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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
STUDY PLAN APPROVAL FORM

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Study Plan Number 8.3.1.2.2.9

Study Plan Title SITE UNSATURATED-ZONE MODELING AND SYNTHESIS

Revision Number 0

Prepared by: UNITED STATES GEOLOGICAL SURVEY

Date: MAY 13, 1993

Approved:

7/1/93
Director, Regulatory and Site Evaluation Division / Date

6/22/93
Director, Quality Assurance Division / Date

Effective Date: 7/2/93

1028

AP-1.10Q

RECORD OF REVISIONS

REVISION NUMBER	REVISION	DATE
R0	Study rationale and plans for five activities: Conceptualization of the unsaturated-zone hydrogeologic system (Section 3.1) Selection, development, and testing of hydrologic-modeling computer codes (Section 3.2) Simulation of the natural hydrogeologic system (Section 3.3) Stochastic modeling and uncertainty analysis (Section 3.4) Site unsaturated-zone integration and synthesis (Section 3.5)	5-13-93

ABSTRACT

This study plan describes five site-characterization activities for site unsaturated-zone modeling and synthesis. The primary objectives of these activities are to develop and refine site-scale conceptual and numerical models of moisture flow and solute transport in the unsaturated zone and to integrate data and analyses to synthesize a comprehensive description of the site unsaturated-zone hydrogeologic system. The activities include:

- Conceptualization of the unsaturated-zone hydrogeologic system,
- Selection, development, and testing of hydrologic-modeling computer codes,
- Simulation of the natural hydrogeologic system,
- Stochastic modeling and uncertainty analysis, and
- Site unsaturated-zone integration and synthesis.

The rationale for the site unsaturated-zone modeling and synthesis study is described in Sections 1.3 (regulatory rationale) and 2 (technical rationale). Section 3 describes the specific activity plans, including proposed methods for design, refinement, and application of models. Section 4 summarizes the application of study results to other site-characterization investigations. Section 5 consists of the study schedule and milestones. Section 6 is a list of study references, and Section 7.1 covers quality assurance requirements.

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1 PURPOSE AND OBJECTIVES OF STUDY

1.1 Purpose of the study plan

The U.S. Geological Survey (USGS) is conducting studies at Yucca Mountain, Nevada, as part of the Yucca Mountain Project (YMP). The purposes of the USGS studies are to collect and analyze hydrologic, geologic, and geochemical data, which will be used to evaluate the suitability of Yucca Mountain for a high-level nuclear-waste repository and assess the ability of the mined geologic-disposal system (MGDS) to isolate the waste in compliance with regulatory requirements. In particular, the project is designed to acquire information necessary for the U.S. Department of Energy (DOE) to demonstrate in its environmental-impact statement and license application that the MGDS will meet the requirements of federal regulations 10 CFR Part 60, 10 CFR Part 960, and 40 CFR Part 191.

This study plan describes the approach and methods adopted by the USGS, in cooperation with Lawrence Berkeley Laboratory (LBL), for modeling moisture flow and solute transport in the unsaturated zone. The study is organized into five activities:

- 8.3.1.2.2.9.1 - Conceptualization of the unsaturated-zone hydrogeologic system;
- 8.3.1.2.2.9.2 - Selection, development, and testing of hydrologic-modeling computer codes;
- 8.3.1.2.2.9.3 - Simulation of the natural hydrogeologic system;
- 8.3.1.2.2.9.4 - Stochastic modeling and uncertainty analysis; and
- 8.3.1.2.2.9.5 - Site unsaturated-zone integration and synthesis.

The numbers (e.g., 8.3.1.2.2.9.1) used throughout this plan refer to specific sections of the YMP Site Characterization Plan (SCP) (U.S. Department of Energy, 1988). The SCP describes the overall site-characterization program including general descriptions of the activities detailed in Section 3 of this study plan.

Figure 1.1-1 locates the unsaturated-zone synthesis and modeling study within the SCP Geohydrology Program. This study is one of nine planned to characterize the unsaturated zone at Yucca Mountain. Seven of these studies are surface-based evaluations and two studies (Study 8.3.1.2.2.4 - Unsaturated-zone percolation: ESF study, and Study 8.3.1.2.2.5 - Diffusion tests in the ESF), will study the *in situ* hydrologic characteristics of Yucca Mountain from ramps and underground drifts. The five activities in this study were selected on the basis of a number of factors including design/performance-parameter needs, available numerical methods, test scale, and time requirements. (*Parameter* is used in this plan to mean a property, characteristic, and/or the numerical value of a constant that is used to describe the unsaturated-zone hydrologic system). These factors are described in Sections 2 and 3.

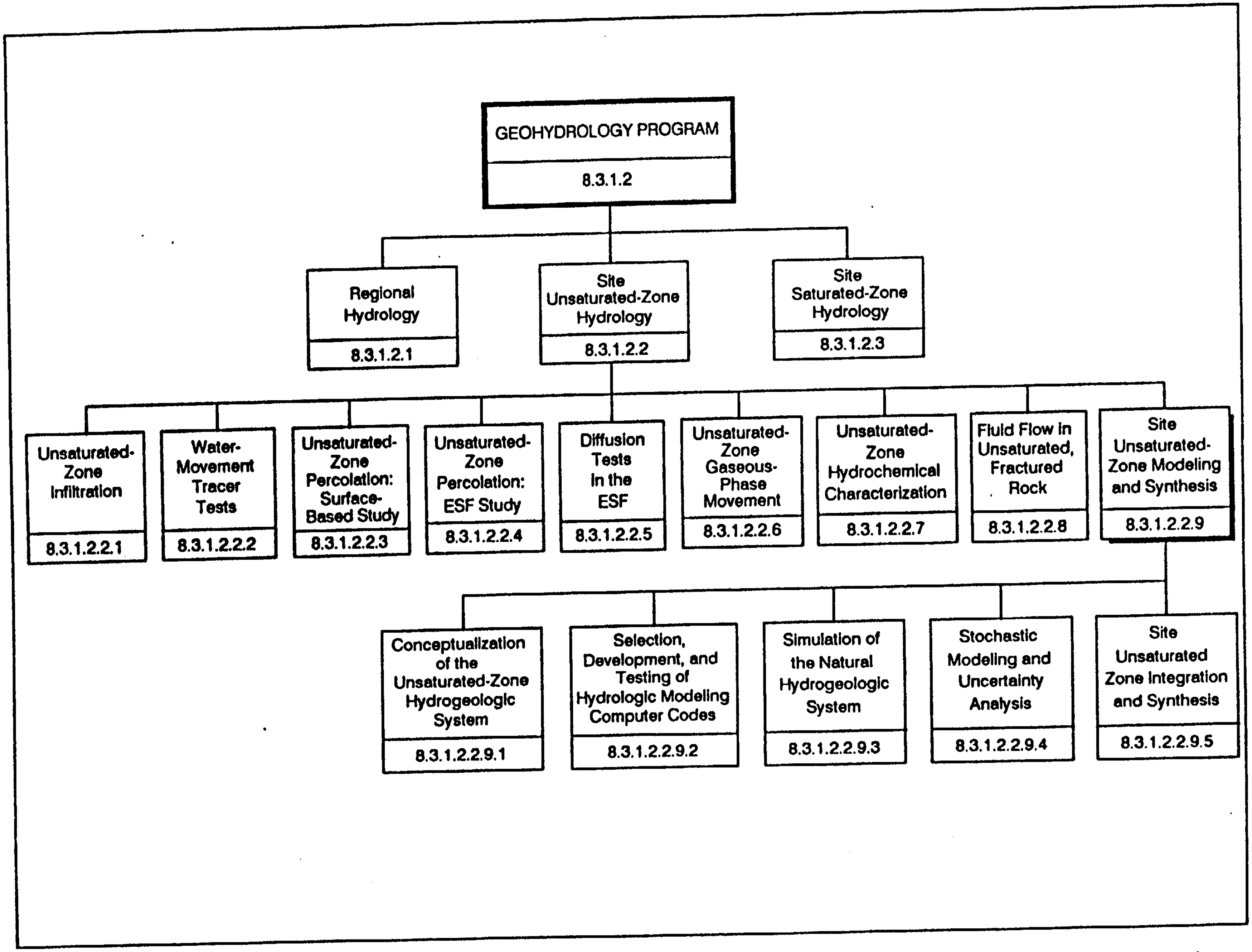


Figure 1.1-1. Diagram showing the location of study within the unsaturated-zone investigation and organization of the Geohydrology Program.

The description and plans for each activity are presented in Section 3. Plans for the conceptualization of the unsaturated-zone hydrogeologic system are discussed in Section 3.1; plans for the selection, development, and testing of hydrologic-modeling computer codes are in Section 3.2; plans for simulation of the natural hydrogeologic system are in Section 3.3; plans for stochastic modeling and uncertainty analysis are in Section 3.4; and plans for site unsaturated-zone integration and synthesis are in Section 3.5. The descriptions include (a) objectives and parameters, (b) technical rationale, and (c) general modeling approach and analytical techniques. Alternate modeling and analytical approaches are also summarized.

Applications of the study results are summarized in Sections 1.3 and 4, schedules and milestones are presented in Section 5, a study-plan reference list appears in Section 6, and quality-assurance requirements are discussed in Section 7.1.

1.2 Objectives of study

The objectives of this study are to (1) develop conceptual models for the site unsaturated-zone hydrogeologic system; (2) select, modify, or develop numerical hydrologic modeling codes to simulate the hydrogeologic system and its component subsystems; (3) apply the models to simulate and investigate the existing system state, and predict the system response to changing external and internal conditions; (4) evaluate the accuracy of the models using stochastic modeling, conventional statistical analyses, and sensitivity analyses; and (5) integrate data and analyses to synthesize a comprehensive qualitative and quantitative description of the site unsaturated-zone hydrogeologic system under present as well as probable, or possible, future conditions. The models developed as part of this study will be used to estimate the quantity and spatial distribution of moisture that can potentially reach the engineered barrier system, test hypotheses concerning the hydrologic behavior of the site, and through calibration against measured state variables, produce estimates of hydrologic parameters that may be useful for design and performance assessment calculations. An integral part of this study is the development of a three-dimensional site-scale model of Yucca Mountain that will consider transport of gases, heat, and environmental tracers; this model will be used to guide in the site-characterization effort. The development of credible quantitative models of the natural flow system (including the movement of environmental tracers) enhances confidence in performance assessment models for which experimental or observational data may be lacking.

The objectives of individual activities in the site unsaturated-zone modeling and synthesis study are as follows:

Activity 8.3.1.2.2.9.1	To develop conceptual models for the overall moisture-flow system within the unsaturated zone at Yucca Mountain.
Activity 8.3.1.2.2.9.2	To select, evaluate, and adapt existing numerical hydrologic modeling codes, or develop new codes, as needed, to simulate particular aspects of the Yucca Mountain system.
Activity 8.3.1.2.2.9.3	To construct appropriate hydrologic models for the natural site hydrogeologic system to simulate and investigate the existing state of the system and predict probable future and past states of the system.
Activity 8.3.1.2.2.9.4	To assess the probable limits of uncertainty of numerical model predictions due to uncertainties in the material-property and boundary-condition data.
Activity 8.3.1.2.2.9.5	To integrate all applicable site data and analyses in order to synthesize a continually updated, comprehensive representation for the site unsaturated-zone hydrogeologic system.

1.3 Hydrogeologic setting

The primary repository area at Yucca Mountain (Figure 1.3-1) is located on a north-trending, eastward-tilted structural block that is bounded on the west by the westward-dipping, high-angle Solitario Canyon fault and on the east by a zone of imbricate high-angle faults (Figure 1.3-2). Vertical displacement along the Solitario Canyon fault decreases from about 200 m at the southern end of the block to about 20 m at the northern end. Strata within the block dip from about 5° to about 10° to the east. The block is transected by north-south trending normal faults, exhibiting westward-dipping fault planes (such as the Ghost Dance fault), of small to moderate displacements (25 m or less). The presence of faults may be of considerable hydrologic significance because, depending on local conditions, they may act either as barriers to or conduits for moisture movement within the unsaturated zone. The eastward tilt of the block also may be hydrologically significant because it establishes the possibility for gravitationally-driven lateral, down-dip movement of moisture, especially along the contacts separating strata whose hydrologic properties differ appreciably. The magnitude and significance of lateral moisture movement also will depend upon the degree of anisotropy of the hydrologic properties within particular hydrogeologic units.

Stratigraphically, Yucca Mountain consists of a layered sequence of principally rhyolitic, ash-flow and ash-fall tuffs of Tertiary age. Individual lithostratigraphic units consist of densely welded to nonwelded, vitric to devitrified tuffs that in the lower part of the unsaturated zone have been altered locally by zeolitization. The densely to moderately welded tuffs tend to be fractured and some contain zones of lithophysal cavities. The vertical sequence of geologically defined lithostratigraphic units can be divided and grouped into functionally defined hydrogeologic units within each of which the hydrologic properties (and, generally, the other material properties as well) can be regarded to be approximately spatially uniform. The hydrologic properties are related, in turn, to petrologic factors such as the grain-size distribution and the degrees of welding and alteration within the rock matrix as well as to fracture aperture, length, orientation, and spacing. The hydrologic properties of individual hydrogeologic units can be determined, in principle, directly or indirectly from field and laboratory measurements. These empirical data are subject to uncertainties due to measurement errors and to the presence of both random and correlated, local and large-scale spatial variability (heterogeneities). The presence of these data uncertainties must be accounted for in assessing the accuracy with which numerical hydrologic models can be expected to simulate the natural hydrogeologic system.

The unsaturated zone within the repository block ranges in thickness from 500 to 750 m (Robison, 1984), and lies wholly within the vertical sequence of tuffaceous rocks. Net infiltration of moisture into the unsaturated zone occurs at land surface and, presumably, is derived solely from precipitation. Average annual precipitation at Yucca Mountain is about 150 mm/yr (Quiring, 1983), most of which probably is returned to the atmosphere by direct evaporation or as

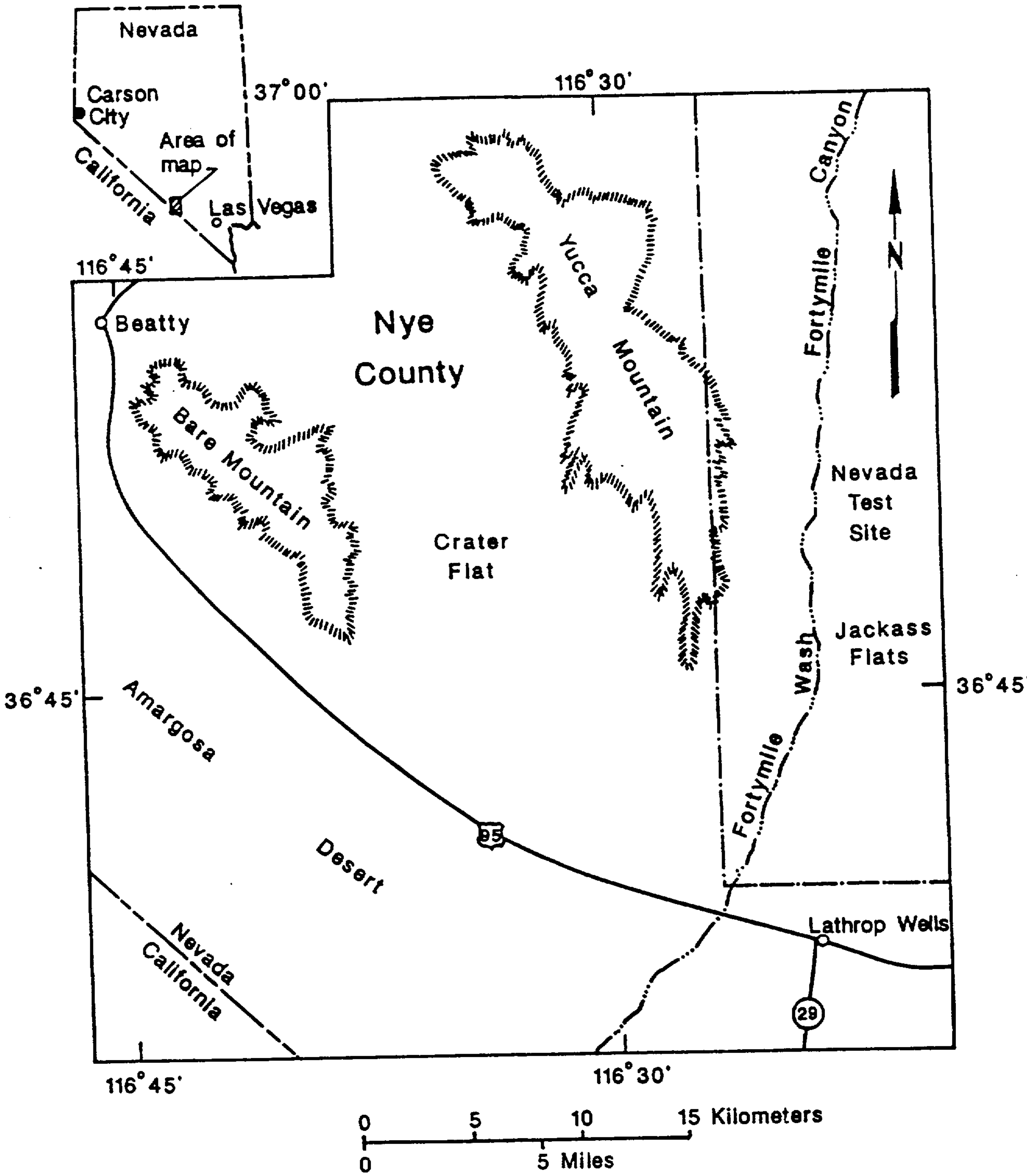


Figure 1.3-1. Location of Yucca Mountain.

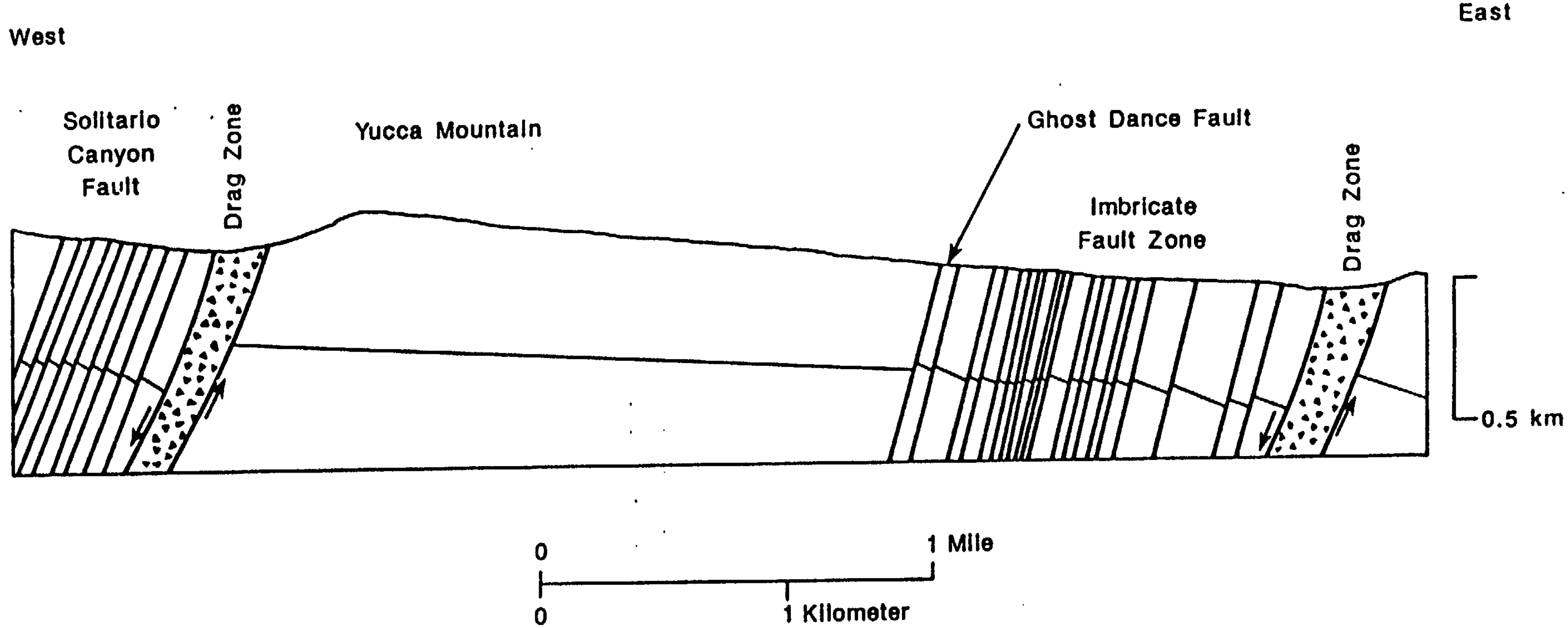


Figure 1.3-2. Schematic cross section of typical structural block at Yucca Mountain.

evapotranspiration from the sparse vegetative cover. Under present climatological conditions, the mean rate of net infiltration of moisture into the unsaturated zone over the repository block is estimated not to exceed 4.5 mm/yr and is probably less than 1 mm/yr (Montazer and Wilson, 1984). Because net infiltration is expected to influence the distribution and flux of moisture within the unsaturated zone, a knowledge of the present, probable past, and expected future rate and spatial distribution of net infiltration of moisture over the Yucca Mountain block is essential for proper and complete hydrologic evaluation of the site. In addition, the rate and spatial distribution of net infiltration is a fundamental input parameter to the numerical hydrologic models that will be constructed for the site. The quantitative evaluation of net infiltration within the primary repository area is one of the principal objectives of the unsaturated-zone infiltration study, as described in YMP-USGS SP 8.3.1.2.2.1. Where predictions regarding future moisture and gas movement are made, best available estimates regarding the thermal output from the potential repository will be used. Although these simulations will not consider moisture redistribution due to thermal loading at the scale of individual canisters, they will consider the effects of thermal loading on flow-path distribution at the site scale. Detailed studies of thermal loading on the near-field are considered in another study plan.

1.4 Regulatory rationale and justification

The present study is directly applicable to the estimation of pre-waste-emplacement ground-water travel time, and secondarily applicable to radionuclide release and repository design through its contributions to activities characterizing the post-emplacement near-field environment. Disturbed zone and thermally altered zone effects may have a significant impact upon ground-water movement and radionuclide transport in terms of overall repository performance. They must be accounted for in assessing total system compliance with EPA requirements, and will be addressed by additional experimentation and modeling in the studies of Issue 1.10. The calibrated models for the natural moisture and gas flow system developed by this study will provide hydrologic data needed for performance-assessment predictions of unsaturated-zone ground-water travel times and rates of radionuclide releases to the accessible environment. Estimates of the quantity and spatial distribution of moisture flux may also be used in design analyses of the underground facility, repository seals, and waste packages.

The overall relations between SCP design and performance information needs and data collected in this study are described in the hydrogeology testing strategy presented in SCP Section 8.3.1.2 and the issue-resolution strategies (repository, seals, waste package, and performance assessment) presented in SCP Sections 8.3.2 - 8.3.5. The description presented below provides a more specific identification of these relations as they apply to this study. A tabulation of some of the design and performance parameter needs and related characterization parameter sources is listed in Table 7.1-1.

In this and other study plans, it has been useful to group the measured or calculated parameters of the various activities (activity parameters) into a limited set of characterization parameters, more broadly defined parameters that encompass activity-parameter data collected in the field and laboratory, or generated by modeling. By introducing these parameters, it becomes easier to demonstrate how the study relates to satisfying the information requirements of parameters in the performance issues. This demonstration is made in Table 7.1-1. In the case of the site unsaturated-zone modeling and synthesis study, the activity parameters (presented in the figures and tables of Sections 3.3 through 3.4) can be grouped under a set of characterization parameters as follows:

Activity 8.3.1.2.2.9.3 - Simulation of the natural hydrogeologic system	Moisture flux, at present state of site unsaturated-zone system
	Pore-gas flux, at present state of site unsaturated-zone system
Activity 8.3.1.2.2.9.4 - Stochastic modeling and uncertainty analysis	Moisture flux, at present state of site unsaturated-zone system
	Pore-gas flux, at present state of site unsaturated-zone system

Activity 8.3.1.2.2.9.5 - Site unsaturated-zone integration and synthesis	Moisture flux, at present state of site unsaturated-zone system
	Pore-gas flux, at present state of site unsaturated-zone system
	Moisture flux, at probable past states of site unsaturated-zone system
	Pore-gas flux, at probable past states of site unsaturated-zone system
	Moisture flux, at possible future states of site unsaturated-zone system
	Pore-gas flux, at possible future states of site unsaturated-zone system

Activities 8.3.1.2.2.9.1 (Conceptualization of the unsaturated-zone hydrogeologic system) and 8.3.1.2.2.9.2 (Selection, development, and testing of hydrologic-modeling computer codes) do not directly generate activity parameters. By their support of the other three activities they contribute indirectly to the evaluation of both activity and characterization parameters of this study.

The grouping of activity parameters according to characterization parameters is given in Table 2.1-1 of Section 2. Characterization parameters are also shown in the logic diagrams accompanying the activity descriptions of Sections 3.3, 3.4, and 3.5.

Project-organization interfaces between the site unsaturated-zone modeling and synthesis study (8.3.1.2.2.9) and the YMP performance and design issues are illustrated in Figure 1.4-1. The figure also indicates project interfaces with other site studies; these relations are described further in Section 4.2. The relations between the design and performance issues noted below and the regulatory requirements of 10 CFR Part 60 and 10 CFR Part 960 are described in Section 8.2.1 of the SCP.

Information derived from the study will principally support the performance determinations of pre-waste-emplacement, ground-water travel time (Issue 1.6) and the predictions of radionuclide releases to the accessible environment (Issue 1.1). Study results also will indirectly support the resolution of issues concerned with waste-package design (Issue 1.10), releases from the repository engineered-barrier system (Issues 1.4 and 1.5), and repository design (Issue 4.4).

The following portion of this section summarizes from the SCP the study-level interfaces between this study and the performance and design issues. The discussion of the uses of site-characterization data from this study in

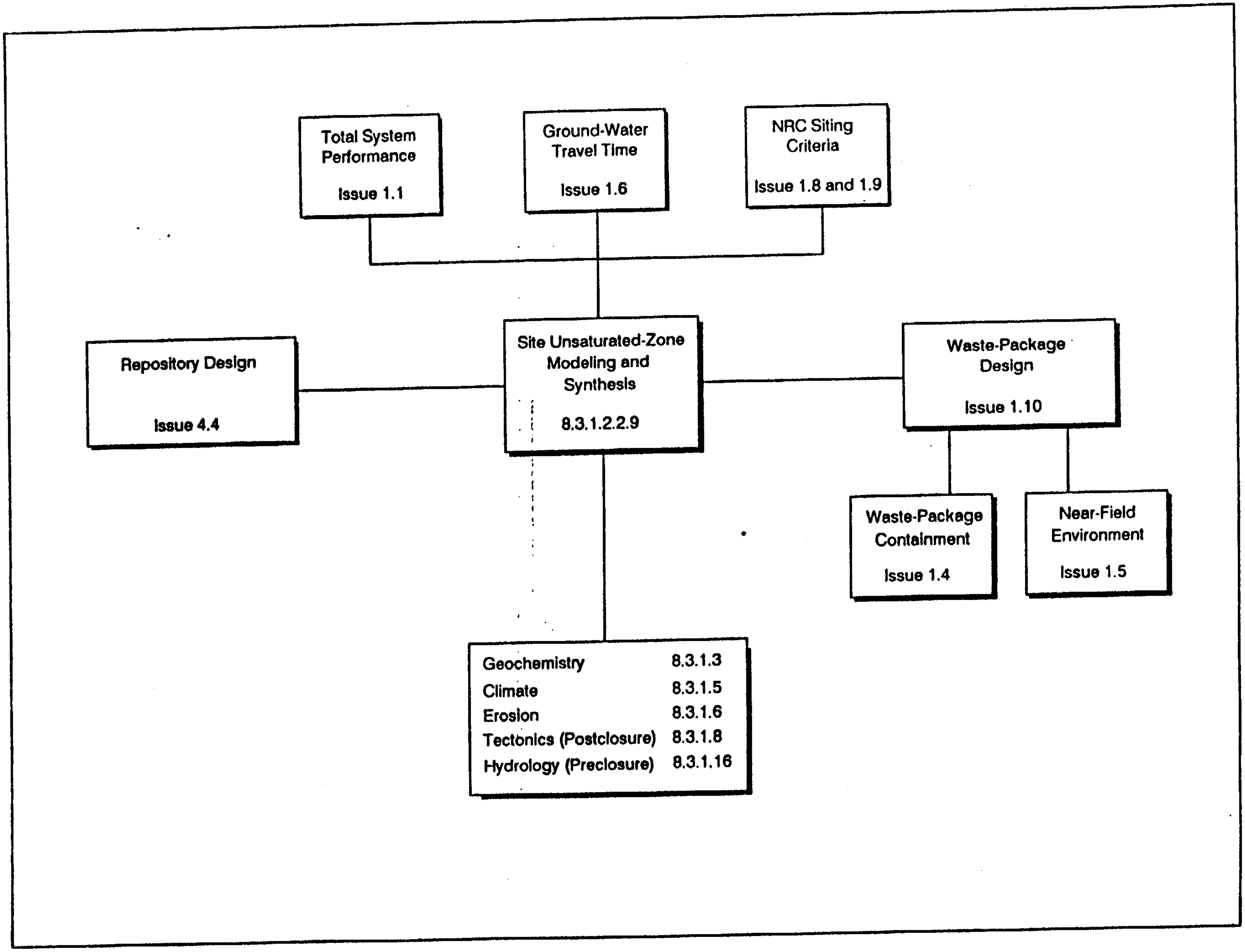


Figure 1.4-1. Interfaces of unsaturated-zone modeling and synthesis with YMP performance and design issues and other site-characterization programs.

resolving those issues is based upon performance measures and performance parameters identified in SCP Section 8.3.5.

Performance Issue 1.1
(Total system radionuclide release to the accessible environment)

This issue is concerned with the total system performance and radionuclide release rates to the accessible environment. The geologic setting, engineered barrier system, ramps, boreholes, and seals are required to be selected and designed so as to limit the cumulative releases of radionuclides for 10,000 years following permanent closure of the repository. Information from site unsaturated-zone modeling and synthesis will be used to evaluate the ability of the site to satisfy the requirements of numerous supporting performance parameters. These will be used to address expected partial performance measures (EPPM's) for the unsaturated-zone liquid pathway and for the gas pathway for the nominal (Class E) scenario in which matrix flow predominates within the undisturbed unsaturated zone.

Performance parameters for the nominal case supported by this study are average flux and effective matrix porosity in the unsaturated-zone rock matrix, fracture networks, and fault-zone rock mass and mean residence time of released $^{14}CO_2$. Other supporting parameters (needed to evaluate the nominal case) are listed in SCP Table 8.3.5.13-17.

Calculations employing supporting parameters for the resolution of Issue 1.1 are: calculation of the specific-discharge fields and moisture contents in the unsaturated-zone units and fault zones; calculation of coupling factors for radionuclide retardation factors; calculation of these coupling factors for model validation; and calculation of gas-phase ^{14}C transport in unsaturated-zone units in conjunction with ^{14}C transport model calibration and verification.

Performance Issue 1.4
(Waste-package containment)

This issue is restricted to assessing waste-package performance for anticipated processes and events during the period not less than 300 years, but not exceeding 1,000 years following closure of the repository. The present study will indirectly contribute to the resolution of Issue 1.4 by providing information on hydraulic parameters and boundary conditions, including fluid fluxes, to those studies involved with modeling near-field processes (SCP Study 1.10.4.2, Hydrologic properties of waste package environment). The chemistry of the water that can contact either the container or the waste can have a large effect on the performance of these materials. For instance the corrosion behavior of the stainless-steel alloys under consideration is sensitive to the chloride content of the water with which it comes in contact. Thus, standards are set for the composition of the water contacting the waste packages so that the water will be similar to that currently thought to exist within the undisturbed environment in the unsaturated Topopah Spring tuff at Yucca Mountain. Similarly, the method by which water is delivered to a waste package can affect both the corrosion rate and mechanisms.

Performance Issue 1.5
(Waste-package and repository engineered-barrier performance)

Issue 1.4, as stated, is restricted to assessing waste package performance for anticipated processes and events for a period of 1,000 years following closure of the repository. The performance of the waste packages during this 1,000 years containment period is intimately linked to the performance required thereafter by the engineered-barrier system in controlling radionuclide releases as addressed in Issue 1.5. Performance Issue 1.5 addresses the regulatory requirement that radionuclide releases from the engineered barrier system not exceed 1 part in 100,000 of the 1000-yr inventory per year after the containment period. Unsaturated-zone fluid flow and transport are part of that issue resolution, and waste degradation and radionuclide release estimates depend upon an estimate of the amount of water reaching the waste form. The present study provides information on the quantity and spatial distribution of moisture that can potentially arrive at the engineered barriers. Studies proposed to resolve this issue may utilize hydrologic properties of the Topopah Spring unit and values of fluid flux estimated from this study to simulate the flow and transport processes in the near-field host rock. The applicable performance measures are water quality and quantity and concentrations of radionuclide species in the liquid and gas phases, and those species absorbed to solid phases within the near-field host rock.

Performance Issue 1.6
(Pre-waste-emplacement ground-water travel time)

The general strategy for resolving this issue entails the definition, characterization, and assessment of multiple barriers to ground-water flow, by identifying and quantifying flow paths and flow processes. In the unsaturated zone, the natural rock barriers have been grouped into distinct hydrogeologic units for which different types of general flow processes may be hypothesized. These processes include dispersive, diffusive, and advective flow in rock pores and fractures, as well as between them. The frequency distribution of calculated ground-water travel times is the performance measure for each hydrogeologic unit. One of the performance goals for the site is a ground-water travel time of 1,000 years or more at a high level of confidence for the combination of hydrogeologic units positioned between the disturbed zone and the accessible environment.

Site information from unsaturated-zone modeling and synthesis will be used to satisfy numerous supporting performance parameters needed to estimate ground-water travel time in individual units within the unsaturated zone, in the saturated zone, and the two combined zones. These supporting parameters (e.g. unsaturated-zone rock-matrix permeability in the repository area) are used to define various aspects of the unsaturated-zone model, saturated-zone model, spatial-correlation structure model, and fracture-hydrologic characteristics model. These aspects include initial and boundary conditions, material properties, system geometry, and validation of model concepts. The present study provides a valid conceptual framework, demonstrated through a favorable comparison between site data and modeling results and through sensitivity analysis (that includes characterization of uncertainty in system parameters), that forms the basis for ground water travel-time calculations. Model calibrations and sensitivity analyses performed as part of the present study will yield performance parameters such as liquid and gas fluxes, unsaturated and saturated hydraulic conductivity, effective porosity, distance along flow paths, and percolation rates within each major unsaturated-zone unit. These performance parameters are further categorized by their fracture, matrix, and fault-zone elements.

Performance Issues 1.8 and 1.9
(Favorable and potentially adverse conditions) (Qualifying and disqualifying conditions)

The results of this study have indirect applications to the NRC siting criteria - Favorable Condition 7 (pre-waste-emplacement, ground-water travel time) through Issue 1.6, and Favorable Condition 8 (unsaturated-zone hydrogeologic conditions) through Issue 1.1. The study also has indirect applications to the higher-level findings for the hydrogeology qualifying and disqualifying conditions through Issues 1.1 and 1.6.

Design Issue 4.4
(Repository design and technical feasibility)

Only the preclosure elements are considered pertinent for resolving Issue 4.4. Single-phase and two-phase fluid flow in the unsaturated zone, as modeled by this study, will be used to characterize the unsaturated-zone fluid flux. This relates to an evaluation of natural-water inflow which will be applied to the repository mining water removal system element. Removal of natural water equal to the rate of inflow is the performance measure. Water and formation chemistry data from this study will be applied to the repository waste-handling retrieval system element. The tentative goal is that a quantitative and qualitative analysis of formation and water chemistry will aid in the understanding of the waste-package liner corrosion.

2 RATIONALE FOR STUDY

2.1 Technical rationale and justification

Quantitative evaluation of the hydrogeologic system encompassing the unsaturated zone at Yucca Mountain is essential to the site-characterization program because it is within this interval of partially saturated rocks that the repository is proposed to be constructed. Because hydrogeologic data are to be obtained directly from only a relatively few surface-based boreholes and from within the exploratory studies facility, the hydrologic evaluation of the site will be based on field data that will be sparsely distributed over the primary repository area. Methodologies are needed to enable interpolation within and extrapolation from this limited body of data to infer the present state of the natural system and to predict probable future states under changing environmental conditions. The accuracy of these inferences and predictions needs to be assessed with respect to the probable errors of measurement of the field and laboratory data as well as to the presence of random or spatially correlated heterogeneities within the system. Deterministic numerical hydrologic models will be constructed to aid in the development of conceptual models, and statistical methods and stochastic modeling procedures will be invoked to estimate the limits of uncertainty attending the deterministic model results.

A knowledge of the present and the expected future spatial distributions of moisture flux within the repository block at Yucca Mountain is of particular importance for repository design and performance assessment as well as for estimating probable ground-water travel times from the repository to the accessible environment. Net moisture flux, occurring in both liquid and vapor phases, is not accessible to direct *in situ* measurement and, therefore, must be inferred from the local potential gradients and hydraulic conductivities or effective vapor diffusion coefficients. Whereas hydraulic conductivities are obtainable from laboratory and field determinations, the spatial distribution of liquid-water matric potential and pore-gas pressure must be inferred or interpolated from sparsely distributed *in situ* measurements. If the overall hydrologic system within the unsaturated zone at Yucca Mountain can be described in terms of existing theories for fluid storage and movement in porous and fractured media, the present and probable future spatial distribution of fluid potential and, subsequently, moisture flux can be predicted from appropriately constructed numerical hydrologic models. Numerical hydrologic models, therefore, are to be constructed specifically to predict moisture flux and its distribution in space and with time as well as to promote an understanding of the hydrogeologic system at the site.

2.1.1 Statement of problem and study justification

The study and quantification of moisture storage and movement within thick, layered sequences of partially saturated, variably fractured tuffs is largely unprecedented. It remains to be demonstrated to what extent such a hydrogeologic system can be represented by commonly accepted theories for fluid storage and movement in variably saturated porous media. The moisture flow and storage within the unsaturated zone of the repository block are controlled by the structural, stratigraphic, and climatological settings. Moisture is presumed to be present both as liquid water and as water vapor within interstitial, fracture, and lithophysal openings. Moisture movement within the unsaturated zone is envisioned to be complexly three dimensional. Specifically, liquid-water flow within interconnected pores and fractures may occur as well as advective and diffusive vapor-phase movement primarily within the interconnected air-filled fracture openings and secondarily within the rock-matrix pore space. Because liquid-water fluxes are assumed to be small under conditions presently existing within the unsaturated zone at the site, the movement of water vapor may contribute significantly to net moisture flow, especially within the highly fractured tuff units. Furthermore, because liquid water and water vapor are expected to be in local thermodynamic phase equilibrium under all but highly transient conditions, liquid-water saturation and water-vapor concentration are coupled through the prevailing geothermal regime. A further complication arises from the need to consider and account for the occurrence of dissolved constituents in both the liquid and gas phases. The concentrations and transport of these solutes within the unsaturated zone are coupled to the occurrence and movement of liquid water and pore gas and, additionally, may be affected by chemical interactions with the enclosing rock matrix. Consequently, hydrologic evaluation of the site, in its most general aspect, constitutes a problem of two-phase, multi-component, coupled heat and moisture flow within a layered sequence of tilted, faulted, and fractured, variably saturated tuffaceous hydrogeologic units of highly dissimilar and variable hydrologic, mechanical, and thermal properties.

The fundamental hydrogeologic data that are required to define the hydrologic system and to validate the numerical hydrologic models will become available only as site characterization proceeds. Consequently, hydrologic evaluation of the site is to be accomplished in an iterative sequence of steps. These steps consist of collecting basic hydrogeologic data and performing tests and experiments to explicate and quantify particular concepts and hypotheses. Numerical hydrologic modeling will be used at many stages to perform preliminary analyses, to design and analyze tests and experiments, and to analyze and interpret field data. The principal hydrologic modeling effort, however, is to construct mathematical representations to simulate the natural hydrogeologic system and its component subsystems. This, too, will be a complex multi-step process that is divided into five activities as follows: (1) Conceptualization of the unsaturated-zone hydrogeologic system, (2) preliminary hydrologic model development and testing, (3) numerical simulation of the natural hydrogeologic system, (4) stochastic modeling and uncertainty analysis, and (5) site unsaturated-zone integration and synthesis. A summary of the multi-step process of model development is illustrated in Figure 2.1-1. The activities are specifically addressed in Section 3 of this study plan.

2.1.2 Hydrologic modeling

The development of credible quantitative models of the natural moisture and gas flow system (including the movement of environmental tracers) enhances the confidence of the scientific commununity, and hence of the public, in models for which no experimental or observational data can be obtained, such as those that predict

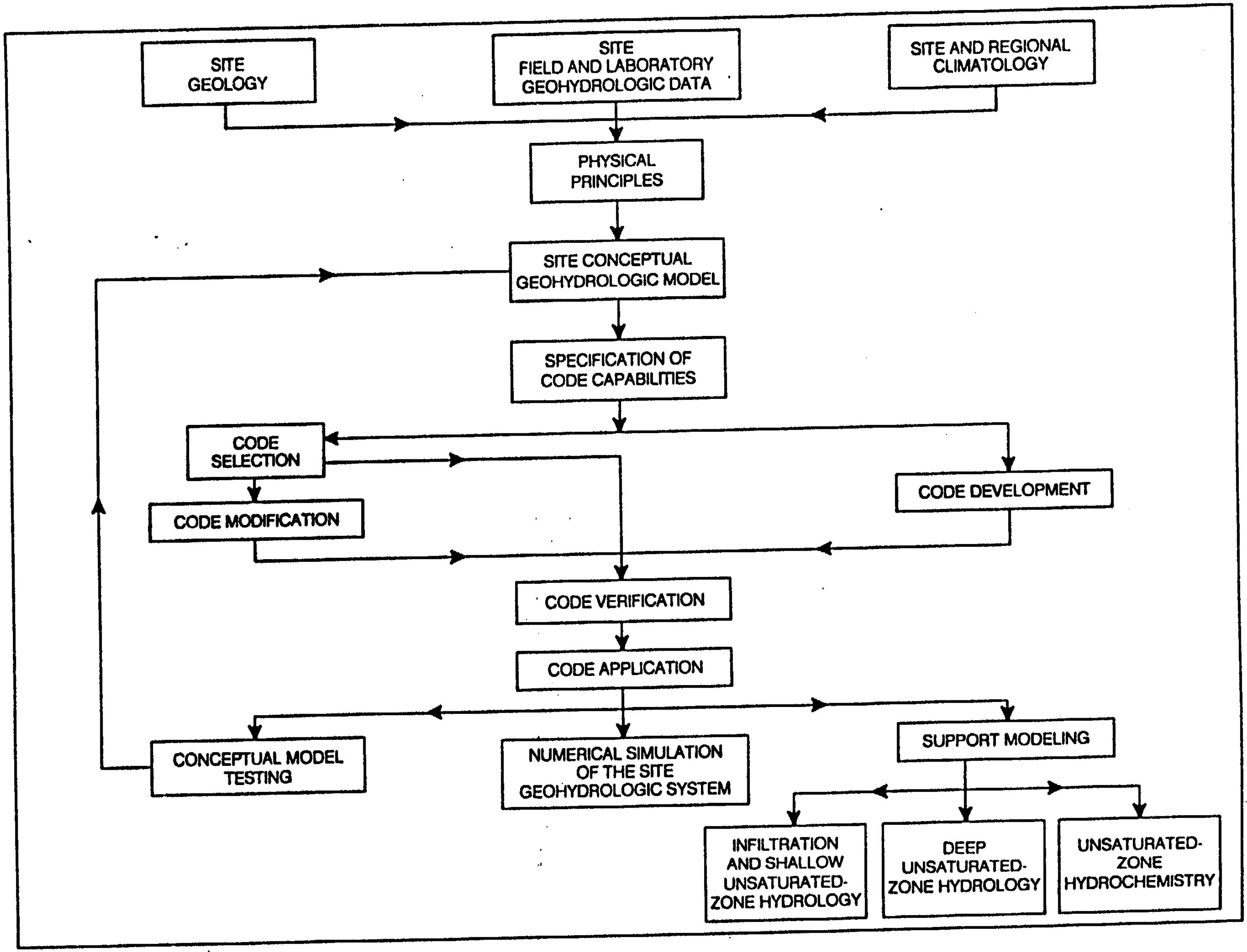


Figure 2.1-1. Block diagram showing iterative hydrologic model development.

radionuclide migration hundreds of years henceforth. Modeling of the natural flow system invariably involves model calibration, which results in parameter estimation; these estimates can subsequently be used in performance-assessment modeling. Numerical models of the site, in addition to guiding data collection and testing of conceptual hypotheses, can also be used to estimate liquid and gas fluxes and their spatial distribution, and identify potential flowpaths along which radionuclide transport may occur. In this regard, results of the proposed modeling may impact drift or canister locations, and, thus, repository design.

A numerical hydrologic model is a mathematical representation for a physical hydrogeologic system. The model is constructed from hydrogeologic data obtained for the system and from conceptual models developed specifically for the system. A conceptual model is an abstract representation of the system that idealizes the underlying geologic framework and identifies the principal hydrologic processes and boundary conditions acting within and on the system. The geologic framework includes the stratigraphic, petrologic, and structural setting. The hydrologic processes include the movement and storage of moisture (occurring as either or both liquid water and water vapor), of pore gas, and possibly of liquid- or gas-phase solutes within the fractures, pores, and lithophysal cavities of the enclosing solid medium. The boundary conditions imposed on the model include the configuration of the water table as well as present and past land-surface climatology. In principle, the construction of a numerical hydrologic model proceeds from the conceptual model as follows:

(1) The geologic framework defines the model geometry and material composition.

(2) Those hydrologic processes assumed by the conceptual model to be operating within the system are formulated mathematically into a set of generally nonlinear integro-differential equations in which the physical hydrologic variables enter as functions of the space-time coordinates. The physical hydrologic variables include, for example, the liquid-water saturation and matric potential, pore-gas pressure, water-vapor concentration, and solute concentrations.

(3) The material-property data (hydrologic, thermal, and mechanical) enter as coefficients in the set of integro-differential governing equations. These data include: (a) the generally nonlinear relations between fluid saturation, relative hydraulic conductivity, and potential under partially saturated conditions; (b) representative values for rock-matrix permeability, porosity, and compressibility; and (c) fracture-length, orientation, and aperture distributions.

(4) Hydrologic boundary conditions are derived from land-surface climatological data, the configuration of the underlying water table, and the geologic framework.

(5) An appropriate numerical procedure is invoked to solve the set of integro-differential equations for the physical hydrologic variables

under the specified model-geometry, composition, and boundary and initial conditions. If the overall problem is mathematically well posed, the resulting numerical solution yields a unique, internally consistent mathematical representation, or simulation, of the system at any instant in time. By extending the numerical solution incrementally in time, the time-evolution of the system can be simulated. Hence, both the existing state of a hydrogeologic system under fixed environmental conditions and possible future states of the system under changing environmental conditions can be predicted. In addition, if it is assumed that the boundary conditions have changed continuously over time, the model calculations can be extended backwards in time to infer the state of the system under past climatological regimes. This will be done by assuming a past state of the system and time dependent boundary conditions, and performing a series of forward calculations to the present time.

2.1.3 Functions of the activities

The conceptualization of the unsaturated-zone hydrogeologic system (Activity 8.3.1.2.2.9.1) is designed to develop conceptual models for the overall moisture-flow system within the unsaturated zone at Yucca Mountain. The conceptualization process is the first step toward developing quantitative models of liquid and pore-gas flow. It includes: (1) evaluation and synthesis of data into conceptual models; and (2) identification of geologic framework controls, hydrologic properties, and boundary conditions.

In the selection, development, and testing of hydrologic-modeling computer codes (Activity 8.3.1.2.2.9.2), existing numerical codes will be selected, evaluated, and adapted for application to the site unsaturated-zone hydrogeologic system. They will also be modified, as needed, to simulate particular problems or aspects of unsaturated-zone flow that are unique to the Yucca Mountain system.

The simulation of the natural hydrogeologic system activity (Activity 8.3.1.2.2.9.3) involves the construction of appropriate unsaturated-zone hydrologic models that will simulate and investigate the site system in its current, probable past, and possible future states. The final model is intended to be comprehensive enough to account for the dominant, controlling hydrologic processes and conditions (identified through sensitivity analyses and hypotheses testing), and to incorporate a degree of complexity consistent with the practical constraints and limitations imposed by the use of finite numerical models to perform mathematical simulations.

The stochastic modeling and uncertainty analysis (Activity 8.3.1.2.2.9.4) is intended to assess the probable limits of the numerical model predictions due to uncertainties in material properties and boundary condition data and as a decision-making aid during the conceptualization process. The complexity of most natural hydrogeologic systems, and the time scales which are required to observe hydrologic response to changing conditions, are obstacles to the direct validation of numerical models. In the case of the unsaturated zone at Yucca Mountain, the model will be calibrated against the observed state variables, such as water potential and saturations obtained from cores (see, for example Kume and Hammermeister, 1990; Loskot and Hammermeister, 1992) or from in situ monitoring. Models can also be calibrated against geochemical data, such as distributions of environmental isotopes. It is not expected that experimentally induced perturbations can practically be included in the calibration process because of the large time factors involved. In addition, this activity will therefore develop indirect methods to assess model accuracy and validity as a function of measurement error, spatial variability, and conceptual model error.

The site unsaturated-zone integration and synthesis (Activity 8.3.1.2.2.9.5) is the culminating effort of the study. It is designed to integrate all applicable site data and analyses in order to synthesize a comprehensive representation for the site unsaturated-zone hydrogeologic system. It will address the present, probable past, and possible future states of the system. The effort will be an ongoing one, continually reviewing the validity of the prevailing conceptual models as well as the contributing data acquisition and experimental program.

2.1.4 Parameters and analytical strategies

In SCP usage (U.S. Department of Energy, 1988) hydrologic activity parameters are those parameters that are generated by testing and analysis in the field, laboratory, or office; they represent the most basic measurements that will be used to characterize the hydrogeology of Yucca Mountain and vicinity. Many of the activity parameters are building blocks to support various aspects of the project. Some, such as hydraulic conductivity, support design and performance issues directly. Others primarily provide bases for analyses and evaluations to be conducted within the Geohydrology Program or within other characterization programs.

In SCP Table 8.3.1.2-1, activity parameters for the Geohydrology Program are grouped according to parameter categories. The activity parameters associated with activities of this study also appear in the figures and tables of Section 3 of this study plan. Parameter categories serve to group similar types of performance and design parameters supporting design and performance-assessment issues resolutions (SCP Sections 8.3.2-8.3.5) and match them with groups of similar types of activity or characterization parameters to be obtained during site characterization. Parameter categories in the SCP were introduced as a classification scheme to aid in assessing the appropriateness and completeness of the data-collection program. In Figure 2.1-2, the parameter categories are shown supporting specific model components that make up the unsaturated-zone model. This figure corresponds to SCP Figure 8.3.1.2-3, and in that document is accompanied by parallel logic diagrams for the surface-water and saturated-zone components of the Geohydrology Program.

Table 2.1-1 groups the activity parameters of the present study according to characterization parameters. In SCP usage, a characterization parameter is a parameter, obtained by a

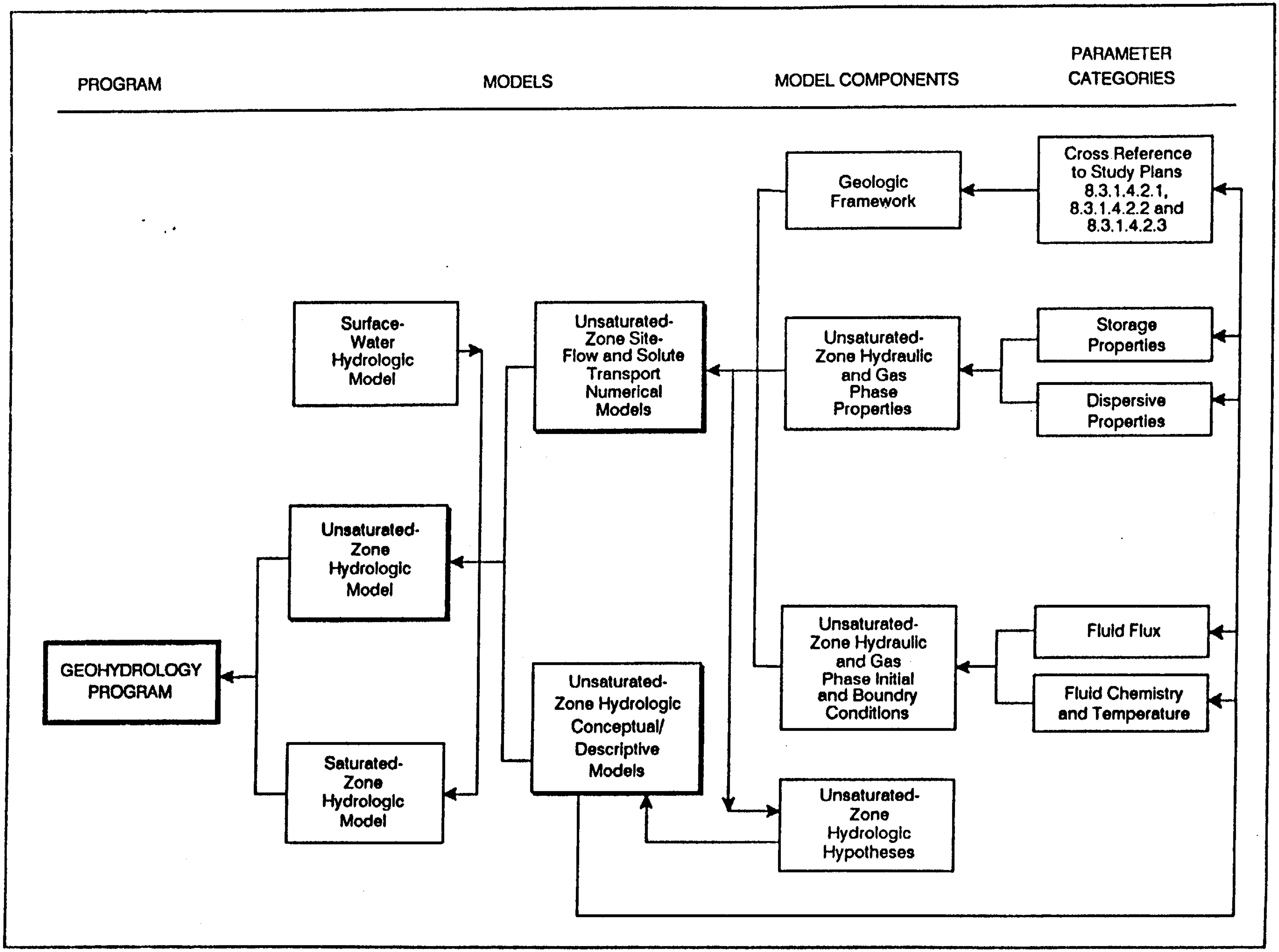


Figure 2.1-2. Logic diagram of the unsaturated-zone investigation within the Geohydrology Program, including model components and parameter categories.

Table 2.1-1 Association of activity parameters with characterization parameters

Activity	Characterization Parameter	Activity Parameters
Simulation of the site natural hydrogeologic system (Activity 8.3.1.2.2.9.3)	Moisture flux, at present state of site unsaturated-zone system	Liquid matric potential, time-dependent spatial distribution Liquid saturation, time-dependent spatial distribution Temperature, time-dependent spatial distribution Relative hydraulic conductivity, time-dependent spatial distribution Moisture flux, time-dependent spatial distribution
	Pore-gas flux, at present state of site unsaturated-zone system	Pore-gas pressure, time-dependent spatial distribution Water-vapor concentration, time-dependent spatial distribution Temperature, time-dependent spatial distribution Relative hydraulic conductivity, time-dependent spatial distribution Pore-gas flux, time-dependent spatial distribution
Stochastic modeling and analysis (Activity 8.3.1.2.2.9.4)	Moisture flux, at present state of site unsaturated-zone system	Variability of hydrologic properties Large-scale heterogeneity of hydrologic properties within hydrogeologic units Critical model parameters Effects of parameter variability or uncertainty on model results
	Pore-gas flux, at present state of site unsaturated-zone system	Variability of hydrologic properties Large-scale heterogeneity of hydrologic properties within hydrogeologic units Critical model parameters

Table 2.1-1 Association of activity parameters with characterization parameters

Activity	Characterization Parameter	Activity Parameters
		Effects of parameter variability or uncertainty on model results

characterization program, that has a logical, direct tie to a performance or design parameter, and for which a testing basis can be defined. Most characterization parameters will be developed from some combination of activity parameters, and will be the products of data reduction, tests and analyses, and modeling. Some of the activity parameters listed in Table 2.1-1, although not required directly for resolving performance or design issues, are required to accomplish satisfactory hydrologic modeling, which in turn increases confidence in the accuracy of the characterization parameters that are required for performance and design analyses. Hydrologic analyses generated in this study can be traced from activity parameters through characterization parameters and to their intended use in satisfying performance and design-parameter requirements for issues resolutions. This last step is addressed by Table 7.1-1.

Characterization parameters will be expressed as functions of space and (or) time and will be presented in formats that will facilitate use of the data in resolving design and performance issues. In future SCP progress reports, a testing basis will be developed for each characterization parameter, and will consist of some means of expressing the goals, confidence limits, and accuracy associated with each characterization parameter, so that requirements of performance and design parameters can be satisfied. An example of a testing basis could be that some statistical measure of the parameter, such as the mean, be known to a specific degree of accuracy.

In addition to supporting design and performance parameters, the activity parameters listed in Table 2.1-1 and Section 3 are needed to test hypotheses that support conceptual models and model components. A sufficient level of confidence in parameter values must exist for the analyses of this study to be employed for this purpose. The approaches to modeling analysis selected for the present study have been chosen to minimize uncertainty in parameter values and in the understanding of parameter interrelations, within the constraints of available resources. Where possible, multiple approaches within an activity are directed toward evaluating the value of a parameter by different means. The combined effect of using multiple approaches (or analyses) will be to increase the level of confidence in the parameter, because reliance will not be placed exclusively in one approach. Within a particular activity, some approaches may provide only partial information, while others will provide extensive information necessary for modeling analysis. By combining the analytical results and studying their relations, a greater understanding and confidence of modeling results can be achieved.

Because of the nonstandard nature of some of the analyses, the possibility that one or more analyses may fail in achieving the desired objectives is recognized. The use of multiple approaches for modeling analysis increases confidence that the failure or the partial failure of one or more analyses will not severely inhibit the ability of the characterization activities in providing the required information.

2.1.5 Contributions from other studies

The site unsaturated-zone models of the present study will incorporate the final models of two-phase flow in unsaturated, fractured rock developed in Study 8.3.1.2.2.8 (Fluid flow in unsaturated, fractured rock). These models will be used to help assess the conceptual uncertainty associated with the simplifications of flow and transport processes and system geometry that may be necessary to perform modeling at the site scale. They will also build upon and be evaluated against the hydrogeological data collected and interpreted in the following unsaturated-zone Studies: 8.3.1.2.2.1 (Unsaturated-zone infiltration), 8.3.1.2.2.2 (Water-movement tracer tests), 8.3.1.2.2.3 (Unsaturated-zone percolation - surface-based study), 8.3.1.2.2.4 (Unsaturated-zone percolation - ESF study), 8.3.1.2.2.5 (Diffusion tests in the ESF), 8.3.1.2.2.6 (Unsaturated-zone gaseous-phase movement), and 8.3.1.2.2.7 (Unsaturated-zone hydrochemistry). The geologic framework for the models will be contributed by Studies 8.3.1.4.2.1 (Vertical and lateral distribution of stratigraphic units within the site area) and 8.3.1.4.2.2 (Structural features within the site area). In characterizing probable unsaturated-zone hydrogeological conditions associated with past climatic episodes, the present study will employ paleoclimatic interpretations generated in Study 8.3.1.5.1.5 (Paleoclimate-paleoenvironmental synthesis), and paleohydrological interpretations from Study 8.3.1.5.2.1 (Quaternary regional hydrology). To evaluate the response of the unsaturated zone to possible future climate change, the present study will use the descriptions of expected future climate scenarios to be provided from Study 8.3.1.5.1.6 (Future regional climate and environments). In addressing possible tectonically induced changes in the average percolation flux rate at the top of the Topopah Spring welded unit, the present sudy may employ analyses and assessments generated in Study 8.3.1.8.3.1 (Effects of tectonic processes and events on average percolation flux rates over the repository). In addressing the possibility of the creation of perched aquifers in the unsaturated zone in the controlled area over the next 10,000 years, the present study may draw upon the results of Study 8.3.1.8.3.2 (Effect of tectonic processes and events on changes in water-table elevation). In addressing possible tectonically induced local changes in saturated fracture permeability or fracture effective porosity, the present study may use the results of Study 8.3.1.8.3.3 (Effects of tectonic processes and events on local fracture permeability and effective porosity).

2.2 Constraints on the study

2.2.1 Accuracy of models

Because of the need to treat problems that are mathematically tractable, a numerical model rarely can allow for the full range of complexity of the specific physical system that the model is intended to represent. Rather, the numerical model generally is based on a set of simplified and idealized hypotheses abstracted from the conceptual model. In the case of a hydrogeologic system, these hypotheses need to include the essential hydrologic processes, geologic structures, and boundary and thermodynamic (natural state) conditions that control the system. As a result of this simplification, the model yields an approximate representation of the physical system of which the accuracy of the approximation can be assessed through uncertainty analysis. For many systems, model accuracy can be assessed directly by comparing the observed and predicted responses of the system either to naturally occurring or to experimentally induced perturbations. This approach is not practical for most hydrogeologic systems that generally respond slowly to changing boundary conditions. Consequently, indirect methods based on classical-statistical or geostatistical techniques will be used to estimate the probable uncertainties associated with the model results. These uncertainties are due both to the errors of measurement in the input hydrogeologic field and laboratory data and to the presence of random or spatially correlated heterogeneities within the physical system. One such indirect method for evaluating model accuracy is the "bootstrap" approach, discussed more fully in Section 3.4. Additionally, conceptual uncertainty due to idealizations and approximations necessary to simplify the system geometry and processes are to be evaluated by an associated study (Study 8.3.1.2.2.8, Fluid flow in unsaturated, fractured rock).

Demonstrating that a conceptual model, as embodied in a numerical model represents a physical system within determined limits of uncertainty is termed <u>model validation</u>. Assessing the validity and accuracy of the numerical models to be used for hydrologic evaluation of the Yucca Mountain site is an essential task to be performed within this study under Activity 8.3.1.2.2.9.4 (Stochastic modeling and uncertainty analysis).

Because this study will not directly address compliance with regulatory requirements, and will not attempt to quantify the liklihood that performance standards will or will not be met, there is no logically defensible way to set general standards for model accuracy. The application of the model results of the present study in design analyses or to studies designed to assess radionuclide release and migration would require that such standards be set on a case-by-case basis. It is possible to imagine that the required accuracy might also depend on the values of the calculated values themselves. The performance characteristics of the waste packages and engineered barrier system, designs not yet finalized and tested, may also influence requirements for model accuracy. In summary, the accuracy requirements for the models developed by the present study depend on the application of these model results to other studies, and are best determined by peer review on a case-by-case basis.

2.2.2 Potential impacts of activities on the site

This study will have no physical impact on the site. The information generated from this study, however, might influence the performance of a study which would impact the site (i.e., the various data-gathering studies). The impact on the site due to individual studies is addressed within those studies and will not be addressed here.

2.2.3 Time required versus time available

A tentative schedule of work activities and reports is given for each of the five activities in Section 5. This study and its constituent activities rely heavily on the data collected by other studies; therefore the time available to perform the study is dependent on the time schedules of supporting studies. The model development itself will closely follow the schedules specified in Section 5.

2.2.4 Representativeness of repository scale and correlation to repository conditions

The unsaturated-zone modeling study is supported by various collection studies which will collect information directly from the repository area. The conceptual models formulated from these data are representative of the site inasmuch as the data are representative of the site. In the data-collection/conceptual-model portion of this study, certain minor hydrologic characteristics will inevitably not be considered and characteristics which have a negligible effect on the system will be omitted. This will allow simplification of the model so that reasonably accurate simulation can be performed in a timely manner. To this extent, the modeling efforts from the study will be generally representative of the repository site. The degree to which the model will represent a localized subsystem will depend on how influential that subsystem is on the behavior of the unsaturated zone as a whole.

3 DESCRIPTION OF ACTIVITIES

The study is organized into five activities:

- 8.3.1.2.2.9.1 - Conceptualization of the unsaturated-zone hydrogeologic system
- 8.3.1.2.2.9.2 - Selection, development, and testing of hydrologic-modeling computer codes
- 8.3.1.2.2.9.3 - Simulation of the natural hydrogeologic system
- 8.3.1.2.2.9.4 - Stochastic modeling and uncertainty analysis
- 8.3.1.2.2.9.5 - Site unsaturated-zone integration and synthesis

The plans for these activities are described in Sections 3.1 through 3.5. Figure 3-1 shows a simplified schematic of the various activities of the study plan and their interrelations. The emphasis of the study plan is the development of a site-scale model of the natural hydrogeologic system (Activity 8.3.1.2.2.9.3). The site-scale model will be developed in stages, starting with moisture flow and gas flow and adding temperature effects due to the prevailing geothermal gradient and transport of various isotopes and chemical species. The consideration of chemical species in the model allows comparison with field observations on the distribution of chemical isotopes such as tritium and C14, thereby providing constraints on simulations of the flow system. The site-scale model will consider all of the available data (at any given time) through the data integration activity (Activity 8.3.1.2.2.9.5), thereby providing continuous feedback to the conceptual modeling activity (Activity 8.3.1.2.2.9.1). The conceptual model will help determine what processes need to be considered in the site-scale model, which will directly impact the activity of selection, development and testing of hydrogeologic modeling computer codes (Activity 8.3.1.2.2.9.2).

As the site-scale model is being developed it will be used to determine the frequency and amount of various hydrogeologic data that are needed. Sensitivity studies may show that more detailed data for a sensitive parameter is needed or conversely, that a certain parameter does not affect the model results to a great extent. This information will be fed back to the data collectors. Concurrent with the development of the site-scale model, sub-models developed as part of this study and Study 8.3.1.2.2.8 (Fluid flow in unsaturated fracture rock) will be used to test various hypotheses of the conceptual model and their importance in terms of incorporation into the site-scale model. Both internal and external peer reviews will be periodically conducted to ensure that all of the field data are properly used in the site-scale model and that the results, including the conceptual model, are in agreement with all relevant information.

Stochastic modeling and uncertainty analysis will be employed in order to evaluate the sensitivity of the model results to parameter uncertainty and the various numerical approximations that may be required by the model. Model accuracy may be evaluated through several qualitative and quantitative methods, including "hypothesis testing" and "bootstrapping" approaches.

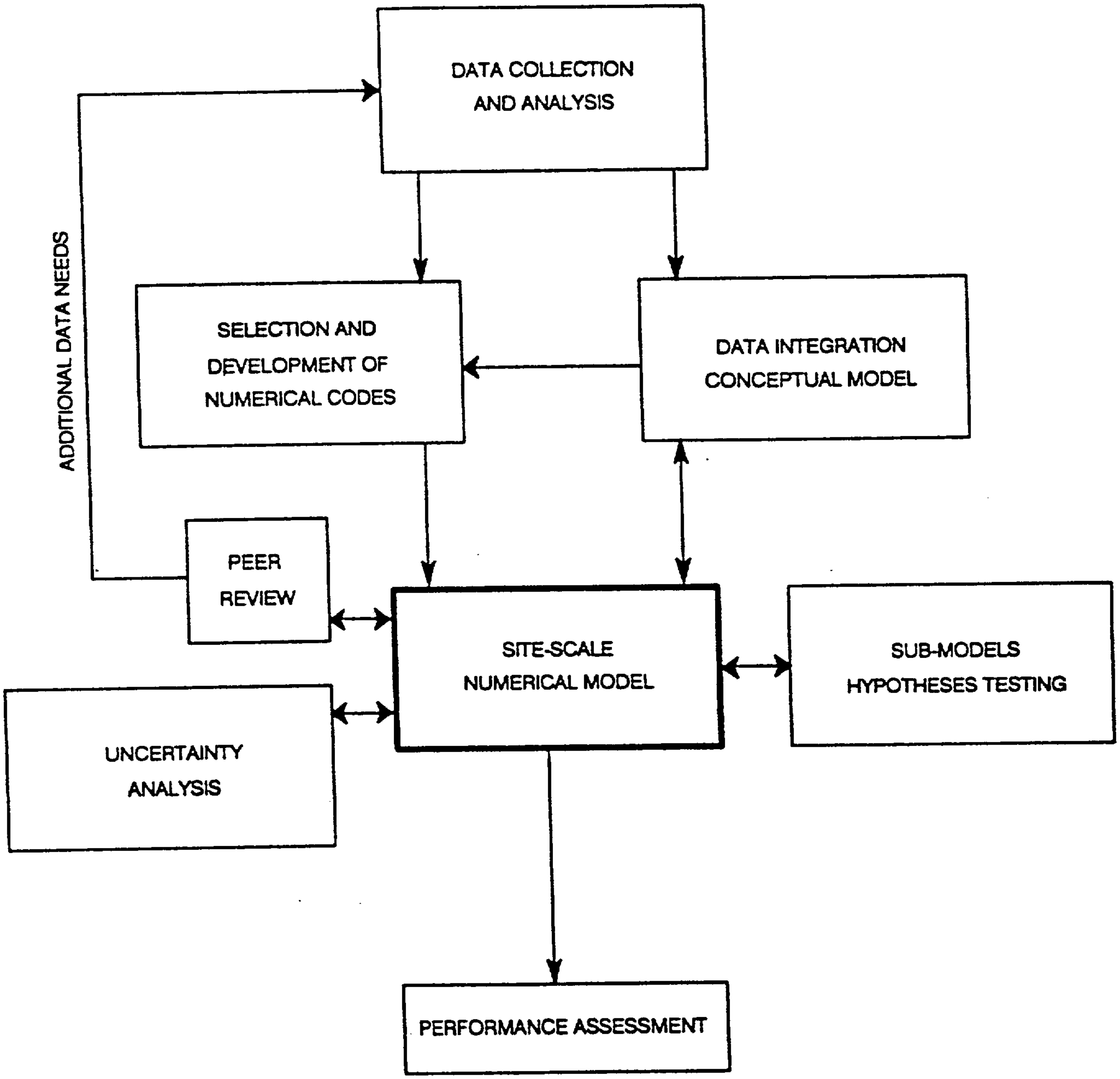


Figure 3-1. Simplified schematic of the overall project approach.

The site-scale model will be developed initially using various assumptions regarding moisture flow and gas flow in the mountain; these assumptions will gradually be verified or discarded as more laboratory and field data become available. For example, the best available assumptions regarding the spatial distribution of infiltration at Yucca Mountain will initially be used, and then later replaced by hard evidence as results from the studies on unsaturated-zone percolation become available (Studies 8.3.1.2.2.3, Unsaturated-zone percolation - surface-based studies; and 8.3.1.2.2.4, Unsaturated-zone percolation - ESF studies). Certain assumptions regarding matrix and fracture flow will also have to be made initially, to be replaced by results from various studies including Study 8.3.1.2.2.8 (Fluid flow in unsaturated, fractured rock).

3.1 Conceptualization of the unsaturated-zone hydrogeologic system

3.1.1 Objectives

The objectives of this activity are to develop conceptual models for the overall moisture-flow system within the unsaturated zone at Yucca Mountain.

3.1.2 Rationale for activity selection

The conceptual models of the system and component subsystems constitute the basis both for the hydrologic testing program at the site and for numerical hydrologic modeling of the site. Conceptual-model development is an ongoing, iterative process by which hypotheses and alternative hypotheses are evaluated and tested using laboratory experiments, field experiments, and analytical and numerical modeling. Hypotheses may be accepted, rejected, revised, or refined. The goal is to develop an internally consistent set of hypotheses that explain the current state of the hydrogeologic system at Yucca Mountain. Conceptual and numerical models that explain and are consistent with hydrologic observations at Yucca Mountain enhance scientific confidence in those models used to assess the capability of the site to isolate nuclear waste for a period of 10,000 years or longer.

3.1.3 General approach

Conceptual models for natural hydrogeologic systems are discussed in general terms in SCP Section 3.9 and are particularized to the Yucca Mountain site in SCP Section 3.9.3. The conceptual model of a system consists of a set of elements that describe the geologic framework for the system, delimit the hydrologic boundary conditions acting on the system, and identify the hydrologic and other related physical processes (e.g., moisture flow, heat flow, tectonic stresses, etc.) operating within the system. The internal system processes operating under the constraints imposed by the geologic framework and the boundary conditions determine the instantaneous state of the system. Because the model elements, in general, tend to change with time, the state of the system also tends to change with time. Consequently, the conceptual model must address the issue of system dynamics and response.

The state of an unsaturated-zone hydrogeologic system is defined, for example, by the spatial distributions of matric potential, liquid-water saturation, pore-gas pressure, temperature, and tectonic stress. The processes operating within the system, together with time-varying internal or external constraints, may cause any one or more of these state variables to change and, in turn, to alter the state of the system. The conceptual model for the system seeks to identify and quantify those principal relations between system processes and constraints that control the state of the system and, thus, govern the performance of the system. In the present context, those elements of system performance that relate to the isolation of high-level nuclear waste are of principal concern, and thus the conceptualization of the system needs to emphasize these elements.

Figure 3.1-1 summarizes the logic for the conceptualization of the unsaturated-zone hydrogeologic system. A descriptive heading for the analysis appears in the box of the second row. Below the analysis is the procedure that will be used. The figure summarizes the overall structure of the planned activity in terms the procedure to be employed.

3.1.3.1 Development of conceptual models

Generalized conceptual models for moisture flow within the unsaturated zone beneath Yucca Mountain have been developed by Montazer and Wilson (1984), Sinnock and others (1986) and Hoxie (1989). In addition, specific hydraulic problems were conceptualized by Peters and Klavetter (1988), and Wang and Narasimhan (1985, 1986). The essential features of these models define the hydrogeologic framework and identify the possible processes of moisture flow and storage that occur under the constraints imposed by the hydrogeologic framework. One conceptual model is illustrated schematically in Figure 3.1-2, which depicts a generalized east-west cross section through Yucca Mountain. The hydrogeologic framework consists of the eastward-tilted Yucca Mountain block, composed of the stratified sequence of hydrogeologic units listed in Figure 3.1-3. The block is bounded on the west by a westward-dipping high-angle normal fault (the Solitario Canyon fault), is transected internally by westward-dipping high-angle faults (for example, the Ghost Dance fault), and is bounded on the east by a set (or zone) of imbricate westward-dipping high-angle normal faults. The upper hydrologic boundary consists of the land surface, across which water enters the unsaturated zone as infiltration directly from precipitation. The lower hydrologic boundary is the water table, whose regional configuration is known. The figure also suggests the potential for the lateral redistribution of moisture within the nonwelded units and at the contacts between the welded and nonwelded units. Water may enter the mountain either through the densely welded, highly fractured tuffs or through the nonwelded tuffs where these crop out along canyons or washes. Faults may disrupt the lateral continuity of the nonwelded units and intercept lateral flow. Perched water zones may occur near faults due to downdip water movement if the faults are sealed or the fault openings are so large that faults are essentially seepage faces. Upward-directed arrows within the highly fractured, welded units represent the potential for upward redistribution of moisture as vapor due to vapor-pressure gradients that result from the geothermal gradient. These and other conceptual uncertainties are discussed more fully in the following sections.

3.1.3.2 Hydrologic hypotheses

The unsaturated-zone hydrologic hypotheses describe in general terms the manner in which water and gases move through the unsaturated zone, including the direction and paths of water flow. The testing and refinement of hydrologic hypotheses provide a logical and systematic approach to improving our understanding of how the hydrologic system functions, the result being an improved

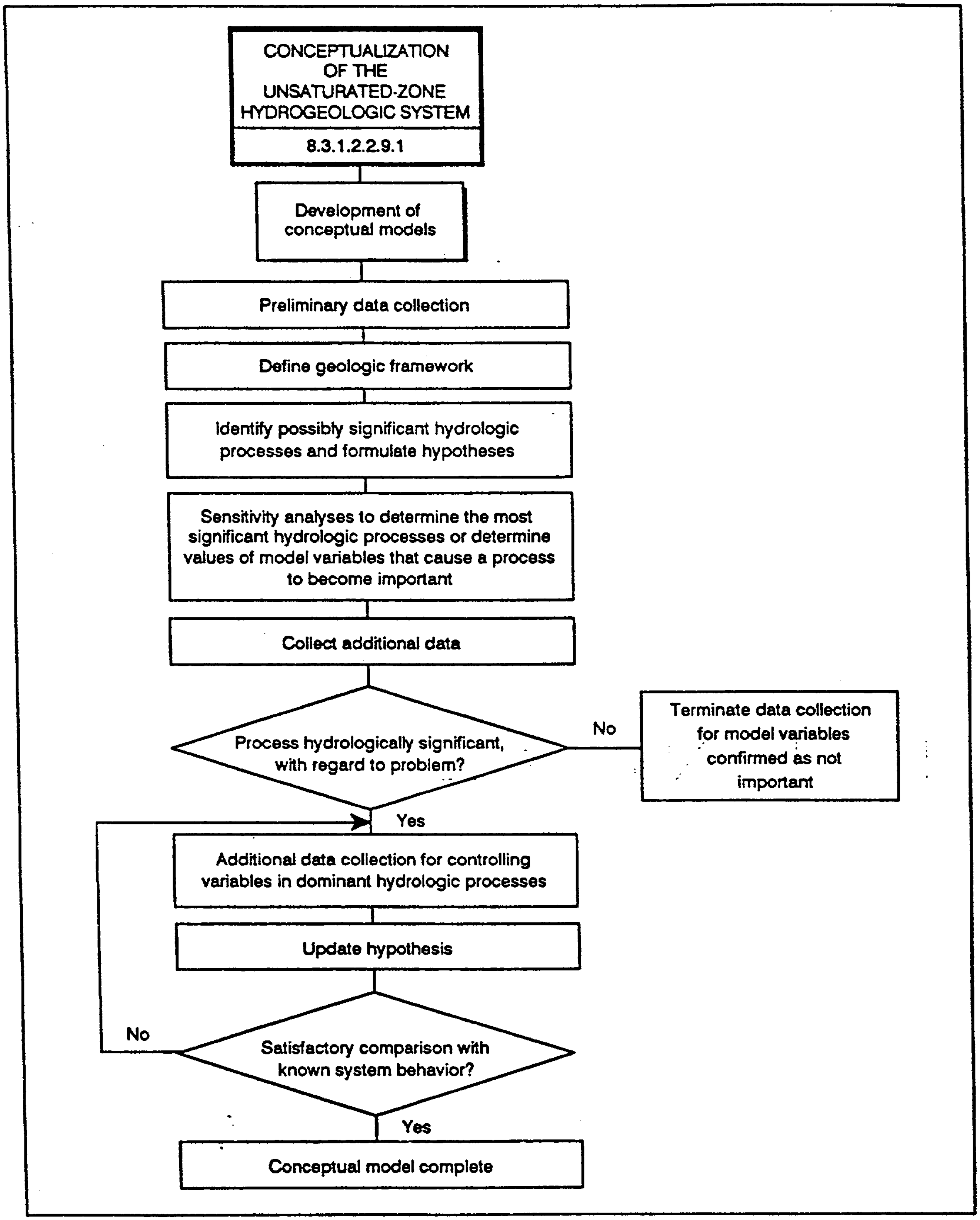
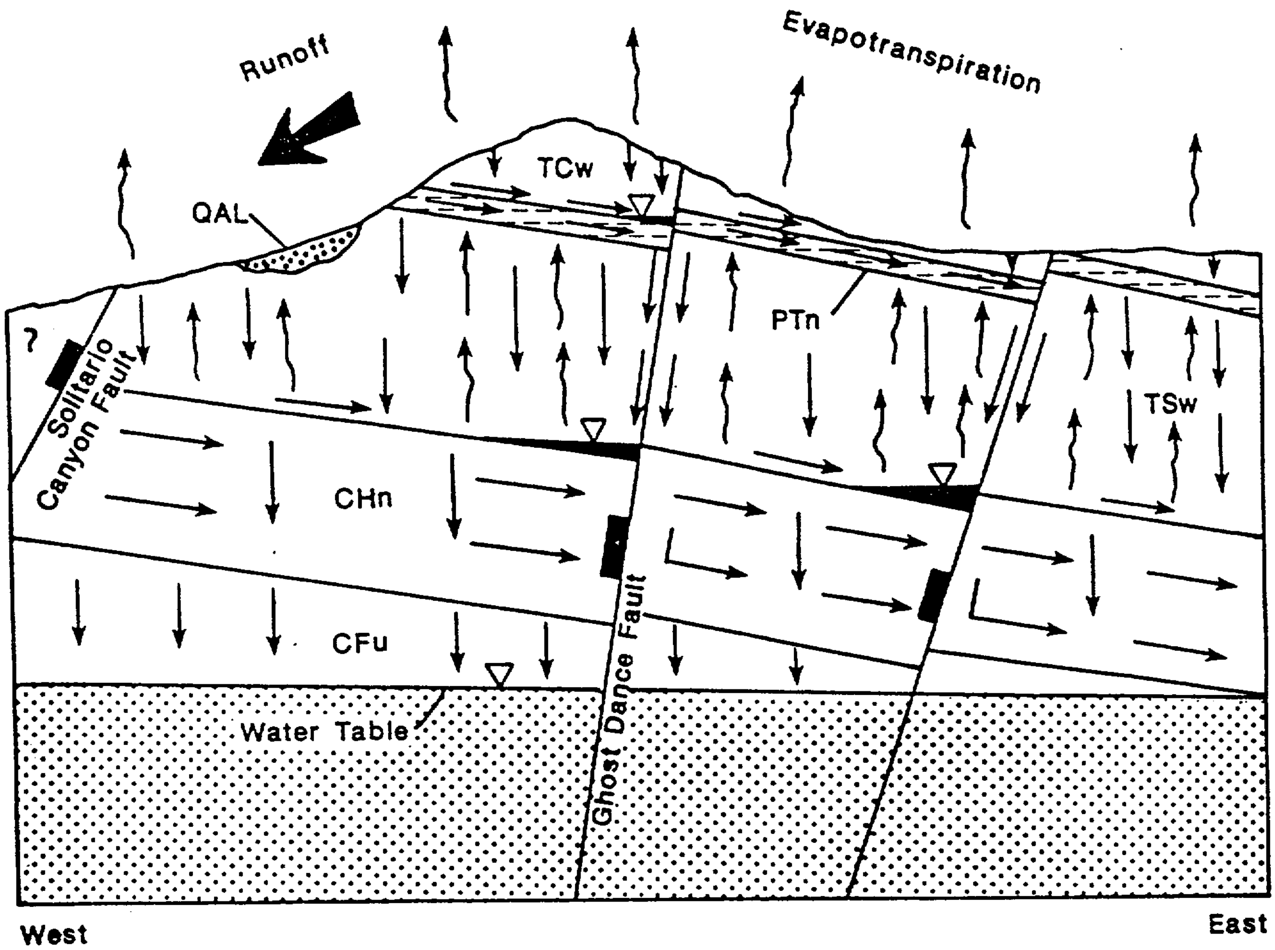


Figure 3.1-1. Logic diagram of the development of the conceptual models activity, showing analyses and methods.



Explanation

QAL	Alluvium
TCw	Tiva Canyon Welded Unit
PTn	Paintbrush Nonwelded Unit
TSw	Topopah Spring Welded Unit
CHn	Calico Hills Nonwelded Unit
CFu	Crater Flats (Undifferentiated) Unit

Liquid-Water Flow

Water-Vapor Flow

Normal Fault

Water Table

Possible Perched-Water Zone

Saturated Zone

? Unit Uncertain

Figure 3.1-2. Generalized west-east section through Yucca Mountain showing the conceptual moisture-flow system under natural conditions. Modified from Montazer and Wilson (1984).

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

[a]Sources: Montazer and Wilson (1984) and as noted in footnotes.

[b]Lithology summarized from Ortiz and others (1985).

Qal – Quaternary alluvium
TCw – Tiva Canyon welded unit
PTn – Paintbrush nonwelded unit
TSw – Topopah Spring welded unit
CHn – Calico Hills nonwelded unit
CHnv – Calico Hills nonwelded vitric unit
CHnz – Calico Hills nonwelded zeolitic unit
CFu – Crater Flat undifferentiated unit

Figure 3.1-3. Relation of unsaturated-zone hydrogeologic units with rock-stratigraphic units.

conceptual model which, in turn, leads to increased confidence in the hydrogeologic program (Figure 2.1-2).

In general, the conceptual model of a system consists of empirical data obtained from the system together with sets of hypotheses corresponding to each of the model elements for the system. A viable conceptual model requires that the hypotheses (1) fit the available data, (2) be as simple as is compatible with the data known, and (3) be mutually consistent. The sets of possible hypotheses satisfying these conditions need not be unique, and the occurrence of conflicting or competing hypotheses gives rise to the notion of alternative conceptual models.

The hypotheses that constitute the current conceptual model for the site unsaturated-zone hydrogeologic system are listed in SCP Table 8.3.1.2-2a.

If competing hypotheses are shown to affect important aspects of system performance, then tests must be devised to select from the competing hypotheses the one hypothesis that best applies to the system. Because complete knowledge of a macroscopic system and its governing processes and constraints is not attainable, formulating a conceptual model includes attempting to develop the simplest set of mutually consistent hypotheses that accounts for the essential aspects of the system.

Even if no internal conflicts exist, a conceptual model is by no means a fixed entity. The acquisition of new or improved data from laboratory or field measurements and tests, the results of numerical experiments, and the reconceptualization of model elements (for example, during peer review) may require that the conceptual model be revised with the addition of new hypotheses and the elimination or revision of previously accepted hypotheses. The development of a conceptual model, therefore, must be regarded as an evolving, frequently iterative process. In general, each hypothesis must be regarded as tentative and subject to continual examination and testing. Many of the field and laboratory experiments and tests of the site-characterization program are directed at examining the validity of hypotheses and at quantifying tenable hypotheses.

Independent peer review will be an important aspect of conceptual-model development. Peer review will be used to examine the completeness and consistency of the conceptual-model hypotheses and to ensure that the physics and mathematics of process hypotheses are formulated correctly. Changes in the conceptual model also should be subjected to appropriate peer review to ensure that the changes are both necessary and compatible with currently existing data.

From Table 8.3.1.2-2a of the SCP, a subset of hydrologic issues have been identified. These are listed in Table 3.1-1. Resolution of these issues may be considered one of the principal objectives of this activity. These are presented below with a discussion of supporting data and analyses. Other hydrologic issues may be found

Table 3.1-1. Current representation and alternative hypotheses for unsaturated-zone hydrologic system conceptual models for the Geohydrology Program

Hydrologic issue	Hypothesis	Research on the issue	Evaluation of the hypothesis
1) The role of faults in the hydrologic system	If faults are sealed or fault openings so large that they function as seepage faces, perched-water bodies or zones of higher saturation may form on the updip sides of the faults. Similar phenomena may occur where strata of vastly different permeability are offset across the fault and a relatively impermeable unit is brought in contact with a permeable unit on the updip side of the fault. Alternatively, if faults are open they may intercept water flowing parallel to unit contacts and redirect this flow downward.	Rulon and others (1986) Thordarson (1965) Wang and Narasimhan (1988)	Single- and cross-hole testing of fault planes or fault zones, characterization of fill materials, and long-term monitoring, in Activity 8.3.1.2.2.4.10 (Hydrologic properties of major faults). Future numerical investigations to test sensitivity of the flow system to the combined capillary and permeability characteristics assumed for the faults.
2) The role of the Paintbrush tuff nonwelded unit on the hydrologic system	Downward-flowing water may be diverted laterally within the Paintbrush Tuff and at the contacts with adjacent units, shedding water around the potential locations of the waste-emplacement drifts. Due to the contrasting permeabilities of its constitient members, the unit as a whole may be anisotropic with respect to permeability, and the permeability parallel to bedding may be many times larger than the permeability transverse to bedding. The Paintbrush tuff is also potentially significant because of its capacity to buffer transient infiltration moving through the fractures of the near-surface welded units.	Wang and Narasimhan (1986) Nitao and others (1992) Wittwer and others (1992) Ross (1990) Kume and Hammermeister (1990) Loskot and Hammermeister (1992) Rautman and Flint (1992) Whitfield (1985)	Numerical simulation to investigate the manner in which the effective properties of the Paintbrush tuff nonwelded unit are related to the unsaturated properties of the sub-units comprising it. This numerical investigation will also examine the potential for the creation of capillary barriers at the interfaces between the various sub-units, using data supplied from Activity 8.3.1.2.2.3.1 (Matrix hydrologic properties testing). Modeling to examine the effects of locally concentrating infiltration in space, and the capacity of the Paintbrush tuff nonwelded unit to redistribute infiltration spatially as well as temporally. Modeling to concentrate flow in both time and space to examine the effects on steady-flow behavior through the underlying Topopah Spring unit.

Table 3.1-1. Current representation and alternative hypotheses for unsaturated-zone hydrologic system conceptual models for the Geohydrology Program (continued)

Hydrologic issue	Hypothesis	Research on the issue	Evaluation of the hypothesis
3) Investigation of the expected relative contributions of liquid-water and water-vapor fluxes to the net moisture flow within the unsaturated-zone system.	In arid environments where potential evapotranspiration greatly exceeds precipitation, average downward moisture fluxes are expected to be relatively small, and much of the pore space is air-filled. Consequently, the movement of moisture as vapor can play a significant role in the redistribution of liquid water. Large daily temperature fluctuations can create temperature gradients in the near surface that create associated gradients in vapor pressure. These temperature fluctuations are dampened with depth in a way that depends upon the amplitude of temperature variations at the surface, the periodicity of the fluctuations, and the thermal diffusivity of the media. Beyond the depth at which these surface fluctuations in temperature are dampened out, the geothermal gradient suggests an upward diffusive vapor flux.	Bedinger (1987) Scanlon (1992) Hillel (1980) Sass and others (1988) Tsang and others (1990) Church and others (1983-1986) Kipp (1987) Weeks (1978)	Examining the potential for moving recently infiltrated water through the unsaturated zone by evaporation at shallow depths and condensation at greater depths, as well as the potential for discharge of recently infiltrated fracture water as water vapor as a result of convective and diffusive processes. Estimation of pneumatic diffusivities by modeling, using barometric pressure-change data collected by pressure transducers in stemmed boreholes, in Activity 8.3.1.2.2.3.2 (Site vertical-boreholes studies).

Table 3.1-1. Current representation and alternative hypotheses for unsaturated-zone hydrologic system conceptual models for the Geohydrology Program (continued)

Hydrologic issue	Hypothesis	Research on the issue	Evaluation of the hypothesis
4) Assessment of the likelihood for the occurrence of geothermally or barometrically-driven convection cells involving the upward flow of water vapor with a corresponding downward return flow of water.	Under steady-state conditions in a closed system subjected to a geothermal gradient, upward vapor flux must be exactly canceled by the net downward liquid-water flux. The Topopah Spring unit may approximate such a closed system with regard to gas and water flow. Geochemical evidence suggests there is little gas communication between the shallow and deep portions of the Yucca Mountain unsaturated zone, a condition that may be due to limited gas permeability within certain horizons of the Paintbrush tuff nonwelded unit at existing water saturations and with the relative sparseness of air-filled fractures intersecting this unit. When the permeability ratio between densely fractured welded units and sparsely fractured nonwelded units equals or exceeds 1000, modeling has predicted the development of convection cells within the Topopah Spring unit under ambient temperatures beneath the east flank of Yucca Mountain. For a permeability ratio of 1, flow lines originating on the flanks of the mountain circulated below the proposed repository horizon and exited along the mountain crest. For permeability ratios of 10 and 100, flow regimes were intermediate between the two cases described above.	Tsang and others (1990) Thorstenson and others (1989) Lu and others (1991)	Building upon prior modeling efforts by considering the potential for downward liquid-water flux to perturb the temperature field and thus patterns of air and vapor movement. Consideration of effects of major structural features on air-movement patterns.

Table 3.1-1. Current representation and alternative hypotheses for unsaturated-zone hydrologic system conceptual models for the Geohydrology Program (continued)

Hydrologic issue	Hypothesis	Research on the issue	Evaluation of the hypothesis
5) The potential for downward flow to bypass the zeolitic facies of the Calico Hills unit	The zeolitic facies of the Calico Hills is considered to be one of the most important natural barriers to potential radionuclide migration because of the tendency for most radionuclides to be absorbed by zeolitic minerals in this facies. The identification of potential flow paths that bypass this facies is therefore considered to be an important goal of this study. The permeability of the CHn vitric facies is substantially greater than the zeolitic facies, and therefore the distribution of the two facies can affect the flow of water below the potential repository horizon.	Montazer and Wilson (1984) Sheppard and others (1988) Thordarson (1965) Rulon and others (1986)	Utilize information on the spatial distribution and hydraulic properties of both the zeolitic facies and structural features to assess the likelihood for downward flow to bypass the zeolitic facies to the water table.

to be important as more data are collected on Yucca Mountain; these will be identified and addresses as needed during their proposed study.

1) The role of faults in the hydrologic system.

Figure 3.1-2 suggests that faults may impact the flow system in a variety of ways. If faults are sealed or fault openings so large that they function as seepage faces, perched-water bodies or zones of high saturation may form on the updip sides of the faults. Similar phenomena may occur where strata of vastly different permeability are offset across the fault and a relatively impermeable unit is brought in contact with a permeable unit on the updip side of the fault. Alternatively, if faults are open they may intercept water flowing parallel to unit contacts and redirect this flow downward. Simulations by Rulon and others (1986) showed that for low fluxes, the PTn unit was effective in diverting water laterally toward the fault, thus reducing the flux that could potentially contact the waste canisters, assuming that waste had not been emplaced near the fault. For relatively large fluxes, perched-water bodies formed at the contact between the TSw and CHn units drained into the fault. Interception of perched water at this depth is potentially of concern because radionuclides leached from the waste canisters might bypass the low-permeability zeolitic units. Because of their sorptive properties, the zeolitic units are considered to be the principal barrier to radionuclide migration. Results of these simulations must be viewed with caution, however, because of the poorly known values for the hydrologic properties employed, especially for the faults. Faults in similar rock types at Rainier Mesa were reported by Thordarson (1965) to be open and water-filled within perched-water zones contained in zeolitic nonwelded tuffs penetrated by tunnels excavated for the first underground nuclear tests. However, faults within the overlying friable nonwelded tuffs were described as being generally sealed with clay gouge. Characterization of hydrologic properties of major faults is described in YMP-USGS SP 8.3.1.2.2.4. Planned activities include single- and cross-hole testing of the fault plane or fault zone; characterization of fill materials, including unsaturated hydraulic properties; and long-term monitoring.

Wang and Narasimhan (1988) examined the effects of faults transverse to layering on the flow system at Yucca Mountain. The fault considered, the Ghost Dance Fault, was assumed to be sufficiently open so that it possessed no capillary properties and thus essentially behaved as a seepage face. Therefore, water did not enter the fault until pressure heads along the interface between the adjaçent formations and the fault became positive. Wang and Narasimhan (1988) found that eastward-tilting of the units at 6 degrees contributes to the redistribution of flow laterally, primarily through the nonwelded units, resulting in larger saturations and greater vertical velocities near the downdip end of the flow system adjacent to the fault. The magnitude of these effects depended on the prescribed flux. For a net infiltration rate of 0.1 mm/yr, the lateral variations in saturation, pressure head, and potential were found to be relatively minor, and nowhere were pressure heads adjacent to the fault sufficiently large that water entered the fault. For a net infiltration rate of 0.5 mm/yr, the lateral variations were more pronounced, the rock matrix in the welded hydrogeologic units nearly saturated, and water was predicted to enter the fault at the interface between the vitric facies and the underlying, relatively less permeable zeolitic facies of the Calico Hills. The work of Wang and Narasimhan (1988) also recognized that the capillary properties attributed to the fault zone have a significant influence on the relative proportion of flow diverted laterally. In particular, lateral flow is enhanced by faults that simultaneously possess high permeability and high suction, a phenomenon which may result if the fault is expressed as either a zone of dense fractures in which individual fractures are of small average aperture, or a zone which consists of a few medium or large aperture fractures which are filled with gouge. Numerical investigations planned in this study plan will further test the sensitivity of the flow system to the combined capillary and permeability characteristics assumed for the faults.

(2) The role of the Paintbrush Tuff nonwelded unit on the hydrologic system.

The hydrogeologic unit PTn, which is composed of a number of mappable stratigraphic members, can be of great hydrological importance in a number of ways. First, as suggested by Figure 3.1-2, downward-flowing water may be diverted laterally within this unit and at the contacts with adjacent units, shedding water around the potential locations of the waste-emplacement drifts. Due to the contrasting permeabilities of its constituent members (Flint and Flint, 1990), the unit as a whole may be anisotropic with respect to permeability, with the permeability parallel to bedding being perhaps many times larger than the permeability transverse to bedding. The degree of anisotropy of a layered sequence of nonwelded tuffs, like that of layered soils (Stephens and Heerman, 1988) is probably also a function of the degree of saturation of the constituent members.

The Paintbrush tuff nonwelded unit is also potentially important hydrologically by virtue of its capacity to buffer transient infiltration moving through fractures of the near-surface welded units. As discussed in Section 3.3, numerical modeling of the Yucca Mountain site could be greatly simplified if it could be demonstrated that the temporal and spatial variations in net infiltration had negligible effect on the long-term behavior of the flow system at depth and the capability of Yucca Mountain to safely isolate nuclear waste. The capacity of the Tiva Canyon and Paintbrush hydrogeologic units to buffer extreme, transient infiltration pulses, so that flow through the underlying Topopah Spring unit remains essentially steady and predominantly matrix-dominated, was examined by Wang and Narasimhan (1986). That numerical study, which utilized both composite and dual-porosity models to represent these hydrogeologic units, found that pulsing infiltration essentially did not perturb the long-term steady-state flow behavior within the Topopah Spring unit, and that liquid-water flow within the fractures of this unit remained insignificant even when the cumulative infiltration resulting from a net infiltration rate of 0.5 mm/yr sustained over a 5,000-year period entered the fractures of the Tiva Canyon unit within a 0.2-year interval. More recently, Nitao and others (1992), showed that most of the drained pore space potentially available to infiltrating water was provided by this unit. The ability of the PTn unit to smooth locally and temporally large infiltration events is probably related to a number of factors, including fracture continuity through this unit, the anisotropy and the thickness of this unit, which vary considerably over the site area (Wittwer and others, 1992).

When materials with relatively small pores overlie material with relatively larger pores, water movement into the underlying material is delayed if matric potentials at the interface between the two materials are low and the effective hydraulic conductivity of the underlying material is too low to accept the flux. This situation may exist between adjacent subunits within the PTn unit, or between the PTn unit and the fractures of the underlying welded units. The formation of capillary barriers in layered sequences can promote the lateral spreading of localized infiltration. When the layers are tilted, gravity promotes movement in the downdip direction. Recent work by Ross (1990) has resulted in analytical expressions for the diversion capacity of capillary barriers and the lateral extent over which they maintain their effectiveness. Both maximum diversion capacity and effective lateral extent were shown to be directly proportional to the saturated conductivity of the upper unit and the tangent of the dip angle of bedding and inversely proportional to the sorptive number as defined by Philip (1969) for the upper unit. Additionally, effective lateral extent was found to be inversely proportional to the flux at the land surface. Additional calculations done by Ross (written communication, 1990) suggested that a capillary barrier capable of diverting 15 to 150 m^3 of water per year per meter thickness along the strike of the beds may be formed between the Paintbrush nonwelded unit and the underlying fractures of the Topopah Spring hydrogeologic unit. Using the value for saturated conductivity and sorptivity provided by Ross (written communication, 1990) for the Paintbrush unit, the effective lateral extent of this capillary barrier was calculated as 600 to 6,000 m for a percolation rate of 0.1 mm/yr, and can be calculated as 13 to 130 m wide for a percolation rate of 4.5 mm/yr, depending on whether the saturated hydraulic conductivity of the Paintbrush nonwelded unit is taken as 3.0 or 30.0 m/yr.

All of the above analyses have assumed uniform properties for the PTn unit. Figures 3.1-4 through 3.1-6 and Table 3.1-2 show water saturation, water potential, and porosity versus depth profiles based on data determined for cores taken from corehole USW UZ-7 (Kume and Hammermeister, 1990). Test hole USW UZ-7 was drilled and cored to a total depth of 62.94 m. The drilling was done using air as a drilling fluid to minimize disturbance to the water content of cores, drill-bit cuttings, and borehole wall rock. The

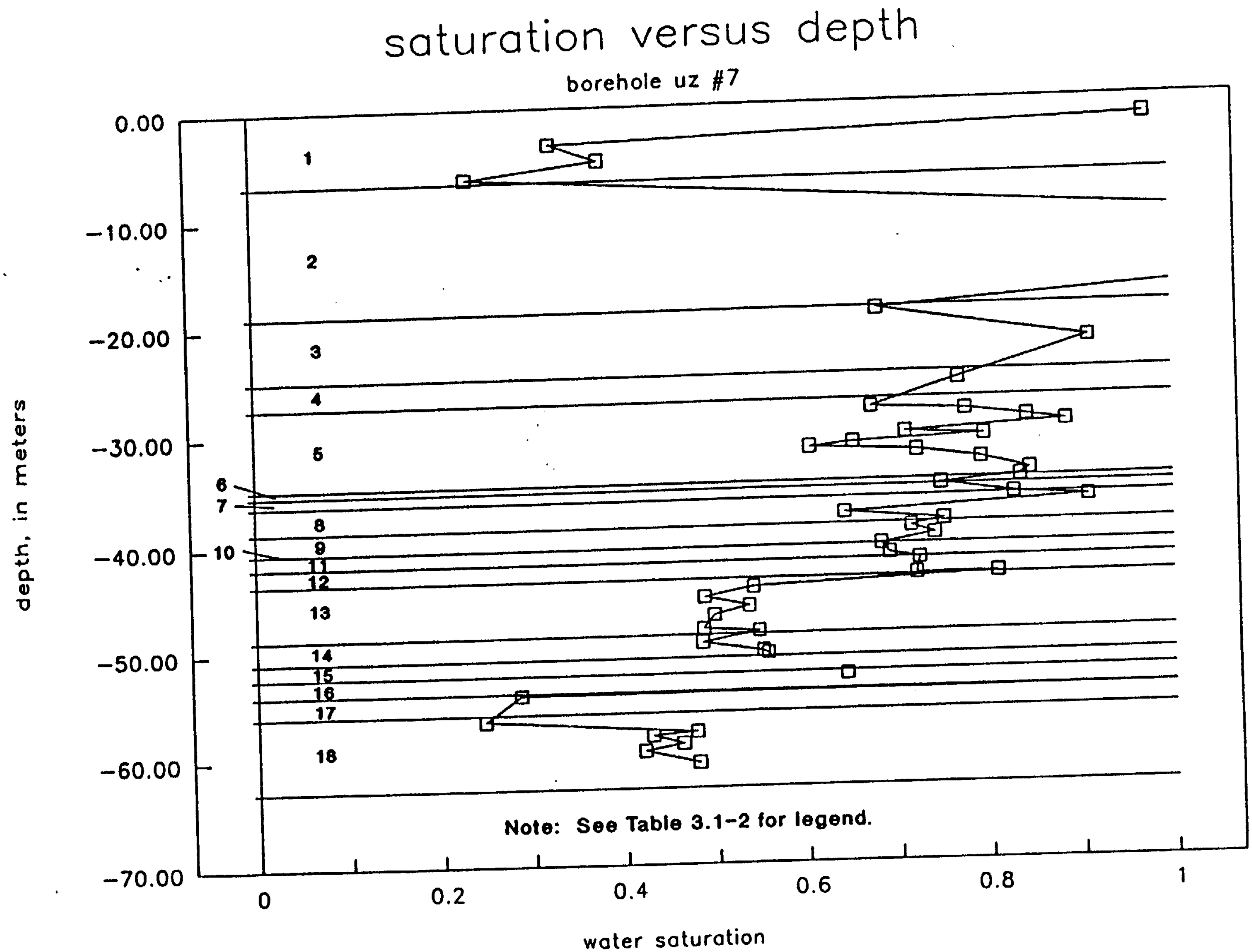


Figure 3.1-4. Saturation of drive cores taken from test hole UZ#7.

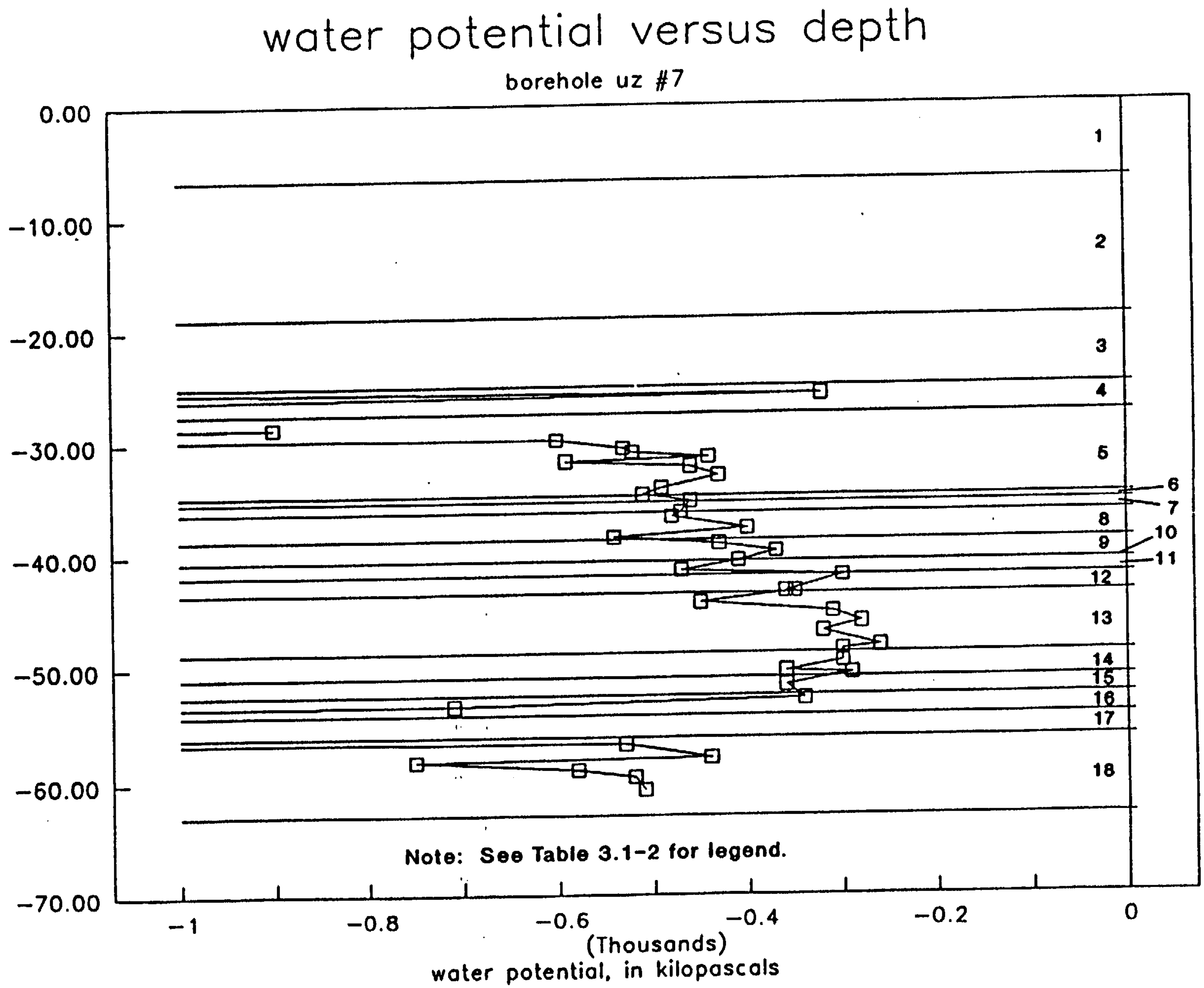


Figure 3.1-5. Water potential of drive cores taken from test hole UZ #7

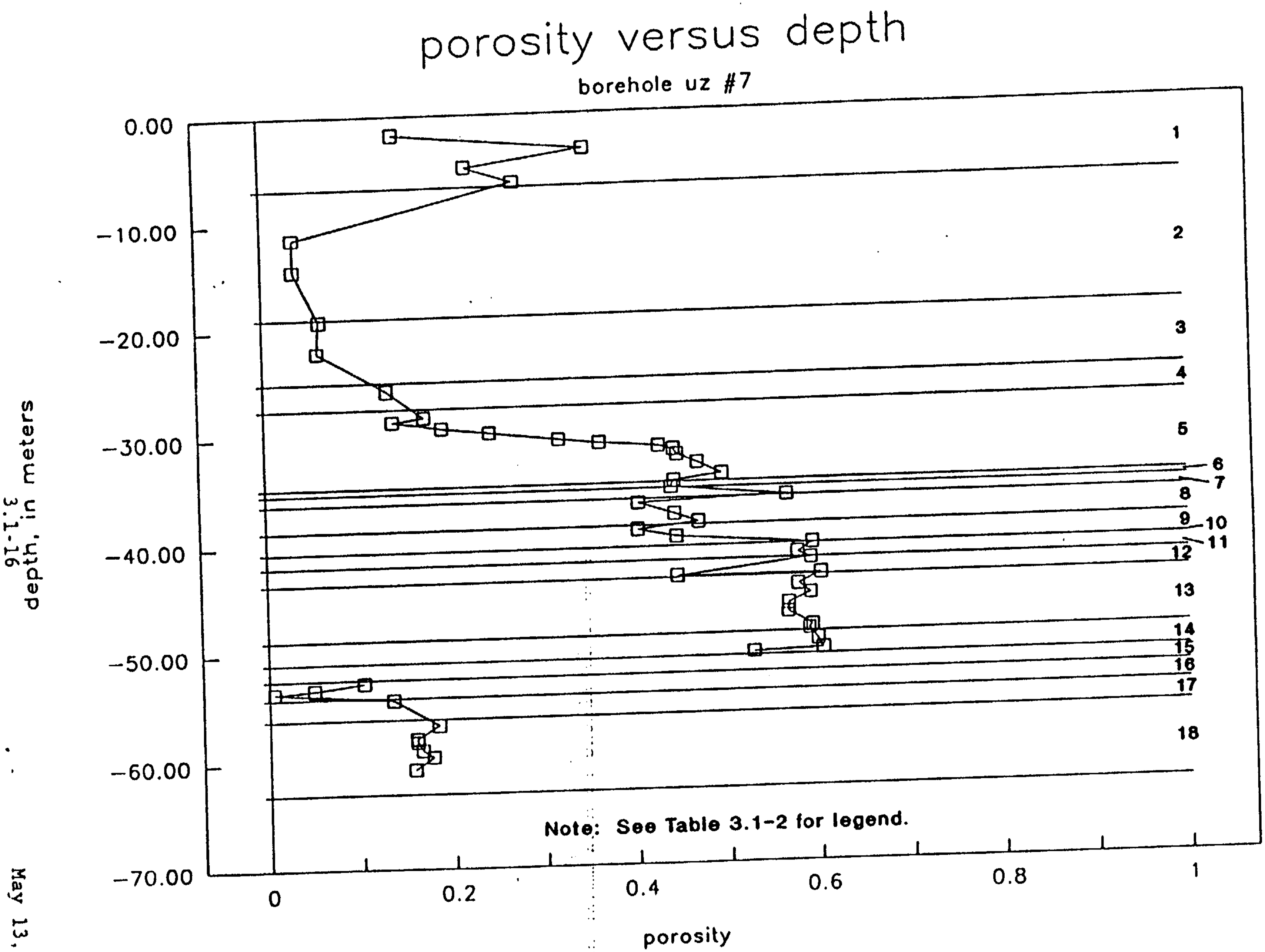


Figure 3.1-6. Porosity of drive cores taken from test hole UZ #7

LEGEND

1	alluvium	
2	tc,dw,dv	(Tiva Canyon, densely welded, devitrified)
3	tc,mdw,dv	(Tiva Canyon, moderately to densely welded,devitrified)
4	tc,mw,dv	(Tiva Canyon, moderately welded, devitrified)
5	tc,npw,v	(Tiva Canyon, non to partially welded, vitric)
6	bd,rw,mi,ms,v	(bedded, reworked, moderately indurated, moderately sorted, vitric)
7	bd,af,mi,mws,v	(bedded, airfall, moderately indurated, moderately to well sorted, vitric)
8	bd,af,si,ss,v,ar	(bedded, airfall, slightly indurated, slightly sorted, vitric, argillic)
9	bd,rw,mi,sms,v	(bedded, reworked, moderately indurated, slightly to moderately sorted, vitric)
10	bd,af,si,ms,v	(bedded, airfall, slightly indurated, moderately sorted, vitric)
11	pc,nw,v	(Pah Canyon, nonwelded, vitric)
12	bd,af,mi,v	(bedded, airfall, moderately indurated, vitric)
13	bd,af,si,ss,v	(bedded, airfall, slightly indurated, slightly sorted, vitric)
14	ts,af?,nw,v	(Topopah Springs, airfall(?), nonwelded, vitric)
15	ts,af,wi,v	(Topopah Springs, airfall, well indurated, vitric)
16	ts,dw,vitro	(Topopah Springs, densely welded, vitrophere)
17	ts,dw,dv	(Topopah Springs, densely welded, devitrified)
18	ts,mw,vpc	(Topopah Springs, moderately welded, vapor phase crystallization)

Table 3.1-2 Legend showing stratigraphic and lithologic information for Figures 3.1-4, 3.1-5, and 3.1-6.

unsaturated-zone rock consisted of alluvium, welded and partially welded to nonwelded ash-flow tuff, bedded and reworked ash-fall tuff, nonwelded ash-fall tuff, and welded ash-flow tuff. Alluvium and welded ash-flow tuffs were cored at selected intervals; nonwelded ash-fall and partially welded to nonwelded ash-flow tuffs, and bedded and reworked ash-fall tuffs were continuously cored. Figures 3.1-4 and 3.1-6 show that saturations and porosity exhibit considerable vertical variability. The stratigraphic units have been sub-divided on the basis of lithologic descriptions provided by the wellsite geologist who examined the core. It is clear that the saturation profiles would be difficult to understand if the microstratigraphy were not considered. Data has also been analyzed for coreholes USW UZ-4 and USW UZ-5 based on data from Loskot and Hammermeister (1992). At these holes, the members comprising the PTn unit are different from those at USW UZ-7. Nonetheless, saturations of the nonwelded units at all three holes are less than 100 percent. At all three locations, the presence of a low porosity (<2 percent), densely welded "vitrophyre", apparently saturated, may restrict downward flow. This low-porosity horizon was also noted by Rautman and Flint (1992) for data collected along a transect and from neutron-hole drilling. The limited data thus suggest that this horizon may be fairly pervasive. Based on linear regression of water potentials between depths of -30.0 and -50.0 m at USW UZ-7 (r^2=0.69), the total head gradient in the 20 m above the vitrophyre is -0.18, indicating upward flow. Varying the slope of the regression by plus or minus twice the standard deviation results in calculated total head gradients of -0.47 (upward flow) and 0.117 (downward flow). The harmonic mean of estimated hydraulic conductivities over this interval is 3.31 mm/yr. Multiplying the values defining the 95% confidence interval for the head gradients by effective hydraulic conductivity results in fluxes ranging from 1.56 mm/yr upward to 0.39 mm/yr downward. Thus, although water saturation over this depth interval may be high, head gradients do not suggest significant downward water movement. Since matrix permeability of the vitrophyre is probably negligible (based on its small porosity), fractures must transmit any downward flux across this unit. Theoretical water permeability versus water-potential curves developed for fractures suggest that water potential in a fracture must be larger than -0.1 MPa (-1.0 bar) to initiate flow in a fracture with apertures averaging even only a few microns (see Section 3.3). Thus, capillary barrier effects may account for the relatively large water potentials near this horizon at all three holes. These data are presented as the types of data that are becoming available for analysis, and conclusions must be considered tentative until many such profiles are examined. Drill cuttings were continually collected and their gravimetric moisture contents measured during the drilling of boreholes USW UZ-1 and USW UZ-6 (Whitfield, 1985), and USW UZ-7 (Kume and Hammermeister, 1990). However, because USW UZ-1 and USW UZ-6 both used air as a drilling fluid and the cuttings were returned to the surface within the air stream, significant drying of the cuttings may have occurred and so estimates of *in situ* saturations remain tentative at present.

Numerical simulation will be employed to investigate the manner in which the effective properties of the Paintbrush nonwelded unit are related to the unsaturated properties of the sub-units comprising it. This numerical investigation will also examine the potential for the creation of capillary barriers at the interfaces between the various sub-units of the Paintbrush hydrogeologic unit using data supplied from SCP Activity 8.3.1.2.2.3.1 (Matrix hydrologic properties testing) in Study 8.3.1.2.2.3 (Unsaturated-zone percolation - surface-based studies).

Analogous to the work of Wang and Narasimhan (1986), it is proposed that future modeling work examine the effects of concentrating infiltration in space so that although the areally averaged net infiltration rates remain at 0.1 or 0.5 mm/yr, locally the infiltration rates can be many orders of magnitude higher. The capacity of the Paintbrush nonwelded hydrogeologic unit to redistribute infiltration spatially as well as temporally will then have been examined. Spatial redistribution may occur because of pronounced capillary pressure gradients which result when recharge to the Paintbrush nonwelded unit occurs at isolated locations. Finally, as a worst-case scenario, flow will be concentrated in both time and space, while respecting the constraints imposed by a temporally and spatially averaged flux value of either 0.1 and 0.5 mm/yr, and the effects on the steady-flow behavior through the underlying Topopah Spring unit observed.

(3) Investigation of the expected relative contributions of liquid-water and water-vapor fluxes to the net moisture flow within the unsaturated-zone system.

In arid environments where potential evapotranspiration greatly exceeds precipitation, average downward moisture fluxes are estimated to be relatively small (Bedinger, 1987), and much of the pore space is air-filled. Consequently, the movement of moisture as vapor can play a significant role in the redistribution of liquid water (see, for example, Scanlon, 1992). Large daily temperature fluctuations can create temperature gradients in the near surface that create associated gradients in vapor pressure. These temperature fluctuations are dampened with depth in a way that depends on the amplitude of temperature variations at the surface, the periodicity of these fluctuations, and the thermal diffusivity of the media (Hillel, 1980). Beyond the depth at which these surface fluctuations in temperature are dampened out, the geothermal gradient suggests an upward diffusive vapor flux. Data published by Sass and others (1988) indicate that temperature gradients within the unsaturated zone in Yucca Mountain range from about 0.015 to 0.060 degrees Celsius per meter. Fifty-seven measurements of thermal conductivity reported on core samples preserved at ambient saturations were observed to be bimodally distributed, with modes of 1.0 and 2.1 watts per meter-degree Kelvin representing the nonwelded and welded tuff units, respectively. Measured thermal conductivities were combined with the observed thermal gradients to estimate heat fluxes within the unsaturated zone. Although data of higher quality are needed to make unambiguous interpretations, heat flow appeared to vary inversely with thickness of the unsaturated zone, and the average heat flow from the unsaturated zone of approximately 0.041 watts per m^2 was approximately 20 percent less than the average heat flow from the saturated zone, suggesting the possibility that heat was being removed nonconductively from the unsaturated zone by vaporization and advective removal of water by air circulating in fractures. Vaporization of 0.1 mm of water per year would consume about 5.8 calories per cm^2 per year, which is about 0.008 watts per m^2 or approximately the unsaturated-zone heat-flow deficiency (Sass and others, 1988, p.47) Using the numerical model TOUGH and assuming an unfractured, homogeneous medium between the water table and ground surface, Tsang and others (1990) showed that for a closed system, net upward vapor flux was exactly canceled by the net downward liquid-water flux when the effects of low atmospheric relative humidity on capillary pressure in the near-surface rock were ignored. However, when capillary pressure in the near-surface rock was fixed at a value corresponding to 50 percent relative humidity by Kelvin's equation and flow across the ground surface permitted to occur, both liquid and vapor fluxes were upward and totaled 0.04 mm/yr, with vapor movement being the dominant mechanism for upward moisture transport.

Air entering the outcropping formations at Yucca Mountain has an estimated mean relative humidity of 0.28 along Yucca Ridge and 0.33 in an alluvial valley to the east of the mountain (Tsang and others, 1990). Once in the rock, the relative humidity of this air becomes greater as liquid and water vapor approach equilibrium in accordance with Kelvin's equation. When atmospheric pressure decreases at a later time, moist soil gas is returned to the atmosphere, resulting in a net loss of formation moisture with each cycle of rise and fall in barometric pressure. Using a simple analytical expression which assumed piston displacement of gas in the unsaturated zone and constant formation properties with depth, Tsang and others (1990) estimated the moisture removal rate by barometric pumping to be approximately 0.32 mm/yr, or on the same order of magnitude as current estimates of liquid-water percolation through the unsaturated zone at Yucca Mountain. These estimates of moisture loss due to barometric pumping were calculated using data from Church and others (1983-1986) which indicated that the average pressure change in a 24-hour cycle is 0.5 kPa for the Ridge Site and 0.8 kPa for the Alluvial Site and that the mean pressure (for the period 1982-1984) was 85.2 kPa.

Barometric pumping may contribute to the convective movement of water vapor in the shallow unsaturated zone, thereby either augmenting or offsetting upward vapor-movement due to temperature and vapor pressure gradients. During summer months, near surface temperatures may be higher than those at depth, resulting in larger vapor pressures in the near surface, whereas the opposite may be true in winter (Kipp, 1987). The potential for moving recently infiltrated water through the unsaturated zone by evaporating it at shallow depths and condensing it at greater depths, as well as the potential for discharging recently infiltrated fracture water as water vapor due to convective and diffusive processes, will be examined as part of this study.

Gas permeability data will be obtained from pneumatic diffusivities which, in turn, will be estimated by locating pressure transducers at various depths within stemmed boreholes (SCP Activity 8.3.1.2.2.3.2, Site vertical-borehole studies, in Study 8.3.1.2.2.3, Unsaturated-zone percolation - surface-based studies). These transducers will record the manner in which barometric pressure changes occuring at the land surface are attenuated and shifted in phase as they propagate through the unsaturated-zone units. From these data, estimates of pneumatic diffusivity may be made using the parameter estimation model described by Weeks (1978).

(4) Assessment of the likelihood for the occurrence of geothermally or barometrically driven convection cells involving the upward flow of water vapor with a corresponding downward return flow of water.

As discussed above, the work of Tsang and others (1990) illustrates that under steady-state conditions in a closed system subjected to a geothermal gradient, upward vapor flux must be exactly cancelled by the net downward liquid water flux. The Topopah Spring unit may approximate such a closed system with regard to gas and vapor flow. Geochemical evidence suggests there is little gas communication between the shallow and deep portions of the unsaturated zone at Yucca Mountain (Thorstenson and others, 1989). Lack of communication may be due to limited gas permeability within certain horizons of the Paintbrush nonwelded hydrolgeologic unit at the existing water saturations and the relative sparseness of air-filled fractures transecting this unit. Recent modeling (Lu and others, 1991) has suggested that the shallow and deep air-circulation systems remain relatively isolated from each other when the permeability ratio between the densely fractured welded units and the sparsely fractured nonwelded units equals or exceeds 1,000. Furthermore, at these permeability ratios, convection cells within the Topopah Spring unit were predicted to develop at ambient temperatures beneath the east flank of Yucca Mountain. For a permeability ratio of 1, flow lines originating on the flanks of the mountain circulated below the horizon of the proposed repository and exited along the crest of the mountain. For permeability ratios of 10 and 100, flow regimes were intermediate between the two cases described above.

Whereas the work of Tsang and others (1990) employed a highly simplified stratigraphy and assumed the system to be either open or closed, the work of Lu and others (1991) and Thorstenson and others (1989) clearly indicates that both shallow open and deep closed air-circulation systems may exist at Yucca Mountain, depending on the permeability to gas of the Paintbrush unit. On the other hand, neither the work of Lu and others (1991) nor Tsang and others (1990) examined the potential for downward liquid-water flux to perturb the temperature field and, hence, the patterns of air and vapor movement. The patterns of air movement through Yucca Mountain are also expected to be altered by the presence of major structural features such as the Ghost Dance fault. This study proposes to build on the work of Tsang and others (1990) and Lu and others (1991) by considering these complicating factors.

(5) The potential for downward flow to bypass the zeolitic facies of the CHn unit.

The zeolitic facies of the Calico Hills is considered to be one of the most important natural barriers to potential radionuclide migration because of tendency for most radionuclides to be adsorbed by zeolitic minerals in this facies. The identification of potential flow paths that bypass this facies is therefore considered to be an important goal of this study. As noted by Montazer and Wilson (1984), the permeability of the vitric facies of the CHn unit is substantially greater than that of the zeolitic facies, and therefore the distribution of the two facies can be expected to affect the flow of water below the potential repository horizon. The thickness of the zeolitic facies generally increases from the southwest to northeast beneath Yucca Mountain. Beneath the southern two-thirds of the central block, the lower part of the CHn unit is zeolitized and the upper part is vitric. Beneath the northern and northeastern parts of the central block, the entire unit is zeolitized (Montazer and Wilson, 1984, Figure 4). Sheppard and others (1988, Figure 3) showed diagenetic zonation among different zeolite minerals in the central and northern parts of Yucca Mountain.

Because the intrinsic permeability of the zeolitic tuffs is comparable to that of densely welded tuff (roughly on the order of 10^{-18} m^2), but the zeolitic tuffs are thought to be relatively unfractured, perched water within Yucca Mountain may be most likely to occur within and above the zeolitized facies of the CHn unit. At Rainier Mesa, zeolitic-bedded tuffs of the Indian Trail Formation restrict downward flow and both matrix pores and fractures within the zeolitic-bedded tuffs were completely saturated at the time they were penetrated by tunnels (Thordarson, 1965). Measurements of specific conductance on both interstitial water and water that entered the drifts through faults suggested that the salinity of the interstitial water was much greater than that of the fracture water (Thordarson, 1965, p. 76). It was not clear whether differences in specific conductance were due to "addition of ions to pore water by ionization of clay particles in the rock", or to differences in residence time. If the latter, the data indicate relatively little communication between matrix water and fracture water, suggesting that much of the effective porosity and adsorptive capacity of the zeolitic facies may be bypassed by water moving through structural features. Preliminary modeling of Yucca Mountain by Rulon and others (1986) indicated that for flux rates in excess of the saturated matrix hydraulic conductivity of the zeolitic tuff, water flowed downdip along the contact between the TSw and CHn units, until intercepted by a fault and redirected downward. Thordarson (1965, p. 45) noted that in U12e tunnel at Rainier Mesa, water did not appear to be flowing downdip within the matrix toward the axial trace of a local syncline, although he acknowledged the possibility that air circulation within the tunnel might evaporate interstitial water as fast as it reaches the tunnel walls.

This study will utilize information on the spatial distribution and hydraulic properties of both the zeolitic facies and structural features to assess the likelihood for downward flow to bypass the zeolitic facies to the water table.

3.1.4 Quality assurance requirements

Technical procedures do not apply to this activity because: (1) documentation and control of the quality of software used for modeling are subject to the requirements set forth in YMP-USGS QMP-3.03 (Software Quality Assurance); (2) modeling is an analytical and interpretive process, the appropriate application of which is assured by technical review as set forth in YMP-USGS QMP-3.04 (Technical Review, Approval, and Distribution of YMP-USGS Publications); and (3) data used in modeling are collected under other studies (listed in Section 2.1.6).

3.2 Selection, development, and testing of hydrologic-modeling computer codes

3.2.1 Objectives

The objectives of this activity are: (1) to select, evaluate, and adapt existing numerical hydrologic-modeling computer codes for application to the site unsaturated-zone hydrogeologic system and (2) to modify existing codes or develop new codes, as needed, to simulate particular problems or aspects that are unique to the Yucca Mountain system.

3.2.2 Rationale for activity selection

Numerical flow and transport models are constructed to represent hydrogeologic systems that are too complex to be analyzed quantitatively using analytical methods. This study does not propose to model the transport of radionuclides. Some transport capability is needed, however, to evaluate the distribution of environmental isotopes within the mountain, and the implications this distribution may have for flow mechanisms (diffusion versus advecton, matrix flow versus fracture flow, etc.) and flow path definition. In view of the diversity of hydrologic problems that are expected to be encountered within the unsaturated zone, a repertoire of general and site-specific codes will be required to meet all of the anticipated hydrologic-modeling needs. A number of computer codes are available from which flow and transport models can be constructed for natural hydrogeologic systems composed of variably saturated porous media. However, individual codes within this set of available codes differ considerably in their capabilities to model highly complex systems and processes. These existing codes may require modification and new codes may need to be developed in order to meet specific requirements and objectives peculiar to the Yucca Mountain site. Testing and verifying these codes and code modifications will be the major task to be performed as part of this activity.

3.2.3 General approach

Figure 3.2-1 summarizes the organization of the selection, development, and testing of the hydrologic-modeling computer codes activity. A descriptive heading for each analysis appears in the shadowed boxes of the second row. Below each analysis are the individual methods that will be utilized. The figure summarizes the overall structure of the planned activity in terms of methods to be employed. The descriptions of the following sections are organized on the basis of this chart.

The methods utilized in this activity will provide information that is approximately representative of the repository area. The existing conditions within the repository area and correlations to present and potential future repository conditions are addressed by this activity.

The codes developed as part of this activity will be capable of implementing the conceptual models that result from the activities described in Section 3.1. The conceptual model will constantly be

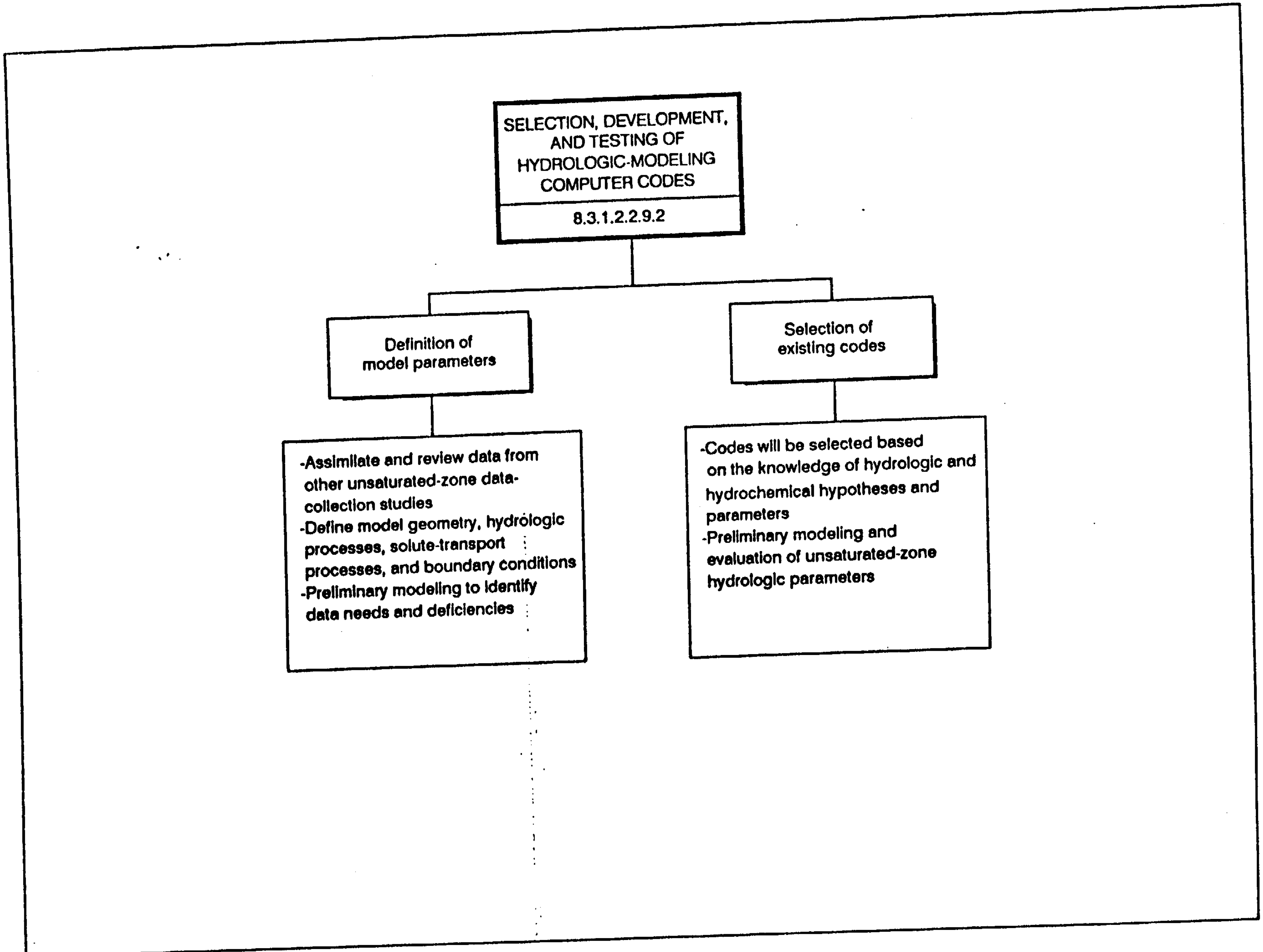


Figure 3.2-1. Logic diagram of selection, development, and testing of hydrologic-modeling computer codes activity, showing analyses and methods.

checked with regard to new data as site characterization proceeds, therefore the developed conceptual model will be representative of the repository site in as much as the current data base is representative of the site. Existing computer codes that numerically simulate unsaturated-zone systems will be selected and used to evaluate the developing conceptual model and to test unsaturated-zone hypotheses. Ultimately the application of these codes will assist in developing a general model for Yucca Mountain (Section 3.3).

The Yucca Mountain site is a highly complex hydrogeologic site which will require numerical modeling to describe the hydrologic system in the unsaturated zone. The numerical models generally solve the appropriate flow and transport equations for a specific system using finite numerical methods on high-speed digital computers. The flow and transport equations originate from conceptual models developed for the site (Section 3.1). The relevant physical processes that may need to be considered would include the storage and flow of moisture, gas, and heat together with the transport of solutes and heat by the movement of either or both liquid-phase and gas-phase pore fluids. Code capabilities, thus, are defined in terms of the underlying physical and mathematical assumptions and approximations on which the codes are based, the numerical procedures that the codes employ, and the computer resources that the codes require for implementation. Most codes have limited capabilities because they are designed to solve only a restricted class of problems.

In general, techniques for modeling moisture flow and solute transport in thick sequences of variably saturated fractured tuffs are not well advanced. Consequently, much of the methodology for constructing hydrologic models in such hydrogeologic systems as well as for obtaining the field and laboratory hydrogeologic data required for input to the models remains imperfectly and incompletely developed. For example, few hydrologic-modeling codes are presently available that can treat the flow of moisture in partially saturated rock matrix and fractures under all of the conditions of transient or steady-state flow that may be encountered within the unsaturated zone at the Yucca Mountain site. Existing codes may require modification and new codes may need to be developed in order to meet specific needs and objectives peculiar to the site. Testing and verifying these codes and code modifications will be a major task to be performed as part of this preliminary modeling activity. Flow and transport equations are obtained by combining general mass and energy balance equations with a set of postulated relationships between fluxes and driving forces. Site-specific forms are obtained by choosing to neglect some terms. Each term neglected represents a hypothesis to be tested against observation. In addition, the requisite procedures to perform the stochastic modeling and uncertainty analyses described in Section 3.4 of this study plan will be developed and tested as part of this preliminary modeling activity.

In addition to constructing hydrologic models for the site hydrogeologic system, numerical hydrologic modeling will be used to support many of the activities being undertaken as part of the overall site hydrologic evaluation. These support-modeling activities include preliminary analyses and calculations, the design and analysis of hydrologic tests and experiments, and the analysis and interpretation of field and laboratory hydrogeologic data. Specific support-modeling applications will be performed independently of the preliminary modeling activity described in this study and are described within the study plans for the studies that the models are to support. However, the selection, adaptation, and verification of appropriate computer codes to perform these support-modeling tasks will be undertaken as part of this preliminary modeling activity. The intent is to assemble a minimal set of versatile, mutually compatible and consistent codes to perform the unsaturated-zone hydrologic modeling tasks required during hydrologic site characterization. Both code modification and code development may be required to meet specific support-modeling objectives. A numerical model embodies both the conceptual model and the computer code used to implement it. Because a numerical model of a hydrologic system includes not only the computer code but also incorporates idealizations of the system geometry, processes, and boundary and initial conditions, it may be improper to speak of a validating a computer code in an absolute sense, independent of its application. A numerical model, including both the conceptual model and the computer code, is considered valid if it represents the hydrologic system at the temporal and spatial scales of interest within the accuracy required for that application.

3.2.3.1 Model parameters

Preliminary modeling of the site hydrogeologic system and its component subsystems will rely heavily on virtually all other studies and activities concerned with hydrologic evaluation of the site. The hydrologic and geologic data generated by these studies will be incorporated into the preliminary models as these data become available during site characterization. The data will be used to define model parameters. The model parameters to be defined in this activity are: model geometry, hydrologic processes, solute-transport processes, and boundary conditions. The geologic data define the model geometries and material compositions. The conceptual models establish the hypotheses for system and subsystem moisture flow and solute transport processes. Borehole cores and cuttings as well as samples taken from within the exploratory studies facility determine the material properties appropriate to hydrogeologic units. The monitoring of ambient conditions within boreholes and the exploratory studies facility together with studies of present and past site and regional climatology provide initial-value and boundary-value data for the models. Preliminary modeling coupled with these data-gathering activities is expected to identify particular data needs and deficiencies that can be addressed subsequently through additional or modified data-acquisition activities. The principal function of the preliminary models is to test continually the integrity of the site hydrogeologic conceptual model and its consistency with accumulating data. In this piecemeal fashion the sequence of preliminary models is expected to converge and evolve into a comprehensive representation of the natural site hydrogeologic system.

3.2.3.2 Selection of existing codes

A major task of this study will be to develop the capability to numerically simulate complex, variably saturated hydrogeologic systems. This capability will be acquired by using currently available hydrologic simulations or by developing new computer codes as needed. This section identifies and summarizes the capabilities of some existing hydrologic simulators that could be used to support this study. Code selection criteria include (1) intended application, (2) process treatment, (3) accuracy, (4) efficiency, (5) stability, (6) dimensionality, and (7) adaptability.

The intended application and purpose of a particular modeling exercise determine what processes need to be addressed by the model. Obviously, if the model does not consider the processes being investigated (e.g. solute transport, coupled heat and moisture flow, etc.), there is no need to consider the subsequent criteria. If, in principle, several codes may be used in a particular application, then the manner in which processes are treated may be the deciding factor in code selection. For instance, some codes may linearize the governing equation for gas flow, while others may solve this equation without simplifying assumptions. Some codes may address the solute transport problem by solving the advection-dispersion equation, others by a particle-tracking method. Particular problems may be inherently easier to solve with one approach or another, or the level of accuracy required may permit simplifying assumptions to be made, with correspondingly less computational effort. Efficiency may be a major consideration in code selection if Monte Carlo simulations are to be done, in which case hundreds of similar, related hydrologic problems are solved repetitively. In this case, the code must converge in relatively few iterations, and the computational effort per iteration should be small. Related to the issues of efficiency and accuracy is the question of code stability. It is important that a code be able to converge on a solution without excessive refinement of the time or space domains.

Additional criteria for code selection are the number of dimensions in which flow processes may be simulated, and the adaptability of the code to treatment of processes in double-porosity media, problems involving temporally-variable boundary conditions, etc.

Clearly, the advantages offered by a particular code with regard to one particular selection criterion may be offset by limitations in other areas, and the process of code selection for a particular application will require a great deal of subjective judgement by the principal investigator.

Examples of typical computer codes which might be used for hydrologic simulations are as follows:

(1) Code name: SAGUARO

Code capabilities: Transport of water and heat through partially or fully saturated porous media in two-dimensional Cartesian coordinates or axially symmetric, three-dimensional cylinders.

Material models: SAGUARO is a finite-element computer program that considers energy transport and the flow of a single-phase incompressible liquid in partiall y or fully-saturated porous media. In addition to capillary and gravitational gradients, liquid water flow may also occur in response to temperature gradients, a phenomena known as the Soret effect. The rock matrix and liquid are assumed to be in thermal equilibrium. Energy transport in the model occurs by conduction, convection, and dispersion. Effective thermal conductivity and thermal capacitance are expressed as functions of local liquid-water saturation. Material properties such as fluid viscosity and thermal conductivity may be expressed as functions of temperature. Principa l directions of the anisotropic permeability tensor need not be aligned with respect to the principal material axes. Volumetric heat sources may be functions of either time or temperature. SAGUARO contains routines for mesh generation, data analysis, and plotting.

Documentation: Eaton and others (1983); Gartling and Hickox (1982).

(2) Code name: NORIA

Code capabilities: Transport of water, air, water vapor and heat in partially saturated porous media in two-dimensio nal Cartesian coordinates or axially symmetric, three-dimensional cylinders.

Material models: NORIA is a finite-element computer code that solves four nonlinear, parabolic differential equations that describe the transport of water, air, water vapor, and heat. Both air and water vapor are taken to be ideal gases and the solid, liquid, and gas phases are assumed to be in local thermal equilibrium. The transfer of sensible heat takes place by conduction and convection. In addition to convective movement, vapor transport can also occur by Knudsen diffusion due to gradients in vapor density, binary diffusion, which results from gradients in the relative concentrations of two species, and thermo-diffusion, in which diffusion of gas species through each other is caused by temperature gradients. Buoyancy forces in the gas phase are also considered. A liquid-vapor nonequilibrium model is also available which assumes the vaporization rate is proportional to the difference between local equilibrium vapor pressure and local partial vapor pressure and the difference between local moisture content and residual moisture content. Material properties can be set to constant values or can be defined as functions of the dependent and independent variables by user-supplied subroutines. Time integration is performed by a third-order predictor-corrector scheme that used error estimates to automatically adjust the time-step size so as to maintain uniform local truncation error throughout the calculation. The predictor-corrector scheme is coupled with a Newton iteration procedure. NORIA performs automatic mesh generation and contains a plotting routine that can generate plots of nodal point locations, the finite element mesh, outlines of materials, dependent variables, and velocities or heat fluxes.

Documentation: Bixler (1985).

(3) Code name: TOSPAC

Code capabilities: Water and solute transport through unsaturated, fractured porous media.

Material models: TOSPAC simulates vertical, one-dimensional steady or transient fluid flow, and solute transport. The flow module assumes water potential equilibrium between fracture- and matrix-pore domains and the applicability of a composite porosity model (Peters and Klavetter, 1988). Transport calculations include advective, dispersive, and diffusional processes, equilibrium adsorption, and three-member decay chains. A matrix-fracture coupling term permits the exchange of solute between fracture- and matrix-pore domains. A solubility-limited-release source term or a congruent-leach model, which assumes that the fractional release rate of radionuclides from the spent-fuel inventory is equal to the fractional leach rate of the waste matrix, can be used to calculate a radionuclide source term. All partial differential equations are solved using finite-difference methods.

Documentation: Dudley and others (1988).

(4) Code name: TOUGH

Code capabilities: Transport of water, water vapor, air, and heat in one-,two-, or three-dimensional, partially saturated porous media.

Material models: Fluid flow in both liquid and gaseous phases occurs under pressure, viscous, and gravity forces according to Darcy's law with interference between the phases represented by means of relative permeability functions. In addition, binary diffusion in the gas phase is considered. No account is made of Knudsen diffusion. Capillary and phase adsorption effects are taken into account for the liquid phase, with allowance for vapor pressure lowering. Provision is made, through an auxiliary program, for hysteresis in both capillary pressure and relative permeability. All thermophysical properties of liquid water and vapor are obtained within experimental accuracy from steam table equations (International Formulation Committee, 1967). Air is treated as an ideal gas, and additivity of partial pressures is assumed for air/vapor mixtures. Air dissolution in water is presented by Henry's law.

Heat transport occurs by means of conduction with thermal conductivity dependent on water saturation, convection, and binary diffusion, which includes both sensible and latent heat.

The governing equations used in TOUGH, and their numerical implementation, are applicable to one-, two- or three-dimensional anisotropic porous or fractured media. TOUGH does not perform stress calculations for the solid skeleton, but it allows for porosity changes in response to changes in pore pressure (compressibility) and temperature (expansivity). Through entry of appropriate input data created by a preprocessor (Pruess and Narasimhan, 1985), TOUGH can be employed to simulate fluid flow and heat transport in double-porosity media.

Documentation: Pruess (1987).

(5) Code name: **TRACER3D**

Code capabilities: Transport of water, air, and reactive chemical species through fractured or unfractured porous materials in one, two, or three dimensions.

Material models: Problems ranging from steady, single-phase one-dimensional flow to transient, three-dimensional two-phase (gas and liquid) flow and tracer transport in fractured, porous media may be solved with TRACER3D. The equations that comprise the TRACER3D model are the mass and chemical species conservation equation, a reduced form of the momenta equation, and an equation of state plus several constitutive relations. Momenta conservation equations are solved in a reduced form known as the Forchheimer equation. At low Reynolds numbers (<10), this expression reduces to the Darcy equation; at higher Reynolds numbers, the nonlinear term becomes important. Tracer transport occurs through advection, mechanical dispersion, and molecular diffusion. Radioactive decay may be simulated in n-member chains, and sorption to the solid materials can be accommodated by either a simple, linear equilibrium sorption model, or by a nonequilibrium saturable sorption model in which sorption can be either reversible or irreversible. Fractures may be specified explicitly in the mesh definition by the user, specified implicitly by the user through a distribution of fracture width and spacing parameters, or a random network of fractures can be generated. Flow equations are solved with a fully implicit, centered-in-space, backward-in-time finite-difference scheme. A time step different than that used for the solution of the flow equation may be used for solution of the transport equation. An active-zone calculator is used to limit computations only to those computational cells that are experiencing significant changes in the dependent variables.

Documentation: Travis (1984); Travis and Birdsell (1991).

(6) Code name: UNSAT2

Code capabilities: Unsaturated, partially saturated, and saturated flow in porous media in two dimensions, or axially symmetric three-dimensional coordinates.

Material models: USAT2 utilizes a lumped-mass Galerkin finite-element scheme using quadrilateral and triangular elements, in combination with the Picard iteration method, to solve the nonlinear unsaturated-flow equation. Simulations can be conducted in a vertical plane, in a horizontal plane, or in a three-dimensional region exhibiti ng radial symmetry about a vertical axis. In addition to conventional prescribed head or flux boundaries, UNSAT2 can also accommodate boundari es controlled by atmospheric conditions such as seepage faces and evaporation or infiltration surfaces. Water uptake by plants is simulated in a manner that accounts for both soil and atmospheric conditions and allows for plant growth. A special algorithm permits analysis of flow to a partially- or fully-penetrating well of finite radius that pumps at an arbitrary rate. This analysis takes full account of wellbore storage.

Documentation: Davis and Neuman (1983).

(7) Code names: **VS2D, VS2DT**

Code capabilities: Single-phase flow and solute transport in one- or two-dimensional, variably saturated porous media.

Material models: The mathematical model for variably saturated fluid flow is developed for VS2D by combining the law of conservation of fluid mass with a nonlinear form of Darcy's law. The resultant mathematical model, or flow equation, is written with total hydraulic potential as the dependent variable. This allows straightforward treatment of both saturated and unsaturated conditions. The spatial derivatives in the flow equation are approximated by central differences written about grid-block boundaries. Time derivatives are approximated by a fully implicit backward scheme. Nonlinear storage terms are linearized by an implicit Newton-Raphson method. Nonlinear conductance terms, boundary conditions, and sink terms are linearized implicitly. Relative hydraulic conductivity is evaluated at cell boundaries by using full upstream weighting, the arithmetic mean, or the geometric mean of values from adjacent cells. Saturated hydraulic conductivities are evaluated at cell boundaries by using distance-weighted harmonic means. The linearized matrix equations are solved using the strongly implicit procedure.

Nonlinear conductance and storage coefficients are assumed to be represented by one of three closed-form algebraic equations. Alternatively, these values may be interpolated from tabulated data. Nonlinear boundary conditions treated by the code include infiltration, evaporation, and seepage faces. Extraction by plant roots is included as a nonlinear sink term.

VS2DT uses a finite-difference approximation to the advection-dispersion equation to solve problems of solute transport in variably saturated porous media. The program is an extension to the computer program VS2D. Simulated regions can be one-dimensional columns, two-dimensional vertical cross-sections, or axially symmetric, three-dimensional cylinders. Program options include: backward or centered approximations for both space and time derivatives, first-order decay, equilibrium adsorption as described by Freundlich or Langmuir isotherms, and ion exchange (Healy, 1990).

Documentation: Lappala and others (1987); Healy (1990).

(8) Code name: HST3D

Code capabilities: Coupled heat, solute and single-phase fluid flow in three dimensions.

Material models: The equations governing single-phase fluid flow, and heat and solute transport, are coupled through the dependence of advective transport on the interstitial fluid-velocity field, the dependence of fluid viscosity on temperature and solute concentration, and the dependence of fluid density on pressure, temperature, and solute concentration. Finite-difference techniques are used to discretize the governing equations using a point-distributed grid. Two techniques are available for solution of the finite-difference matrix equations. One is a direct elimination solver, using equations reordered by alternating diagonal planes. The other technique is an iterative solver, using two-line successive relaxation. Solute transpor t is governed by the advective-dispersive equation and allows for the transport of a single species, with possible linear-equilibrium adsorption and first-order decay.

Documentation: Kipp (1987).

(9) Code name: FEHMN

Code capabilities: Non-isothermal multiphase multicomponent flow in two-dimensional, two-dimensional radial, or three-dimensional geometries.

Material models: FEHMN (Finite Element Heat and Mass Nuclear) code uses the Galerkin finite element method to discretize the governing equations that result from combining the nonlinear form of Darcy's Law with the equations of mass conservation. Moisture movement occurs in both liquid and vapor phases. Heat transport occurs as a result of convection in both the liquid and gas phases, as well as by conduction. Tracer movement is modeled with a form of the convection-dispersion equation, and may occur in both the liquid and gas phases. The movement of up to 10 different tracers may be simulated. Adsorption of tracers may occur according to linear, Freundlich, modified Freundlich, or Langmuir isotherm models. Upwind weighting is available for both the flow and transport equations. The pressure- and temperature-dependent behavior of the liquid-phase density, enthalpy, and viscosity are represented with polynomials. In addition to simulating the movement of moisture as both vapor and liquid, the model is also capable of simulating noncondensible gas (air) flow. The density of air is assumed to obey the ideal gas law; the enthalpy of air is a function of temperature only. The mass fraction of air in the liquid phase is assumed to obey Henry's Law and the viscosity of air is assumed constant. Porosity may vary either because of changes in fluid pressure or thermal expansion; permeability is assumed to vary with the cube of porosity. Solution of the nonlinear algebraic equations that result from application of the finite element method is done using a Newton-Raphson iterative procedure. An option is available to consider dual-porosity effects. The code can generate computational meshes automatically. Results can be displayed in three dimensions using a post-processing capability.

Documentation: Zyvoloski, Dash and Kelkar (1992).

Of the hydrologic simulators described above, TOUGH and FEHMN have sufficient geometric flexibility to allow their use in discrete fracture simulations. The FRACMAN code (Dershowitz and others, 1991), which performs discrete fracture data analysis, geometric modeling and exploration simulation in rock with discrete features, has recently been adapted to generate computational meshes compatible with TOUGH and FEHMN. Coupling of these multiphase flow and heat simulators with the discrete features analysis and generation capability offered by FRACMAN can offer a potentially valuable alternative to the porous media representation of unsaturated fractured rock in those cases where discrete features need to be considered.

Of the numerical codes described in this section, only TRACER3D, HST3D, and TOUGH presently have the capability to perform calculations in three-dimensional cartesian coordinates. Modification of the remaining codes to three-dimensional simulation capabilities is not anticipated to become part of this study. The primary constraints in applying TRACER3D, HST3D or TOUGH are expected to be the increased storage requirements and execution times that are associated with the larger number of nodes involved in three-dimensional problems, particularly if it is necessary to have a high degree of refinement in the time and space domains. If discretization of the time or space domains is too coarse, ambiguous or improper conclusions may be drawn from the simulation results if they lack sufficient detail or contain excessive numerical error.

Because TOUGH is potentially the most versatile code, both with regard to its treatment of coupled liquid, gas, and heat flow and its dimensionality, emphasis will be placed on exploring its applicabilty to three-dimensional site-scale problems. Beginning with a relatively crude mesh, progressive refinement will be made in the time and space domains until simulation results are no longer sensitive to continued refinement of the temporal and spatial discretization, or until the code- and machine-dependent execution times and storage limitations prohibit further refinement. This portion of Activity 8.3.1.2.2.9.2 will also involve the development and linkage of the appropriate pre-processing and post-processing software, including that software dealing with three-dimensional graphics capabilities.

3.2.3.3 Methods summary

A major task of this study will be to develop the capability to simulate fluid flow and tracer transport in variably saturated fractured rock. Such a capability requires not only conceptual models but also computer codes capable of implementing them. Because the conceptual model will continue to evolve throughout the project, continued refinement of the associated computer codes may be required. Based on current conceptual models, a set of hydrologic simulators has been identified, each member of which provides a potentially useful platform from which to develop a numerical code that addresses modeling requirements specific to the Yucca Mountain site. The codes are similar in that the governing equations are obtained by combining general mass and energy balance equations with a set of postulated relationships between fluxes and driving forces. They differ in the types of processes they address and in their treatment of these processes, as well as their dimensionality, efficiency, and adaptability to site-specific conditions, such as the existence of primary and secondary porosity. It is likely that no single computer code will be the optimal choice for all applications, as desirable as this may be. Some applications of these models are undoubtedly unforeseen at this time. The hydrologic simulators described above provide logical starting points for the development of site-specific codes.

3.2.4 Quality assurance requirements

Technical procedures do not apply to this activity because: (1) documentation and control of the quality of software used for modeling are subject to the requirements set forth in YMP-USGS QMP-3.03 (Software Quality Assurance); (2) modeling is an analytical and interpretive process, the appropriate application of which is assured by technical review as set forth in YMP-USGS QMP-3.04 (Technical Review, Approval, and Distribution of YMP-USGS Publications); and (3) data used in modeling are collected under other studies (listed in Section 2.1.6).

3.3 Simulation of the natural hydrogeologic system

3.3.1 Objectives

The objectives of this activity are to construct appropriate hydrologic models for the natural site hydrogeologic system to (1) simulate and investigate the existing state of the system, and (2) predict expected future and past states of the system under changing environmental conditions.

3.3.2 Rationale for activity selection

Based on the preliminary hydrologic modeling activity described in Section 3.2, a set of one or more numerical hydrologic models will be constructed to mathematically simulate the hydrogeologic system within the unsaturated zone at the site. This simulation will be comprehensive in that it will need to account for all of the dominant, controlling hydrologic processes and conditions and to incorporate a degree of complexity consistent with the practical constraints and limitations imposed by the use of finite numerical methods to perform the mathematical simulations.

3.3.3 General approach

In order to achieve maximum simplification and economy, the final model for the site will be constructed incrementally, proceeding to greater complexity and refinement as the conceptual model for the site hydrologic system is developed and revised during site characterization.

Initially, a coarse three-dimensional model (main model) of the site will be developed that incorporates some of the major processes known to be of importance. This model will be designed so that it can readily be refined everywhere in space and additional complexities and processes incorporated. Numerical submodels will be developed to investigate specific hypotheses and approximations of the main model. These submodels will be one- or two-dimensional depending on the nature of the hypothesis or the approximation. For example, a one-dimensional model may be sufficient to investigate how fine a numerical grid is required near boundaries between different geologic strata. On the other hand, a two-dimensional model will be needed to investigate the importance of accurate representation of spatial variations of the land-surface net-infiltration rates. The results of the submodel investigations are then used to appropriately modify or enhance the main site-scale model.

As part of this stepwise process of model construction, a number of specific hypotheses related to the conceptual model will be tested. These include: (1) investigation of the expected relative contributions of liquid-water and water-vapor fluxes to the net moisture flux within the unsaturated-zone system; (2) assessment of the likelihood for the occurrence of geothermally or barometrically driven convection cells involving the upward flow of water vapor with a corresponding downward return flow of liquid water; (3) investigation of the limiting conditions under which capillary barriers and perched-water zones can be expected to occur; (4) assessment of the effects produced by spatial and temporal variations in assumed values for land-surface net-infiltration rates; (5) assessment of the complicating effects of allowing for a three-dimensional flow-system geometry; and (6) incorporation of the effects of moisture storage and flow within and between rock matrix and fractures. Some of these hypotheses were discussed in Section 3.1 and presented in Table 3.1-1. A most important task of this activity is to identify and include those hydrologic processes and concepts that are essential for a valid mathematical representation and to exclude those that can be shown to be of negligible importance.

The output generated by the model for a specified set of input data consists of predicted time-dependent spatial distributions of liquid-water matric potential and saturation, pore-gas pressure, water-vapor concentration, temperature, and moisture and pore-gas fluxes. To the extent that the mathematical formulation on which the model is based incorporates all the hydrologic processes and conditions that control the physical hydrogeologic system, the flow model yields an internally self-consistent mathematical representation of the hydrologic system and its evolution over time. The probable accuracy and validity of this representation is considered in Section 3.4 (Stochastic modeling and uncertainty analysis). The final flow model will be consistent with the observed spatial distributions of water potential, pneumatic pressure and temperature, as well as with the flow paths and flow mechanisms suggested by the spatial distributions of the above-mentioned environmental tracers.

Figure 3.3-1 summarizes the organization of the numerical simulation of the natural hydrogeologic system activity. A descriptive heading for each analysis appears in the shadowed boxes of the second row. Below each analysis are the individual methods that will be utilized during testing. Figure 3.3-2 summarizes the objectives of the activity, characterization parameters which are addressed by the activity, and the activity parameters calculated by modeling. These appear in the boxes in the top left side, top right side, and below the shadowed analysis boxes.

The two figures summarize the overall structure of the planned activity in terms of methods and analyses to be used and calculations to be made. The descriptions of the following sections are organized on the basis of these charts. Methodology and parameter information are tabulated as a means of summarizing the pertinent relations among (1) the activity parameters to be modeled, (2) the information needs of the performance and design issues, (3) the technical objectives of the activity, and (4) the methods to be used.

The methods utilized in this activity will provide information that is approximately representative of the repository area. The existing conditions within the repository area, and correlations to present and potential future repository conditions are addressed by this activity. Numerical simulations of the site hydrogeologic system will be performed by solving the appropriate governing set of equations, subject to boundary conditions, using numerical procedures. The governing equations are formulated from a conceptual model which has been based upon observations and data gathered from the repository area. The

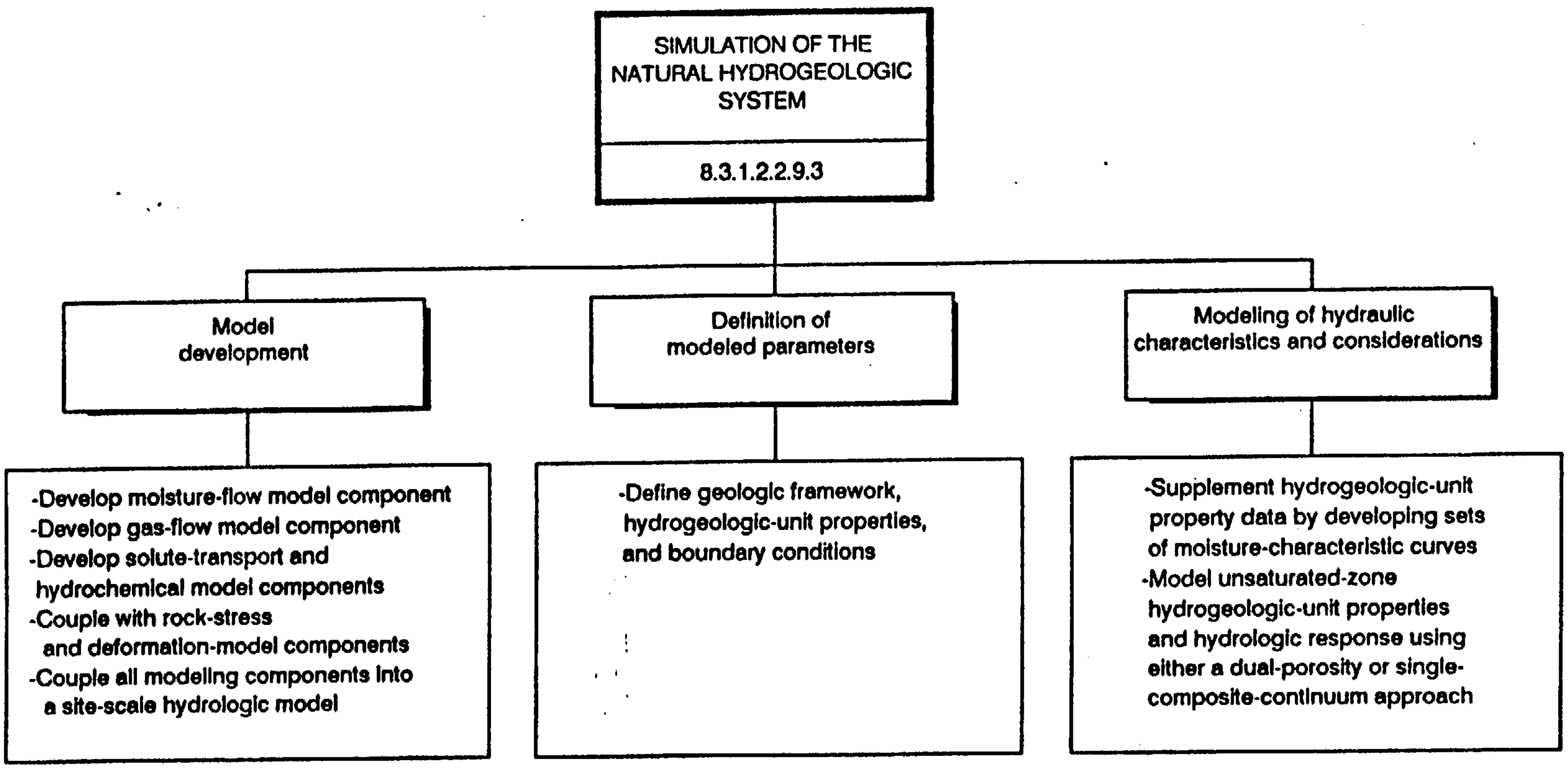


Figure 3.3-1. Logic diagram of the simulation of the site natural hydrogeologic system activity, showing analyses and methods.

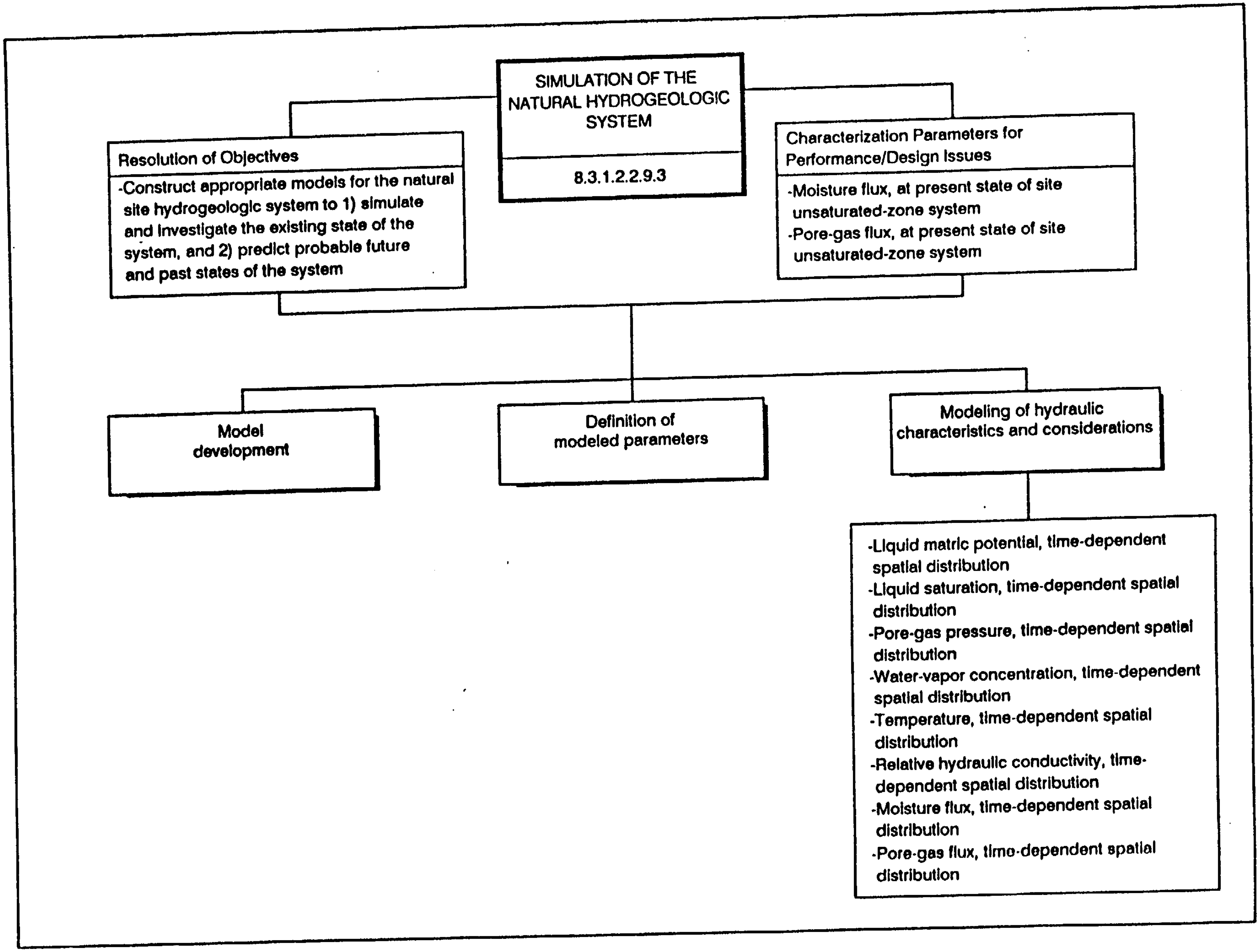


Figure 3.3-2. Logic diagram of the simulation of the site natural hydrogeologic system activity, showing analyses and activity parameters.

adequacy of the conceptual models and the associated numerical procedures can be assessed by comparing simulations to actual field observations. The conceptual model and hence the numerical simulations will be constantly refined as site characterization proceeds and the unsaturated-zone database is updated.

3.3.3.1 Model development

Site characterization studies at Yucca Mountain are expected to yield a description of a highly complex hydrogeologic system. Due to the system complexity, a single numerical model may not consider in sufficient detail and generality all of the significant aspects of the site. Therefore, a set of hydrologic models may be needed. A possible breakdown may be as follows:

1. A moisture-flow model will be constructed initially to simulate the flow and storage of moisture, both as liquid water and as water vapor, within the system. In some instances, water-vapor may not need to be considered explicitly, which would yield a considerably simplified representation that could be decoupled from the pore-gas and geothermal systems.

2. If there is significant pore-gas movement within the system, a gas-flow model constructed under the assumption of constant or slowly changing liquid-water saturation may be adequate for predicting net water-vapor flux the movement of both natural and introduced gas-phase tracers.

3. General solute-transport and hydrochemical modeling will of necessity be performed following construction of the appropriate moisture-flow or gas-flow models.

4. The hydrologic models may be coupled to rock stress and deformation models to assess the effects produced by changing rock and fracture hydrologic properties under changing mechanical stress fields.

Certain model applications, including studies which examine the relative contributions of the liquid and water-vapor fluxes, the effects of repository heating on the large-scale flow system, or thermally-driven convection cells, will require the use of models which consider nonisothermal effects. Solute-transport models may be useful for interpreting the spatial distribution of environmental tracers such as tritium and carbon-14 in order to better understand both flow paths and the factors which affect the manner in which these tracers are partitioned between fractures and matrix. Simple hydrochemical models coupled to the transport models could provide insight as to how carbon-13 and carbon-14 are partitioned between the gas, liquid, and solid phases as air flows through Yucca Mountain. Solute-transport models which account for the movement of tracers in the gas phase may also aid in the determination of values for effective transport porosity and dispersivity from cross-hole tracer tests (e.g. Study 8.3.1.2.2.3, Unsaturated zone percolation - surface-based studies).

Stress/deformation models may be used to predict the manner in which stress changes occurring at some time in the future at Yucca Mountain, due to either thermal loading caused by repository heating or tectonic events, may affect fracture apertures and hence fracture permeability. These analyses may constrain scenarios which consider the hydrologic impact of future tectonic stresses, where modification of the permeability field occurs due to deformation of existing fractures rather than the introduction of new ones. Although it may not be possible to predict the location and magnitude of permeability changes within the unsaturated zone following a major tectonic event, it is possible to perform a sensitivity study to examine the practical consequences of varying the saturated permeability by several orders of magnitude relative to what will be current best estimates, at various locations in the system. In addition to examining the effect of altered permeability due to tectonic events, we would also, in effect, be examining the effect of having failed to identify an existing zone of large or small permeability. One could examine the effect of additional tectonic-related fracturing on any perched-water bodies identified within the unsaturated zone at Yucca Mountain. Based on current understanding, it is anticipated that because fracture storage is probably small, flow through the fractures recently formed by a tectonic event would be initially large, but short-lived, with the welded tuff matrix draining slowly, if at all. Additional fractures might also enhance gas flow and the transport of gaseous contaminants. The consequences of this could also be examined through a sensitivity analysis. Similarly, while it may be difficult to predict the magnitude of changes in water table elevation following a tectonic event, we can evaluate the hydrologic consequences of a water table elevation changes of a given magnitude.

The effects of future nuclear weapons testing on faults and fractures within the unsaturated zone also introduce additional uncertainty. However, this uncertainty is expected to be minor relative to existing and expected future uncertainty concerning fault and fracture locations and hydrologic properties. Furthermore, emplacement of waste at Yucca Mountain would impose thermally-induced stresses that would probably alter the fracture and fault properties more persistently than stresses associated with nuclear tests. The latter are expected to be transient, as evidenced by data from the saturated zone at Yucca Mountain. There, water levels tend to return to pre-test conditions within minutes to hours following nuclear events, suggesting no permanent changes in fracture and fault properties. Following the June, 1992, 5.6-magnitude earthquake at Little Skull Mountain, Nevada, approximately 30 km from Yucca Mountain, persistent changes in water-level altitude occurred at only one of the several dozen wells monitored (O'Brien and Tucci, 1992). Water levels at this well required 6 months to recover, which is nonetheless short relative to the period of waste isolation. The magnitude of this earthquake is large relative to what has been observed at Yucca Mountain following nuclear tests (4.0 or less). As indicated above, stress-deformation models will be used in conjunction with sensitivity analysis to bound expected changes in fracture permeability due to thermal, tectonically and blast-induced stresses.

3.3.3.2 Modeled parameters

The input and output for the model(s) define the parameters for this activity. Requisite input data include (1) the geologic framework for the site, which determines the model geometry and spatial distribution of material types, (2) the hydrologic, thermal, and mechanical properties of the hydrogeologic units that make up the unsaturated zone at the site, (3) the existing boundary conditions, which are determined by the flux, water-potential, and pneumatic-pressure distributions on the spatial boundaries of the model, and (4) specification of the present state of the system. In general, the land surface will define the upper spatial boundary, and the water table will define the lower boundary for the model; the lateral hydrologic boundaries must enclose the primary repository area and remain to be established. The material property data for the hydrogeologic units will be obtained from field and laboratory measurements that will become available during site characterization. The environmental conditions establish the hydrologic boundary conditions and will be determined by the present and past site climatology. Expected output data include values of liquid- and gas-phase pressure, saturation, fluid fluxes, and seepage velocities, solute concentrations and temperature at various locations throughout the mountain. Additional output will include estimates of model parameters determined through calibration of the model against observed data, including characterization of the uncertainty of these estimates.

3.3.3.3 Hydraulic characteristics and considerations of the unsaturated zone

The approach to numerically model a hydrologic system is based on the conceptual models developed for the system as derived from field and experimental data. The following paragraphs summarize some of the characteristics known about the unsaturated zone at Yucca Mountain and some considerations on how to model them.

3.3.3.3.1 Hydraulic characteristics

The hydraulic characteristics of the unsaturated zone include effective porosity, saturated matrix and fracture hydraulic conductivities, and moisture-characteristic relations for the rock-matrix and fracture systems. Mean values of rock-matrix hydrologic properties for most of the hydrogeologic units at the site are listed in Table 3.3-1. The compilation of Montazer and Wilson (1984) includes data from several sources (Anderson, 1981; Peters and others, 1984; Rush and others, 1983; Thordarson, 1983; and Weeks and Wilson, 1984). The data of Anderson (1981) were from core samples collected from well UE25a #1; the data of Peters and others (1984) were based on analyses of core samples from test wells USW G-1, USW G-4, and USW GU-3; the data of Rush and others (1983) were obtained from well USW

Table 3.3-1 Summary of compilation of hydrogeologic properties of hydrogeologic units within the unsaturated zone, Yucca Mountain

Hydrogeologic unit[a]	Source of data	Range of thickness (m)[b]	Grain density (kg/m^3)	Fracture density (no./m^3)[c]	Porosity	Saturated matrix-hydraulic conductivity (m/s)
TCw	(d)	0-150	ND	10-20	0.12	2×10^{-11}
	(e)	ND	1,390	ND	0.08	9.7×10^{-12}
	(f)	0-170	ND	ND	0.1-0.15	1×10^{-11}
PTn	(d)	20-100	ND	1	0.46	1×10^{-7}
	(e)	ND	2,350	ND	0.40	3.9×10^{-7}
	(f)	60-340	ND	ND	0.2-0.4	1×10^{-6} to 1×10^{-8}
TSw	(d)	290-360	ND	8-40	0.14	3.5×10^{-11}
	(e)	ND	2,580	ND	0.11	1.9×10^{-11}
	(f)	ND	ND	ND	.15-0.2	1×10^{-11}
CHnv	(d)	100-400	ND	2-3	0.37	5×10^{-8}
	(e)	ND	2,370	ND	0.46	2.7×10^{-7}
	(f)	ND	ND	ND	0.2-0.5	1×10^{-8} to 1×10^{-10}
CHnz	(d)	100-400	ND	2-3	0.31	9×10^{-11}
	(e)	ND	2,230	ND	0.28	2.0×10^{-11}
	(f)	ND	ND	ND	0.2-0.5	1×10^{-10} to 1×10^{-11}

[a]Hydrogeologic units are defined in Figure 3.1-2
[b]Scott and Bonk (1984)
[c]Scott and others (1983)
[d]Montazer and Wilson (1984)
[e]Peters and others (1984) and Peters and others (1986)
[f]Wittwer and others (1992)
ND - no data available

H-1; the data of Thordarson (1983) were obtained from well J-13; and the data reported by Weeks and Wilson (1984) were obtained from core samples from well USW H-1. The range of mean values among the references cited for each property within each hydrogeologic unit reflects the effects of lateral and vertical spatial heterogeneity within each unit and experimental error resulting from differences in applied measurement techniques. Table 3.3-1 provides only values typical of the samples tested for hydrologic properties. These data are based, in general, on insufficient sampling (several cores for the entire unsaturated zone at Yucca Mountain) to permit meaningful statistical analyses to be performed for each hydrogeologic unit. An indication of the variance within and between sample sets is shown by the saturated matrix-hydraulic conductivity, whose values listed in Table 3.3-1 range over an order of magnitude.

The discrepancy in the values reported in Table 3.3-1 for saturated matrix-hydraulic conductivity for the Calico Hills non-welded hydrogeologic unit reflects, in part, the current uncertainty in the position of hydrogeologic unit contacts and, in part, the heterogeneity of the units. Rock-sample collection for the measurement of hydrologic properties is to be done through the program of surface-based borehole drilling and coring and of sampling within the exploratory studies facility, as described in Section 8.3.1.4 of the SCP. Plans to define the hydrogeologic framework are described in Section 8.3.1.2 of the SCP.

The hydrogeologic property data of Table 3.3-1 needs to be supplemented by developing moisture-characteristic curves for the functional dependence of liquid-water saturation and relative hydraulic conductivity on the liquid-water potential within the rock matrix and fractures appropriate for each hydrogeologic unit. In unfractured rocks, these relations refer to the storage and movement of liquid within and through the interstitial pore space. In fractured rocks, allowance must be made for the storage and movement of water within the interconnected fracture openings as well as for the movement of water between the fracture openings and the rock-matrix pore space.

A set of moisture-retention curves under drainage conditions relating matric-potential and saturation is shown in Figure 3.3-3 and was developed by Peters and others (1984) for the matrix properties of most of the hydrogeologic units listed in Table 3.3-1. These curves were obtained by fitting the van Genuchten (1978) analytic representation to laboratory psychrometric data obtained for unfractured samples extracted from cores from test wells USW G-4 and USW GU-3. Because psychrometric techniques are appropriate only for matric potentials less than -3 bars (-0.3 MPa), the moisture-retention curves reported by Peters and others (1984) are not well determined for matric potentials that exceed this value. In lieu of direct measurements, the van Genuchten (1978) representation can also be used to estimate

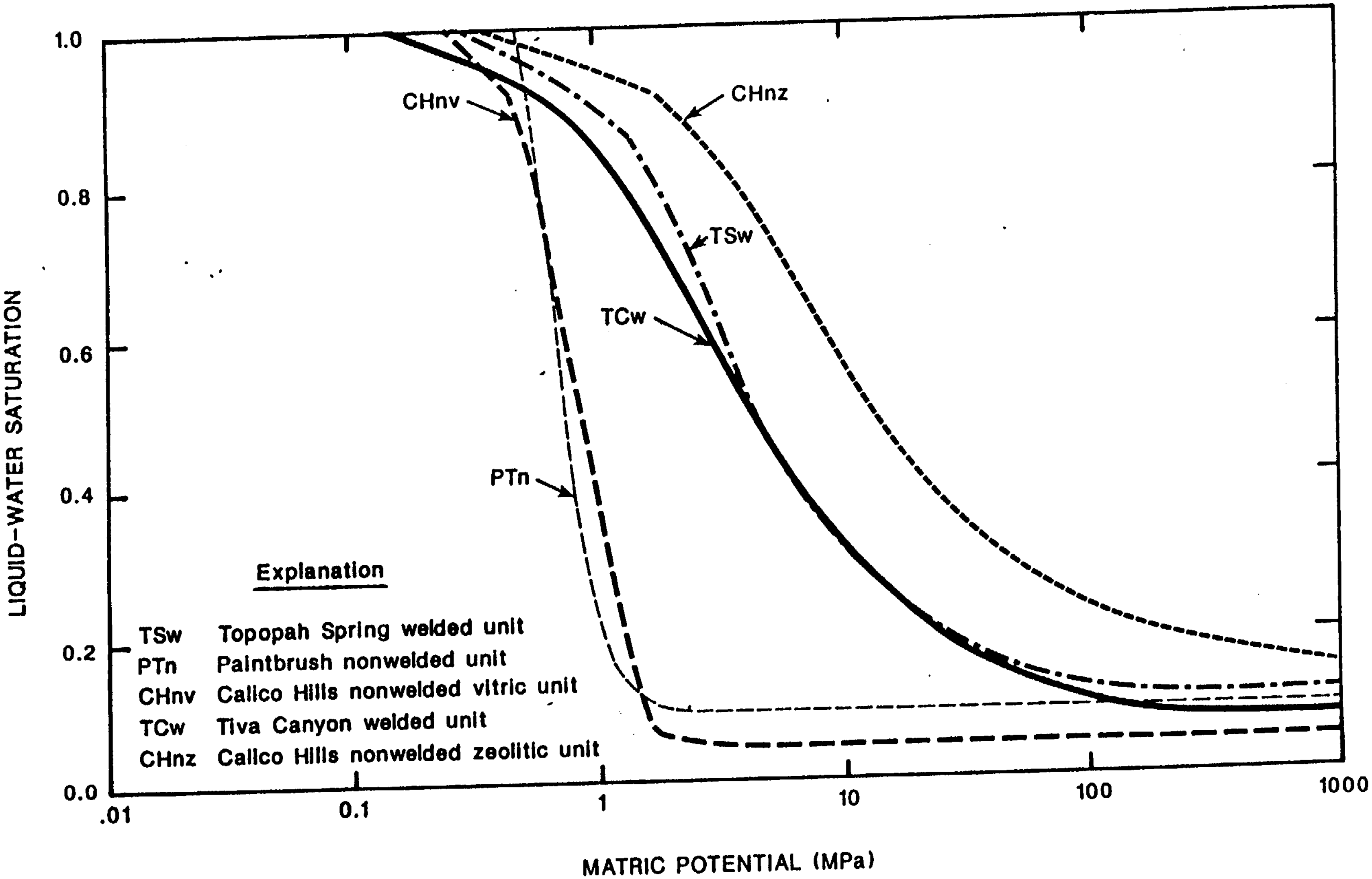


Figure 3.3-3. Moisture-retention curves for the hydrogeologic units within the unsaturated zone at Yucca Mountain. Modified from Peters et al. (1984).

matrix relative hydraulic conductivity for these units. Such estimates must be regarded as highly tentative, however, because it is not known to what extent this analytic representation for relative hydraulic conductivity is appropriate for the tuffs at Yucca Mountain (SCP Section 8.3.1.2.2). Furthermore, the curves in Figure 3.3-3 are based on laboratory determinations on small sample sets from only two locations, and the curves may not be representative of the units at Yucca Mountain as a whole. Additional measurements of saturation versus capillary pressure, as well as measurements of relative permeability as a function of saturation, were provided for nonwelded tuffs from various stratigraphic intervals in Flint and Flint (1990). However, measurements of the same quantities by different techniques show considerable differences. Direct measurements of relative permeability for intact matrix materials will be performed as part of Activity 8.3.1.2.2.3.1 (Matrix hydrologic-properties testing) in Study 8.3.1.2.2.3 (Unsaturated-zone percolation - surface-based studies).

Standard laboratory methods are not yet available by which to determine the moisture-characteristic relations for fractures and fractured rocks, and reliance must be made on theoretically based models and approximations. Liquid-water storage within fractures probably is insignificant, but the flow of liquid water within and across fractures is not yet well understood. Theoretical models for liquid-water flow (Wang and Narasimhan, 1985; Montazer and Harrold, 1985) and two-phase (water and air) flow (Pruess and Tsang, 1990) in single, variably saturated fractures have been developed, but have not yet been laboratory- or field-tested. These models generally assume that fracture apertures vary within the plane of the fracture. Based on capillary theory, it is hypothesized that because of this variation in apertures, individual fractures drain or fill over a range of matric potentials, rather than a single value, and thus may possess flow and storage properties that can be represented by functional relations similar to those that have been developed for porous media. These theoretical studies have concluded that compared with the intact rock, fractures drain or fill over a relatively narrow range of matric potentials and at matric potentials generally larger than those at which the intact matrix fills or drains. Consequently, it has been hypothesized that if fractures are locally in matric potential equilibrium with the surrounding matrix, liquid water flow within the fracture does not become significant volumetrically until the enclosing matrix is nearly saturated. As pointed out by a number of authors (Peters and Klavetter, 1988; Nitao and Buschek, 1991; Pruess and others, 1990a,b), the assumption of fracture-matrix potential equilibrium breaks down under certain conditions, as discussed below. Figures 3.3-4 to 3.3-6 show water saturation versus matric potential, water permeability versus matric potential, and air-permeability versus matric potential curves calculated using a numerical model conceptually similar to that described by Pruess and Tsang, (1990). Curves are shown for fractures with average physical apertures of 25.0

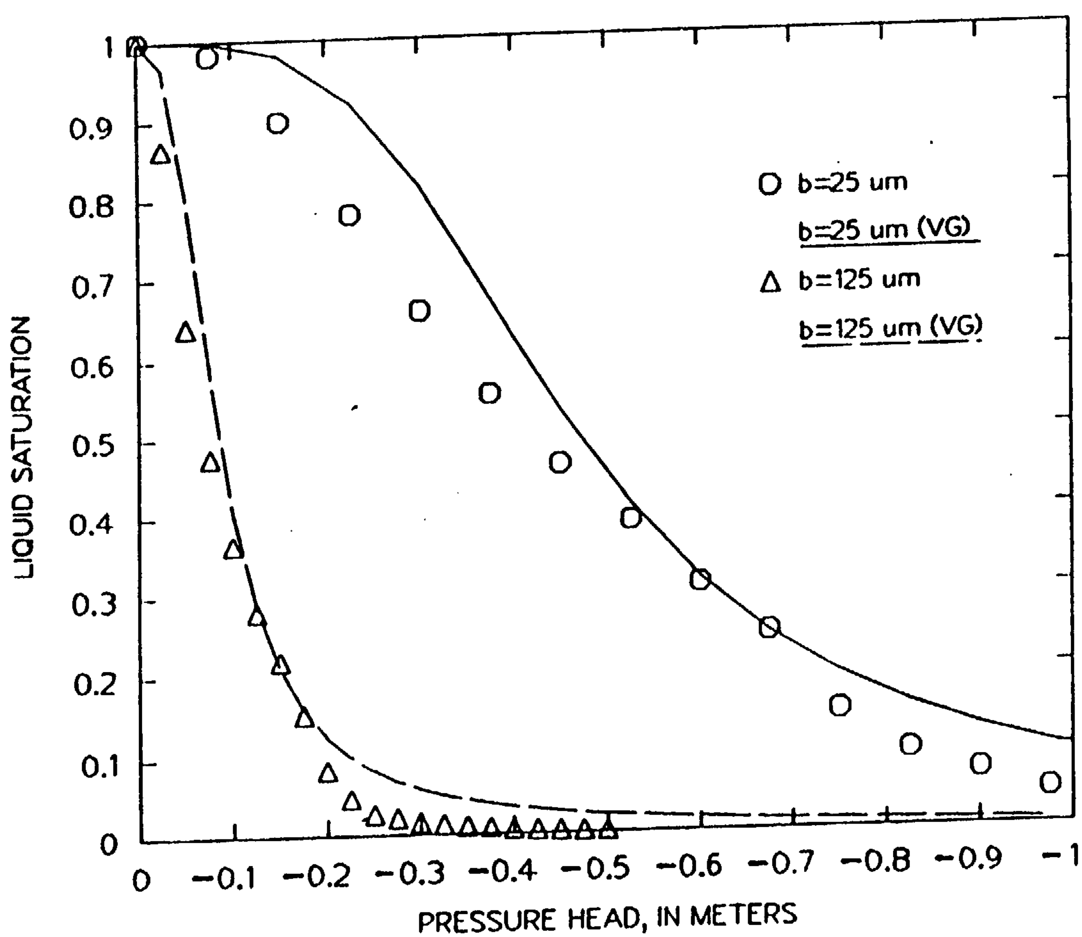


Figure 3.3-4. Theoretical moisture retention curves calculated for single fractures with average physical apertures of 25.0 and 125.0 microns. (After Kwicklis and Healy, 1993)

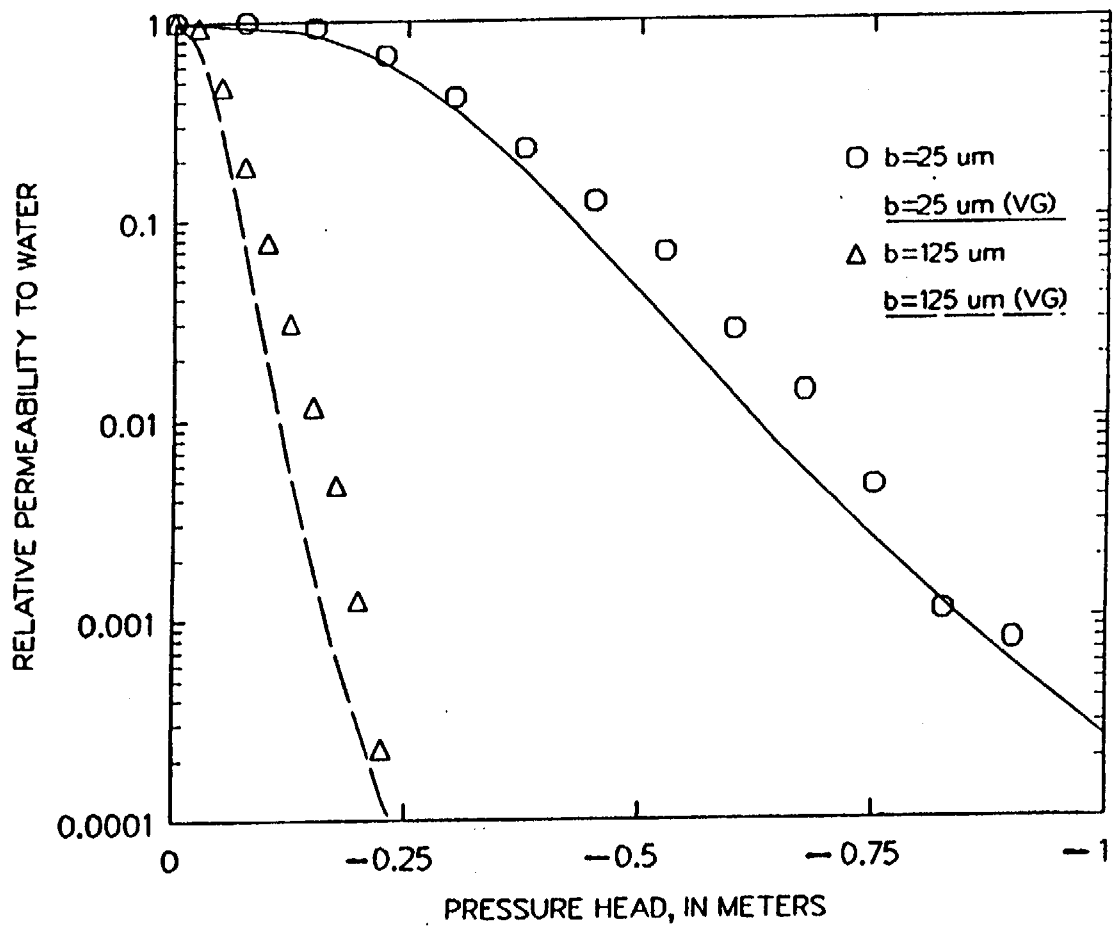


Figure 3.3-5. Theoretical water permeability versus pressure head curves calculated for single fractures with average physical apertures of 25.0 and 125.0 microns. (After Kwicklis and Healy, 1993)

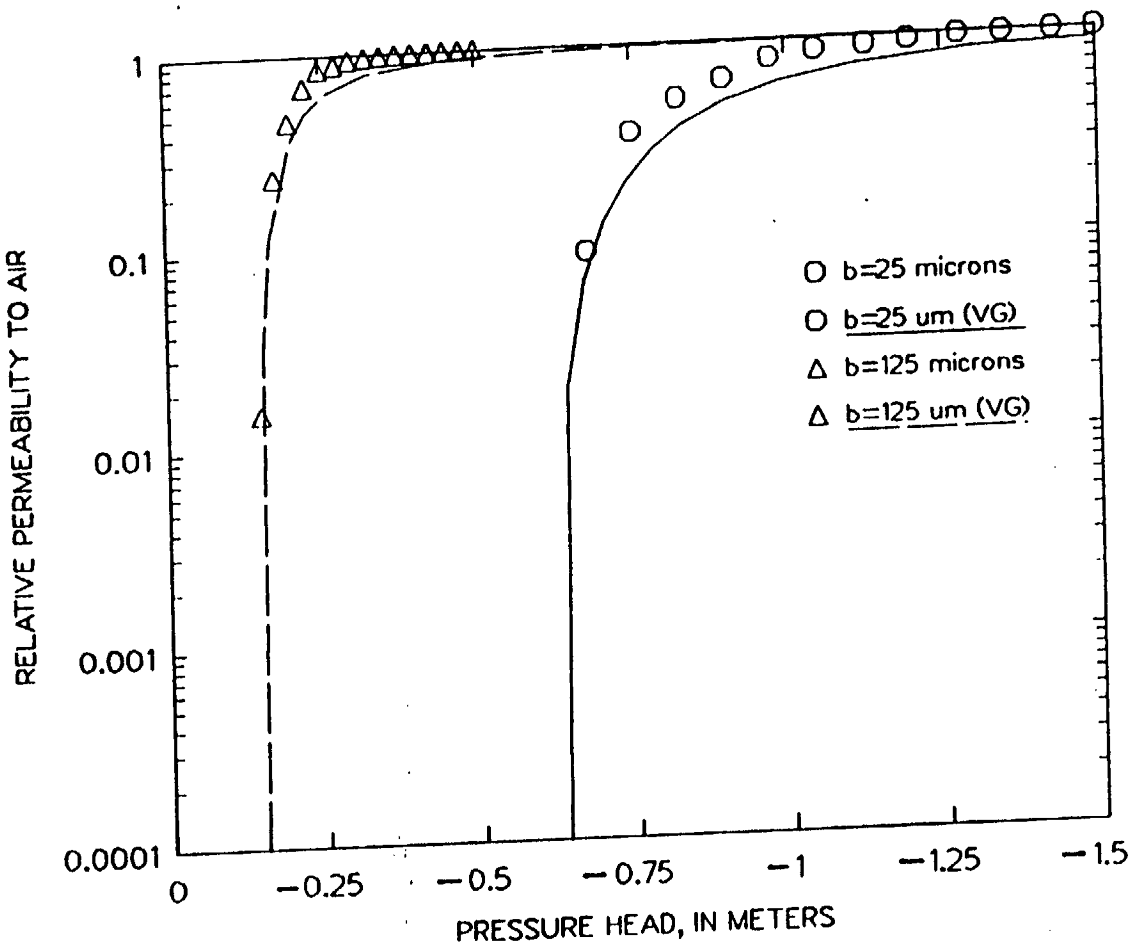


Figure 3.3-6. Theoretical air permeability versus pressure head curves calculated for single fractures with average physical apertures of 25.0 and 125.0 microns. (After Kwicklis and Healy, 1993)

and 125.0 microns. Each point in these figures represents the average of 10 stochastic realizations of the aperture field. The solid curves represent fits of the analytical functions of Luckner and others (1989) to the numerically generated data. The figures give an idea of the matric potentials at which fractures of various average apertures might be expected to become water-filled and conductive to either water or air. The fit of analytic functions originally developed for porous media to data generated by the numerical model support the use of these functions to represent the unsaturated hydraulic behavior of variable aperture fractures. The intact-fracture test to be performed in the exploratory studies facility at Yucca Mountain (Study 8.3.1.2.2.4, Unsaturated-zone percolation - ESF studies) is designed to investigate in detail the mechanics of flow in a single fracture under variable conditions of saturation and stress.

3.3.3.3.2 Matrix versus fracture flow

Considerable attention must be given to the problem of how best to represent the hydrologic properties and hydrologic response of a highly fractured porous medium. Explicit representation of individual fractures in numerical models is not considered feasible, except possibly for small volumes of rock, and unless some simplifying assumptions are made concerning fracture network geometry. In the first place, the generation of a complete set of fracture location and geometry data is, at best, difficult. Secondly, if the Topopah Spring welded unit has a mean fracture density of 20 fractures/m^3 and has a mean thickness of 300 m over the approximately $7x10^6$ m^2 area of the central Yucca Mountain block, then one would have to consider flow in approximately $4x10^{10}$ discrete fractures. One approach to modeling variably saturated fractured rock has been to explicitly represent a single fracture in the computational mesh, and invoke the symmetry of highly idealized fracture-network geometries, such as parallel fracture systems, to predict network behavior (Nitao and Buschek, 1991; Pruess and others, 1990a,b). This approach has provided useful insights regarding how fluids are exchanged between fractures and intact matrix, but has ignored potentially important issues such as network connectivity, and the dispersive effects on flow due to intersecting fractures. Conceptual approaches for modeling variably saturated fractured rock to be considered by this study include: a) representation of fracture and matrix pore domains as two separate but overlapping continua; (b) representation of fractures and matrix as a single "composite" continuum (Montazer and Wilson, 1984; Peters and Klavetter, 1988), whose properties are calculated from the combined contributions of the fracture and matrix pore domains under the assumption of <u>local</u> fracture-matrix matric potential equilibrium (which requires slowly changing conditions, but not necessarily steady-state flow conditions; and (c) a hybrid approach, wherein fracture and matrix continua are treated conceptually as separate continua where field or theoretical evidence (discussed below) suggest that fracture-matrix equilbrium is a poor assumption, and as a composite continuum elsewhere (for computational efficiency). Each of these approaches allows for the possibility that the properties of the matrix or fracture continuua vary in space. Neuman (1987) has described the use of fixed-interval packer tests to define the structure of the permeability field for the fracture continuum at spatial scales amenable to testing.

Additionally, relatively infrequent, potentially highly transmissive and areally extensive fractures (essentially faults) may be represented as distinct entities in the models. Ubiquitous small-aperture fractures or microfractures, or less areally extensive features, are lumped into the fracture continuua, and treated as described above in approaches (a) through (c). This approach captures some of the flow irregularity seemingly characteristic of fractured environments, yet reduces the number of fractures that need to be considered as discrete entities by the model. The objective of models to be developed by this study is to create an artifical system that displays flow and transport behavior approximately equivalent to the real system. The methodology required to do this is, in part, the subject of this and a related investigation (Study 8.3.1.2.2.8, Fluid flow in unsaturated, fractured rock).

Preliminary results based on a composite porosity, porous-medium-equivalent representation for fractured hydrogeologic units have been reported by Peters and Klavetter (1988). The dependence of hydraulic conductivity on liquid-water potential in a fractured porous medium such as the TSw hydrogeologic unit under the composite porosity continuum hypothesis may be expected to exhibit the qualitative appearance shown in Figure 3.3-7. At low pressure heads, or correspondingly for welded tuffs at low matrix saturations, little or no water moves longitudinally within the fracture openings, and the effective hydraulic conductivity is controlled by the fracture-bounded matrix blocks. As pressure head increases and the matrix approaches complete saturation, however, the movement of water within and along the fracture aperture rapidly becomes more efficient so that at complete saturation the fractures may be dominant contributors to the net hydraulic conductivity. If the matric potentials in the rock matrix and within the fractures are equal, a condition which may occur if moisture conditions within the rock change only slowly with time and, the properties for the fracture and matrix continua may be combined to produce the hydraulic conductivity-matric potential relationship for the composite continuum or bulk rock-mass.

Many of the theoretical aspects of unsaturated fracture flow, fracture-matrix interactions, flow within variably saturated fracture networks are being addressed in an associated study plan, YMP-USGS SP 8.3.1.2.2.8 (Fluid flow in unsaturated, fractured rock). That study plan also proposed to investigate, through comparison with fracture-network models ("synthetic data"), the adequacy of many of the alternative modeling

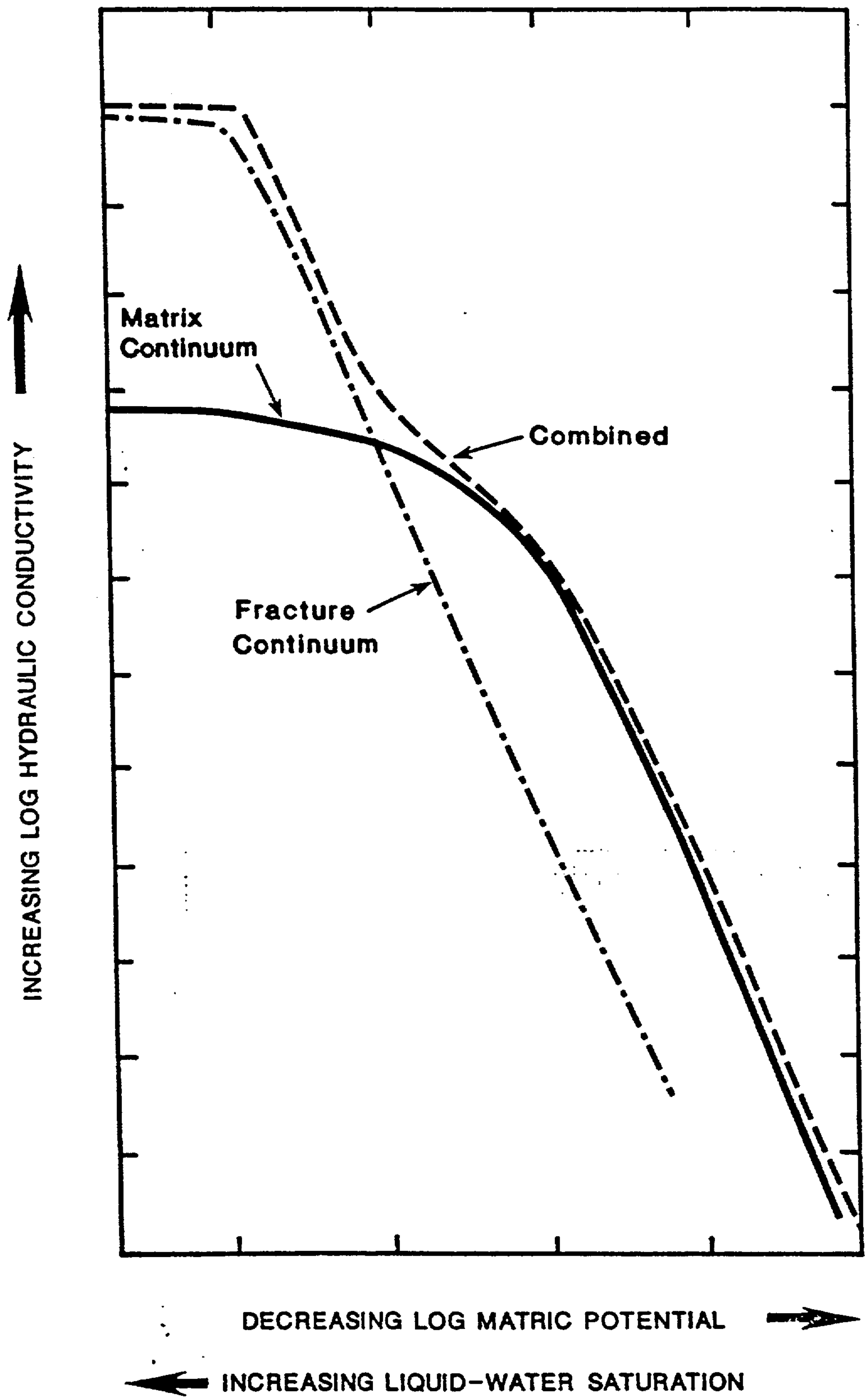


Figure 3.3-7. Idealized hydraulic-conductivity characteristic curve for a composite (fracture-matrix) porous medium. Modified from Montazer and Wilson (1984).

approaches considered by the present study plan for the site model. Conceptual uncertainty concerning simplifying assumptions made about stratigraphy, fracture-matrix interactions, and other processes will also be examined using submodels developed by this study. Examples of how submodels might be used to evaluate assumptions made in the site models are provided by Wang and Narasimhan (1986), who used dual-porosity models to evaluate the penetration depths of temporally varying infiltration events, and Nitao and others (1992). The results of Wang and Narasimhan (1986) suggested that dual-porosity treatment of the fracture and matrix continua may be necessary above and within the PTn unit, but that below this horizon the temporal effects of cyclically varying inflows are effectively dampened by the PTn unit, implying that the composite-porosity model may be applicable at greater depths. Nitao and Buschek (1991) and Nitao and others (1992) developed analytical and numerical models that explicitly accounted for water movement in single fractures, and between fractures and matrix, to investigate depths of water penetration in fractures of various hydraulic apertures. They found that water could penetrate hundreds of meters in a time period of hours when large-aperture fractures embedded in low-permeability, densely welded tuff are subjected to ponded conditions, and that for a low-permeability matrix with widely spaced fractures the assumption of fracture-matrix potential equilibrium was a rather poor one. However, their analysis ignored enhanced matrix permeability due to extensive microfractures, and the dispersion of the wetting pulse within the fracture network due to other fractures intersecting the source fracture. Their analysis was also very conservative in that unlimited amounts of water were available. The results of their analysis did, however, suggest caution be used in assuming fracture-matrix potential equilibrium throughout the mountain and that the composite-porosity approach not be applied uncritically. Field evidence that would, if found, discredit the assumption of fracture-matrix potential equilibrium at depth includes the presence of tracers of anthropogenic origin, such as tritium or chlorine-36, at depths incompatible with purely matrix-flow pathways, and water inflows into drifts of the underground facility whose volumes fluctuated cyclically or in some other manner that indicated intimate and immediate connection to surface events.

The relative contributions of fractures and matrix to the net effective hydraulic conductivity depend, in part, on the fracture frequency, aperture-size distribution, and degree of interconnectivity. The Topopah Spring welded unit exemplifies the extremes that may be encountered. This unit has a matrix saturated hydraulic conductivity of about 10^{-11} m/s and a fracture density of 8 to 40 fractures /m^3. In well J-13, where it is fully saturated and is the major source of water to the well, the Topopah Spring unit has an estimated hydraulic conductivity of about 8×10^{-6} m/s (Thordarson, 1983). The difference between the laboratory-derived matrix saturated hydraulic conductivity and the value estimated from aquifer tests conducted at well J-13 presumably represents the contribution of fractures to the bulk permeability of the Topopah Spring unit.

A further complication arises because the hydrogeologic units are likely to be anisotropic with respect to intrinsic permeability and, thus, to hydraulic conductivity. When, for the purposes of modeling, multiple layers are grouped into a single hydrogeologic unit, the resulting unit will display anisotropic behavior even if the constituent layers are isotropic with respect to hydraulic conductivity. The fracture and fault systems within the densely welded units may also introduce an inherent anisotropy wherever they are present and contribute significantly to moisture or pore-gas flow. Data are presently insufficient to perform quantitative assessment of the possible anisotropic behavior of these units.

Two principal fracture sets have been identified within the Yucca Mountain block (Scott and others, 1983). One set strikes north-northwest and the other strikes north-northeast, and both fracture sets exhibit steep to vertical dips. Most of the faults bounding and within the Yucca Mountain block are typical Basin and Range style high-angle normal faults that dip to the west, strike to the north, and exhibit small individual displacements (2 to 5 m). The Solitario Canyon fault, which bounds the proposed repository block on the west, is a north-striking high-angle normal fault that dips to the west and has a displacement ranging from 20 to 200 m along its trace. The Ghost Dance fault within the Yucca Mountain block is likewise a west-dipping, north-striking normal fault with a maximum displacement of about 25 m. These faults and their associated fracture zones in the more competent hydrogeologic units probably introduce a fundamental preferential directional control on moisture movement, whether these fault zones act as conduits for, or barriers to, flow. Quantitative data by which to characterize rock-matrix and fracture-induced anisotropy is currently lacking but will be examined by field testing in surface-based boreholes and in the underground facility (SCP Activity 8.3.1.2.2.4.4, Radial bore/bulk permeability testing in Study 8.3.1.2.2.4, Unsaturated-zone percolation - ESF studies), and by laboratory measurements on cores and on rock samples obtained during excavation of the exploratory studies facility, as described in SCP Section 8.3.1.2.

Estimates of effective block size and skin effects due to fracture coatings are considered to be important data in evaluating the interactions between fracture and matrix continua. These may be evaluated by adapting techniques originally developed for water-saturated dual-porosity media (for example, Moench, 1984) for use with highly compressible fluids such as air. Techniques for modeling variably saturated flow in dual-porosity media include those described by Pruess and Narasimhan (1985), and Zimmerman and others (1990).

Many of the field tests currently planned for the highly fractured, densely welded units from the surface-based boreholes and boreholes drilled from the underground facility will provide estimates of the intrinsic permeability of the fracture continuum, under the assumption that fractures are the dominant contributors to flow, and that within the unsaturated zone they are largely drained under current moisture conditions. Because of the experimental difficulty involved in conducting controlled unsaturated-flow experiments in large volumes of fractured rock, direct measurement of the unsaturated hydraulic properties of fractured rocks at scales relevant to site modeling may not be feasible. Indirect methods involving laboratory testing of individual fractures (SCP Activity 8.3.1.2.2.4.1), fracture mapping (SCP Activity 8.3.1.4.2.2.4), hydraulic or pneumatic testing (SCP Activity 8.3.1.2.2.4.4 and SCP Study 8.3.1.2.2.3) and fracture-network modeling (SCP Study 8.3.1.2.2.8) may prove to be the only means of estimating the unsaturated hydraulic properties of fractured rock at large scales. In brief, the strategy requires that the gross fracture geometry (orientations, lengths, and termination characteristics) be obtained from drift-wall mapping. A three-dimensional fracture-network model will be used to deduce the statistical distribution of hydraulic apertures that reproduces the observed distribution of pneumatic and hydraulic packer-injection test results, given fracture statistics consistent with the mapped geometry. Laboratory testing of individual fractures, and associated modeling of these tests with models that consider aperture variability, allow the unsaturated hydraulic properties of a fracture of a given pneumatic (or hydraulic) aperture to be estimated and bounded. Estimation of the large-scale hydraulic properties under variably saturated conditions is accomplished by incorporating unsaturated hydraulic properties typical of each hydraulic aperture size (based on laboratory testing and associated modeling) into the fracture-network model. The accuracy of this approach can be evaluated by comparing model predictions with observed flow (and transport) behavior for fracture networks of limited size (SCP Activity 8.3.1.2.2.4.2, Percolation tests in the exploratory studies facility). Estimation of the unsaturated hydraulic properties of rock at spatial scales compatible with the site model will be conducted as part of the calibration process, as described in Section 3.4 of this study, and with fracture-network models developed as part of Study 8.3.1.2.2.8.

Under transient conditions, moisture enters or is released from storage within the system, and the parameters describing the moisture-storage properties of the system must be supplied as part of the hydrologic properties. Storativity is defined by Bear (1972) to be change in volume of liquid-water storage per unit volume of bulk rock mass upon unit change of liquid-water potential. The rate at which the quantity of water held in storage changes with time is equal to the product of storativity and the time rate of change of liquid-water potential. In partially saturated media, storativity depends upon (1) the relations between ambient matrix and fracture saturations and the liquid-water potential in the matrix and fractures, (2) the liquid-water compressibility, and (3) the effective bulk compressibility appropriate to the rock matrix and the fractures. Consequently, specification of moisture storage and movement within the unsaturated zone requires the availability of hydro-mechanical-thermal properties and their spatial variation for each hydrogeologic unit. These data are to be determined through the field, laboratory, and theoretical studies that are described in SCP Sections 8.3.1.2 and 8.3.1.15. Thermomechanical data presently available for the rocks composing the hydrogeologic units at Yucca Mountain have been compiled and summarized in SCP Section 2.4.

Using approximate values for the rock-matrix and fracture mechanical properties, Peters and Klavetter (1988) have performed a preliminary analysis of capacitance (conceptually similar to storativity but with different dimensions) for the hydrogeologic units in the unsaturated zone at Yucca Mountain. They regarded each fractured unit to be represented as a composite porous medium in which the matric potential in the fractures is equal to that in the rock matrix. Their results for the TSw unit are summarized in Figure 3.3-8, which shows the contributions to the total capacitance due to a number of independent storage mechanisms. The results plotted in Figure 3.3-8 are typical of those for the other hydrogeologic units under the assumed conditions and indicate that changing fracture and rock-matrix saturations dominate storage capacity with decreasing matric potential while the bulk rock-matrix compressibility becomes the dominant contributor near complete saturation.

3.3.3.3.3 Hysteretic effects

It may be important to account for hysteretic effects when modeling the hydrologic system at Yucca Mountain. In hydrologic systems, hysteresis is the dependence of hydraulic pamameters on the past state of the flow system, specifically, whether the system is wetting or drying. Fundamentally, hysteresis is a consequence of media heterogeneity. Because heterogeneity may exist over a large range of spatial scales, from the pore scale to the formation scale, it is logical to assume that hysteresis also occurs over the same range of scales. Historically, more attention has been given to hysteresis at the pore scale (see, for example, Kool and Parker, 1987). However, it has recently been recognized that effective unsaturated hydraulic conductivity and effective moisture retention properties for heterogeneous soil volumes are hysteretic, when expressed as a function of mean pressure head, because of spatial variability in local hydraulic soil properties (Mantoglou and Gelhar, 1987a,b,c). Moreover, Mantoglou and Gelhar (1987a,b,c) showed that in a stratified system effective hydraulic conductivities are anisotropic, with a degree of anisotropy that depends on whether the system is wetting or drying. At Yucca Mountain,

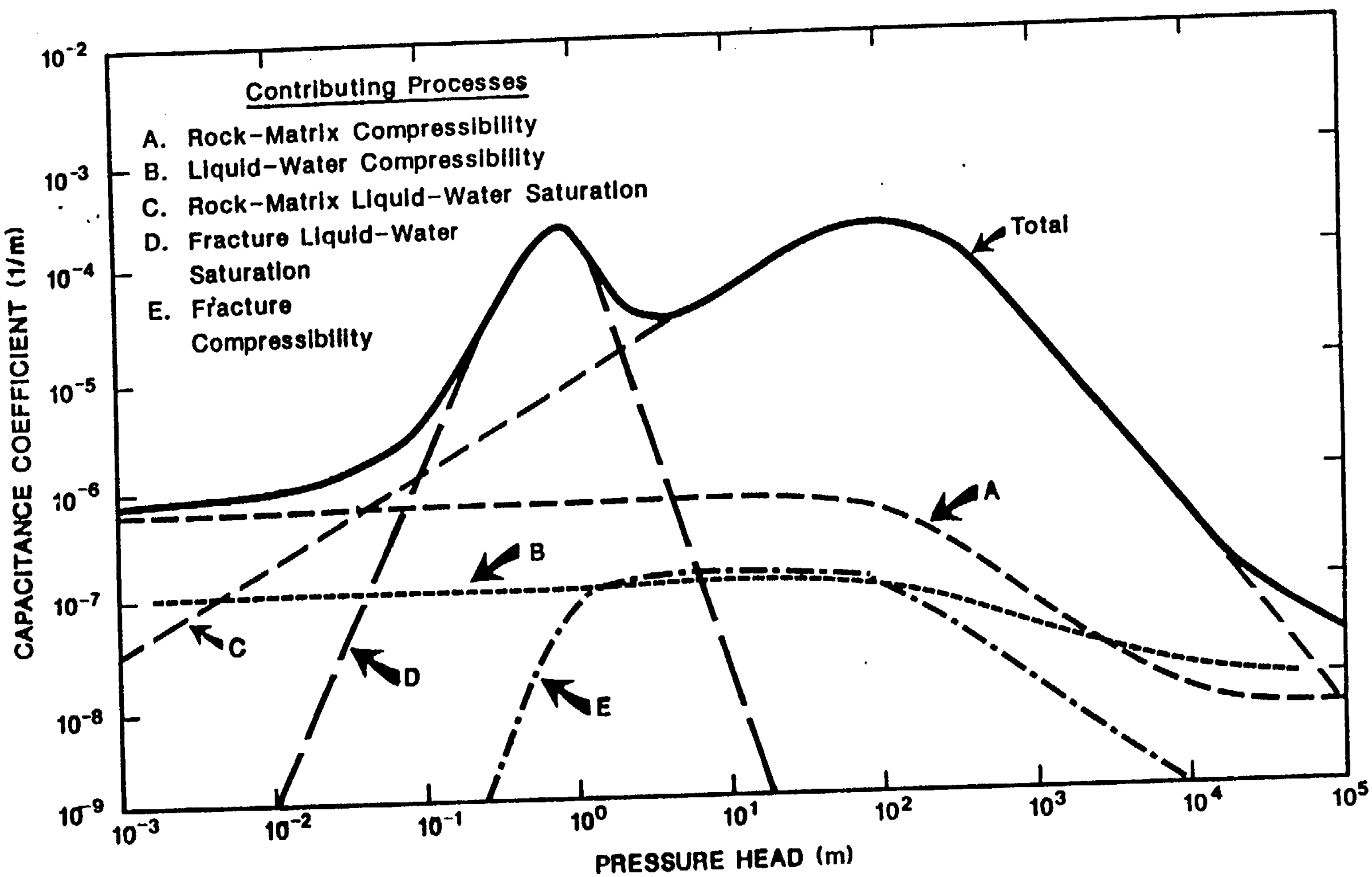


Figure 3.3-8. Computed capacitance coefficient versus pressure head for the Topopah Spring welded hydrogeologic unit. Modified from Kalavetter and Peters (1986).

such large-scale hysteresis could potentially be important in explaining the current distribution of moisture. For instance, if the mountain was once much wetter, drainage of fractures within the underlying densely welded units could trap water which entered the PTn unit under wetter climatic conditions, but which cannot drain because of the low permeability of the underlying welded tuff matrix.

3.3.3.3.4 Gas flow

Fundamental pneumatic-property data for the bulk-gas flow system within the unsaturated zone are presently lacking. Highly preliminary estimates of *in situ* air permeability in the TCw and TPn units at boreholes USW UZ-1 and USW UE-25a #4 have been reported by Montazer and others (1985). Downhole pore-gas pressures are being monitored at regular intervals in borehole USW UZ-1 (Montazer and others, 1985; see also SCP Section 3.9.1.1.1), and the results of pore-gas sampling and chemical analyses have been reported by Yang and others (1985a) (SCP Section 3.9.1.3) and Thorstenson and others (1989). Thorstenson and others (1989) have concluded on the basis of ^{13}C and ^{14}C data of gas samples that there is little communication of gas between the shallow and deep portions of the unsaturated zone beneath Yucca Crest in the vicinity of UZ-6 and UZ6-S. An extensive program of gas-phase monitoring, chemical sampling, gas-tracer studies and pneumatic-property determinations is planned as part of the surface-based, exploratory studies facility and laboratory investigations within the unsaturated zone and are described in SCP Section 8.3.1.2.2.

3.3.3.3.5 Chemical transport

In order to be able to utilize important constraining information provided by environmental tracers about flow paths and times of travel (see, for example, Yang, 1992), some capability for simulating the movement of these tracers will be coupled to the flow models for both liquid and gas. Transport models for saturated, fractured rock that employ a discrete-fracture approach (see, for example, Nordqvist and others, 1992) have shown that on the relatively small scale at which tracer experiments have been conducted from underground drifts, variability in fracture-wall separation in addition to network connectivity exerts an important influence on the simulated breakthrough of a tracer. While such models might be adapted for use helping interpret tracer experiments conducted within the exploratory studies facility, their utility for transport studies conducted at the site scale remains uncertain. At this time, both the small- and large-scale transport behavior of variably saturated fractured, porous rock is subject to considerable conceptual and parameter uncertainty. Based on analogy with saturated systems, if advective fluid movement within the fractures is significant, transport behavior may differ considerably from that thought to occur in porous media in that fluid flow may be occurring predominantly within a few structural pathways that bypass much of the available pore space (see, for example, Neretnieks and others, 1987; Cacas and others, 1990a,b). Transport porosities may therefore depend on the extent to which the tracer interacts with the matrix. In unsaturated, fractured, porous rock, tracers moving within the liquid phase may diffuse from water moving within the fractures into the matrix, or vice-versa, or be carried along advectively with water imbibed into the matrix. Numerical models employing dual-porosity concepts (see, for example, Neretnieks and Rasmusson, 1984) can theoretically account for these effects, given estimates of effective matrix block size based on fracture maps or pump-test data. However, the degree to which these interactions occurs depends on the wetted surface area of the fractures actively participating in the flow processes, among other factors, all of which may be difficult to characterize even under water-saturated conditions. For variably saturated conditions under which flow paths may change as a function of the boundary fluxes, characterization of these processes may be even more difficult.

In addition to treating fracture-matrix interactions, transport models will need to account for heterogeneity in properties in both the fracture and matrix continua. As described previously in the discussion on hydraulic behavior, it may be possible to treat the fracture system as a heterogenous porous continuum, with a permeability structure defined on the basis of packer-injection tests. The matrix continua is treated in a similar way. This approach allows the spatial distribution of permeability to dictate the characteristics of the breakthrough curve, and avoids assumptions about the large-scale dispersive properties of the medium. As was demonstrated by the numerical transport experiments of Smith and Schwartz (1980) for heterogeneous saturated media, and shown by recent field and modeling studies of nonreactive tracer movement through agricultural soils (Butters and others, 1989; Butters and Jury, 1989), fitted dispersivities may change in a complex way with travel distance as a tracer plume encounters local heterogeneities.

The matrix continua and the fracture continua defined on the basis of packer tests interact hydraulically in the numerical model through one of the approaches outlined above. Some modification of the transport capabilities of the codes listed in Section 3.2 may be required to account for the potential double-porosity effects on tracer transport. Alternatively, seepage velocities calculated by one of these codes may be used in conjunction with particle tracking algorithms such as that described by Pollock (1989). Seepage velocity is typically calculated from the fluid flux and an effective transport porosity. It has been suggested that seepage velocities necessary for transport calculations for both the fracture and matrix continua be calculated by dividing fracture and matrix fluxes within a computational cell by the mobile (non-residual) fracture and matrix water contents calculated for those cells (see, for example, Dudley and others, 1988).

3.3.3.4 Methods summary

The activity parameters to be determined by the tests and analyses described in the above sections, and the selected methods for evaluating the parameters, are summarized in Table 3.3-2. Alternate methods may be utilized only if selected methods are impractical to evaluate the parameter(s) of interest. The USGS investigators have selected modeling approaches which they believe are suitable to provide reliable data within the expected ranges of the activity parameters.

3.3.4 Quality-assurance requirements

Technical procedures do not apply to this activity because: (1) documentation and control of the quality of software used for modeling are subject to the requirements set forth in YMP-USGS QMP-3.03 (Software Quality Assurance); (2) modeling is an analytical and interpretive process, the appropriate application of which is assured by technical review as set forth in YMP-USGS QMP-3.04 (Technical Review, Approval, and Distribution of YMP-USGS Publications); and (3) data used in modeling are collected under other studies (listed in Section 2.1.6).

Table 3.3-2. Summary of analyses and methods for simulation of the natural hydrogeologic system (SCP 8.3.1.2.2.9.3)

Methods	Activity parameter
Model development	
Develop moisture-flow models	(Does not directly generate activity parameters)
Develop gas-flow model	"
Develop solute-transport model	"
Couple with rock-stress and deformation models	"
Definition of modeled parameters	
Define geologic framework, hydrogeologic-unit properties and boundary conditions	(Does not directly generate activity parameters)
Modeling of hydraulic characteristics and considerations of the unsaturated zone	
Supplement hydrogeologic-unit property data by developing sets of moisture characteristic curves	Liquid matric potential, time-dependent spatial distribution
"	Liquid saturation, time-dependent spatial distribution
"	Pore-gas pressure, time-dependent spatial distribution
"	Water-vapor concentration, time-dependent spatial distribution
"	Relative hydraulic conductivity, time-dependent spatial distribution
Model unsaturated-zone hydrogeologic-unit properties and hydrologic response using either a dual-porosity or single-composite-continuum approach	Liquid matric potential, time-dependent spatial distribution
"	Liquid saturation, time-dependent spatial distribution
"	Pore-gas pressure, time-dependent spatial distribution

Table 3.3-2. Summary of analyses and methods for simulation of the natural hydrogeologic system (SCP 8.3.1.2.2.9.3) - continued

Methods	Activity parameter
Modeling of hydraulic characteristics and considerations of the unsaturated zone - continued	
Model unsaturated-zone hydrogeologic-unit properties and hydrologic response using either a dual-porosity or single-composite-continuum approach	Water-vapor concentration, time-dependent spatial distribution
"	Temperature, time-dependent spatial distribution
"	Relative hydraulic conductivity, time-dependent spatial distribution
"	Moisture flux, time-dependent spatial distribution
"	Pore-gas flux, time-dependent spatial distribution

3.4 Stochastic modeling and uncertainty analysis

3.4.1 Objectives

The objective of this activity is to assess the probable limits of uncertainty of the numerical model predictions resulting primarily from uncertainties in material property and boundary-condition, initial-condition, and other auxiliary data.

3.4.2 Rationale for activity selection

Numerical models are mathematical approximations to physical systems and can simulate the systems that they are intended to represent only to within finite limits of accuracy. These models require that flow and transport variables be defined at discrete locations within the flow domain, including those that have not been sampled. Uncertainty in input variables due to natural variability and limited sampling results in uncertainty in the output variables (pressure head, saturation, seepage velocity, Darcy flux, solute concentration, etc.) produced by these models. Through analysis of the statistical properties of the input variables and their spatial structure, and the use of Monte Carlo methods, the uncertainty associated with various outcomes may be characterized by generating distributions of output variables and assigning probabilities to the possible outcomes (see for example, Smith and Schwarz, 1980; Smith and Schwarz, 1981). In theory, the accuracy with which a numerical hydrologic model represents an actual hydrogeologic system can be measured quantitatively by comparing the values calculated or predicted by the model for the physical hydrologic variables with those values actually measured within the system. A model is considered to be validated if it represents a system and its response to changing external conditions to within determinable and acceptable limits of accuracy. In practice, numerical models of complex natural hydrogeologic systems rarely can be validated directly because these models usually are calibrated on the basis of available hydrogeologic data for the system and hence are consistent with these data. Also, because the state of most natural hydrogeologic systems changes very slowly with time, it usually is not possible to compare model predictions with observed system response under changing environmental conditions. Consequently, practical considerations require that indirect methods be developed by which to assess model accuracy and validity. One such possible method for accomplishing this is the "bootstrap" approach, discussed below, which uses subsets of available data to calibrate the model and the remaining data to evaluate model accuracy.

3.4.3 General approach

The accuracy of a model representation depends on the adequacy and completeness of the underlying conceptual model as well as on the presence of computational and data-related error. The sources of error include: (1) discretization and truncation errors introduced by the finite numerical solution procedures; (2) round-off error inherent to the numerical calculations; (3) experimental errors of measurement associated with field and laboratory determinations of the hydrogeologic input data; (4) scale effects -- parameters are incorporated into model at one scale but measured at a different scale, or output is at one scale but is compared with data collected at another scale; and (5) random or spatially correlated heterogeneity of material properties within hydrogeologic units that introduces uncertainty in parameter values at those locations that have not been measured. The adequacy and completeness of the conceptual model is to be established as part of the conceptual-modeling and preliminary-modeling activities prior to construction of a final hydrologic model for the site, and through comparison with fracture network models developed as part of Study 8.3.1.2.2.8. Mass-balance error associated with model simulations may also aid in evaluation of the model representation. Although discretization, truncation, and round-off errors will be assessed and minimized as part of computer-code verification, these computational errors are almost always very much smaller than the errors introduced by uncertainties in the hydrogeologic input data. Consequently, an assessment of hydrologic-model accuracy and validity reduces to that of evaluating the overall effect of hydrogeologic-data variability and uncertainty on the hydrologic model results and predictions. Approximate quantitative bounds of uncertainty for the site moisture-flow model are to be estimated through a combination of classical-statistical and geostatistical data analyses, sensitivity-analysis studies, and stochastic modeling.

Deterministic models presume that all quantitative input data are known virtually to an infinitely high degree of accuracy. Stochastic models, on the other hand, consider the input data and parameters to be random variables that, however, can be characterized by appropriately defined probabilistic distribution functions or by low-order statistical moments. The probabilistic properties of the input random variables may be independent of spatial location, thus exemplifying a stationary stochastic process, or they may be the realization of non-stationary processes. In either case, these variables may be subject to varying degrees of spatial auto-correlation and cross-correlation. Although the statistical properties of the input data can be incorporated, in principle, directly into the governing set of integro-differential equations of a hydrologic model, this approach is rarely practical computationally for large-scale, complex hydrogeologic system. An alternative approach that is computationally tractable but frequently time consuming considers the overall statistical features of the hydrologic-model results to be characterizable through a finite set of Monte Carlo probabilistic-model simulations, or realizations. However, it is not known at this time whether it is either possible or necessary to perform Monte Carlo simulations for the Yucca Mountain site in three-dimensions, incorporating all of the known processes. This is because the relative importance of different processes, the hydrologic effects of local-scale heterogeneity, and the necessity of including these processes and effects in the site model, are still being investigated. Stochastic analysis and Monte Carlo simulation may be possible and perhaps only necessary for sub-system models. For instance, a stochastic approach for modeling the temporal variability in infiltration rates may be adopted by a subsystem model in order to investigate if transient and sporadic infiltration pulses are damped with increasing depth to result in approximately steady flow. Depending on the outcome of the results of the subsystem model, it may not be necessary to consider the temporal variability in infiltration rates in the three-dimensional site model.

Monte Carlo simulation can be used to examine the uncertainty in the output of the numerical models, given the uncertainty in the value of input parameters that results from spatial variability and a finite number of sampling locations. Techniques for assessing model accuracy are not well established. For instance, no quantitative methodology has yet been universally accepted for validating stochastic models that generate distributions of values at a given point in space or time when only one measured value at that value of space or time is available for comparison. One possible approach would be to test if the measured data fall within the interval containing some arbitrarily large percentage, say 95 percent, of the generated values at that location.

Another possible approach for assessing model accuracy may be some variant of the so-called "bootstrap" approach. Models of the unsaturated zone at Yucca Mountain will be calibrated, in part, on measured state variables such as water potential, saturation, temperatures, and the concentrations of environmental isotopes. In the bootstrap approach, the calibration is done on the basis of data collected at all but a relatively few locations. Numerical simulations are then conducted to produce output at various locations in the flow domain, including those locations not used in the calibration. By comparing measured and predicted values at locations omitted from the calibration process, and sequentially omitting various locations from one simulation run to the next, an assessment can be made concerning model predictions at locations were no measurements have been made. Ideally, scatterplots of predicted versus measured data at locations omitted from the calibration process plot as a one-to-one line, and have uncorrelated residuals and a large value for goodness-of-fit (r^2). Sensitivity of the results to omitted data indicates the value of that data. High sensitivity suggests the need for additional data.

A third, more qualitative technique for assessing model validity is the hypotheses testing approach. In this approach, the existence of significant hydrologic phenomena (such as perched water bodies, seeps, the spatial distribution of "young" or "old" water, etc.) predicted to occur on the basis of modeling are confirmed or refuted by field investigations. The numerical models may suggest if and where such phenomena should occur and hence guide field investigations. Alternatively, numerical models should be consistent with such "soft" data. Parameter values needed to reproduce such observations with numerical models can be compared with available data to assess if model parameters are reasonable. If so, confidence in the model is enhanced.

Figure 3.4-1 summarizes the organization of the stochastic modeling and uncertainty analysis activity. Descriptive headings for the analyses appear in the shadowed boxes of the second row. Below each analysis are the individual methods that will be utilized during testing. Figure 3.4-2 summarizes the objectives of the activity,

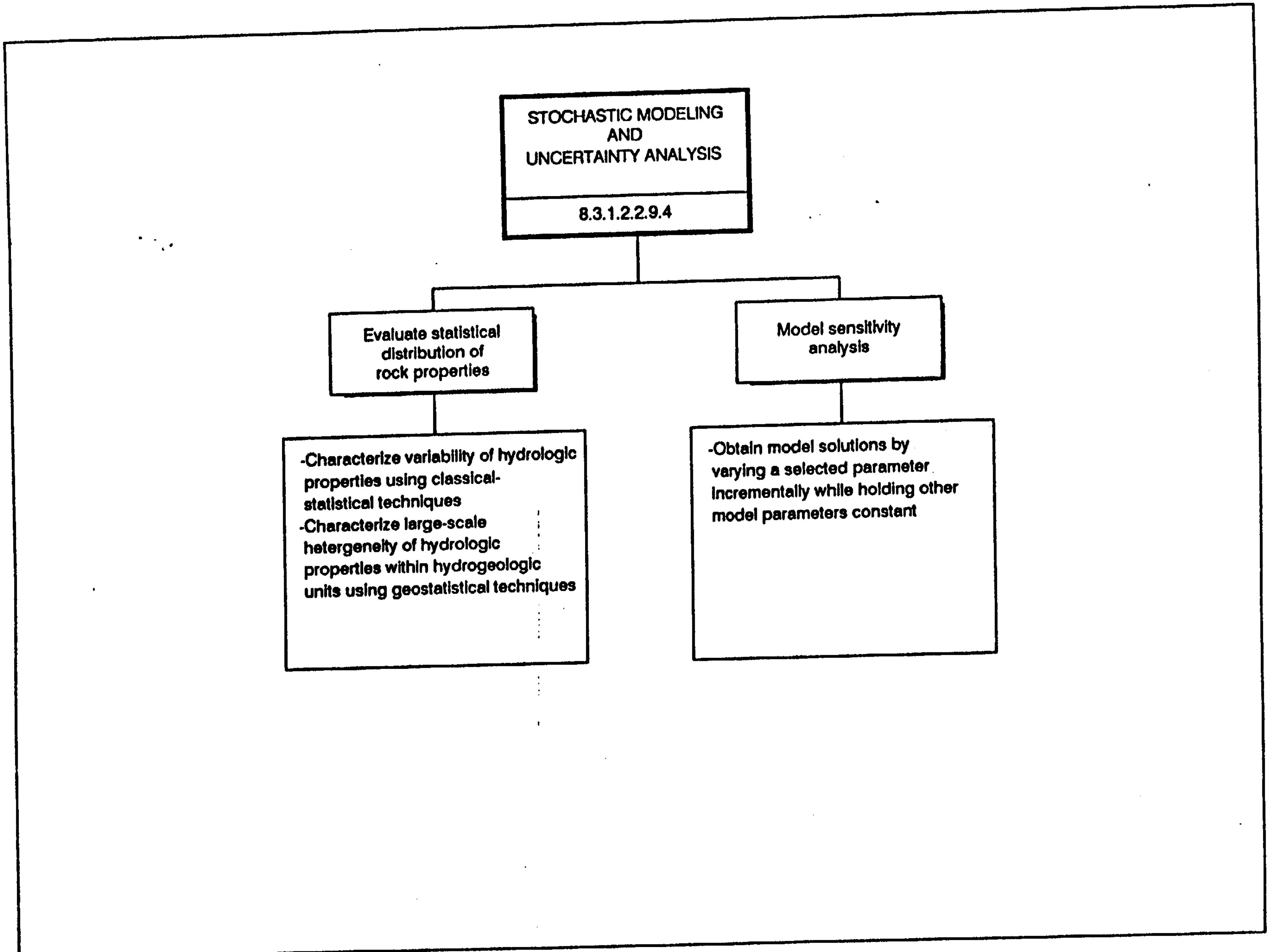


Figure 3.4-1. Logic diagram of the stochastic modeling and uncertainty analysis activity showing analyses and ...thods.

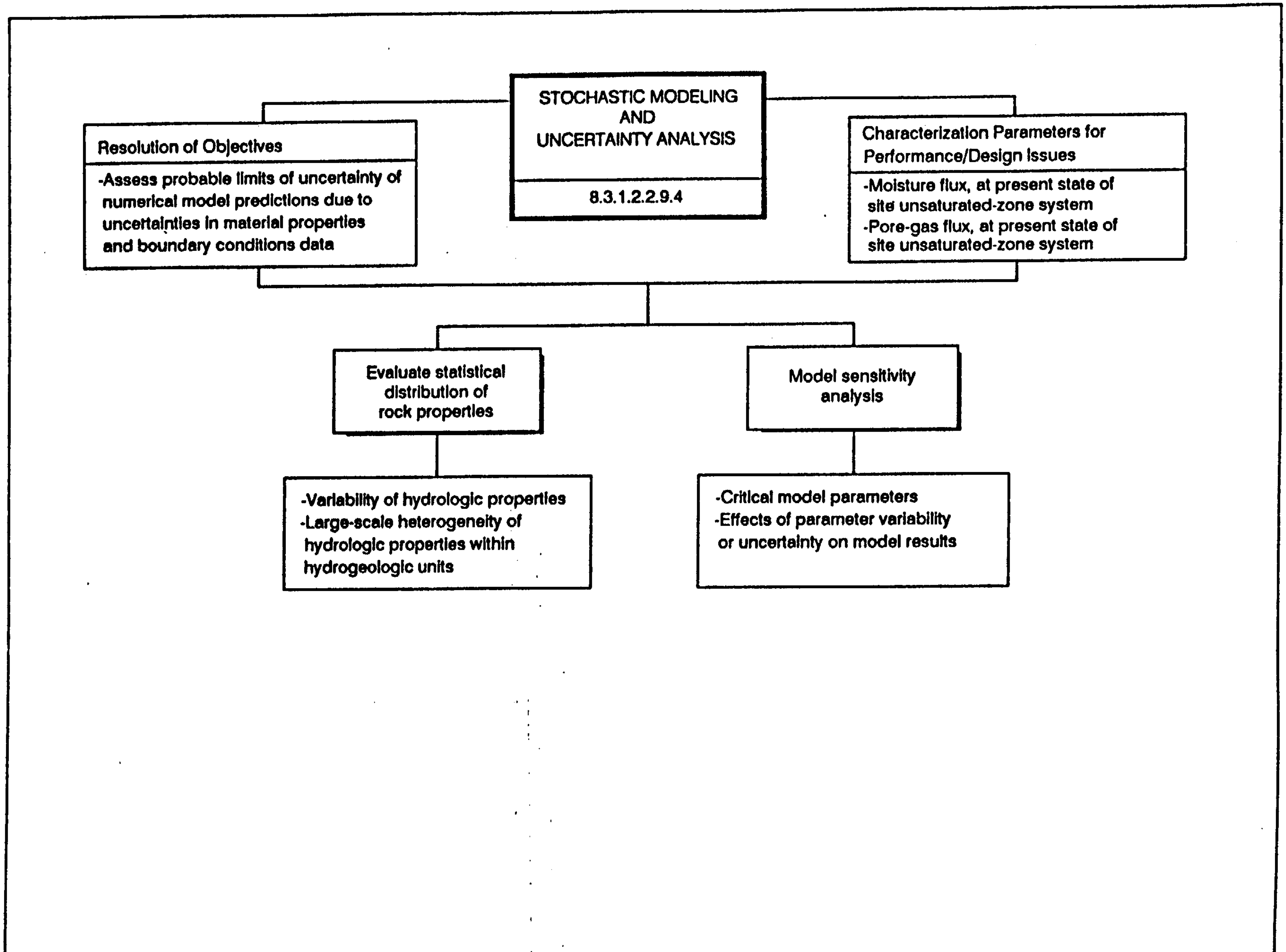


Figure 3.4-2. Logic diagram of the stochastic modeling and uncertainty analysis activity showing analyses and activity parameters.

characterization parameters which are addressed by the activity, and the activity parameters measured during testing. These appear in the boxes in the top left side, top right side, and below the shadowed analysis boxes.

The two figures summarize the overall structure of the planned activity in terms of methods to be employed and calculations to be made. The description of the following sections is organized on the basis of these charts. Methodology and parameter information are tabulated as a means of summarizing the pertinent relations among (1) the activity parameters to be determined, (2) the information needs of the performance and design issues, (3) the technical objectives of the activity, and (4) the methods to be used.

3.4.3.1 Statistical distribution of rock properties

Fundamental hydrologic, thermal, and mechanical rock-matrix properties to be used in model development are to be measured in the laboratory on cores and cuttings obtained from boreholes and on rock samples collected from within the exploratory studies facility. By performing repeat measurements on sufficiently large numbers of replicate samples, the variability of properties within each sample set can be characterized using classical-statistical techniques.

In particular, statistical distribution functions can be developed to represent the variability due to measurement error and local nonhomogeneities in measured values of porosity, saturated hydraulic conductivity, air-permeability, and the parameters defining the moisture-characteristic relations for each hydrogeologic unit within the unsaturated zone at the site. Similarly, fracture properties, specifically fracture frequencies, orientations, and apertures, can be characterized by appropriate statistical distribution functions. Also, where feasible, statistical representations can be developed for the bulk-hydrologic properties as inferred from large-scale borehole testing (Activity 8.3.1.2.2.3.2, Site vertical-borehole studies) and from testing and experimentation within the exploratory studies facility (Activity 8.3.1.2.2.4.4, Radial borehole/bulk-permeability test). Mean values computed for the properties comprise the input hydrologic data for the deterministic hydrologic models; whereas the statistical distribution functions provide the basis for the stochastic models.

A hydrogeologic unit is defined to be: a continuous body of rock to which approximately spatially uniform mean values of hydrologic and other material properties can be assigned or in which the mean properties vary within a specified limited range over the extent of the unit. A hydrogeologic unit may include all or parts of one or more geologically defined rock-stratigraphic units (Figure 3.1-3). The division of a hydrogeologic system into distinct hydrogeologic units is based on the criterion that the spatial variability of properties within each unit must be very much less than the variability between the unit and adjacent hydrogeologic units. If a hydrogeologic unit is statistically homogeneous, then its properties can be characterized in terms of a set of mean values and associated statistical distribution functions describing the errors of measurement and the effects of local, small-scale heterogeneity. If large-scale heterogeneity is present within a hydrogeologic unit, locally determined mean values for some or all of the properties will be spatially dependent. Depending on the distance over which the observations are made, trends can be considered as either drift in the mean or as correlated variation with a spatially constant mean. To the extent that the spatial distribution of data collection will allow, established geostatistical techniques can be used to analyze and develop statistical models for any large-scale heterogeneity that may be present within hydrogeologic units at the Yucca Mountain site. The results of these geostatistical investigations provide input data for subsequent stochastic modeling of the site hydrogeologic system. The statistical characterization of the hydrogeologic properties of the hydrogeologic units underlying Yucca Mountain will use both classical statistical and geostatistical methods, as part of Study 8.3.1.2.2.3 (Unsaturated-zone percolation -- surface-based studies).

Data on the spatial structure of important hydrologic parameters and on cross-correlations between parameters have begun to emerge. Rautman and Flint (1992) have reported that there are both distinct stratigraphic layers and gradational variations within and between layers. These variations were explained in terms of processes related to the emplacement and alteration of the tuffaceous materials. Rautman and Flint (1992) interpreted the observed variability as a result of random processes superimposed on the deterministic ones. Variograms with ranges of 200 m and 900 m were calculated for porosity for the Topopah Spring caprock and the zeolitic beds of the Calico Hills. Rautman and Flint (1992) also reported that the natural logarithm of saturated conductivity is correlated with porosity across a range of conductivities from 10^{-13} to 10^{-4} m/sec, with a correlation (r^2) of approximately 0.8. Wang (1992) showed that among tuffs with various degrees of welding, there appears to be a good correlation between flow parameters (intrinsic permeability) and pore-geometry parameters (capillary radius, or equivalently, air-entry pressure head).

Geostatistical analyses and classical statistical analyses can be done on parameters that characterize the unsaturated hydraulic functions that describe the relation between saturation, water potential and effective hydraulic conductivity. Characterization of the spatial distribution of these parameters through first-order methods such as geostatistics therefore provides information how these nonlinear relations change in space. For example, correlation of the van Genuchten (1980) fitting parameters α and n with porosity, and a knowledge of the spatial distribution of porosity through geostatistical methods provides information on the manner in which the moisture retention relations change spatially.

Appropriate numerical procedures will have to be devised to perform the stochastic modeling tasks. These procedures are intended to be generic so that they may be used in conjunction with any computer code used to construct numerical hydrologic models of the site hydrogeologic system or its component subsystems. In addition to the geostatistical approaches for characterizing media heterogeneity described previously, it is possible that the spatial structure of important rock characteristics will be better described using fractal geometry (see, for example, Hewett, 1986; Hewett and Behrens, 1990). This approach for representing variability in rock properties will also be investigated. The development, testing, and verification of these procedures will be completed as part of the code development and verification described in Section 3.2.

3.4.3.2 Model sensitivity analysis

Model sensitivity analyses are performed to identify critical model parameters and to assess the effects of parameter variability or uncertainty on the model results. A sensitivity analysis consists of obtaining model solutions by varying a selected model parameter incrementally while holding other model parameters constant. Sensitivity analyses will be performed on the site moisture-flow model with respect to those model parameters whose inherent variability or uncertainty cannot be characterized by statistical distribution functions because of insufficient or inadequate data. For example, the magnitude and areal distribution of the net infiltration rate at land surface over the Yucca Mountain block is unknown and inaccessible to direct measurement. The net infiltration rate is of critical importance, however, because it ultimately controls the magnitude and spatial distribution of moisture flux within the unsaturated zone. Not only must the sensitivity of the site moisture-flux model be evaluated with respect to the present rate and areal distribution of net infiltration but, because the unsaturated-zone hydrologic system is likely to respond slowly to changing environmental conditions, the sensitivity of the model also must be assessed with respect to probable past and future net infiltration rates. Rainfall simulation studies being conducted at the site as part of Study 8.3.1.2.2.1 (Unsaturated-zone infiltration) will permit an assessment of likely present-day net infiltration rates whereas probable past and future rates must be inferred from the paleoclimatology and the future-climates studies (see Section 2.1.6).

3.4.3.3 Methods summary

The activity parameters to be estimated by the tests and analyses described in the above sections are summarized in Table 3.4-1. The selected methods were chosen wholly or in part on the basis of the Principal Investigator's knowledge and experience with uncertainty analysis and stochastic modeling.

3.4.4 Quality-assurance requirements

Technical procedures do not apply to this activity because: (1) documentation and control of the quality of software used for modeling are subject to the requirements set forth in YMP-USGS QMP-3.03 (Software Quality Assurance); (2) modeling is an analytical and interpretive

Table 3.4-1. Summary of analyses and methods for stochastic modeling and uncertainty analysis (SCP 8.3.1.2.2.9.4)

Methods	Activity parameter
Evaluate statistical distribution of rock properties	
Characterize variability of hydrologic properties using classical-statistical techniques	Variability of hydrologic properties
Characterize large-scale heterogeneity of hydrologic properties within hydrogeologic units using geostatistical techniques	Large-scale heterogeneity of hydrologic properties within hydrogeologic units
Model sensitivity analysis	
Obtain model solutions by varying a selected parameter incrementally while holding other model parameters constant	Critical model parameters
"	Effects of parameter variability or uncertainty on model results

process, the appropriate application of which is assured by technical review as set forth in YMP-USGS QMP-3.04 (Technical Review, Approval, and Distribution of YMP-USGS Publications); and (3) data used in modeling are collected under other studies (listed in Section 2.1.6).

3.5 Site unsaturated-zone integration and synthesis

3.5.1 Objective

The objective of this activity is to integrate all applicable site data and analyses in order to synthesize a continually updated, comprehensive representation for the site unsaturated-zone hydrogeologic system. Attention will focus both on the present state of the system as well as on the implications concerning probable, or possible, future and past states of the system.

3.5.2 Rationale for activity selection

As site characterization progresses, a diverse set of empirical data, quantitative analyses, and interpretations will become available for the site unsaturated-zone hydrogeologic system. These data, analyses, and interpretations will be continually integrated with the prevailing conceptual model for the system in order to synthesize overall representations of the system. These representations will be examined for internal consistency and completeness. Consequently, system integration and synthesis are envisioned to be an ongoing activity that will review the validity of the prevailing conceptual model as well as the data acquisition and experimental program to ensure that, to the extent possible, all critical hydrogeologic data are being collected, and the appropriate hypotheses are being tested.

3.5.3 General approach

The synthesis performed at the end of the site-characterization program is intended to yield a best-possible representation of the current state of the hydrogeologic system together with inferences concerning past states of the system. This information will be used to extrapolate from the system behavior as observed during the performance-confirmation period. Predictions of long-term system performance will have been made before and possibly during the licensing process. Performance-confirmation monitoring will provide a partial set of confirmatory data that can be integrated into the system synthesis to provide a partial test of the validity of the synthesis. Further numerical modeling can be performed to check specific aspects of observed performance-confirmation system dynamics and response.

Assessments of the current state of system integration and synthesis are to be presented as progress and status reports to be issued periodically. Peer review will be an important aspect to ensure the integrity of the system integration and synthesis process. By issuing progress reports, not only will the process of system integration and synthesis be formalized, but implementation of the peer review process also will be facilitated. Other peer review will consist of periodic meetings with principal investigators of several other study plans to ensure (1) that the data collected from those studies are properly utilized in the site-scale model and (2) that further data needs for the site-scale model are identified and requested from the appropriate principal investigators.

Figure 3.5-1 summarizes the organization of the conceptualization of the unsaturated-zone hydrogeologic system. A descriptive heading for the analysis appears in the box of the second row. Below the analysis are the individual methods that will be utilized. The figure summarizes the overall structure of the planned activity in terms of methods to be employed. Figure 3.5-2 summarizes the objectives of the activity, the analysis to be used in the activity, and the characterization parameters addressed by the analysis. These appear in the boxes in the top left side, second row, and third row, respectively. The description in the following section is organized on the basis of these charts.

3.5.4 Quality-assurance requirements

Technical procedures do not apply to this activity because: (1) documentation and control of the quality of software used for modeling are subject to the requirements set forth in YMP-USGS QMP-3.03 (Software Quality Assurance); (2) modeling is an analytical and interpretive process, the appropriate application of which is assured by technical review as set forth in YMP-USGS QMP-3.04 (Technical Review, Approval, and Distribution of YMP-USGS Publications); and (3) data used in modeling are collected under other studies (listed in Section 2.1.6).

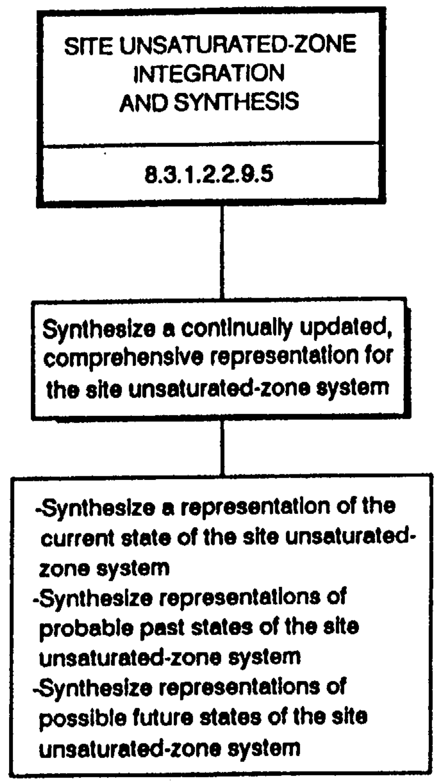


Figure 3.5-1. Logic diagram of the site unsaturated-zone integration and synthesis activity, showing analyses and methods.

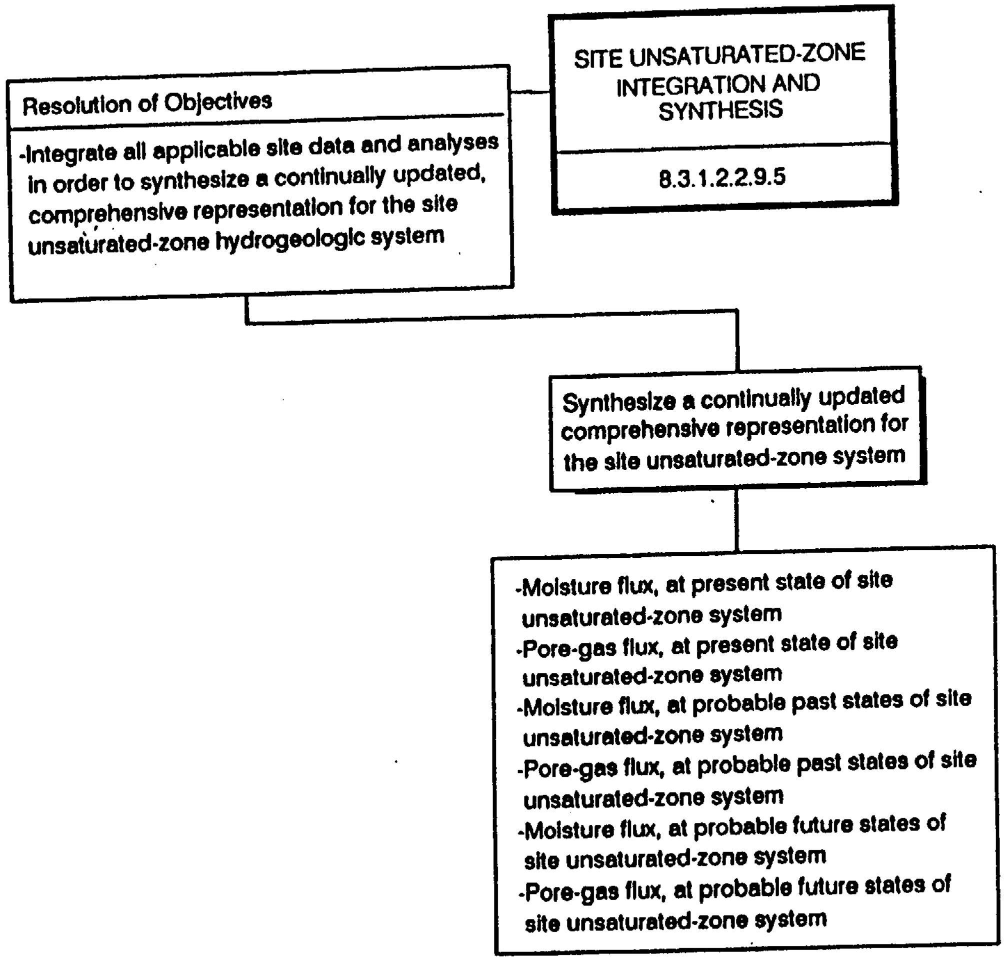


Figure 3.5-2. Logic diagram of the site unsaturated-zone integration and synthesis activity, showing analyses and characterization parameters.

4 APPLICATION OF STUDY RESULTS

4.1 Application of results to resolution of design and performance issues

The results of this study will be used in the resolution of YMP design and performance issues concerned with the fluid flow in the unsaturated zone of the Yucca Mountain site. The principal applications will be to support assessment of ground-water and gas travel times (Issues 1.1 an 1.6), design analysis and operating procedures related to the underground-repository facilities and waste packages (Issues 4.4 and 1.10), and the total performance of the containment system and repository engineered-barriers (Issues 1.4 and 1.5).

The application of site information from this study to design and performance-parameter needs required for the resolution of design and performance issues is addressed in Section 1.3. Sections 2 and 3 use logic diagrams and tables to summarize specific relationships between design and performance parameter needs and site-characterization parameters determined from this study.

4.2 Application of results to support other site-characterization investigations and studies

The models and codes collected and developed from this study will be utilized in other studies in Investigation 8.3.1.2.2 (Description of the unsaturated-zone hydrologic system at the site), as well as other studies in the following investigations:

- 8.3.1.2.1 - Description of the regional hydrologic system;
- 8.3.1.2.3 - Description of the saturated-zone hydrologic system at the site;
- 8.3.1.3.1 - Studies to provide the information on water chemistry within the potential emplacement horizon and along potential flow paths;
- 8.3.1.3.4 - Studies to provide information required on radionuclide retardation by sorption processes along flow path to the accessible environment;
- 8.3.1.3.5 - Studies to provide the information required on radionuclide retardation by precipitation processes along flow paths to the accessible environment;
- 8.3.1.3.6 - Studies to provide the information required on radionuclide retardation by dispersive/diffusive/advective transport processes along flow paths to the accessible environment;
- 8.3.1.3.7 - Radionuclide retardation by all processes along flow paths to the accessible environment;
- 8.3.1.3.8 - Studies to provide the required information on retardation of gaseous radionuclides along flow paths to the accessible environment;
- 8.3.1.5.1 - Nature and rates of change in climatic conditions to predict future climates;
- 8.3.1.5.2 - Potential effects of future climatic conditions on hydrologic characteristics;
- 8.3.1.6.4 - Potential effects of erosion on hydrologic characteristics;
- 8.3.1.8.3 - Potential effects of igneous and tectonic activity on hydrologic characteristics;
- 8.3.1.16.3 - Ground-water conditions within and above the potential host rock.

The final product of Study 8.3.1.2.2.9 is a model or set of models to describe the three-dimensional, two-phase, coupled heat- and moisture-flow for the Yucca Mountain hydrogeologic site. The final flow model(s) will be used to perform a set of baseline simulations of the natural hydrogeologic system. Using the simulation of the presently existing natural system as initial conditions, a sequence of simulations will be obtained to extrapolate the system both forward and backward in time. The forward extrapolation will be based on expected changes in the site climatological regime derived from Study 8.3.1.5.1.6 (Future regional climate and environments); whereas the backward extrapolations will be based on past climatological conditions and variations inferred from Study 8.3.1.5.1.4, (Synthesis of the paleoenvironmental history of the Yucca Mountain region). The sequence of baseline simulations constitutes a standard set against which the effects of extreme or episodic changes in environmental conditions at the site may be assessed. The most-probable limits of uncertainty attaching to the baseline simulations is to be estimated as part of Section 3.4 (Stochastic modeling and uncertainty analysis). This flow model will be used to define flow paths and calculate fluxes and velocities within the unsaturated zone, as described in Section 3.5 (Site unsaturated-zone integration and synthesis). The use of the model(s) and computer code(s) will have direct application to the previously cited investigations in the following manner:

The unsaturated-zone flow and transport modeling study interfaces with several other studies and investigations to provide an understanding of the hydrology and chemistry beneath Yucca Mountain. In Investigation 8.3.1.2.1 (Description of the regional hydrologic system), results from the flow and transport modeling will be applicable to the characterization of the regional ground-water flow system and the development of numerical models of regional ground-water flow (8.3.1.2.1.4). The data from these studies will be used in conceptual-model, mathematical-model, and computer-code development. In turn, the computer codes will be used to identify deficiencies in the database and assist in other site-characterization studies.

The data acquired in this study will complement data from Investigation 8.3.1.2.3 (Description of the saturated-zone hydrologic system at the site). Chemical and isotopic analyses of unsaturated-zone interstitial waters will be used specifically in Study 8.3.1.2.3.2 (Site saturated-zone hydrochemistry). Also, in order to calculate flow paths, fluxes, and velocities within the saturated zone, input from unsaturated-zone flow and transport models will be required. Study 8.3.1.2.3.3 (Site saturated-zone synthesis and modeling) defines model and computer code development for the saturated-zone system. In order to model this system the unsaturated-saturated zone interface boundary conditions must be defined. These boundary conditions will be better defined by unsaturated-zone models developed in the present study.

Investigations 8.3.1.3.1, 8.3.1.3.4, 8.3.1.3.5, 8.3.1.3.6, 8.3.1.3.7, and 8.3.1.3.8 deal with providing information on water chemistry; radionuclide retardation by sorption, precipitation, dispersive/diffusive/advective transport, and all processes; and gaseous radionuclide transport along possible flow paths to the accessible environment. The codes in this study will assist in defining the possible flow paths in the unsaturated zone.

Investigation 8.3.1.3.1 (Water chemistry within the potential emplacement horizon and along potential flow paths) will receive direct input from the activities in this study plan. The ground-water chemistry study (Study 8.3.1.3.1.1) will employ results from modeling generated in the present study.

In Investigations 8.3.1.3.4, 8.3.1.3.5, and 8.3.1.3.6 the hydrochemical and flow characteristics researched in this study will contribute to sorption, precipitation, and dispersive/diffusive/advective transport studies. The modeling will provide information relevant to water-rock interactions and, consequently, to radionuclide migration and retardation by all processes along flow paths to the accessible environment (Investigation 8.3.1.3.7). Data from the unsaturated-zone hydrochemical modeling will be used in retardation sensitivity analyses (Study 8.3.1.3.7.1), geochemical models of Yucca Mountain (Study 8.3.1.8.7.2), and transport modeling (Study 8.3.1.3.7.3). Similarly, the gaseous-phase chemical data evaluated in this study plan will be used in Investigation 8.3.1.3.8 to provide information on the retardation of gaseous radionuclides along flow paths to the accessible environment.

Investigations 8.3.1.5.1, 8.3.1.5.2, 8.3.1.6.4, and 8.3.1.8.3 are concerned with the potential effect of climatic, erosional, and tectonic activities on the hydrologic system. The conceptual models and computer codes developed in this study will be used to evaluate these effects for the unsaturated zone. Interpretation of data from this study will provide estimates of pore-water ages and insight as to recharge to and flow within the unsaturated zone. In Investigation 8.3.1.5.1, unsaturated-zone modeling hydrochemistry data will be used in comparison with the isotopic content of regional storms (Activity 8.3.1.5.1.1.1), paleoclimate geochemistry (Activity 8.3.1.5.1.2.3), and in the modeling of future climates (Study 8.3.1.5.1.6). Unsaturated-zone flow and transport information will also support the Quaternary regional hydrology study (8.3.1.5.2.1) of Investigation 8.3.1.5.2 by providing isotopic and water flow and composition data to determine pore-water residence times and travel paths. The modeled results of the forward extrapolation of unsaturated-zone conditions may contribute to the modeling of future saturated-zone hydrology in Study 8.3.1.5.2.2 (Future regional hydrology due to climate changes).

The understanding of unsaturated-zone hydrologic properties developed by the modeling efforts of this study will support Investigation 8.3.1.16.3, which outlines studies to be used in evaluating ground-water conditions within and above the potential host rock. Study 8.3.1.16.3.1 (Determination of the preclosure hydrologic conditions of the unsaturated zone at Yucca Mountain) will compile and synthesize data collected in this study pertinent to unsaturated-zone characterization. These data will be used in addressing repository design requirements, design analyses, and underground facilities technology.

5 SCHEDULES AND MILESTONES

5.1 Schedules

Figure 5.1-1 presents an integrated schedule for the site unsaturated-zone modeling and synthesis study. The proposed schedule summarizes the logic network and reports for the activities in the study, and represents a summary of the schedule information which includes the sequencing, interrelations, and relative durations of the activities described in this study. Specific durations, and start and finish dates for the activities are being developed as part of ongoing planning efforts. The development of the schedule for the present study has taken into account how the study will be affected by contributions of data or interferences from other studies, and also how the present study will contribute or may interfere with other studies.

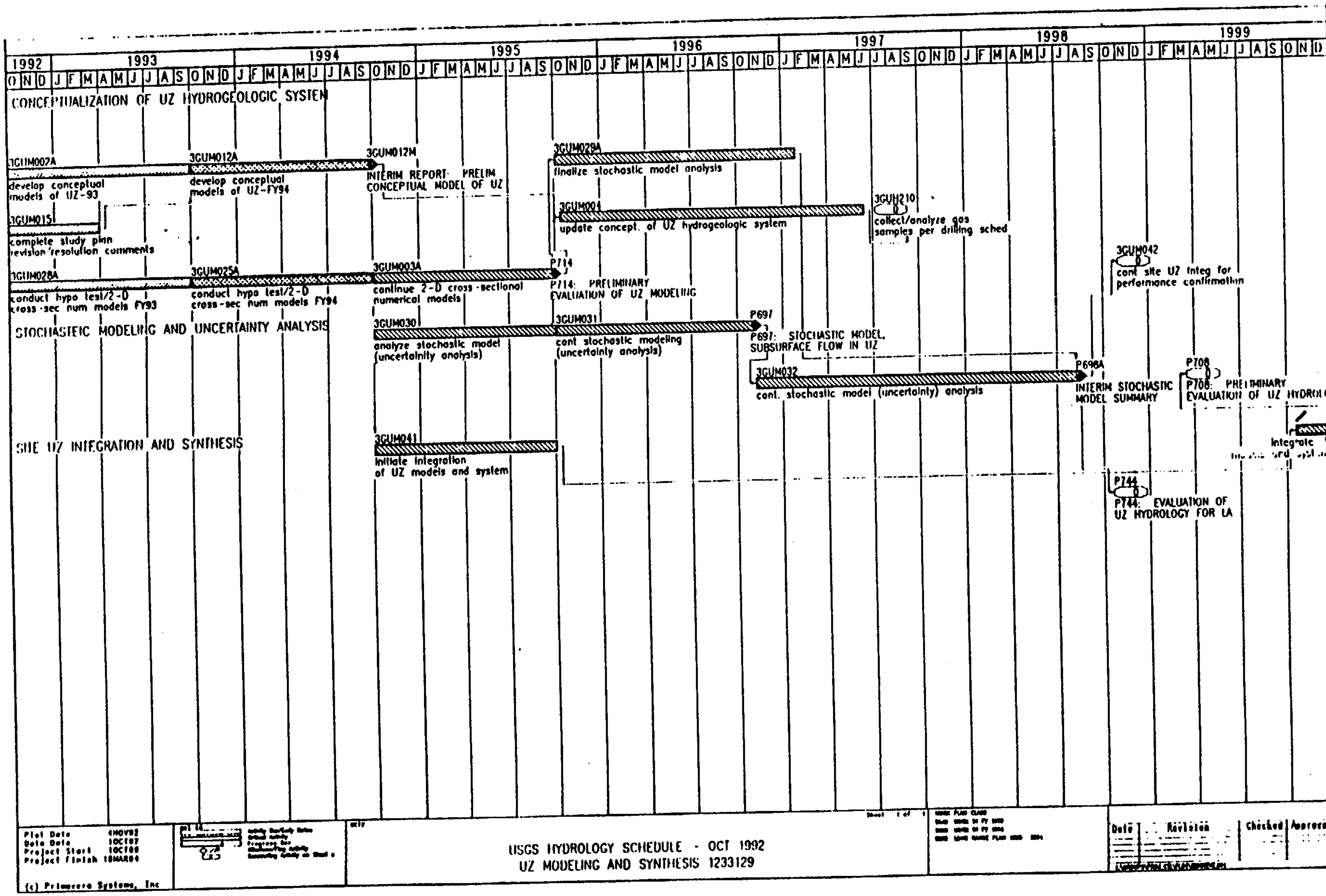


Figure 5.1-1a. Summary logic network for the unsaturated-zone modeling and synthesis study

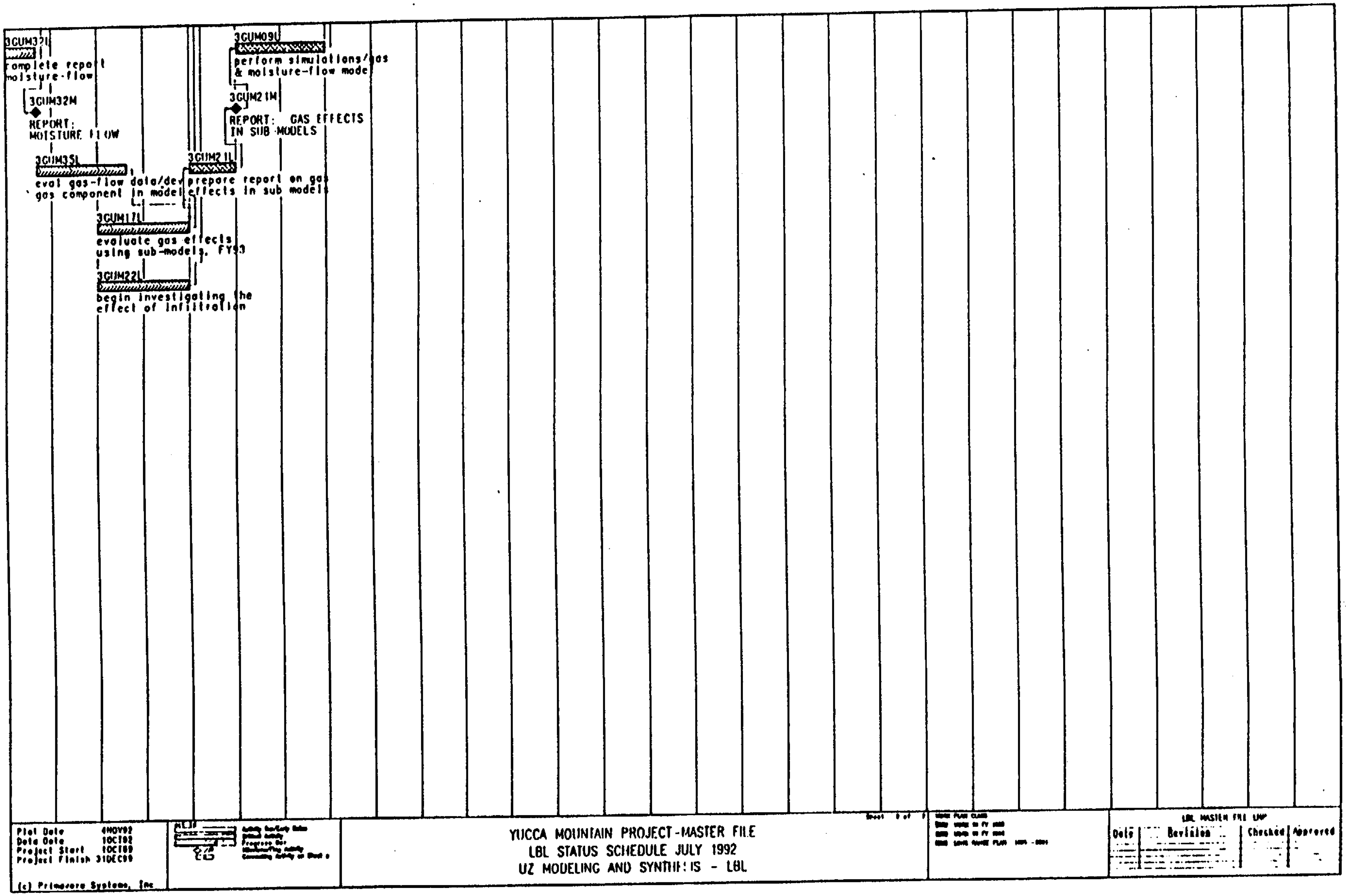


Figure 5.1-1b. Summary logic network for the unsaturated-zone modeling and synthesis study

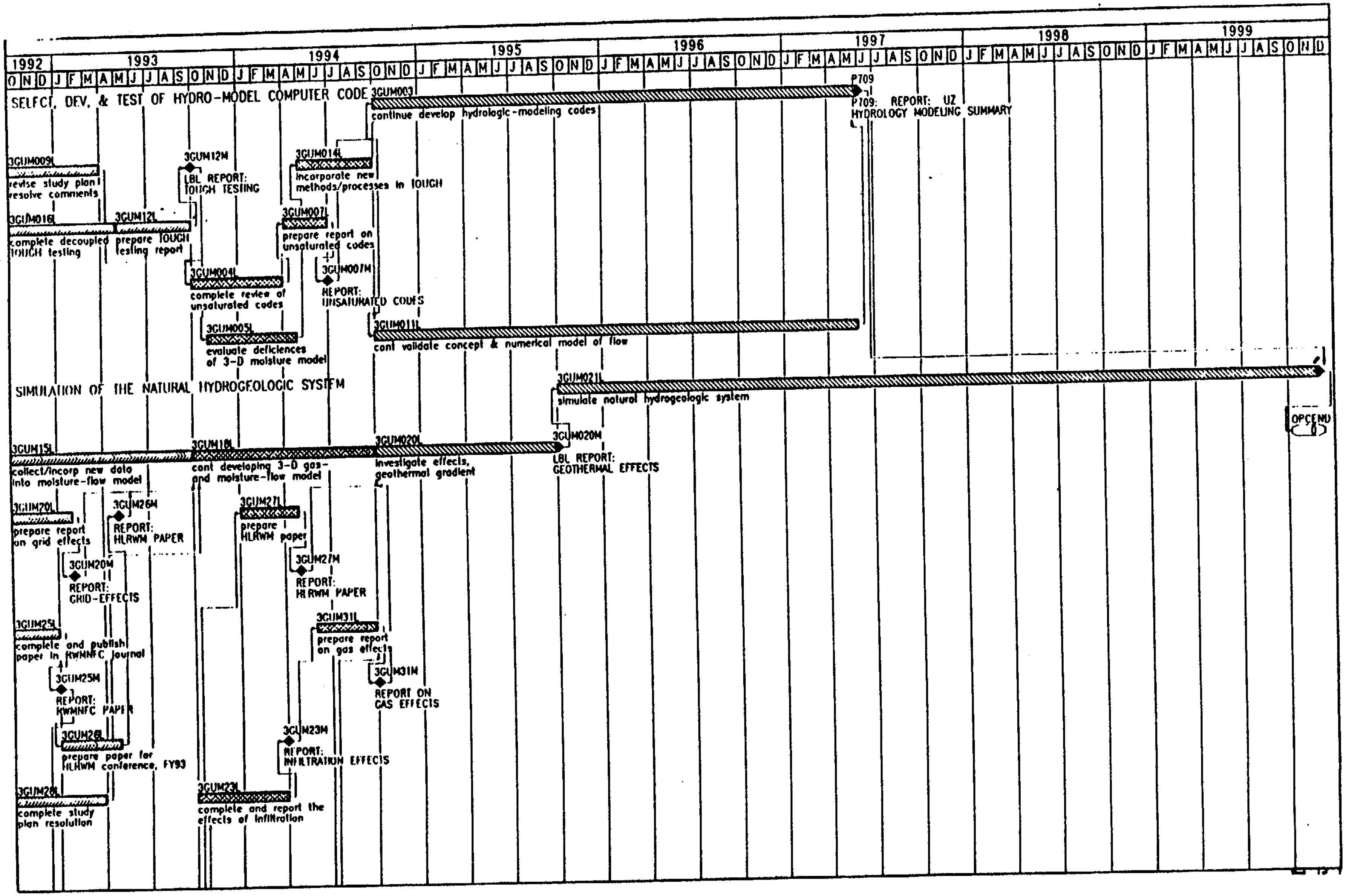


Figure 5.1-1c. Summary logic network for the unsaturated-zone modeling and synthesis study

5.2 Milestones

The milestone numbers and titles associated with the activities of the unsaturated-zone flow and transport modeling study are summarized in Table 5.2-1. The information presented in Table 5.2-1 represents major events or important summary milestones associated with the activities presented in this study plan as shown in Figure 5.1-1. Specific dates for the milestone are not included in the tables as these dates are subject to change due to ongoing planning efforts.

Table 5.2-1. Milestone list for Study 8.3.1.2.2.9

Milestone Number	Milestone	Milestone Level
Conceptualization of the unsaturated-zone hydrogeologic system: Activity 8.3.1.2.2.9.1		
P714	Preliminary evaluation of UZ modeling	2
3GUM012M	Interim Report: Preliminary conceptual model of UZ	3
Selection, development, and testing of hydrologic-modeling computer codes: Activity 8.3.1.2.2.9.2		
P709	Report: UZ hydrology modeling summary	2
3GUM007M	Report: Unsaturated codes	3
3GUM12M	LBL Report: TOUGH testing	3
Simulation of the natural hydrologic system: Activity 8.3.1.2.2.9.3		
3GUM020M	LBL Report: Geothermal effects	3
3GUM20M	Report: Grid-effects	3
3GUM21M	Report: Gas effects in sub-models	3
3GUM23M	Report: Infiltration effects	3
3GUM25M	Report: RWMNFC paper	3
3GUM26M	Report: HLRWM paper	3
3GUM27M	Report: HLRWM paper	3
3GUM31M	Report on gas effects	3
3GUM32M	Report: Moisture-flow	3
M036	Preliminary hydrologic model of the UZ	3

Table 5.2-1. Milestone list for Study 8.3.1.2.2.9)--*Continued*

Milestone Number	Milestone	Milestone Level
Stochastic modeling and uncertainty analysis: Activity 8.3.1.2.2.9.4		
P697	Stochastic model, subsurface flow in UZ	2
P698A	Interim stochastic model summary	3
Site unsaturated-zone integration and synthesis: Activity 8.3.1.2.2.9.5		
P708	Preliminary evaluation of UZ hydrology	2
3GUM043M	Final hydrologic description of UZ	3
P744	Evaluation of UZ hydrology for LA	3

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7 APPENDIX

7.1 Relations between the site information to be developed in this study and the performance and design information needs specified in the SCP

This section tabulates in Table 7.1-1 the specific technical information relations between SCP design/performance-parameters needs and characterization parameters to be determined in this study. The relations were developed using model-based parameter categories (See Figure 2.1-1) that provide common terminology and organization for evaluation of site and design/performance information relations.

Performance and design issues that obtain data from this study are noted in the table. For each issue, the characterization parameters (from SCP 8.3.1.2) are related to the design/performance parameters reported in the design/performance allocation tables (from SCP 8.3.2 - 8.3.5). At the beginning of each issue group, the performance measures addressed by the design/performance parameters for the issue are listed. Parameter categories, as noted above, are used to group the design/performance parameters with the characterization parameters so that comparisons of information requirement (performance) with information source (site study) can be made.

For each design/performance parameter noted in the table, the associated goal and confidence (current and needed) and site location are listed. For each parameter category, the associated characterization parameters are listed with information about the site location and the site activity providing the information.

Note - Comparison of the information relations (site parameters with design/performance parameters) must be done as sets of parameters in a given parameter category. Line-by-line comparisons from the left side of the table (design/performance parameters) with the right side of the table (characterization parameters) within a parameter category should not be made.

Table 7.1-1 Design and performance issues and parameters supported by results of this study

Design and Performance Parameters	Parameter Goal and Confidence (Current and Needed)	Characterization Parameters	Site Activity
			(SCP 8.3.5.13)
Issue 1.1	Total system performance		
Performance Measures:	(Supporting parameters needed to evaluate the nominal case and as baseline data for the disturbed cases.) EPPM[a], nominal case, release scenario class E, water and gas pathway releases		
q_u: average flux through repository area in unsaturated zone	Goal: <0.5 mm/yr Current: Medium Needed: High	Moisture flux, at present state of site unsaturated-zone system	8.3.1.2.2.9.3 8.3.1.2.2.9.4 8.3.1.2.2.9.5
n_e: average effective matrix porosity, repository area unsaturated zone	Goal: >0.1 Current: Low Needed: High	Pore-gas, at present state of site unsaturated-zone system	"
Mean residence time of released carbon-14 dioxide in unsaturated-zone units	Goal: Show residence time >10,000 yr Current: Low Needed: High	Moisture flux, at probably past states of site unsaturated-zone system	8.3.1.2.2.9.5
		Pore-gas flux, at probably past states of site unsaturated-zone system	"
		Moisture flux, at possible future states of site unsaturated-zone system	"
		Pore-gas flux, at possible future states of site unsaturated-zone system	"

Table 7.1-1 Design and performance issues and parameters supported by results of this study

Design and Performance Parameters	Parameter Goal and Confidence (Current and Needed)	Characterization Parameters	Site Activity
Issue 1.5	Waste package and repository engineered-barrier system release rates		(SCP 8.3.5.10)
Performance Measures:	Concentrations of radionuclide species in gas phase, liquid water, and adsorbed to solid phases within the near-field host rock.		
Host-rock hydrologic properties (waste package environment)	Goal: Properties known with accuracy sufficient to calculate difference in flow through the near-field rock resulting from anticipated and unanticipated events Current: Low Needed: High	Moisture flux, at present state of site unsaturated-zone system	8.3.1.2.2.9.3 8.3.1.2.2.9.4 8.3.1.2.2.9.5
		Pore-gas, at present state of site unsaturated-zone system	"
		Moisture flux, at probably past states of site unsaturated-zone system	8.3.1.2.2.9.5
		Pore-gas flux, at probably past states of site unsaturated-zone system	"
		Moisture flux, at possible future states of site unsaturated-zone system	"
		Pore-gas flux, at possible future states of site unsaturated-zone system	"

Table 7.1-1 Design and performance issues and parameters supported by results of this study

Design and Performance Parameters	Parameter Goal and Confidence (Current and Needed)	Characterization Parameters	Site Activity
			(SCP 8.3.5.12)
Issue 1.6	Pre-waste-emplacement, ground-water travel time		
Performance Measures:	(Supporting parameters used in calculating performance parameters for ground-water travel time.)		
Flux (q)	Goal: <0.5 mm/yr Current: Medium Needed: High	Moisture flux, at present state of site unsaturated-zone system	8.3.1.2.2.9.3 8.3.1.2.2.9.4 8.3.1.2.2.9.5
Effective porosity and porosity of the fracture network, fault zones, rock mass, and matrix	Goal: -- Current: -- Needed: --	Pore-gas, at present state of site unsaturated-zone system	"
q/K_s where K_s is hydraulic conductivity of saturated-matrix zones	Goal: <0.95 Current: Medium Needed: High	Moisture flux, at probably past states of site unsaturated-zone system	8.3.1.2.2.9.5
		Pore-gas flux, at probably past states of site unsaturated-zone system	"
		Moisture flux, at possible future states of site unsaturated-zone system	"
		Pore-gas flux, at possible future states of site unsaturated-zone system	"

Table 7.1-1 Design and performance issues and parameters supported by results of this study

Design and Performance Parameters	Parameter Goal and Confidence (Current and Needed)	Characterization Parameters	Site Activity
Issue 4.4	Repository construction, operation, closure, and decommissioning technologies		(SCP 8.3.2.5)
Performance Measures:	Removal rate equal to rate of inflow		
Host rock hydrologic properties (waste package environment)	Goal: Properties known with accuracy sufficient to calculate differences in flow through the near-field rock resulting from anticipated and unanticipated events Current: Low Needed: High	Moisture flux, at present state of site unsaturated-zone system	8.3.1.2.2.9.3 8.3.1.2.2.9.4 8.3.1.2.2.9.5
		Pore-gas, at present state of site unsaturated-zone system	"
		Moisture flux, at probably past states of site unsaturated-zone system	8.3.1.2.2.9.5
		Pore-gas flux, at probably past states of site unsaturated-zone system	"
		Moisture flux, at possible future states of site unsaturated-zone system	"
		Pore-gas flux, at possible future states of site unsaturated-zone system	

SP 8.3.1.2.2.9, R0

United States Department of the Interior

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IN REPLY REFER TO:

June 16, 1993

WBS: 1.2.9.1.2
QA: N/A

1-343484

Carl P. Gertz, Project Manager
Yucca Mountain Site
Characterization Project Office
U.S. Department of Energy
P.O. Box 98608
Las Vegas, Nevada 89193-8608

SUBJECT: U.S. Geological Survey (USGS) Detailed Monthly Status Report for April, 1993

Dear Carl:

Enclosed is the USGS detailed monthly status report for April, 1993. If you have any questions or comments, please contact Raye Ritchey at 303-236-0517.

Sincerely,

Raye E. Ritchey
for Larry R. Hayes
Technical Project Officer
Yucca Mountain Project Branch
U.S. Geological Survey

Attachment

DIVISION: Lau
CC: Simecka-w/o
CC: Dyer
CC: Dixon
CC: Schreiner/gost
CC: Brodsky
CC: Jones, S
CC: Lyman
CC: Stucker-ew22 / Gertz
Wallace-ew22
Smith, L-w/o

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