)	1.5	1.98 ±0.014
MQ Leached Pore Water (DSB core from 14 m)	10			1.97 ±0.016
MQ Leached Pore Water (DSB core from 17 m)	12			2.26 ±0.032
MQ Leached Pore Water (DSB core from 24 m)	17			2.23 ±0.045
MQ Leached Pore Water (DSB core from 35 m)	25			4.79 ±0.024
Sample replicate of above.				4.89 ±0.024
MQ Leached Pore Water (DSB core from 45m)	32			4.67 ±0.23 ⁽⁷⁾
MQ Leached Pore Water (DSB core from 45 m)	32	317 ^(1,6)	29.2	5.23 ±0.026
MQ Leached Pore Water (DSB core from 83 m)	58	58 ^(1,6)	4.2	4.22 ±0.021
MQ Leached Pore Water (DSB core from 149 m)	106			5.16 ±0.026
MQ Leached Pore Water (DSB core from 192 m)	147			4.72 ±0.024

Figure 6.1. Schematic of sampling locations at the ALRS for uranium geochemistry investigations.

fractionation in deeper waters (Figure 6.2).

6.3. Pore Water Sampling by Flushing of Preserved Cores

A previously described method (Bassett et al., 1995) for flushing preserved core samples with Milli-Q water was modified to increase injection pressure to 70 bars. Each core sample was enclosed by Teflon endcaps and a vinyl sleeve, placed inside a hydrostatic pressure vessel, and injected with Milli-Q through one end. Samples with saturated hydraulic conductivity as low as 0.01 mm/yr were flushed, and recovered U mass for isotopic analysis was as low as ~1 ng. Control and measurement of contamination were critical as previously reported. Useful results were obtained and earlier data were replicated, however, changes to the method of core confinement would be appropriate if the method is to be used at greater pressures.

Using the flushing method at 70 bars, core samples from the perched zone were sampled and the AR transition at about 20 m depth was sampled in more detail. Chemical processing and isotopic analysis of water samples was done at the Clean Chemistry and Mass Spectrometry Facility at the Los Alamos National Laboratory (LANL). Water samples were acidified, spiked with U-233 and U-236 where appropriate, evaporated, and separated chemically using a two-column anion exchange procedure described by Goldstein et al. (1989). The U-234/U-238 and isotope dilution analyses were performed using the VG Sector 54 thermal ionization mass spectrometer at the LANL facility. The smallest U samples were not spiked because the standard contains U-234 thus increasing the number of isotopes to be counted for analysis of U-234 during the limited life of such samples in the instrument. The observed AR is a lower bound on actual pore water composition since the sample may acquire less fractionated U from the solid phase, or from the U blank.

Above the AR transition (Figure 6.2) activity ratios from flushing were indistinguishable from ratios for squeezed pore waters (Table 6.1). New, duplicated analyses from 25 m vertical depth show that the AR transition occurs within a depth range of about 8 m (between 17 and 25 m). The single pore water AR analysis from the perched zone has a value $AR=4.72$ which is significantly lower than the perched water ($AR=6.23$). This datum could be important for interpreting fractionation mechanisms, but it was a small U mass sampled over many weeks from impermeable core samples, and could have been contaminated. Additional study is underway to evaluate this datum using a different leaching procedure. Perched water sampled in April, 1990 during drilling of the Oak Flat borehole was also analyzed, and found to have an AR very similar to perched water in the DSB, although the U concentration is three times greater (Table 6.1).

6.4. Fractionation Mechanisms

Selective leaching of U-234 from recoil-damaged sites apparently occurs in surface soils and near-surface fracture zones, given the short residence time and the relation between total U and the AR for these waters (Figure 6.2). A wide range of concentration was observed in squeezed near-surface pore waters, all with $AR \sim 2$ (Table 6.1).

The three perched water samples were analyzed for C-14 activity in earlier studies and

Figure 6.2. Summary of U-234/U-238 isotopic analyses on water samples from the ALRS, plotted against vertical depth.

found to have similar apparent ages of about 3,000 yr (Davidson, 1995; Bassett et al., 1994). The AR values reported in Table 6.1 for these waters are also similar. In the Oak Flat perched water the AR differs from the DSB value by only 1%, yet the U concentration is three times greater. This is probably related to the stratigraphic position of the perched water table at Oak Flat, which lies within the near-surface porous tuff layer. At the ALRS the perched water table lies deeper in the tuff section where hydraulic conductivity is dominated by fractures. A similar statement can be made about the tunnel discharge water, which probably originates as recharge in Oak Flat. The slightly lower AR of the tunnel discharge water suggests mixing with modern recharge, consistent with the presence of anthropogenic sulfate (Bassett et al., 1994). Where the same AR occurs over a wide range of concentration the predominant mechanism is probably selective leaching.

As pointed out by Petit et al. (1985) congruently dissolving mineral phases that contain U-238 tend to dilute the excess U-234 derived from selective leaching, limiting fractionation. They argued that this always occurs given the U abundance and etching rates of rock-forming minerals. Attributing the observed perched water fractionation at the ALRS to selective leaching could imply unrealistically low rates of congruent dissolution for U bearing minerals (e.g. $< 10^{-13}$ m/yr). They proposed an auto-oxidative leaching mechanism instead, in which minerals can dissolve more congruently. In this widely accepted conceptual model, primary U-238 existing as U(4+) decays down to U-234(6+) and fractionation occurs principally because U(6+) is more soluble.

If sampled near-surface fracture waters represent recharge, then a selective leaching model for perched water at the ALRS requires a highly fractionated leaching "end member." The needed selectivity is directly related to the U-238 contributed by recharge, and the intensity of isotopic exchange with an adsorbed phase. Secondary minerals are present which tend to be good adsorbents but such partitioning could also produce conditions favoring direct recoil fractionation, in which U-238 at the solution:solid interface decays and the α -recoil leads to the accumulation of U-234 in the mobile phase. Recoil from U-238 adsorbed to secondary oxides was once suggested as the operant fractionation mechanism for perched waters from tuffs on the Nevada Test Site (Zielinski and Rosholt, 1978).

In the vadose zone at the ALRS, pore water residence time controlled by matrix K_{sat} might be a determinant of the direct recoil effect. Contrary evidence may be found in the C-14 apparent ages reported by Davidson (1995) which ranged from 1,000 yr in the upper part of the tuff section to 3,000 yr in the perched zone, showing that some form of mass transport between recharge and matrix pore waters is ongoing, and suggesting that residence time does not vary enough to account for the observed AR transition. Alternatively, increased fractionation with depth could be caused by increased leaching selectivity at a horizon representing the maximum depth to which weathering has penetrated and the rock is substantially oxidized, in accordance with the auto-oxidative mechanism.

The AR transition at the ALRS correlates closely with steeply decreasing K_{sat} and a transition in magnetic susceptibility caused by oxidative weathering (Hardin and Bassett, 1995; Bassett et al., 1995). At the nearby Oak Flat borehole, similar transitions in hydraulic properties and magnetic susceptibility occur at about the same stratigraphic horizon, near the modern perched water table. Vadose zone pore water AR's are less than the perched water AR,

suggesting that the AR transition actually represents a former high stand of perched water table up to 10^5 yr ago. However, this possibility is contradicted by the C-14 apparent ages reported by Davidson (1995), so it is evident that fractionation in the vadose zone pore waters at the ALRS developed independently of the perched water table.

The remainder of this paper evaluates the relative contributions from direct recoil and selective leaching in the perched zone at Apache Leap. This requires a model that integrates mass balance, radioactive decay, sorption, isotopic exchange, and direct recoil. The strategy was to describe the fractionation and total U in DSB and Oak Flat perched waters using selective leaching only, and then to use these parameters in the same model with direct recoil activated.

6.5. Steady State Model for Fractionation in the Perched Zone at the ALRS

Matrix hydraulic conductivity at the ALRS declines sharply with depth so that below a depth of 20 to 30 m recharge must move through fractures. Surface waters apparently move downward through fractures without acquiring much solute from vadose zone pore waters, as evidenced from differences between chloride analyses for vadose zone pore waters and the perched water (Davidson, 1995). Recharging waters from the surface are relatively unfractionated (AR~2) so it may be inferred that fractionation in perched water (AR~6.3) occurs mostly in the perched zone. Also, the similar C-14 ages obtained for perched waters from three different sampling locations indicate uniformity of the hydraulic and chemical conditions of recharge. These arguments form the rationale for a lumped parameter approach to modeling perched water fractionation.

The model is based on a system of equations (Figure 6.3) that includes U leaching from a rock phase, partitioning to an adsorbent phase, and transfer of ^{234}U from the adsorbed phase to the mobile phase by direct recoil. Model parameters include partition coefficient, rate constant for sorption (and isotopic exchange), residence time, leaching rate, and leaching selectivity. Constraints include residence time from ^{14}C apparent age, U concentration and $^{234}\text{U}/^{238}\text{U}$ AR in perched waters from different locations, and matrix partitioning from studies of whole rock composition. A steady state solution was derived algebraically, and a transient solution was computed using a Runge-Kutta method with adaptive step size (Press et al., 1989).

Selective extraction of Mn from pulverized tuff showed that as much as half the whole rock Mn exists as MnO_2 (depending on the extent of oxidative weathering) containing about 50 ppm U (Figure 6.4). Assuming typical values for MnO_2 abundance and pore water U concentration the whole-rock U partition coefficient is about $K=100$ mL/g. The effective value for isotopic exchange is probably smaller because of desorption hysteresis and because only part of the MnO_2 phase is accessible. The effective K for direct recoil is probably smaller still, since this involves only U adsorbed within recoil range (tens of nanometers) of fluid-filled pores in communication with the mobile phase.

Residence time can be estimated from C-14 apparent age (3,000 yr), and leaching rates from U concentration and residence time under the assumption of a chemical steady state (Table 6.1). For the DSB the corresponding perched zone leaching rate is 0.033 ppt/yr, and for the Oak

$$\frac{dC_{238}}{dt} = -\frac{1}{T}(C_{238} - C_{238,0}) - \frac{\rho_b k}{\theta \rho_w}(KC_{238} - S_{238}) + \frac{l R_{238}}{R_{238,0}} - \lambda_{238} C_{238}$$

$$\begin{aligned} \frac{dC_{234}}{dt} = & -\frac{1}{T}(C_{234} - C_{234,0}) - \frac{\rho_b k}{\theta \rho_w}(KC_{234} - S_{234}) + \frac{L_{AR} \lambda_{238} l R_{234}}{\lambda_{234} R_{234,0}} \\ & - \lambda_{234} C_{234} + \frac{\rho_b f}{\theta \rho_w} \lambda_{238} S_{238} \end{aligned}$$

$$\frac{dS_{238}}{dt} = k(KC_{238} - S_{238}) - \lambda_{238} S_{238}$$

$$\frac{dS_{234}}{dt} = k(KC_{234} - S_{234}) - \lambda_{234} S_{234} + (1 - f) \lambda_{238} S_{238}$$

$$\frac{dR_{238}}{dt} = -\frac{\theta \rho_w l R_{238}}{\rho_b R_{238,0}} - \lambda_{238} R_{238}$$

$$\frac{dR_{234}}{dt} = -\frac{L_{AR} \theta \rho_w l R_{234}}{\rho_b R_{238,0}} + \lambda_{238} R_{238} - \lambda_{234} R_{234}$$

- C,S,R = mobile phase, adsorbent phase, and leachable phase concentrations
 k = first order rate constant for noncompetitive sorption (sec⁻¹)
 K = mobile:adsorbent phase partition coefficient (g/g)
 l = leaching rate (ppt solution concentration/yr)
 L_{AR} = leaching selectivity
 T = residence time
 λ = decay constants for ²³⁴U and ²³⁸U
 f = efficiency of direct recoil

Figure 6.3. System of equations describing fractionation model (nomenclature matches text).

Figure 6.4. Uranium vs. Mn extracted from pulverized rock core.

Flat borehole it is 0.25 ppt/yr. This does not constrain the leaching selectivity, defined as the AR of leached U.

A key parameter for which few constraints are available is k , the rate constant controlling isotopic exchange. Whole rock U and Th analyses by fusion and ICP/MS show that the Th/U ratio changes little through the tuff section, therefore the rate constant must be large enough to permit local redistribution of leached U. Thus $k > 10^{-14} \text{ sec}^{-1}$ otherwise more than a few percent of the whole rock U would be lost over the age of the Apache Leap Tuff at modern leaching rates, which would give rise to anomalous whole rock U/Th ratios which are not observed. An upper bound estimate on k was derived by running the transient model with the initial condition of zero adsorbed U, showing that isotopic exchange begins to predominate and conditions approach equilibrium sorption within one half life of U-234 for $k > 5 \times 10^{-13} \text{ sec}^{-1}$ (Figure 6.5).

The curves plotted in Figure 6.6 were computed using the steady state solution to show the relation between the proportion of perched water U contributed by recharge at AR~2, leaching selectivity, and effective partitioning in the perched zone. For a given perched water AR, strong partitioning requires greater selectivity because of decay and isotopic exchange.

The isotopic mass balance represented by Figure 6.6 can be used to constrain formation scale steady state partitioning behavior when the sampling locations differ with respect to the proportion of U contributed by recharge. Recharge at both the DSB and Oak Flat locations

Figure 6.5. (upper) Ratio of actual to potential sorption as a function of time for a system starting at zero initial concentration, for different values of rate constant k . (lower) Decreasing mobile phase AR for a system starting at chemical and isotopic equilibrium with input having $AR=AR_0$, representing the effect of isotopic exchange with an adsorbent phase undergoing radioactive decay.

Figure 6.6. Plots representing the steady state isotopic mass balance, and showing the leaching selectivity required to maintain the mobile phase $AR=6.3$, given a proportion of U contributed by recharge with $AR=2$. The resulting constraint on effective partitioning scales to the rate constant, which is assigned values of (upper) $k=10^{-14} \text{ sec}^{-1}$, and (lower) $k=5 \times 10^{-13} \text{ sec}^{-1}$.

percolates through at least 20 m of weathered tuff, which has been identified with AR~2 in the DSB. Perched water from Oak Flat has about three times more U with nearly the same AR as in the DSB, from which it is inferred that the proportion of U contributed by recharge is significantly smaller.

Davidson (1995) estimated from a mixing model of contributions to perched zone tritium and C-14 observations that about 50% of perched water at the DSB location is contributed by fracture flow. The C-14 composition of fracture flow was represented by distillation of core samples originating near the perched water table. With 50% of U from recharge with AR~2, the minimum selectivity that can produce the perched water AR (6.3) at the DSB location is about 10 (Figure 6.6). Applying the same selectivity to the Oak Flat location ("isoselectivity") and requiring that the proportional contribution of recharge is significantly smaller implies that $K \geq 2$ mL/g on a whole rock basis ($k=5 \times 10^{-13}$ sec⁻¹). From Figure 6.6 it is apparent that the rate constant is critical for determining effective partitioning. Partitioning at the DSB location cannot be similarly constrained because that datum was used to estimate selectivity.

Adding direct recoil to the model (Figure 6.7) confirms that the incremental fractionation is important only for larger values of K and small values of k. The figure was calculated with recoil efficiency $f=50\%$, which is high especially for large K. Within the likely range of partitioning behavior the contribution from direct recoil to observed activity ratios is probably minor (< 1 AR unit) under the model assumptions.

Figure 6.7. Incremental mobile phase fractionation obtained by differencing steady state model results with and without direct recoil ($f=0.5$ and $f=0$). Computed for different values of the rate constant. The isotopic mass balance model is linear, so that the magnitude of the mobile phase AR and the leaching selectivity do not affect the results of this calculation.

6.6. Conclusions

Fractionation in perched waters from the Apache Leap Tuff is attributable to selective leaching with a minor contribution from direct recoil. Fractionation in surface and near-surface waters from the ALRS (AR~2) is attributable to less selective leaching from weathered rock. Activity ratios up to 5 were found in deep vadose pore waters, correlated with trends in magnetic susceptibility and hydraulic conductivity representing the penetration of oxidative weathering from the surface. From apparent C-14 ages (Davidson, 1995) it is evident that this transition does not reflect a former high stand of the perched water table.

Using a mechanistic model it was shown that leaching selectivity is probably significantly greater than the observed mobile phase AR. Assuming a minimum value for selectivity consistent with the observed AR, the model constrains effective in situ partitioning. Model assumptions include a hydraulic steady state, first-order isotopic exchange kinetics, and chemical equilibrium with respect to U-238.

Fractionation encountered in perched water at Yucca Mountain (AR~7.5, J. Stuckless, personal communication) is probably not limited to perched zones but exists in vadose zone pore waters as well. Fractionation can be interpreted in terms of conditions that promote or inhibit retardation of natural U. These results in conjunction with the C-14 data of Davidson (1995) show that rapid recharge pathways through the vadose zone can be identified from the isotopic character of pore waters.

7. TRACER TESTS AND FRACTURE FLOW AND TRANSPORT MODELING ON THE 100m SCALE AT THE QUEEN CREEK RESEARCH SITE (Subtask 2.2)

7.1 Queen Creek/Haulage Tunnel Tracer Tests to Investigate Rapid, Focused Fracture Flow *by D.M. Stephens, D.L. Thompson and R.L. Bassett*

7.1.1 Introduction

Among the views of the infiltration process at Yucca Mountain is the concept of episodic focused flow which stands in contrast to uniformly distributed infiltration to explain subsurface hydrologic conditions. Focused flow has been observed at ALRS, for example, by means of single fractures or fracture networks and the consequence is deeper penetration (on the scale of tens of meters) of liquid water over a relatively short time frame (on the order of days). Focused recharge may be initiated by episodic events such as storm runoff on mountain slopes which enters fractures exposed in bare rock, fractures subcropping below alluvium at the mountain base, or fractures below washes on valley floors. Flow into fractures is driven by temporary conditions of full saturation at land surface allowing for either fingering or complete saturation conditions to occur in the fracture network. Similarly, in the subsurface, focused flow occurs in fractures below zones of local saturation, such as the case in which water drains from perched water zones into underlying fractures. This is analogous to the non-isothermal conditions which will undoubtedly exist as water redistributes around a repository.

There is the need to define, characterize, and simulate the rapid movement of both fluid and solute in focused flow scenarios, a process which requires a coupled modeling approach between hydrologic and chemical processes. To date flow and transport models have not been tested against such flow scenarios, primarily due to the lack of data from either laboratory or field experiments. In addition, models have not yet emerged that are clearly appropriate for simulating multicomponent speciation and transport for the fractured-unsaturated environment. The proposed tracer tests for the Queen Creek location are designed to test the concepts of long distant transport of water and solute in a tuff environment dominated by fractures. The transport of both conservative and non-conservative tracers will be tested, methods and techniques for monitoring and sample collection will be evaluated, and various modeling approaches will be compared.

7.1.2 Field Setting and Pre-Test Experimentals

The network of fractures in the section of tuff connecting Queen Creek and Magma Mine Haulage Tunnel provides the field environment for meeting components of the Task objective: 1) to experimentally determine the rate, degree of interaction between fracture and matrix, and pathway of solute flux; 2) to investigate the additional support gained by the use of isotopic tracers, and 3) to extend the hydraulic transport simulations by coupling the physical flow simulations with geochemical modeling.

The hydrologic depiction (Fig. 7.1) illustrates the fracture network of interest. Access to

Figure 7.1. Three dimensional diagram illustrating the location of the fracture network relative to the Queen Creek Valley.

the tunnel is provided by Magma Copper Company. Prior work has verified the fracture hydraulic connection between the land surface and the tunnel fracture sets (Bassett et al., 1994b). The vertical distance from the fracture site in Queen Creek to the fracture in the haulage tunnel is 120 m. (Fitzmaurice, 1994).

The subtask is proceeding in three distinct phases: 1) pre-test computer simulations to define the geologic framework of the site in a 3D visualization model and simulate flow and transport results using a dual continuum transport code; 2) design and conduct a multi-element tracer test in collaboration with CNWRA and the Magma Copper Company, and 3) simulate the results of both tests using several modeling approaches and conduct an intercomparison of the resultant simulations for accuracy and usefulness especially for performance assessment work. At present two codes selected by the UA to be used for post test simulations are: HYDROGEOCHEM (Yeh, 1992) a multi component speciation and transport code, and DCM3D (Updegraff et al., 1991) a dual-porosity model. Output from the codes used by the UA can be linked to the 3D visualization code STRATAMODEL.

To prepare for the tracer tests in Queen Creek and the Haulage Tunnel, a calibrated, sharp crested weir was installed under the fracture that discharges into the tunnel. A pressure transducer was installed in the weir to measure the height of water resulting from fracture flow. The weir was calibrated in the lab and a head versus flow rate curve was established to calculate the flow rate from the fracture. An electrical conductivity (EC) probe was also installed in the weir. The probe was calibrated using a standard KCl solution (Wood, 1976) and corrections to the reported conductivity values at 25°C are made using a temperature curve constructed by Campbell Scientific for the probe. The probe and pressure transducer are connected to Campbell Scientific Data Loggers. Data are periodically downloaded onto portable computers and processed for interpretation. Figure 7.2 illustrates the arrangement of the weir and data logger in the Never Sweat Tunnel.

A pressure transducer used to measure stage height at the fracture in Queen Creek and an EC probe have been installed. The probe and transducer are used for continuous monitoring of the surface water conditions for comparison with the EC and flow rate of the fracture in the tunnel. The fracture site in Queen Creek and the fracture in the Never Sweat Tunnel are now both be equipped for continuous monitoring of EC and flow rates. A quantitative comparison, as well as a comparison of EC can be made to further understand the connection between Queen Creek and the haulage tunnel.

Prior to the installation of the pressure transducer and EC probe in the creek, EC and stage height data from Queen Creek were not available. The height of water in the flume located at the Deep Borehole Site (DBS) was used to compare flow events with changes in EC in the tunnel. The flume at DBS is installed on a tributary to Queen Creek and is approximately 3 km upgradient from the fracture site. It has been observed that any rain event large enough to induce flow in the flume will also induce flow in Queen Creek. Therefore, a flow event in the flume can indicate flow in Queen Creek. Until the equipment was in place, however, a quantitative analysis could not be done on flow at the fracture site.

Figure 7.2. Arrangement of sharp-crested weir, electrical conductivity probe, pressure transducer for measuring head, and data logger in the Never Sweat Tunnel.

Since the EC probe and pressure transducer have been in place in Queen Creek, flow and EC in the creek have been compared directly with EC and flow in the Never Sweat Tunnel. During January, 1995 the fracture in the tunnel went completely dry due to a long period of no precipitation in the area. This presented the opportunity to monitor the breakthrough of the first water to arrive in the tunnel due to precipitation at the surface. On February 1, 1996, a precipitation event generated runoff in Queen Creek. The EC probe installed on the fracture set in the creek indicates that water first arrived at the fracture at approximately 5:00 p.m. The EC reading in the tunnel shows that the water arrived at the weir installed on the fracture on February 3, 1996 at approximately 9:00 p.m. Figure 7.3 shows the breakthrough of water in the creek and tunnel due to this rain event. This breakthrough time of 2 days further validates earlier estimates of the travel time.

The focus of study has been on identifying which fracture set in the creek is connected to the fracture being monitored in the tunnel. A connection between the creek and the tunnel has been shown, but in order to complete the tracer test it is necessary to identify the fracture at the surface. STRATAMODEL (LGC) has been used along with fracture mapping at the surface and in the tunnel to model the fracture plane. Two preliminary injection tests have been conducted. One was done using approximately 300 gallons of water collected from the tunnel. The water was ponded on a suspected fracture set in the creek. The second test ponded approximately 800 gallons of deionized water on the fracture. The deionized water has a very low EC and should cause a low spike in EC in the tunnel when it arrives. Because neither test had any affect on EC or flow rate in the tunnel, further efforts are being made to verify that the correct fracture set is being used on the surface.

Future efforts include continuous monitoring of the tunnel and creek, further fracture mapping and modeling, and more injection tests using deionized water. Once the fracture set is correctly identified and confirmed, a tracer study can be conducted and results modeled as mentioned earlier.

Figure 7.3. Breakthrough of the first water in Queen Creek and the Never Sweat Tunnel due to a precipitation event after the tunnel and creek were dry.

7.2 Modeling Efforts at Apache Leap Research Site

by M.J. Thomasson and R.L. Bassett

7.2.1 Introduction

Two computer codes, HYDROFLOW (Yeh, 1992a) and HYDROGEOCHEM (Yeh, 1992b), are being utilized to simulate episodes of focused flow through fracture networks at the Apache Leap Research Site (ALRS). The model HYDROFLOW is a finite element model capable of simulating subsurface flow through saturated or unsaturated porous media. HYDROGEOCHEM is a model that combines hydrologic transport with geochemical reactions in saturated or unsaturated media.

These models have been chosen to model this site because of their unique ability to handle both saturated and unsaturated conditions, the ability to specify different material types with their own properties for specific sections in the region being modeled and most importantly HYDROGEOCHEM's approach of coupling hydrologic transport with the geochemical reactions.

7.2.2 HYDROFLOW

7.2.2.1 General Model Features

HYDROFLOW is a finite element model derived from FEMWATER (Yeh, 1988) capable of simulating subsurface flow through saturated or unsaturated porous media. HYDROFLOW simulates flow only and generates the vector and moisture content field that is required for the solute transport code HYDROGEOCHEM. Due to the unsaturated conditions that exist most of the time at ALRS the flow simulation within HYDROGEOCHEM is unable to adequately conform to the unsaturated conditions that predominate in the ALRS tuff section; consequently HYDROFLOW with its more robust flow characteristics is used as a preprocessor. The vector and moisture content field are stored in a specific output file for input directly into HYDROGEOCHEM. In addition to the ability to provide direct input for HYDROGEOCHEM HYDROFLOW is unique in that it can simulate regions of irregular dimensions, fluxes through a variety of boundary conditions, and allows for a variety of media properties in either tabular or analytical form. Key features of HYDROFLOW are summarized in Table 7.1.

7.2.2.2 Input specifications for HYDROFLOW

Required input to HYDROFLOW includes the control indices, properties of the porous media in either tabular or analytical form, the geometry as specified by the elements and nodes, and the initial and boundary conditions.

The model of Apache Leap Research Site was discretized using 30 rectangular elements constructed as three vertical columns comprised of 10 elements each and 44 nodes as shown in Figure 7.4. The dimensions of the elements in the center column are 2 mm wide by 120 dm long and are modeled to represent the highly fractured tuff. The adjacent elements are 5 dm wide by 120 dm long and represent the surrounding unfractured tuff. Using the model's material

7.1 Key Features of HYDROFLOW

Models characteristics and features: HYDROFLOW
Features: The ability to:
Handles heterogeneous & anisotropic media
Specify spatially & temporally distributed sources & sinks as well as point source & sinks
Prescribe initial conditions or obtain initial conditions by simulating the steady-state version of system
Prescribe transient heads distributed over a Dirchlet boundary
Handle time dependent fluxes due to pressure gradient varying along a Neumman boundary
Handle time dependent total fluxes (i.e. sum of gravitational fluxes and pressure gradients) over a Cauchy boundary
Automatically computes variable boundary conditions of evaporation, infiltration, or seepage on the soil-air interface
Include off-diagonal hydraulic conductivity when coordinate system conflicts with hydraulic conductivity tensor
Treat mass matrix either as consistent or lumping
Provides three alternatives to approximating the time derivative: Crank-Nicholson, backward and mid-difference
Provide three options , exact relaxation, under & over relaxation for estimating the non-linear matrix
Include both quadrilateral and triangular elements to discretize the region
Automatically reset the time step size when boundary conditions or source/sinks abruptly change
Checks the mass balance over the entire region for every time step
Input:
Geometry of the system
Spatial distribution of finite elements and nodes
Properties of the media
Initial conditions
Boundary conditions
Output:
Spatial distribution of pressure head, total head, moisture content, and Darcy velocity components at any time step

Figure 7.4. Representation of the three-column grid for the tracer experiment.

correction facility, material type of 1 was assigned to the elements adjacent to both sides of the elements representing the heavily fractured tuff. Material type 2 was assigned to the fractured tuff. This distinction is necessary to allow the user to specify different material properties for each material such as saturated moisture content (θ_s), residual moisture content (θ_r), pressure head (h) at the surface as well as through the porous media, and the intrinsic permeability (k). The values used for the material types are shown in Table 7.2.

Table 7.2 Input specifications to HYDROFLOW

Material Property	Material 1: Unfractured	Material 2: Fractured
Saturated Moisture Content	0.07	0.001
Residual Moisture Content	0.013	0.001
Pressure Head, Surface	100 dm	100 dm
Pressure Head, in Media	-10 dm	-10 dm
Intrinsic Permeability	$4.3\text{e-}16 \text{ m}^2$	$1.16\text{e-}14 \text{ m}^2$

The process under investigation is focused flow through a fracture network; the initial and boundary conditions are specified as follows: The initial conditions are specified as a pressure head of -10 dm at the surface, 0 dm at the bottom of the tuff, and -11 dm throughout the domain. The boundary conditions are specified as no flux on the left, right, front, and back of the modeled region, a dirchlet condition is imposed on the bottom with a specified pressure head of 0 dm, and variable conditions on the top three elements. Due to the short, very intense nature of the storms in this region a rainfall of 10 dm/day for three days with ponding allowed up to 1500 dm above the base of the tuff. A potential evaporation of 5 dm/day is specified for the remaining time of the simulation. Due to the constant head condition that develops after a rain storm event the model is being modified to simulate a dirchlet condition at the upper boundary for future simulations.

7.2.3 HYDROGEOCHEM

7.2.3.1 General model features

Using an iterative process, HYDROGEOCHEM solves one or two-dimensional transport and geochemical equilibrium equations. Table 7.3 provides an overview of HYDROGEOCHEM's characteristics and features.

HYDROGEOCHEM allows the user comprehensive control in defining both the hydrology and the chemistry of the region being modeled as well as options for the numerical scheme used to solve the system of equations.

Table 7.3 Key Features of HYDROGEOCHEM

Models characteristics and features: HYDROGEOCHEM
Features: The ability to:
Solve 2-D transport & geochemical equilibrium equations
Handles heterogeneous & anisotropic media
Specify spatially & temporally distributed sources & sinks as well as point source & sinks
Prescribe initial conditions or obtain initial conditions by simulating the steady-state version of system
Prescribe transient concentrations distributed over a Dirchlet boundary
Handle time dependent fluxes over variable boundaries
Handle time dependent total fluxes over Cauchy boundaries
Include off-diagonal dispersion coefficient when coordinate system conflicts with dispersion tensor
Treat mass matrix either as consistent or lumping
Provide three options , exact relaxation, under & over relaxation for estimating the non-linear matrix
Include both quadrilateral and triangular elements to discretize the region
Automatically reset the time step size when boundary conditions or source/sinks abruptly change
Include simultaneous chemical processes of aqueous complexation and precipitation/dissolution reactions
Include simultaneous chemical processes of ion exchange, redox and acid-base reactions
Input:
Geometry of the system
Spatial distribution of finite elements and nodes
Properties of the media
Potential chemical reactions
Initial conditions
Boundary conditions
Output:
Spatial distribution of chemical element concentrations as a function of time and space
The chemical speciation at user-specified nodes

Options available to the user concerning the hydrology of the region include both one and two-dimensional flow in heterogeneous and anisotropic media, distributed as well as point sources and sinks which can be varied both spatially and temporally. Initial conditions can either be prescribed or obtained by running the steady-state version of the system. Options are available to prescribe boundary conditions as well as transient concentrations distributed over a Dirchlet boundary can be defined, as well as, time dependent fluxes over both variable and Cauchy boundaries.

Options for defining the chemistry of the region are as follows. As mentioned above transient concentrations distributed over a Dirchlet boundary can be defined as well as variable boundaries. The user has the ability to include an off-diagonal dispersion coefficient when the coordinate system conflicts with the dispersion tensor due to the finite element construction. The user can also specify simultaneous chemical processes of aqueous complexation, precipitation-dissolution reactions, ion exchange, redox and acid-base reactions.

7.2.3.2 Input specifications for HYDROGEOCHEM

Input data needed to run HYDROGEOCHEM include the geometry of the system, spatial distribution of the finite elements and nodes, properties of the media, potential chemical reactions, initial conditions, and boundary conditions.

For the pre-test series of simulations, the region is being modeled using an average porosity of 0.07 for the surrounding tuff and 0.001 for the fractured tuff. Dry bulk density is set at 2.37 g/cm³. The fractured tuff elements were modeled employing a longitudinal dispersivity of 10.0. A longitudinal dispersivity of 1.0 is assigned for the adjacent elements. The chemistry of the system is simplified with only sodium, chloride, and hydrogen being defined to allow verification that the transport portion of the input data set is properly constructed. All chemistry is modeled using variable boundary conditions which allows the concentration to vary over time at specified nodes and element sides. Since unsaturated conditions exist the velocity vectors and moisture content field are computed using the model HYDROFLOW and directly input via logical unit one. The initial conditions for sodium and chloride was specified to be 10⁻³ M while the pH was held at 7.6 to 7.9.

Electrical conductivity readings analyzed in Fitzmaurice (1994) reflect a breakthrough within two to six days following a rainstorm event. Accordingly, HYDROFLOW and HYDROGEOCHEM were calibrated to allow sodium to breakthrough in approximately two to six days; that is, approximately 14% of the initial concentration breaks through at the regions endpoint (120 meters) as shown in Figure 7.5. Figure 7.6 reflects the overall sodium breakthrough curve with respect to time at the endpoint of the domain (120 m), as can be seen 50% of the initial concentration breaks through in 5.5 days.

7.2.4 Conclusion

The pre-test simulations illustrate HYDROGEOCHEM's ability to simulate focused flow through partially saturated, fractured rock. As can be seen in Figures 7.5 and 7.6, initial results

indicate that numerically stable solutions can be obtained when calibrating the model to simulate breakthrough curves on the order of 2 to 4 days total travel time. Future tracer test data will allow the model to be optimized to provide calibration and sensitivity analysis for hydraulic parameters, and to access their effect on the total travel time simulation.

Figure 7.5 Preliminary simulation of sodium breakthrough at the tracer site.

Figure 7.6 Sodium breakthrough versus time at the tracer site.

8. THE EFFECT OF FRACTURES ON THE FORMATION AND RECHARGE OF
PERCHED WATER ZONES AT THE ALRS (Subtask 3.1)
by E.G. Woodhouse, R.L. Bassett, and D.L. Thompson

Perched water has been identified at both the Apache Leap Research Site (ALRS) near Superior, Arizona, and in various locations at Yucca Mountain. A major goal of this part of the investigation is to narrow the list of all possible perching mechanisms into those most likely to cause perching in fractured, welded tuff. A second goal of this research is to determine the quantity of water available for recharge to the perched water zone, and to determine the relative importance of the predominant pathways. Fractures may provide significant pathways for water flow, but the depth, frequency, and magnitude of such flow are not yet quantified. Fractures may also determine quantity and rate of water accumulation, possibly affecting the spatial distribution and residence time of perched water zones. This investigation recently has focused on the role of fractures with respect to the formation of, and recharge to, the uppermost perched water zone at ALRS.

8.1 The Formation of Perched Water Zones

Perched water is a zone of saturated soil or rock separated from a regional, or at least more significant, zone of saturation by a section of partially saturated rock. Perched water has been defined in ALRS borings as depths at which water flowed freely into the borehole, indicating zones of local saturated conditions, beneath which water did not appear to flow. Most commonly, perched water is associated with a stratigraphic change, whereby material of relatively high hydraulic conductivity overlies material of lower hydraulic conductivity. The results of an investigation by Schneider and Luthin (1978) showed that if the ratio of the recharge rate (or hydraulic conductivity of the upper layer) to the hydraulic conductivity of the semi-pervious (perching) subsurface layer were less than 10, perching was not likely to occur. If that ratio were greater than 25, perching was highly likely; a ratio of between 10 and 25 gave a weak perching condition. The hydraulic conductivity of the upper layer is a function of moisture content, however, therefore changes in the degree of saturation will directly affect this ratio. A second, and essentially inverse, perching mechanism exists beneath a saturated zone, such as fine-grained sediment within an alluvial fan deposit (Schneider and Luthin, 1978), in which the coarser alluvium simply drains faster.

Regardless of whether the lower unit has higher or lower hydraulic conductivity, the change in hydraulic conductivity could be the result of a number of different processes, including changes in the original depositional environment, non-uniform diagenetic alteration, lithologic change, or, in volcanic rocks, cooling and degassing. On a larger scale, perched water could also result from phenomena such as a reduction or change in the fracture density or pattern, or from faulting, whereby fault planes create either conduits for, or impedances to, flow. Figure 8.1 illustrates some potential mechanisms for perching water at ALRS, which will be discussed separately below.

a. Perching between flow units

b. Perching related to cooling zones

c. Perching due to faulting and nonuniform weathering

d. Perching due to disconnected fracture sets

Figure 8.1. Possible perching mechanisms.

The Apache Leap tuff consists of an undetermined number of individual flows deposited in rapid succession, which then cooled as a single unit. Slight changes in hydraulic conductivity due to minor variations in the composition or texture between flows could perhaps cause water to perch. This mechanism would support the presence of several perched zones at different depths (Figure 8.1-a), as were identified in the Oak Flat core at ALRS.

Perched water in volcanic rock could also result from cooling and degassing processes, or changes in the degree of welding. The basal vitrophyre is typically one of the most impermeable zones of a cooling unit, and could be expected to be sufficiently less permeable to support a perched zone (Figure 8.1-b). This mechanism could explain the existence of some perched zones, but would not account for those in the upper part of the Apache Leap tuff, nor would it account for the stacked perched water zones.

Changes in hydraulic conductivity might also result from nonuniform weathering of minerals. Feldspars are especially susceptible to weathering, and the smectite clays that result would tend to reduce pore size and permeability. Clays are present in both the Apache Leap and Yucca Mountain tuffs; their location and abundance relative to past or present saturated zones may provide further information regarding perching conditions. If the presence of clays can be correlated to perched water, then the question of whether their presence resulted from, or was responsible for, perched water must be also be addressed.

Both the Apache Leap and Yucca Mountain deposits have been highly faulted and fractured. Faulting could create pathways for flow by grinding up otherwise dense, crystalline rock, allowing it to reach deeper inhomogeneities rapidly. Alternatively, faults could also impede flow if they are filled by secondary minerals precipitating from solution (Figure 8.1-c).

Variations in either fracture densities or in the connectivity of fracture sets could also provide conditions for perched water. Vertical fracture sets present at both sites would allow water to move down rapidly, but if the fracture sets die out or are not connected to deeper sets, hydraulic conductivity could be reduced enough to perch water (Figure 8.1-d).

Several of these mechanisms combined may also be responsible for perched water zones. At ALRS, a zone immediately above the uppermost perched water zone has been identified as having a higher fracture and/or fault density and greater alteration indicative of water flow (Figure 8.2). At some distance beneath this zone, the tuff becomes more densely welded and less fractured. Perhaps the more densely welded zone is in fact also saturated, but does not contain the fracture network sufficient to produce significant quantities of water into the borehole, and therefore only appears to be an unsaturated zone, while in fact it just does not hold very much water. The next stage of this aspect of the investigation will attempt provide greater insight into the role of fractures in the location of the perched water zone at ALRS, and to eliminate some of these proposed mechanisms through correlation between the physical characteristics of the rock and the location of the perched water zone.

Figure 8.2. Analysis of number of fractures with various characteristics per 10-ft interval in Deep Slant Borehole. Linear depth in feet along DSB shown on y-axis.

8.2 Measurement of Hydrologic Parameters

This portion of the investigation was designed to test the hypothesis that the perched water zone is fracture-dominated. In addition, the data collected could provide estimates of the hydraulic parameters of such a fracture system. Furthermore, data were desired that might indicate whether the perched water zone is influenced by boundary conditions, such as a limited extent of the zone.

In September 1995, COLOG logged sections of the vertical observation borehole (VOB) at ALRS using their Borehole Image Processing System (BIPS). The product of this work shows specific locations and orientations of fractures in the vertical borehole (Figure 8.3) which could be sources of water to the perched zone.

In March, 1996, an 18.8-hour aquifer test was conducted in the vertical borehole to measure the hydrologic response in the well, including the fracture shown in Figure 8.2. The borehole setup is shown in Figure 8.4. The vertical borehole extends to a depth of 170.7 m below the surface; static water level is approximately 23 m above the bottom. The deepest part of the borehole, approximately 7 m, appeared in the COLOG imaging run to contain large amounts of suspended silt, so the pump was placed above that interval to avoid clogging. A 1-horsepower, 10-cm diameter, submersible domestic pump was used to withdraw water. A 50-psi absolute pressure transducer sensitive to 0.03 m was placed 1.5 m above the pump intake to measure drawdown and recovery. Therefore, at the start of the test, 12.5 m of head sat above the transducer. A second transducer was installed in the deep slant borehole, which, at the depth of the top of the static water level, is approximately 150 m horizontally away from the vertical borehole. No response was ever seen in the deep slant borehole. The discharged water was routed by hose to a location approximately 160 m downgradient of the wellheads, and downgradient of any vertical fractures that could potentially recharge into the deep slant borehole.

Early pumping tests in the vertical borehole indicated that at a pumping rate of about 13 L/min, the water level would drop to just above the transducer in approximately 35 minutes; complete recovery took about 2 hours. This pumping rate was too high to see any other than well storage effects. A three-hour test was run at 4.5 L/min, and showed a distinct change in drawdown rate after 48 min; however, the water level was dropping too far at that rate to continue the test. The 18.8-hour (1127-min) test was run at a discharge rate of 3.56 L/min. Discharge rate was monitored visually with a flowmeter installed in the discharge plumbing, which was calibrated using a 1-L graduated cylinder and stopwatch. Flow was adjusted manually using a diaphragm valve installed downstream of the flowmeter. Flow was monitored frequently, but not continually, and was adjusted as deemed necessary. Following numerous slight adjustments during the first 10 min of the test, flow adjustments were made at 19, 32, 78, 104, 182, 460, 472, 742, and 997 minutes into the test.

Figure 8.5 shows the results of the pumping test. The drawdown and recovery observed in the vertical observation well are shown as symbols, matched to a theoretical type curve. Some of the flow adjustments, such as those at 78, 182, 460-472, and 742 minutes, may have been significant enough to affect the drawdown curve at those times. The type curve is derived from

Figure 8.3. Image of fracture in the Vertical Observation Borehole at 165.3 m. Source: COLOG, Inc.

Figure 8.4. Schematic of Aquifer Test Setup.

horizontal fracture model

Figure 8.5. Type drawdown and sample recovery curves plotted as log dimensionless time (t_D) versus log dimensionless drawdown (s_b) from Gringarten and Ramey, 1973 (solid line). Overlain is data from VOB pumping test fit to the type curve, plotted as log time (minutes) versus log drawdown (feet).

Gringarten and Ramey's (1973) method of using an appropriate Green's function to solve unsteady flow problems. The analytical expression that was used represents the aquifer system as the intersection of an infinite solid cylinder source, with an infinite horizontal slab source in an infinite horizontal slab reservoir with impermeable upper and lower boundaries, as sketched in Figure 8.6, modified from Gringarten and Ramey (1974). The matrix region may include fractures that are not as significant to fluid flow as the primary fracture or fracture zone. This model was chosen as the one likely to most closely fit the conditions in the ALRS system.

Figure 8.6. Cross-section of horizontal fracture model, modified from Gringarten and Ramey (1974).

The following equations were applied:

$$s_D(t_D) = \frac{4\pi b \sqrt{k_f k_m}}{Q} s(t) \quad (8.1)$$

$$t_D = \frac{k_f t}{S_{sm} x_f^2} \quad (8.2)$$

$$s_D(t_D) = 2\pi\sqrt{t_D} \operatorname{erf}\left(\frac{1}{2\sqrt{t_D}}\right) + E_1\left(\frac{1}{4t_D}\right) \quad (8.3)$$

$$E_1(u) = \int_u^{\infty} \frac{e^{-y}}{y} dy, \quad \text{where} \quad u = \frac{1}{4t_D} \quad (8.3a)$$

where:

- s_D = dimensionless drawdown
- t_D = dimensionless time
- b = aquifer thickness
- k_f = hydraulic conductivity of the fracture zone
- k_m = hydraulic conductivity of the matrix
- Q = pumping rate
- $s(t)$ = drawdown at time t
- S_m = specific storage of the matrix
- x_f = thickness of the fracture
- erf = error function, obtained from Abramowitz and Stegun, (1967)
- $E_1(u)$ = Theis model, obtained from Abramowitz and Stegun, (1967)

Equation 8.3 was used to plot s_D versus t_D , generating the drawdown portion of the curve shown in Figure 8.5. Then, a recharge well was superimposed to obtain recovery curves from:

$$s(t) = \frac{Q}{4\pi b \sqrt{k_f k_m}} [s_D(t_D) - s_D(t'_D)] \quad (8.4)$$

$$s_D(t'_D) = 0 \quad \text{for} \quad t \leq t_s \quad (8.5)$$

$$t'_D = \frac{k_f (t - t_s)}{S_m x_f^2}; \quad t_s = \text{shut in time (end of pumping)} \quad (8.6a,b)$$

Recovery type curves were obtained by plotting $s_D(t_D) - s_D(t'_D)$ versus t_D on the same graph as the drawdown curve, for various shut in times.

The fit of the data onto the type curve is fair, and improves with increasing time. The deviations due to flow adjustment affect discrete time intervals but do not invalidate the observed trend. At times where the drawdown data more closely approximated the type curve, the recovery data was a poor match, and vice versa. The use of an analytical solution such as this incorporates certain assumptions which may not reflect the conditions of the natural system. Deviations in the natural system from the model could include a greater contribution to flow from fractures in the matrix, or from more than one major fracture system; or aberrations in the aquifer such that it does not meet the assumed boundary conditions. In spite of such potential errors in

the approach, the reasonable fit between the data and type curve does support the theory that fracture flow is dominant in the system, even if it is not as precisely defined as the model.

From a match point on the type curve, an effective transmissivity was calculated from Equation 8.1 of $0.161 \text{ m}^2/\text{day}$. A fracture hydraulic conductivity was then obtained from approximations of aquifer thickness and matrix hydraulic conductivity. The aquifer region was estimated to be 18 m thick, based on drilling observations, borehole imaging, and water level measurements. The matrix hydraulic conductivity was estimated to be 10^{-4} m/day , based on estimates for fractured tuff (Driscoll, 1986) and site data. These values gave an estimated fracture hydraulic conductivity of 0.80 m/day , which also supports the significance of fracture flow in this system.

8.3 Recharge to the Perched Water Zone

As described in detail in Woodhouse et al. (in press), field data have been collected over the past two years to determine a water budget for a watershed at ALRS (Figure 8.7). The component of greatest interest in the water budget is infiltration, for that parameter will allow some estimation to be made of the quantity of water entering the subsurface, to potentially recharge the perched water zone. As expected in an arid to semi-arid environment such as at ALRS, most precipitation is lost to evapotranspiration (Harshbarger et al., 1966). However, the surface at ALRS contains a large proportion of exposed fractured rock, and the hypothesis is that fractures enable greater volumes of water, than would otherwise be expected, to enter the subsurface. Devices such as infiltrometers or lysimeters that are traditionally used to measure infiltration generate point measurements in space and time. The water budget method represents an average over the area of the watershed, and over the time of data collection, on the order of years. This method seems more suitable for natural terrain where large variation exists in surface cover, slope, aspect, and seasonality.

The results presented in Woodhouse et al. (1997) showed that while infiltration may be as much as 13% of the water budget on a seasonal scale, on an annual scale it is less than 10%. These data suggest that the exposed fractured rock did not significantly reduce the large fraction of water lost to evapotranspiration, and that relatively small amounts of water reach the subsurface. Data collection has continued in an effort to more precisely quantify the contributions of the various components of the water budget.

Figure 8.7. Watershed at the ALRS for which water budget is being determined. AWS = location of the recording micrometeorological station.

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BIBLIOGRAPHIC DATA SHEET

(See instructions on the reverse)

1. REPORT NUMBER
(Assigned by NRC. Add Vol., Supp., Rev.,
and Addendum Numbers, if any.)

NUREG/CR-6497

2. TITLE AND SUBTITLE

Data Collection and Field Experiments at the Apache Leap
Research Site
May 1995 - 1996

3. DATE REPORT PUBLISHED

MONTH YEAR

August 1997

4. FIN OR GRANT NUMBER

W6387

5. AUTHOR(S)

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6. TYPE OF REPORT

Technical Report

7. PERIOD COVERED (Inclusive Dates)

5/95 - 5/96

8. PERFORMING ORGANIZATION - NAME AND ADDRESS (If NRC, provide Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address; if contractor, provide name and mailing address.)

Department of Hydrology and Water Resources
University of Arizona
Tucson, Arizona 85721-0011

9. SPONSORING ORGANIZATION - NAME AND ADDRESS (If NRC, type "Same as above"; if contractor, provide NRC Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address.)

Division of Regulatory Applications
Office of Nuclear Regulatory Research
U. S. Nuclear Regulatory Commission
Washington, DC 20555-0001

10. SUPPLEMENTARY NOTES

T. J. Nicholson, NRC Project Manager

11. ABSTRACT (200 words or less)

This report documents the research performed during the period May 1995-May 1996 for a project of the U.S. Nuclear Regulatory Commission (sponsored contract NRC-04-090-051) by the University of Arizona. The project manager for this research is Thomas J. Nicholson, Office of Nuclear Regulatory Research. The objectives of this research were to examine hypotheses and test alternative conceptual models concerning unsaturated flow and transport through fractured rock, and to design and execute confirmatory field and laboratory experiments to test these hypotheses and conceptual models at the Apache Leap Research Site near Superior, Arizona.

Each chapter in this report summarizes research related to a specific set of objectives and can be read and interpreted as a separate entity. Topics include: crosshole pneumatic and gaseous tracer field and modeling experiments designed to help validate the applicability of continuum geostatistical and stochastic concepts, theories, models, and scaling relations relevant to unsaturated flow and transport; use of geochemistry and aquifer testing to evaluate fracture flow and perching mechanisms; investigations of uranium isotopes to evaluate leaching selectivity; and transport and modeling of both conservative and non-conservative tracers.

12. KEY WORDS/DESCRIPTORS (List words or phrases that will assist researchers in locating the report.)

air permeability, infiltration, geostatistics, perched water,
radiocarbon, tracers, uranium

13. AVAILABILITY STATEMENT

unlimited

14. SECURITY CLASSIFICATION

(This Page)

unclassified

(This Report)

unclassified

15. NUMBER OF PAGES

16. PRICE