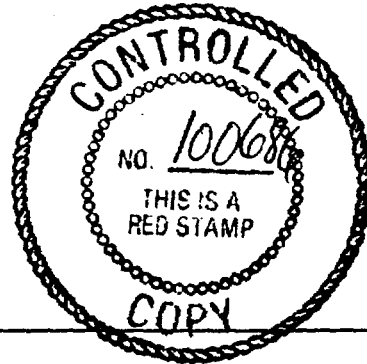


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LABORATORY THERMAL PROPERTIES

Site Characterization Plan Study 8.3.1.15.1.1

**Performance Assessment Applications Department
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ABSTRACT

Licensing of a nuclear-waste repository by the Nuclear Regulatory Commission requires, among other things, demonstration of the long-term usability of the underground portion of the repository. Such a demonstration involves analysis of the thermal response of the rock to the presence of heat-producing waste, which in turn requires data on the thermal properties of the rock. This document describes (1) the rationale for obtaining thermal-properties data; (2) the determination of specific requirements for the data (e.g., number of samples, experiment conditions); and (3) specific experimental plans for obtaining data on each thermal property (bulk density, thermal conductivity, and heat capacity).

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1.0 INTRODUCTION

This Study Plan describes the experiments planned to obtain the data on thermal properties of tuff units as required by repository design and performance assessment to support the license application process. The data base will contribute to the estimation of the thermal properties of the rock mass, which in turn will be used in analyses of heat transfer in and around a repository located in the lower part of the Topopah Spring Member of the Paintbrush Tuff. These estimated thermal properties of the rock mass will be compared and, if appropriate, combined with information on thermal properties of the rock mass obtained directly from in situ measurements. In addition, the thermal property information will be used to determine the temperature distributions required as input to thermal-stress analyses.

To date, emphasis has been placed on properties that contribute to conductive heat transfer because this mechanism is assumed to dominate heat transfer in the unsaturated tuffs in which a repository would be located. Therefore, this Study Plan is directed primarily toward plans to obtain data on thermal conductivity (in some cases, effective thermal conductivity because of incorporation of heat-transfer mechanisms such as latent-heat transfer), heat capacity, and bulk density (thermal diffusivity, the ratio of thermal conductivity to the product of density and heat capacity, can be calculated from these properties). The possibility remains, however, that other heat transfer mechanisms (e.g., radiation or convection) may be locally significant in the rock mass in the vicinity of a repository. The heat-transfer mechanisms will be studied during a number of in situ experiments (discussed in other Study Plans as summarized in Table 1.0-1). Mechanisms other than conduction are not discussed in this document except in cases where effects on heat transfer are relevant to the main objective of this Study Plan.

Table 1.0-1
Summary of In Situ Experiments Obtaining Information Related
to Data for the Thermal Properties of the Rock Mass

Study Plan	Experiment
8.3.1.15.1.6	Heater Experiment in Unit TSw1 Canister-Scale Heater Experiment Yucca Mountain Heated Block Thermal-Stress Measurements Heated-Room Experiments
8.3.4.2.4.4	Engineered-Barrier-System Field Tests

1.1 Objectives of Laboratory Thermal-Properties Study

The experiments discussed in the Laboratory Thermal-Properties Study are intended to provide all of the data on thermal properties required by repository design and performance assessment that can be obtained in the laboratory. Described in the Study Plan are experiments designed to (1) determine the effects of variations in environmental parameters on thermal properties; and (2) determine whether the thermal properties vary as a function of spatial location, and if so, to obtain quantitative estimates of the spatial variability. Estimates of rock-mass thermal properties will be based on the intact-rock data obtained in the laboratory and information to be obtained from other studies (as described in Section 2.3.8) on fracture porosity, lithophysal-cavity abundance, mineralogy and bulk chemistry, and the in situ saturation of the rock mass.

Laboratory data will be obtained for the following parameters: matrix porosity, grain density, bulk density, heat capacity, and thermal conductivity. Data on matrix porosity and grain density will be obtained in order to calculate in situ bulk densities at any given saturation state. For each parameter, variability in the parameter as a function of lithology and spatial location will be examined. Variability in parameters associated with variations in environmental conditions will be studied, as follows:

<u>Thermal Property</u>	<u>Variable Environmental Parameter(s)</u>
Bulk density	Saturation
Heat capacity	Saturation, temperature
Thermal conductivity	Saturation, temperature

Stress/confining pressure is not expected to have a significant effect on any of these thermal properties and so does not need to be considered as an environmental variable (Lappin, 1981).

An environmental condition that may change during the operational lifetime of a repository but which has not been considered above is mineralogic change within the tuffaceous rocks in response to elevated temperatures, changing saturations, and long periods of time. Mineralogic change might include (1) dissolution, precipitation, or both; or (2) conversion of an initial assemblage of minerals to a different assemblage (e.g., devitrification of glass, conversion of cristobalite or tridymite to quartz). Such changes involve both the thermodynamics and kinetics of mineral reactions; the changes considered to be of potential concern are being evaluated for Studies 8.3.1.3.2.1 (Mineralogy, Petrology and Chemistry of Transport Pathways) and 8.3.1.3.3.2 (Kinetics and Thermodynamics of Mineral Evolution).

Another potential change in environment is dehydration of glass, zeolite, and clay resulting from drying of the rock by elevated temperatures. Such dehydration is a kinetic process that depends on temperature and time. Rather than attempting to evaluate the specifics of the kinetics of dehydration for individual minerals, consideration of the process will be included in procedures for any oven drying of samples that is a part of the experimental plan. Any information about dehydration that is obtained as a part of Study 8.3.1.3.2.1 (Mineralogy, Petrology, and Chemistry of Transport Pathways) will be included in the development of procedures when such information is available.

1.1.1 Use of Results of Laboratory Thermal-Properties Study

The principal information requirements for resolving preclosure issues related to repository design (addressing nonradiological health and safety as well as the feasibility of waste retrieval) center on the question of adequate support for the underground openings. The design of these openings and the supports to keep them open must take into consideration the rock-mass characteristics, the pre-existing in situ stress state, the redistribution of stresses due to the excavation of the opening, the changing temperature field, and the geometry of the openings and their spatial relationship with each other. Experiments to be conducted for the Laboratory Thermal-Properties Study will contribute primarily to calculation of temperature increases caused by the presence of heat-producing waste; the temperature changes then will be used in the calculation of the resulting thermally induced stresses. A secondary design consideration that is affected by the thermal properties is the ventilation system for the repository. The thermal properties will affect the temperatures in the repository, which will in turn be a constraint on the airflow required through the underground openings in order to maintain an adequate working environment. Additional discussion of this topic is provided in Section 8.3.2.4 of the Site Characterization Plan (SCP) (DOE, 1988) and in SNL (1987).

For performance assessment, data on the thermal properties will contribute in several ways to resolution of post-closure issues. First, the properties will affect the maximum temperatures expected in the underground portion of a repository and the time interval over which the waste canisters can be expected to be isolated from liquid water (by temperatures that exceed the local boiling temperature). Second, interaction of the elevated temperatures with the hydrologic regime may affect the estimated ground-water travel time, travel path, or both. (In addition, the thermal pulse may cause geochemical changes within the boundary of the disturbed zone that may need to be considered even though water and radionuclide movement through the disturbed zone are not pertinent to travel-time calculations.) Finally, waste-package performance will depend, in part, on heat transfer in the surrounding rock because of the effects of the resulting thermally induced stresses on emplacement-hole stability.

Experiments for the Laboratory Thermal-Properties Study will be conducted on samples taken from thermal/mechanical units (a brief discussion of these units is provided in Section 2.2) that are expected to affect the temperatures calculated in the vicinity of the underground portion of a repository. At present, these units include all material from the ground surface (except for recent unconsolidated sediments) down to the static water level. For units that occur at deeper levels, thermal properties for tuffs of similar lithology will be assumed when these deeper units are included in an analysis. (The units for which data are required have been selected by repository-design and performance-assessment personnel; future analyses may indicate that data for some of the units also could be estimated rather than measured. Experiment plans will be adjusted accordingly if scheduling permits.)

1.2 Rationale and Justification for Information to be Obtained

1.2.1 Resolution of Performance and Design Issues

Performance Allocation was used by the Yucca Mountain Site Characterization Project (YMP) to establish appropriate issue resolution strategies (the issues to be resolved are presented in Section 8.2.1 of the SCP). A general discussion of the performance-allocation approach is provided in Section 8.1 of the SCP. Issue resolution strategies for each Site Program are provided in Section 8.3 of the SCP.

Sections 6.4 and 8.3 of the SCP provide detailed discussions of the approach that will be used in the design of the underground openings. This approach emphasizes the need to ensure that openings associated with the underground facility will remain usable throughout the retrieval period (Section 6.4.8 of the SCP). The ability to predict the magnitudes of stress and displacement is fundamental to the ability to ensure the retrievability of waste for up to 50 years after emplacement begins and to demonstrate that an underground facility can be constructed in welded tuff using reasonably available technology.

The design, construction, and operation of the underground facility must comply with applicable health and safety standards (e.g., 30 CFR 57) and the underground openings must remain usable for the operational period of the facility. The initial design of the facility will be based on empirical design guidelines as well as the results of mechanical, thermal, and thermomechanical analyses. These analyses will be refined as the input data base, the design, or both evolve, and will not only allow estimation of the rock-mass response to repository-induced loads but also will allow assessment of the performance of the repository relative to the standards mentioned above. The ground control-strategy concept (Hoek and Brown, 1980) initially establishes limiting values on the amounts of displacement and induced stress that cannot be exceeded during construction and operation for the proposed design of the underground openings. This design approach then uses Tunnel-Index methods (Barton et al., 1974; Bieniawski, 1976) to establish the initial requirements for the

ground-support system. These methods then are supplemented with an in situ monitoring system to assess the performance of the support system selected.

Information Need 4.4.1, "Site and Performance Assessment Information Needed for Design," (Section 8.3.2.5.1 of the SCP), which includes the data needs of Issues 2.4 (Waste Retrievalability), 4.2 (Nonradiological Health and Safety), and 4.4 (Preclosure Design and Technical Feasibility), identifies the site parameters that must be obtained to design the repository and to develop the repository operating procedures to assure the nonradiological safety of the worker. A similar set of parameters are identified in Information Need 1.11.1, "Site Characterization Information Needed for Design," (Section 8.3.2.2.1 of the SCP) as necessary for analysis of the thermal and thermomechanical response of the tuffs after closure of the repository and in Issue 1.12 [Seal Characteristics (Section 8.3.3.2 of the SCP)] as necessary for analysis of seal response to the thermal and thermomechanical environment. The thermal properties required by these two Information Needs are thermal conductivity and heat capacity. Information Need 1.11.1 subsumes several data requirements from performance assessment Issues, including 1.1 [Total System Performance (Section 8.3.5.13 of the SCP)], Issue 1.2 [Individual Protection (Section 8.3.5.14 of the SCP)], and 1.6 [Ground-Water Travel Time (Section 8.3.5.12 of the SCP)].

Issue 1.6 (Ground-Water Travel Time, Section 8.3.5.12 of the SCP) addresses ground-water travel time. In order to perform the necessary calculations, the boundary of the disturbed zone must be estimated [see Langkopf (1988)]. This estimation requires an estimate of the location of selected isotherms surrounding a repository, which in turn requires a knowledge of the thermal properties of the relevant units.

Proper design of a waste package for emplacement in welded tuff relies on an evaluation of the environment to which the waste package will be subjected in situ. Temperature is an important part of the waste-package environment. Thus, Issue 1.10 [Waste Package Characteristics (Post-closure), Section 8.3.4.2 of the SCP], which addresses the approach to waste-package design for post-closure performance, requires data on the thermal properties of the host rock.

Issue 2.7 (Repository Design Criteria for Radiological Safety, Section 8.3.2.3 of the SCP) discusses the approach to be followed in ensuring the radiological safety of the worker. Part of the approach is to estimate the radiologic shielding properties of the host rock. One of these properties is bulk density, which will be determined as part of the Laboratory Thermal-Properties Study. Requirements in Issue 2.2 [Worker Radiological Safety – Normal Conditions (Section 8.3.5.4 of the SCP)] also will be met when meeting the requirements from Issue 2.7.

1.2.2 Regulatory Requirements

This study will provide some of the information required to demonstrate compliance with several key regulations outlined in 10 CFR Part 60 (NRC, 1986) ("Disposal of High-Level Radioactive Wastes in Geologic Repositories; Licensing Procedures"). These regulations form the basis for the requirements outlined in 10 CFR Part 960 (DOE, 1984). Performance objectives as stated in 10 CFR Part 60 require demonstration that: (1) waste retrieval shall be feasible starting at any time up to 50 years after waste emplacement begins [60.111(b)]; and (2) the overall system performance of the geologic repository shall be such as to ensure that releases of radioactive material to the accessible environment conform to applicable Environmental Protection Agency requirements (60.112).

Experiments conducted for the Laboratory Thermal-Properties Study will provide data that will contribute to calculation of temperature increases induced by the heat-producing waste. These temperatures will be used in the evaluation of retrievability through: (1) the design of a ventilation system that will aid in keeping the underground openings sufficiently cool for retrieval operations to proceed; and (2) allowing calculation of expected thermally induced stresses and resulting design of a ground-support system that will be sufficient to withstand the maximum expected stresses around an opening. Predicted temperatures also will be used in the evaluation of the disturbed zone boundary and of the time interval during which the waste package will not be in contact with liquid water; the latter will contribute to estimates of ground-water travel time (10 CFR 60.113) and total system performance (10 CFR 60.112).

The Nuclear Regulatory Commission (NRC) describes as one potentially adverse condition the presence of geomechanical properties that do not permit the design of underground openings that will remain stable through permanent closure [10 CFR 60.122(c)(21)]. 10 CFR 60.133(e)(1) and 60.133(e)(2) specify that openings in the underground facility shall be designed for safe operations, to maintain the option of retrievability of the waste, and to reduce the amount of deleterious rock movement or fracturing of overlying or surrounding rock. Potentially adverse conditions outlined in 10 CFR Part 960.4-2-3(c)(1) and 960.5-2-9(c)(3) (rock characteristics) include in situ characteristics that could necessitate extensive maintenance during repository operation and closure and in situ conditions that require engineering measures beyond reasonably available technology during the construction of the underground facility. Thermally induced stresses and displacements must be estimated in order to ascertain the expected need for maintenance of openings or the viability of reasonably available technology.

1.3 Definitions and Symbols

To avoid confusion, all properties and symbols discussed or used in this Study Plan are defined below or in Table 1.3-1.

Density: the mass per unit volume of material (kg/m^3).

bulk density: the density of material, including any pore space within the volume.

- **dry bulk density:** the density of material when the pore spaces contain only gas (usually air).
- **natural-state bulk density:** the density of material when the pore spaces contain a volume fraction of liquid equivalent to that found in situ.
- **saturated bulk density:** the density of material when the pore spaces contain only liquid (usually water).

grain density: the density of solid, essentially nonporous material

Heat Capacity: the energy (in the form of heat) required to change the temperature of a unit mass of material one degree at constant pressure (J/kg-K).

Lithophysae: Ash-flow components having an approximately concentric sequence consisting of (1) a central cavity, with or without a lining of secondary minerals; and (2) an outer "shell" of variable thickness consisting of relatively coarse alkali feldspar and silica minerals. The shapes of the lithophysae range from quasi-spherical to strongly elliptical.

Porosity: The part of the volume of a material that is occupied by non-solid material (i.e., voids). Expressed as a volume fraction in this document.

matrix porosity: the portion of porosity the size of which is approximately described by "microscopic" or "submicroscopic." Specifically excludes void space contributed by fractures or lithophysal cavities.

total porosity: total void space, equivalent to the sum of matrix porosity, fracture porosity, and volume of lithophysal cavities.

Saturation: the volume fraction of the porosity (usually the matrix porosity) that is occupied by liquid (usually water).

Thermal Conductivity: the quantity of heat conducted through a unit area (perpendicular to the direction of heat transfer) per unit time when the temperature gradient is one degree, per unit thickness (W/m-K).

Table 1.3-1
Definition of Symbols

Symbol	Definition
c	fitting parameter in Asaad's thermal conductivity equation (Table 3.4-2)
C_p^{air}	heat capacity of air (J/kg-K)
$C_p^{H_2O}$	heat capacity of liquid water (J/kg-K)
C_p^{rock}	heat capacity of rock mass (J/kg-K)
C_p^{solid}	heat capacity of solid (essentially nonporous) material (J/kg-K)
K	thermal conductivity (W/m-K); also parameter used in expressing tolerance limits (Section 2.2.1)
K_a	thermal conductivity of air (W/m-K)
K_c	thermal conductivity of composite [i.e., solid plus fluid (W/m-K)]
K_f	thermal conductivity of fluid (W/m-K)
K_s	thermal conductivity of solid (essentially nonporous material (W/m-K)
K_{vac}	thermal conductivity of composite when the material is subjected to a vacuum (W/m-K)
K_w	thermal conductivity of water (W/m-K)
n	number of samples [Also a fitting parameter in the thermal conductivity equation of Sugawara and Yoshizawa (Table 3.4-2).]
S	saturation (volume fraction); also, standard deviation
\bar{X}	mean value
α	level of significance; $(1 - \alpha)$ is the confidence level associated with a data request (Section 2.2.1)
γ	probability that a given proportion of a population is located within specified tolerance limits (Section 2.2.1)

Table 1.3-1
Definition of Symbols (Concluded)

Symbol	Definition
ρ_b	bulk density (kg/m ³)
ρ_{db}	dry bulk density (kg/m ³)
ρ_g	grain density (kg/m ³)
ρ_{sb}	saturated bulk density (kg/m ³)
ϕ_f	porosity occurring in fractures (volume fraction)
ϕ_L	porosity occurring in lithophysal cavities (volume fraction)
ϕ_m	matrix porosity (volume fraction)

2.0 RATIONALE FOR LABORATORY THERMAL-PROPERTIES STUDY

Experiments are planned to measure three thermal properties for the Laboratory Thermal-Properties Study. The primary emphasis in each group of experiments is to obtain data in the laboratory that can be used to estimate the thermal properties of the rock mass throughout the area within the boundary of the underground facilities for the relevant thermal/ mechanical units. These rock-mass properties then will serve as primary input to thermal calculations performed in support of repository-design and performance-assessment activities.

2.1 Rationale and Justification for Laboratory Thermal-Properties Experiments

Heat-transfer calculations of temperature increases resulting from waste emplacement require as input the thermal properties of the rock mass. The performance-allocation process resulted in the definition of both preferred limits for each thermal property and confidence in those limits.

The rock-mass properties will be measured in situ during a number of experiments (Table 1.0-1). Data gathered in the small number of in situ experiments are unlikely to have narrow confidence intervals even for the two thermal/mechanical units (TSw1 and TSw2) in which such experiments will be performed. In addition, the in situ experiments will be unable to provide data either to examine spatial variability within the relevant thermal/mechanical units (because the number of experiments will be insufficient) or to provide rock-mass thermal properties for units in which no in situ thermal experiments are to be conducted.

As a result of these limitations for the in situ experiments, a program of laboratory experiments is necessary as a first step in obtaining rock-mass thermal-properties data. Laboratory determinations of grain density, matrix porosity, heat capacity, and thermal conductivity can be combined with information on fracture porosity, in situ saturation state, and lithophysal-cavity abundance to estimate rock-mass thermal properties. In addition, correlation of thermal properties with mineralogic or petrologic information may be useful in estimating thermal properties for the rock mass. (Additional discussion of the methods of calculating in situ thermal properties are provided in a number of sections later in this document.) The laboratory program can be designed to provide both the proper number of samples and the proper distribution of sampling locations to enable the limitations mentioned previously to be overcome. In addition, laboratory experiments will examine thermal properties under controlled conditions, thus permitting the effects of parameters (e.g., saturation level) to be studied.

Figure 2.2-1 is a flow chart that summarizes the sequence of events that is to be followed in obtaining rock-mass thermal properties for this study. [Note: Contacts between thermal/mechanical units will be defined at each location before sampling occurs; definition of the contacts is part of Study 8.3.1.4.3.2 (Three-Dimensional Rock Characteristics Models.)]

2.2 Rationale for the Number of Planned Experiments, Sampling Locations, and the Selection of Test Techniques

Preliminary data for a number of thermal and mechanical properties have been obtained for various tuffaceous units at Yucca Mountain. These data have permitted definition of a thermal/mechanical stratigraphy, in which units are distinguishable based on differences in one or more of the thermal and mechanical properties. A comparison of these units with the formal stratigraphic units is provided in Figure 2.2-2.

Because the thermal/mechanical units have been defined based on differences in thermal properties, mechanical properties, or both, each of the units is assumed to be independent in terms of sampling. Thus, the performance-allocation process has resulted in data requirements for each pertinent thermal/mechanical unit separately.

The existing version of the thermal/mechanical stratigraphy does not include material found between Units TSw2 and TSw3 that is characteristic of neither unit. This material is extremely variable in lithology (usually rich in clay and zeolite) and in thickness [usually less than 10 ft (3 m)]; the variable lithology is the reason the material has not been treated as a thermal/mechanical unit. Brief discussions of the material are provided by Nimick and Schwartz (1987) and by Levy and O'Neil (1989).

Although neither repository-design nor performance-assessment issues contain explicit requests for data on this material, data should be acquired because (1) thermal-property data from other units cannot be used for the material and (2) the material would be sufficiently close to the waste canisters that the thermal properties of the material might affect the heat pulse from emplaced waste. Thus, this document includes plans for determining the thermal properties of what will henceforth be called "altered TSw3."

The following sections discuss the number (Section 2.2.1) and the location (Section 2.2.2) of experiments planned to characterize the thermal properties of the tuffs at Yucca Mountain. Section 2.2.3 discusses additional thermal-conductivity experiments planned to examine, in a scoping fashion, the effects of saturation level, sample size, and the presence of fractures on thermal conductivity.

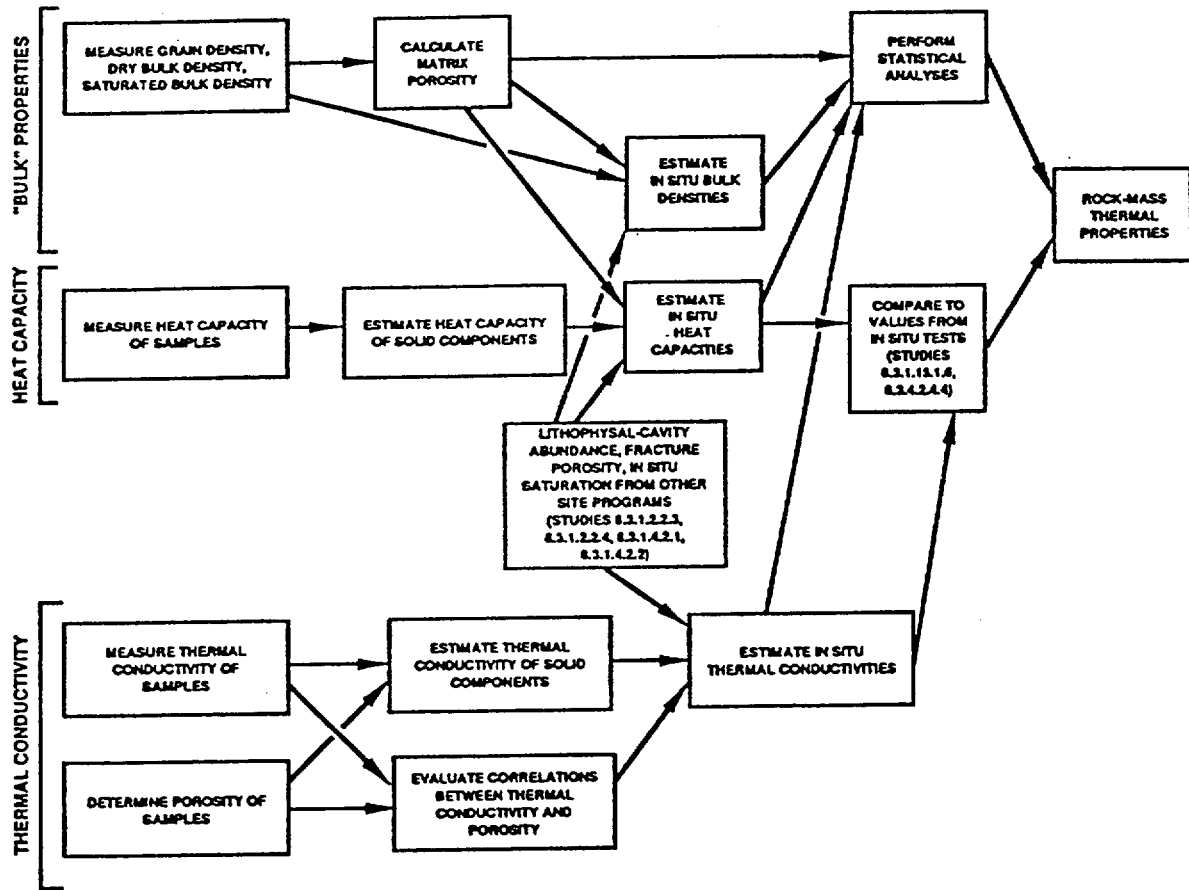
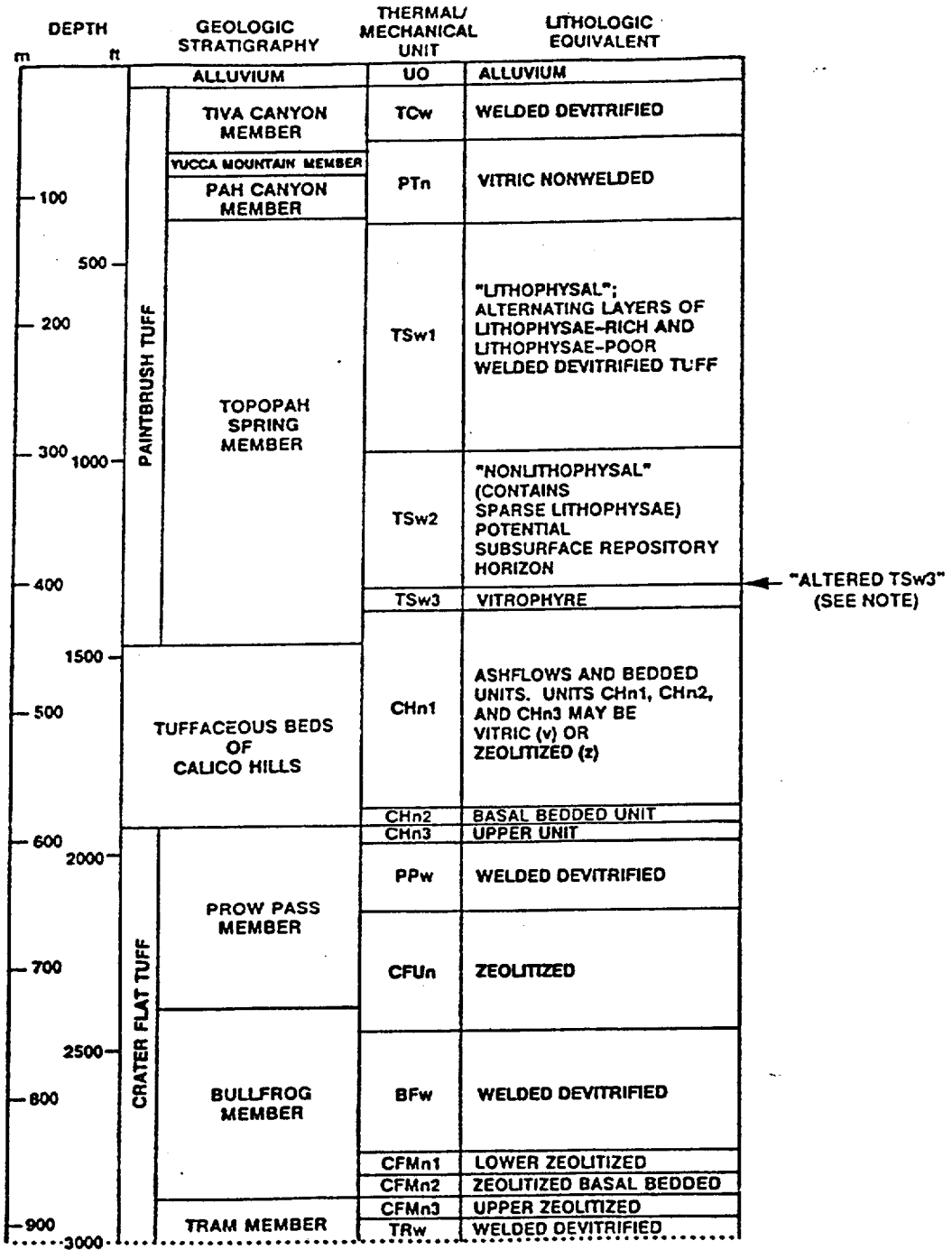


Figure 2.2-1. Flow-Chart Depicting Sequence of Activities Leading to Establishment of a Set of Rock-Mass Thermal Properties.



← "ALTERED TSw3" (SEE NOTE)

NOTE: Altered TSw3 is not included; it is a zone of variable lithology and thickness (see text).

Figure 2.2-2. Comparison of Thermal/Mechanical and Formal Stratigraphies, Including General Lithologic Descriptions and Representative Thicknesses for the Yucca Mountain Area (DOE, 1993).

In order to formulate the plans discussed in these sections, preliminary assumptions were made about the spatial variability of the thermal properties. Existing data are insufficient to analyze large-scale horizontal variability (e.g., between existing core holes) or vertical variability within each thermal/mechanical unit at any given core hole location. Thus, it has been assumed that little is known about the spatial variability of the thermal properties. Section 2.2.1 addresses the number of experiments and Section 2.2.2 discusses sampling locations. Taken together, these sections present the plans to assess the issue of spatial variability.

Given the lack of information, existing data have been used to provide information with which to estimate numbers of samples (Section 2.2.1) which, if there is spatial variability between core holes (i.e., horizontally), would be sufficient to satisfy the data requests of performance assessment and repository design at any single sampling location. In addition, if variability is random and uncorrelated both horizontally and vertically, present sampling plans will provide data that are more than sufficient to satisfy data requirements.

2.2.1 Number of Samples

In general, the minimum number of samples for laboratory thermal-properties experiments that will be necessary for site characterization will be different for each property considered. A preliminary estimate of the necessary number of experiments for each thermal property can be obtained using information provided by repository design and performance assessment through the performance-allocation process. A compilation of the data requirements from a number of design and performance-assessment issues is provided in Table 2.2-1. Before beginning the detailed discussion of estimating the number of samples, it should be noted that the identification of the data requirements and associated qualitative confidence levels has been done with little or no support in the form of sensitivity analyses. Often, the specification of tolerance limits and confidence levels has been made based solely on the expert judgment of repository design personnel. As additional analyses are performed, it is possible that some aspects of the repository design will prove to have a different sensitivity to thermal properties than has been assumed to date. Whenever analyses do indicate changed sensitivity relative to that assumed for the preliminary estimates given in the SCP, the estimated numbers of samples required for experiments will be reevaluated appropriately.

The repository-design and performance-assessment activities express the data requirements in the following form:

We want a proportion, (γ), of the data population to fall within the limits $\bar{X} \pm K\bar{X}$ with a $(1-\alpha)$ level of confidence.

Table 2.2-1

**Summary of Data Requirements for Repository-Design and Performance-Assessment
Activities (Synopsised from Table 8.3.1.15-1 of the SCP)**

Property	SCP Issue	Thermal/Mechanical Unit	Required Interval	Required Confidence Level	
In situ bulk density	1.6	Not specified	Not specified	Not specified	
	1.10	TSw2	$\bar{X} \pm 0.1\bar{X}$	Medium	
	2.2	TSw2	Existing Range	High	
	2.7	TSw2	Existing Range	High	
Thermal Conductivity	1.6	Not specified	Not specified	Not specified	
	1.10	TSw2 (Intact)	$\bar{X} \pm 0.1\bar{X}$	Medium	
		TSw2 (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$	Medium	
	1.11	TSw2 (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	High	
		TSw1 (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	Medium	
		TSw3 (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	Medium	
	1.12	CHn1 (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	Medium	
		TCw (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	Low	
		PTn (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	Low	
		CHn2 (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	Low	
		TSw2 (Rock Mass)	Not Specified	Medium	
		CHn1 (Rock Mass)	Not Specified	Medium	
		4.4	TSw2 (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	Medium
			TSw1 (Rock Mass)	$\bar{X} \pm 0.2\bar{X}$	Medium
	TCw (Rock Mass)		$\bar{X} \pm 0.2\bar{X}$	Low	
	PTn (Rock Mass)		$\bar{X} \pm 0.2\bar{X}$	Low	
	Heat Capacity	1.6	Not Specified	Not Specified	Not Specified
		1.10	TSw2 (Intact)	$\bar{X} \pm 0.2\bar{X}$	Medium
			1.11	TSw2 (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$
		1.11	TSw1 (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$	Medium
TSw3 (Rock Mass)			$\bar{X} \pm 0.1\bar{X}$	Medium	
CHn1 (Rock Mass)			$\bar{X} \pm 0.1\bar{X}$	Medium	
TCw (Rock Mass)			$\bar{X} \pm 0.1\bar{X}$	Low	
PTn			$\bar{X} \pm 0.1\bar{X}$	Low	
CHn2 (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$		Low		

Table 2.2-1

**Summary of Data Requirements for Repository-Design and Performance-Assessment
Activities (Synopsised from Table 8.3.1.15-1 of the SCP)
(Concluded)**

Property	SCP Issue	Thermal/Mechanical Unit	Required Interval	Required Confidence Level
Heat Capacity (contd.)	1.12	TSw2 (Rock Mass)	Not Specified	Medium
		CHn1 (Rock Mass)	Not Specified	Medium
	4.4	TSw2 (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$	Medium
		TSw1 (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$	Medium
		TCw (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$	Low
		PTn (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$	Low
		TSw1 (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$	Low
		TSw2 (Rock Mass)	$\bar{X} \pm 0.1\bar{X}$	Low

NA: Not available (see Table 2.2-2 for reason for lack of availability).

(Note that this requirement is a request for statistical tolerance limits within which the proportion (γ) is expected to occur, not for a confidence interval around \bar{X} .) Ideally, the design requirements specify values for γ and α (which expresses the degree of conservatism in the design), and K (a constant for specific combinations of γ, α) from which the sample size, n , can be estimated for a given population distribution of the data.

Insufficient thermal-properties data are available to determine the population distribution. Although it is preferable to determine sample sizes based on an approach that makes no assumptions about the underlying population distribution, the sample sizes obtained using distribution-free tolerance limits are impractical when scheduling and budgeting also are considered. Therefore, a normal population distribution is assumed for calculating initial sample sizes.

For this study, the method of Bowker and Lieberman (1972) that is based on an assumed normal distribution is used to design the initial sampling program. In this method,

"...statistical tolerance limits for a normal distribution are given by $[L = \bar{X} - KS, U = \bar{X} + KS]$ and have the property that the probability is equal to a preassigned value that the interval includes at least a specified proportion $1 - \alpha$ of the distribution."

(Bowker and Lieberman, 1972, p. 310)

This definition of statistical tolerance limits can be used to estimate the value of n required to obtain tolerance limits of predefined size if values for \bar{X} , S , γ , and α are established. Since repository-design and performance-assessment activities do not establish numerical values for α and γ , values must be assigned.

As shown in Table 2.2-1, one of three qualitative levels of confidence has been associated with each data request — high, medium, or low. In general, the closer the thermal/mechanical unit is to the repository horizon, the greater the level of confidence required for the data from that unit. For this study, the following numerical values of α (the level of significance) have been assigned to each of the qualitative confidence levels:

Qualitative Confidence Level	α
High	0.05
Medium	0.10
Low	0.25

The qualitative levels of confidence were assigned by different individuals, all of whom have different problems to address. Thus, the values of α given above may be more restrictive than is necessary for some applications. However, the values have been selected in an attempt to satisfy even the most stringent of the qualitative requirements.

Values for γ have been assigned based on the assumption that the proportion of the population (γ) required to lie within the statistical tolerance limits (defined as $B\bar{X}$) is the same as the confidence interval ($1 - \alpha$):

Qualitative Confidence Level	γ
High	0.95
Medium	0.90
Low	0.75

Thus, the higher the level of confidence required in the data, the higher the proportion of the data population that must lie within the tolerance limits.

A preliminary estimate of the number of samples required for each thermal property (Table 2.2-2) can be determined by using existing data for \bar{X} and S and calculating K by equating KS and the specified value for $B\bar{X}$ from a repository-design or performance-assessment issue (Table 2.2-1). For many of the entries in Table 2.2-2, no existing data are available with which to calculate \bar{X} and S , so that a preliminary number of required samples cannot be estimated. For other entries, the data requirements from repository design and performance assessment may be unrealistic given the high variability of existing data (equating KS and $B\bar{X}$ yielded a value of K that is not realizable no matter how many samples are tested). In both cases, an alternative approach is necessary that, although arbitrary, will allow a preliminary sampling strategy to be formulated.

Table 2.2-2
Preliminary Estimates of Numbers of Samples* Required for
Thermal-Properties Determination

Unit	Bulk Density	Heat Capacity	Thermal Conductivity
TCw	NA(2)	NA(1)	NA(1)
PTn	NA(2)	NA(1)	NA(1)
TSw1	NA(2)	>50	>50
TSw2	7	>50	>50
Altered TSw3	NA(1)	NA(1)	NA(1)
TSw3	NA(2)	4	10
CHn1v	NA(2)	NA(1)	NA(1)
CHn1z	NA(2)	NA(1)	>50
CHn2v	NA(2)	NA(1)	NA(1)
CHn2z	NA(2)	NA(1)	6

*These numbers of samples pertain to each core hole to be sampled.

NA(1): Data are insufficient to obtain a mean value or a standard deviation.

NA(2): Data requirements expressed in repository design and performance assessment issues are incomplete.

The alternative approach selected involves finding the number of samples required at each confidence level that will provide the same statistical tolerance limits [i.e., the same (arbitrary) value of K]. Some of the data requirements in Table 2.2-1 demand narrower tolerances than others. The initial sampling estimates that are discussed below are based on narrower tolerances (i.e., the greater number of samples). Two-sided statistical tolerance limits are used in the estimation.

The number of samples (n) are 3 [$\gamma = (1-\alpha) = 0.75$ (low confidence)], 11 [$\gamma = (1-\alpha) = 0.90$ (medium confidence)], and 34 [$\gamma = (1-\alpha) = 0.95$ (high confidence)], for a value of $K = 2.5$. These three values have been rounded to 5, 10, and 35 for this study. (For the more rigorous confidence levels, the rounding does not change the value of K except in the third significant digit. For the lowest sample number, rounding will result in an increased amount of data.)

The initial estimates of number of samples are summarized in Table 2.2-3. Suppose that the requirements stated above resulted in n samples for a given thermal/mechanical unit (based on existing data and the assumption that all data are for random, uncorrelated samples). These n samples, taken from numerous core holes and scattered vertical locations within the unit, would be sufficient in the absence of spatial variability. However, thermal properties may be dependent on spatial location. Thus, rather than selecting n samples for the entire area (or volume) to be characterized, n samples will be taken from each selected (horizontal) sampling location, and will be distributed vertically in a manner that any systematic vertical variability should be detectable. Additional details on the locations for sampling are provided in Section 2.2.2.

It is emphasized that the numbers given in Table 2.2-3 are those with which the initial sampling program will be designed. Once the site-characterization testing begins, the resulting data will be examined periodically to assess whether the assumption of normality is justified. If the data do not represent a sample from a normal distribution, the actual distribution will be evaluated, a new sample size will be estimated based on data requirements, and this sample size will be compared to the number of samples already tested. If additional tests are required, more samples will be tested to provide the necessary data.

2.2.2 Sampling Locations

Samples will be taken from the following locations: (1) existing core holes from which samples have been obtained previously for thermal- properties measurements; (2) main accesses of the Exploratory Studies Facility (ESF); (3) main drifts to be excavated within Unit TSw2 of the ESF; and (4) new core holes proposed as part of the surface-based exploration program described in Sections 8.3.1.4.1 and 8.3.1.4.3.1.1 of the SCP.

Table 2.2-3
Initial Estimates of Numbers of Samples^a Required
for Site Characterization of Thermal Properties

Unit	Bulk Density ^b	Heat Capacity	Thermal Conductivity
TCw	10	5	5
PTn	10	5	5
TSw1	10	10	10
TSw2	35	35	35
Altered TSw3	10 ^c	10 ^c	10 ^c
TSw3	10	5	10
CHn1v	10	10	10
CHn1z	10	10	10
CHn2v	5	5	5
CHn2z	5	5	5

- a: These numbers of samples pertain to each core hole to be sampled. Six new core holes are planned for testing.
- b: The numbers of samples listed for bulk density dictate the numbers of samples on which matrix porosity and grain density will be measured.
- c: This number of samples will be tested if sufficient material is available.

A discussion of the number of samples required for site characterization is provided in Section 2.2.1. The discussion does not address the possibility that one or more of the thermal properties vary as a function of spatial location, either horizontally within the boundary of the underground facilities or vertically within a given thermal/mechanical unit. Given the number of cases in which little or no experimental data have been obtained (most of which are represented by "NA" in Table 2.2-2), it is assumed that nothing is known about spatial variability of thermal properties before site characterization begins. Thus, the number of samples discussed in Section 2.2.1 applies for each sampling location employed in site characterization. Additional detail is given in the following subsections.

Not all of the relevant thermal/mechanical units will be penetrated by the subsurface excavations that will provide access to material for sampling. New core holes are planned to extend to depths 200 ft (61 m) below the static ground-water level, so that most of the thermal/mechanical units of interest should be sampled in each core hole.

2.2.2.1 Sampling in New Core Holes

Although a quantity of data on thermal properties has already been obtained for samples from existing core holes, only one of the existing core holes (USW G-4) (Spengler and Chornack, 1984) is located within the main area for site characterization. Thus, data from additional locations are necessary in order to examine the spatial variability of thermal properties within the boundary of the underground facilities as well as to ascertain whether the existing data are representative of the tuffs within the area. In order to coordinate with core holes planned for other YMP activities, six of the core holes suggested as part of a systematic drilling program (SCP Section 8.3.1.4.3.1.1) are anticipated to be used for sampling for the Thermal-Properties Study. Data from these holes should enable an analysis of the lateral variability of thermal properties to be made; additional discussion of the planned analyses is presented in Section 3.5.

It is possible that areas outside the boundary of the underground facilities will be evaluated as potential extensions of the main area will be made in the future. If this evaluation includes new core holes, the sampling program discussed in this section also would be applied to one or more of these additional holes.

As stated earlier, each thermal/mechanical unit will be considered as an independent entity in terms of sampling. In each core hole, the thermal/mechanical units each will be divided into n potential sampling intervals, where n is the number of samples given in the summary at the end of Section 2.2.1. In each of these intervals, a sample will be selected from a location as close to the center of the interval as possible. [Preliminary analysis has shown that the average Kriging variance (a common criterion for optimizing a sampling strategy) will be lower using this sampling strategy rather than a fully random strategy.]

An attempt will be made to avoid any bias in sampling to the extent practicable. Thus, rather than selecting the material that appears to be the best candidate for a sample, the only criterion applied will be that a sample be of sufficient size to meet any size requirements imposed by the type of experiment. If a fragment or piece of core of sufficient size is not available within any given interval, the number of samples estimated as necessary for a given property and unit may not be achievable. Adjustments to the sampling program may be necessary so that the statistical basis of the program will be maintained while still acquiring as close to n samples as possible. The nature of these adjustments will depend on the situation. For example, if suitable samples cannot be obtained from some of the predefined intervals, redundant samples could be selected from one or more of the remainder of the sampling intervals to ensure that sufficient measurements could be made. (The fact that a fragment or piece of core was not available in a given interval may be useful information in the analysis of spatial variability of thermal-property data or of the material on which the data were gathered. Thus, such information will be retained for use after sampling has been completed.)

The thermal conductivity of Unit TSw2 potentially is a function of orientation (i.e., may be anisotropic). The presence or absence of anisotropy in thermal conductivity will be examined by taking two samples of different orientations at 10 of the 35 sampling locations in Unit TSw2 in each core hole.

2.2.2.2 Sampling in the ESF Main Accesses

Samples from the ESF main accesses will be obtained in several ways. First, samples will be taken from core obtained from the multiple point borehole extensometer (MPBX) holes that are planned as part of the access-convergence test (Study 8.3.1.15.1.5, Excavation Investigations). Six samples for each thermal property will be taken from each of the access-convergence stations within the main accesses. A minimum of three access-convergence stations is planned for study.

The second sampling location for thermal properties will be the upper Demonstration Breakout Room (DBR), to be located within the lithophysae-rich portion of Unit TSw1. Three evenly-spaced samples will be taken for each of the thermal properties from each of the MPBX holes from the upper DBR; ten holes are planned as part of Study 8.3.1.15.1.5. In addition, five larger diameter samples will be obtained to examine sample size effects on the thermal conductivity of lithophysae-rich tuff. These samples will be a subset of the sampling in the upper DBR for Study 8.3.1.15.1.3 (Laboratory Determination of the Mechanical Properties of Intact Rock.)

If core from MPBX holes is insufficient in either quality or quantity to provide samples for all thermal-property tests, additional samples will be obtained from horizontal boreholes located in the ESF main accesses. Rubble obtained during excavation of the main accesses also may be used to provide samples, if suitable. Core for thermal-property sampling would be allocated to thermal conductivity first; heat-capacity and bulk-property samples would have equivalent and lower priority. If rubble is required, samples would be obtained from levels close to the access-convergence station for consistency.

2.2.2.3 Sampling in the ESF Main Drifts

The sampling strategy in the main drifts to be excavated at the main test level in the ESF will be similar to that employed for the main accesses (i.e., samples will be taken from core obtained from MPBX holes or horizontal boreholes located in the ESF main drifts). In this case, the MPBX holes will be cored for Study 8.3.1.15.1.8 (In Situ Design Verification). Current plans are that three evenly-spaced samples will be obtained for each hole. By the time core is available from these MPBX holes, additional data on thermal properties will be available with which to define the optimum number of samples in a more rigorous fashion.

As described for the main accesses (Section 2.2.2.2), rubble may be used to obtain thermal-properties samples if MPBX core is insufficient. Sampling locations will be close to the MPBX locations.

2.2.2.4 Additional Sampling

2.2.2.4.1 Additional Sampling for Bulk Properties

The three preceding subsections describe the sampling strategy for all thermal properties; a similar strategy will be followed for sampling for thermal properties and mechanical properties. In each case, random selection of samples will allow relatively accurate estimates to be made of the statistical distribution of the population of each property. However, the scale of any spatial correlation of the data will not be well known. In order to ascertain whether small-scale spatial correlation is significant, additional measurements of bulk properties (matrix porosity and density) will be made.

There are three reasons for selecting bulk properties for this examination: (1) samples do not need to be large or regularly shaped; (2) the measurements are relatively easy, quick, and inexpensive; and (3) heat capacity, thermal conductivity, compressive strength, tensile strength, Coulomb parameters (cohesion and angle of internal friction), and Young's modulus are correlated to matrix porosity (e.g., Nimick and Schwartz, 1987). This last reason is perhaps the most important, because estimates of the small-scale spatial variability (e.g., correlation length) for thermal and mechanical properties can be made based on the small-scale variability observed for matrix porosity. The mineralogy of these bulk property samples will be determined so that small-scale variability of thermal-expansion behavior can be assessed; additional details are given in Study Plan 8.3.1.15.1.2.

In order to evaluate the presence or absence of small-scale correlation in each thermal/mechanical unit, additional sampling intervals will be randomly selected in each new core hole (the method of defining sample intervals in core holes is discussed in Section 2.2.2.1). The number of such intervals will be governed primarily by the location of the unit relative to Unit TSw2. Initially, five intervals will be selected for Unit TSw2, three each for Units TSw1, TSw3, CHn1v, and CHn1z, and two each for Units TCw, PTn, CHn2v, and CHn2z. (If data resulting from this portion of the work suggest that additional small-scale sampling is advisable, the number of intervals will be increased.) Each additional sampling interval will be subdivided into ten sections, and four of these ten sections will be randomly selected. Because of the nature of bulk-property measurements, no problems are anticipated with finding suitable material in each selected section.

The small-scale spatial correlation of bulk properties in the vertical direction will be evaluated using the sampling program described in the preceding paragraph. For most thermal/mechanical units, small-scale spatial correlation in the horizontal direction cannot be examined. The ESF will provide an opportunity to look at the horizontal component for Units TSw1 (upper DBR) and TSw2 (main test level and associated main drifts). Core will be obtained from MPBX holes in these locations; two cores will be examined from the upper DBR and one from each of the main drifts. Each length of core will be divided into n sampling intervals (where n is the number of samples given in Table 2.2-3) and a bulk-property sample will be obtained from the center of each interval. As was described for the core hole sampling, if data suggest that additional small-scale sampling is advisable, the number of cores to be examined will be increased.

2.2.2.4.2 Additional Sampling in Support of In Situ Experiments

As mentioned earlier, rock-mass thermal properties will be determined as part of several in situ experiments to be conducted in the ESF (Table 1.0-1). Laboratory values for the thermal properties of intact rock are required to aid in the interpretation of the results of the experiments. The laboratory values will be determined from samples taken from the vicinity of the relevant in situ experiments. These samples are not considered to be a part of the systematic sampling program described earlier, nor is the number of these supporting measurements governed by the estimates made for the systematic sampling. Instead, the number and location of these samples will be determined by the Principal Investigator (PI) for an in situ experiment in consultation with the PI for laboratory determination of thermal properties. The results of these thermal-properties tests, however, will be incorporated into this study.

2.2.2.4.3 Additional Sampling of Anomalous Material

The possibility exists that, during excavation of the main accesses or associated underground openings, material may be encountered that cannot be considered to be representative of the thermal/mechanical unit in which it is located. An example of such material would be fault gouge. If such material is encountered, appropriate repository-design and performance-assessment personnel will determine whether data on the thermal properties of the material are necessary to their work. If so, samples will be collected under constraints imposed by the data requirements (e.g., confidence level, tolerance limit) for the unit in which the material is located.

2.2.3 Effects of Test Parameters on Thermal Conductivity

Several parameters selected by an experimenter before measuring thermal conductivity have the potential to affect the observed data. These include sample size and the saturation level of the samples. The

existing state of knowledge does not allow conclusions to be drawn concerning the importance of these parameters. As a result, scoping studies to establish baseline test conditions will be performed to assess whether any important effects on thermal conductivity would occur. These studies will not include tests at all combinations of conditions, but instead are designed to examine potential effects of each condition separately. The ranges of each parameter are given below.

Sample Size: 5.1 to 20.3 cm (diameter), 1.3 to 5.1 cm (thickness)

Saturation Level: 0.0 to 1.0

The tests for sample-size effects will be performed using two nominal sizes: 5.1 cm (diameter) by 1.3 cm (thickness) and 20.3 cm (diameter) by 5.1 cm (thickness). Saturation effects will be examined using five different saturation levels — oven-dry, air-dry, saturated, and two other intermediate levels.

To incorporate some of the potential variability between samples, five samples will be tested at each set of conditions. Initially, samples will be taken only from Unit TSw2; the need for sampling of other units will be assessed based on the results for Unit TSw2. Thus, these scoping studies will require only ten samples; the smaller size-effect samples can be used for the saturation-level study also.

Fracture effects on the thermal conductivity of Unit TSw2 also will be examined in a scoping study. The general approach to this study will involve the following steps:

- 1 Measure thermal conductivity of intact sample;
2. Introduce an artificial fracture (e.g., saw cut perpendicular to sample axis);
3. Roughen fracture surface; and
4. Measure thermal conductivity of fractured sample as a function of stress applied normal to the fracture surface (the degree of contact of opposing fracture surfaces as a function of normal stress will be studied as part of Study 8.3.1.15.1.4, Laboratory Determination of the Mechanical Properties of Fractures).

This study will use five air-dry samples, and fracture surfaces will be dry. The range in applied normal stress is expected to be 0 to 10 MPa.

The effects of any natural fracture fillings need not be studied explicitly. Clean, dry fractures will have a greater thermal resistance (e.g., lower thermal conductivity) than would occur with any filling because air has a lower thermal conductivity than any mineral. At the other end of the spectrum, a thin mineral filling

with a thermal conductivity higher than that of the intact rock will provide a thermal short-circuit, so that the measured thermal conductivity would essentially be that measured on the intact sample.

If fracture effects are observed to be significant in this scoping study, there will be two ramifications. First, samples containing natural fractures will be obtained from the ESF and the tests will be repeated. The number of such samples will be defined before sampling. Second, the need to perform similar tests on samples from other units will be assessed, and samples will be obtained if necessary.

If the scoping studies indicate that one or more of the parameters discussed above has a significant effect on the thermal conductivity of tuff, the sampling and testing program described in Sections 2.2.1 and 2.2.2 will be modified to include characterization of the parameter effects. Details of such modification cannot be specified until the results of the scoping studies are available.

2.2.4 Summary of Sampling Plans

There are three sampling groups for this study. First are samples for the scoping studies. These samples will be obtained from existing core or, if no core is available, from outcrop material. The second group of samples will come from the new core holes; the numbers and locations for samples in this group are given in Table 2.2-3 and described in Section 2.2.2.1. The third group of samples will be obtained from the ESF. This group includes samples from the main accesses, from the upper DBR, and from the main drifts. In addition, samples will be obtained to support in situ testing.

A summary of the sampling plans is provided in Table 2.2-4.

2.2.5 Measurement Techniques and Alternatives for Laboratory Thermal Properties

The following subsections briefly discuss the planned approaches for obtaining each of the types of thermal properties and the alternatives, if any, to the approaches. Brief summaries of the actual experimental techniques also are provided.

In addition to the techniques described in the remainder of Section 2.2.5, some mineralogic, petrologic, and petrographic characterization of samples will be performed. The characterization is intended to provide data that can be used to interpret experimental results as well as to examine potential correlations between thermal properties and sample characteristics that might be useful in inferring thermal properties from the results of mineralogic and petrologic studies performed by other project participants. Characterization will be focused on heat capacity and thermal conductivity samples. Bulk-property samples will be characterized if significant

Table 2.2-4 Summary of Sampling Plans

Portion of Study	Sampling Location(s)	Unit(s)	Test Type ^a	Estimated Number of Samples	Section	
Scoping Activities	Existing Core or Outcrop	•TSw2	•TC	5 (size effects, small)	2.2.3	
			•TC	5 (size effects, large)	2.2.3	
			•TC	5 (fracture effects)	2.2.3	
			•TC	3 (saturation effects)	2.2.3	
			•CHnlz	•TC	3 (saturation effects)	2.2.3
Spatial Variability and Site Characterization	New Core Holes	•TCw	•BP	60 (10 per hole)	2.2.2.1	
			•M	48 (8 per hole, small-scale activity)	2.2.2.4.1	
			•M	48 (8 per hole, small-scale activity)	2.2.2.4.1	
			•TC	30 (5 per hole)	2.2.2.1	
			•HC	30 (5 per hole)	2.2.2.1	
			•PTn	•BP	60 (10 per hole)	2.2.2.1
				•M	48 (8 per hole, small-scale activity)	2.2.2.4.1
			•TSw1	•M	48 (8 per hole, small-scale activity)	2.2.2.4.1
				•TC	30 (5 per hole)	2.2.2.1
			•TSw1	•HC	30 (5 per hole)	2.2.2.1
				•BP	60 (10 per hole)	2.2.2.1
			•TSw1	•M	72 (12 per hole, small-scale activity)	2.2.2.4.1
				•M	72 (12 per hole, small-scale activity)	2.2.2.4.1
			•TSw2	•TC	60 (10 per hole)	2.2.2.1
				•HC	60 (10 per hole)	2.2.2.1
			•TSw2	•BP	210 (35 per hole)	2.2.2.1
				•M	120 (20 per hole, small-scale activity)	2.2.2.4.1
			•TSw2	•M	120 (20 per hole, small-scale activity)	2.2.2.4.1
				•TC	210 (35 per hole)	2.2.2.1
			•Altered TSw3	•TC	60 (10 per hole)	2.2.2.1
•BP	60 (10 per hole ^b)	2.2.2.1				
•TSw3	•HC	210 (35 per hole)	2.2.2.1			
	•BP	60 (10 per hole ^b)	2.2.2.1			
•TSw3	•TC	60 (10 per hole ^b)	2.2.2.1			
	•HC	60 (10 per hole ^b)	2.2.2.1			
•TSw3	•BP	60 (10 per hole)	2.2.2.1			
	•M	72 (12 per hole, small-scale activity)	2.2.2.4.1			
•TSw3	•M	72 (12 per hole, small scale activity)	2.2.2.4.1			
	•TC	60 (10 per hole)	2.2.2.1			
•CHnlv	•HC	30 (5 per hole)	2.2.2.1			
	•BP	60 (10 per hole)	2.2.2.1			
•CHnlv	•M	72 (12 per hole, small-scale activity)	2.2.2.4.1			
	•M	72 (12 per hole, small-scale activity)	2.2.2.4.1			
•CHnlv	•TC	60 (10 per hole)	2.2.2.1			
	•HC	60 (10 per hole)	2.2.2.1			

Table 2.2-4 Summary of Sampling Plans (Concluded)

Portion of Study	Sampling Location(s)	Unit(s)	Test Type ^a	Estimated Number of Samples	Section		
Main Drifts	Main Accesses	•CHn1z	•BP	60 (10 per hole)	2.2.2.1		
				72 (12 per hole, small-scale activity)	2.2.2.4.1		
			•M	72 (12 per hole, small-scale activity)	2.2.2.4.1		
		•CHn2v	•TC	60 (10 per hole)	2.2.2.1		
			•HC	60 (10 per hole)	2.2.2.1		
			•BP	30 (5 per hole)	2.2.2.1		
		•CHn2z	•BP	48 (8 per hole, small-scale activity)	2.2.2.4.1		
			•M	48 (8 per hole, small-scale activity)	2.2.2.4.1		
			•TC	30 (5 per hole)	2.2.2.1		
		•CHn2z	•HC	30 (5 per hole)	2.2.2.1		
			•BP	30 (5 per hole)	2.2.2.1		
			•M	48 (8 per hole, small-scale activity)	2.2.2.4.1		
		•CHn2z	•TC	30 (5 per hole)	2.2.2.1		
			•HC	30 (5 per hole)	2.2.2.1		
			•BP	12 (access-convergence)	2.2.2.2		
		Main Drifts	Main Accesses	•TSw1	•BP	30 (upper DBR)	2.2.2.2
						20 (upper DBR, small-scale activity)	2.2.2.4.1
					•M	20 (upper, DBR, small-scale activity)	2.2.2.4.1
•TSw1	•TC			12 (access-convergence)	2.2.2.2		
				35 (upper DBR)	2.2.2.2		
				5 (upper DBR, large diameter)	2.2.2.2		
•TSw1	•HC			12 (access-convergence)	2.2.2.2		
				30 (upper DBR)	2.2.2.2		
	•BP			6 (access-convergence)	2.2.2.2		
•TSw2	•TC			6 (access-convergence)	2.2.2.2		
	•HC			6 (access-convergence)	2.2.2.2		
	•BP			105	2.2.2.3		
•TSw2	•BP	105 (35 per drift, small-scale activity)	2.2.2.4.1				
	•M	105 (35 per drift, small-scale activity)	2.2.2.4.1				
	•TC	105	2.2.2.3				
•TSw2	•HC	105	2.2.2.3				
	•BP	25	2.2.2.4.2				
	•TC	20	2.2.2.4.2				
•TSw2	•HC	20	2.2.2.4.2				

a: BP = bulk properties; TC = thermal conductivity; HC = heat capacity; M = mineralogy.

b: This number of samples will be tested if sufficient material is available.

quantities of clay or zeolite are thought to be present, in order to perform appropriate bulk-property measurements (see Section 2.2.5.1.2). In addition, a few devitrified and vitric bulk-property samples will be characterized to examine potential correlations between bulk properties and mineralogy.

2.2.5.1 Bulk Properties

As mentioned earlier, "bulk properties" is used in the study to indicate matrix porosity and density (including grain density and bulk densities). Porosity (including matrix porosity and lithophysal-cavity abundance), grain density, and bulk density are related by the following equation:

$$\rho_{db} = (1 - \phi_L - \phi_f)(1 - \phi_m)\rho_g + (1 - \phi_L - \phi_f)\phi_m S \quad (2.2-1)$$

where ϕ_m is matrix porosity, ϕ_L is the lithophysal-cavity abundance, ϕ_f is the fracture porosity, ρ_g is grain density, ρ_b is the bulk density, and S is the saturation state for which the bulk density is calculated. (This equation assumes that both the lithophysal cavities and the fractures are dry, which is a reasonable assumption in partially saturated rock.)

If lithophysal cavities are absent (as they will be in most samples used in laboratory experiments) and fracture porosity is insignificant, then Equation 2.2-1 becomes:

$$\rho_b = (1 - \phi_m)\rho_g + \phi_m S \quad (2.2-2)$$

Obviously, if any three of the parameters in Equation 2.2-2 are known, the fourth is easily calculated.

Data requirements expressed by repository design and performance assessment explicitly request data only for in situ bulk density. If all of the tuffs at Yucca Mountain were fully saturated, laboratory measurements could be limited to measurement of saturated bulk densities. However, most of the thermal/mechanical units are partially saturated, and the saturation values for any single unit appear to be quite variable (e.g., Montazer and Wilson, 1984). One possibility for experiments is to attempt to obtain samples that have retained their natural, in situ saturation and to measure the bulk densities thereof. However, the difficulties inherent in obtaining bulk-property samples without disturbing the in situ saturation state (both the in situ value of S and the distribution of water within the rock) and in proving that they have retained their natural-state saturation are greater than the potential increase in accuracy of the data to be obtained. Thus, this option is no longer under consideration for this study. However, data to be gathered for the characterization of the hydrology of the site probably will include bulk properties obtained in the manner described above. If so, comparisons between the two data sets will be made.

The usual approach to be used for this study is to measure the grain density, saturated bulk density (ρ_{sb}), and dry bulk density (ρ_{db}) in the laboratory. (Note: Unless explicitly stated otherwise, ρ_{sb} and ρ_{db} refer to laboratory values, not to in situ data). Matrix porosity will be calculated from these densities using either or both of the following equations:

$$\phi_m = 1 - \left[\frac{\rho_{db}}{\rho_g} \right] \quad (2.2-3)$$

and

$$\phi_m = \frac{\rho_{sb} - \rho_g}{1 - \rho_g} \quad (2.2-4)$$

Measurement of all three density values obviously provides an over-determination of the system. However, the advantage of such a plan is that a valuable check on the validity and self-consistency of the properties is achieved with minimal additional cost in terms of time or money. The data obtained for grain density and matrix porosity will be combined in Equation 2.2-1 with data on the in situ saturation state, fracture porosity, and lithophysal abundance (see Section 2.3.8 for description of which studies will supply these data) to calculate the in situ bulk density for each thermal/mechanical unit.

Data obtained for bulk properties also will be used in other ways. As mentioned earlier, the small-scale correlation of matrix porosity will be used to estimate the small-scale correlations of several other geoen지니어ing properties. In addition, the data for matrix porosity and in situ bulk density can be compared to data obtained by geophysical logging techniques to estimate and improve the accuracy of such techniques (c.f., SCP Section 8.3.1.4.2). Geophysical-logging data then can be used to analyze the spatial variability of density and porosity in more detail than is possible using laboratory data.

The measurement of techniques to be used to obtain bulk properties are summarized in the following sections. Alternative techniques that were considered are mentioned together with the reasons for not selecting those techniques.

2.2.5.1.1 Saturated Bulk Density

Two techniques will be used to obtain data for saturated bulk density. The first technique is to be applied to most of the samples collected for the purpose of obtaining bulk properties. The second technique will be applied to all samples collected for the purpose of obtaining thermal-conductivity, thermal-expansion,

or mechanical-properties data. The difference between the two techniques is in how the volume of a sample is measured.

The methods of volume measurement that involve a displaced volume of liquid (either water or mercury) as described in the following subsections are not designed for samples that have vugs or cavities intersecting the exterior of the sample. For such samples, volume must be calculated using the dimensions of samples that have been machined precisely to shapes such as cylinders or cubes. It is anticipated that approximately 25 percent of the bulk-property samples for Units TCw, TSw1 and TSw2 will contain vugs; occurrences of vugs in samples from other units are expected to be rare.

2.2.5.1.1.1 Water-Displacement Technique

Samples on which saturated bulk densities will be determined by this technique will have a mass of approximately 50 to 100 g; the geometry of the samples is immaterial. Each sample will be saturated with distilled water under a vacuum until constant mass (± 0.05 percent) in air is achieved. (Note: The completeness of the saturation achieved by application of a vacuum will be evaluated before this method of saturation is used routinely. The evaluation will be performed by subjecting vacuum-saturated samples to pressure saturation and observing how much, if any, additional water enters the samples.) The sample then will be weighed while suspended and submerged in distilled water. The difference in the two masses is the mass of the water displaced by the sample. This mass will be used to calculate the volume of the displaced water, which is also the volume of the sample. The mass (weighed in air) will be divided by this volume to obtain the saturated bulk density. This technique follows in a general way the methods described in Hidnert and Peffer (1950), ISRM (1979), Shuri et al. (1981), and in a number of ASTM Standard Test Methods. However, none of the ASTM methods or Hidnert and Peffer (1950) require vacuum saturation to constant mass, so that use of these methods would result in erroneously low values for saturated bulk density. In contrast, ISRM (1979) and Shuri et al. (1981) suggest the vacuum saturation of samples, which should result in a closer approach to complete saturation of pore space and a truer representation of the mass of a saturated sample.

2.2.5.1.1.2 Computed-Volume Technique

Saturated bulk densities will be determined by a second technique on all samples with volumes that can be determined by calculation from easily measured linear dimensions (e.g., right-circular cylinders, rectangular parallelepipeds). (Samples used for determination of mechanical or thermal properties in the past primarily have been cylinders with diameters of 1 to 2 in. (2.5 to 5.1 cm) and lengths of approximately twice the diameter.) The dimensions of a sample will be measured and a sample volume will be calculated using an

appropriate equation. The sample then will be saturated with distilled water under a vacuum until constant mass (± 0.05 percent) is achieved. [As for the smaller samples, the completeness of saturation achieved by application of a vacuum will be evaluated before routine use of this method. Current data suggest that the saturation state will be 0.91 to 0.94 (Nimick and Schwartz, 1987, pp. A-5, A-6)]. This mass will be divided by the sample volume to obtain the saturated bulk density.

This method of determining sample density is discussed in several test methods, including Hidnert and Peffer (1950), ASTM C-134, Lewis and Tandanand (1974), and ISRM (1979). As stated by Lewis and Tandanand (1974), the method is less accurate than other methods of determining volume; Hidnert and Peffer (1950) estimate a probable accuracy of 1 percent for density determined using volumes calculated from sample geometry. This is a convenient method when sample size precludes use of the more standard techniques.

2.2.5.1.1.3 Alternative Technique for Determination of Sample Volume

One additional method for determining sample volume is discussed in ISRM (1979) — that of mercury displacement. The sample volume is equivalent to the volume of mercury that is displaced when the sample is totally submerged in the mercury. This technique is not presently being considered for two reasons: (1) the technique assumes that the mercury does not intrude the sample at all, which may or may not hold true for individual tuff samples; and, more importantly, (2) the method would require acquisition, control, and use of material (mercury) for which stringent safety requirements must be implemented when the material is being used. The relatively small potential increase in accuracy of volume measurement is not considered to be warranted when compared to the large increase in inconvenience associated with the mercury-displacement technique.

2.2.5.1.1.2 Dry Bulk Density

As with saturated bulk density, two techniques will be used to obtain data for dry bulk density. In both cases, measurements complement those described for saturated bulk density; the difference between the two methods is the same difference as for saturated bulk density (i.e., method of volume measurement). Thus, the discussion of supporting standard test methods and alternative techniques provided in Section 2.2.5.1.1 applies for dry bulk density as well. For the primary technique, samples for which saturated bulk densities have been obtained will be dried in air (at ambient pressure) to constant mass (± 0.05 percent) in an oven at approximately 105°C. The mass then will be divided by the sample volume that was determined previously to give a value for the dry bulk density. For the second technique, used for larger and more regularly shaped samples, the samples also will be dried in air (at ambient pressure) to constant mass (± 0.05 percent) at approximately 105°C, with the mass to be divided by the sample volume to get dry bulk density. [Note:

Measurements have shown that the change in sample volume resulting from dehydration is insignificant relative to normal experiment uncertainty (Nimick and Schwartz, 1987)]. If measurements of thermal and mechanical properties of samples are to be performed on saturated samples, oven drying of samples will be deferred until the measurements are completed. For samples to be tested in an oven-dry condition, saturated masses will be obtained first, followed by the oven-drying activity.

Some of the tuff samples are expected to contain significant quantities of clay, zeolites, or both, specifically samples from Units CHn1z and CHn2z and from altered TSw3. Evidence indicates that standard procedures that are designed to remove the water from interstitial pores in a rock also will remove water from the internal channels of the zeolites (Knowlton and McKague, 1976; Knowlton et al., 1981). The amount of such non-pore water that is removed will depend on the intensity and duration of heating and on the quantity and type of zeolite that is present. The effect will always be that too much water will be removed, leading to systematically low sample masses and thus to systematically low values for dry bulk densities of zeolitic tuffs. Because no method has been identified to selectively remove only the pore water from such samples, dry bulk density will not be determined on zeolitic samples. Instead, dry bulk density will be calculated from data for grain density and saturated bulk density using the following equation:

$$\rho_{db} = \frac{\rho_g (\rho_{sb} - 1)}{\rho_g - 1} \quad (2.2-5)$$

The mineralogy of samples that might contain significant quantities of clay or zeolite will be determined before bulk density measurements are performed in order to decide whether measurement of dry bulk density should be made on a given sample.

Equation 2.2-5 is valid as long as all porosity is interconnected and can be saturated before determination of ρ_{sb} . At present, no reason exists to expect isolated pores in the zeolitic material.

2.2.5.1.3 Grain Density

The preferred method for determination of grain density involves the use of a water pycnometer. The sample on which grain density is to be determined in most cases will be the same one used for determination of bulk densities. The sample will be powdered by crushing, grinding, or both. A subsample of the powder (~25-30 g) will be placed in a clean, dry pycnometer with a nominal volume of 100 ml that has been calibrated and weighed before use. (Note: Pycnometers of other sizes can be used; the volume of powder should be adjusted accordingly.) The pycnometer containing the powder will be dried in air at 110°C to constant mass, then cooled and weighed. The mass of the powder will be determined by subtracting the mass

of the empty pycnometer from the mass of the pycnometer containing the powder. Deaerated distilled water will be added to cover the powder, and a vacuum will be applied for at least 24 hours to remove any air in the powder and water. After returning the pycnometer containing the powder and water mixture to ambient temperature, deaerated distilled water will be added to the calibrated fill line on the pycnometer and the pycnometer will be weighed. The volume of the powder will be determined by calculation of the volume of water displaced by the powder. Grain density then will be calculated by dividing the mass of the powder by the volume. This procedure follows the general guidelines provided in Hidnert and Peffer (1950) and in a number of ASTM Standard Test Methods, including C-128, C-135, D-854, and D-2320. [Of these methods, C-128 specifies submersion of the powder without boiling (by application of heat or vacuum) to remove air from powder and water, and thus will produce an apparent grain density rather than a true value.] The other three ASTM methods, as well as Hidnert and Peffer (1950), ISRM (1979), and Shuri et al. (1981), recommend application of a vacuum for different periods of time (all shorter than is planned for this study). The longer time of application of vacuum chosen for this work is based on experience gained from previous work on tuff samples (c.f., Schwartz, 1985).

The major alternative technique for the determination of grain density involves the use of a gas (usually helium) pycnometer (e.g., ASTM C-604). Schwartz (1985) provides a discussion of comparative measurements of the grain densities of tuffs using both types of pycnometer. Several reasons were stated for preferring the water pycnometer, including the fact that the method is more time-effective, because calibration is faster and multiple samples can be run simultaneously. More important, however, is the result that the water pycnometer is more accurate when determining the density of a well-characterized material (α -quartz) and is more precise when determining the density of tuff samples (an average precision of $0.013 \times 10^3 \text{ kg/m}^3$ for the water pycnometer compared to $0.025 \times 10^3 \text{ kg/m}^3$ for the gas pycnometer).

ASTM C-604 states that the precision of specific-gravity data obtained in a single laboratory using a gas pycnometer was 0.0107 for four refractory materials having specific gravities ranging from 2.6 to 4.0. Precision of specific-gravity data for cohesionless soils as obtained in a single laboratory using a water pycnometer is stated to be 0.021 in ASTM D-854. This reversal of the relative precisions of the two techniques compared to the data obtained by Schwartz (1985) suggests that gas pycnometry should be retained as an option for grain-density measurements on devitrified tuff samples. However, for tuff samples that contain more than 10 percent glass, zeolite, clay, or a combination of the three phases, gas pycnometry is not a viable option because of the potential for evaporative water loss during the grain-density measurement.

The measurement technique to be used for most tuff samples involves heating the powdered sample in air to constant mass (± 0.05 percent) at 110°C . As discussed in Section 2.2.5.1.2, such heating is inappropriate for clay-rich or zeolitic samples. Removal of water from the channels in the zeolites would lead to

systematically high grain densities. Alternative approaches for zeolitic samples are being evaluated; these approaches include equilibration with air with a high relative humidity or heating the sample at an as yet unspecified temperature that is less than 100°C. The validity of one or more of these alternative approaches will be evaluated before routine measurements begin.

In order to obtain powders for grain-density measurements, larger rock samples must be crushed, ground, or both. These processes are heat-producing, and zeolitic samples may be dehydrated by a finite amount during powder preparation. Equilibrations of the powders with a high-relative-humidity atmosphere until constant mass is achieved should offset such dehydration.

The grain density of samples to be used in thermal and mechanical experiments usually will not be determined directly because ensuring that the correct value was obtained would require crushing and grinding of the entire sample; archiving of the post-test samples would no longer be possible. Instead, the saturated and dry bulk densities will be used to calculate grain densities using the following equation:

$$\rho_g = \frac{\rho_{db}}{1 + \rho_{db} - \rho_{sb}} \quad (2.2-6)$$

The grain densities obtained by using Equation 2.2-6 will be compared to values obtained by direct measurement to evaluate the relative merits of the two different approaches.

As mentioned in Section 2.2.5.1.2, dry bulk densities will not be determined for zeolitic samples. For many of the zeolitic samples used in thermal and mechanical experiments, representative material will be taken from the post-test sample and grain density will be determined directly using the method described earlier in this section.

2.2.5.1.4 Matrix Porosity

As mentioned earlier, matrix porosity will usually be calculated from the values obtained for the densities of the tuff samples. The primary equation to be used to calculate the matrix porosities will be

$$\phi_m = 1 - \left[\frac{\rho_{db}}{\rho_g} \right] \quad (2.2-3)$$

This equation is preferred because the accuracy and precision of determinations of saturated bulk density are expected to be slightly worse than those for the other two densities. Nonetheless, matrix porosities also will be calculated using the following equation as a check on the consistency of the density measurements:

$$\phi_m = \frac{\rho_{sb} - \rho_g}{1 - \rho_g} \quad (2.2-4)$$

As discussed in Section 2.2.5.1.2, dry bulk densities will not be determined for zeolitic samples. Thus, Equation 2.2-4 will be used to calculate the matrix porosities of these samples.

Discussion in Sections 2.2.5.1.1 and 2.2.5.1.2 provides information on the determination of saturated and dry bulk densities of samples to be used in thermal and mechanical experiments. Matrix porosities of these samples will be calculated using the following equation:

$$\phi_m = \rho_{sb} - \rho_{db} \quad (2.2-7)$$

The matrix porosities obtained by using Equation 2.2-7 will be compared to porosity data obtained for smaller samples (Equations 2.2-3 and 2.2-4) to evaluate the relative merits of the different approaches.

An obvious alternative to the calculation of matrix porosity is the direct determination thereof. Such determinations can be made using a gas permeameter (gas pycnometer used with a solid sample rather than powder) (Lewis and Tandanand, 1974; ISRM, 1979) or by the water-absorption method. The experimental uncertainties associated with the pycnometer measurements are expected to be of the same magnitude as the uncertainties in matrix porosities calculated from density data. Several direct determinations of matrix porosity will be made to test this expectation. If the comparison between calculated and measured values of porosity shows a significant difference, matrix porosities will be both measured and calculated for all subsequent samples.

Several non-standard methods have the potential to provide a direct determination of matrix porosity. These include nuclear magnetic resonance, X-ray transmission, and use of a VHF-resonance cavity. As yet, none of these techniques has been used for tuff samples; data on achievable accuracies and precisions are unavailable. These techniques are not expected to be used routinely because of the cost and time required to perform non-standard measurements. However, several zeolitic samples may be examined by one or more of these techniques in an attempt to assess the accuracy with which standard techniques determine intergranular (matrix) porosity in zeolitic rocks.

2.2.5.2 Heat Capacity

The partial saturation of the tuffs in situ at Yucca Mountain plays a major role in the determination of an approach to obtaining heat capacity data. The in situ heat capacity of a rock (C_p^{rock}) can be expressed as follows:

$$C_p^{rock} = (1 - \phi_L - \phi_f)(1 - \phi_m)C_p^{solid} + (1 - \phi_L - \phi_f)\phi_m S C_p^{H_2O} + [\phi_L + \phi_f + (1 - \phi_L)\phi_m(1 - S)]C_p^{air} \quad (2.2-8)$$

where C_p^{solid} is the heat capacity of the solid material, and $C_p^{H_2O}$ and C_p^{air} are the heat capacities of water and air, respectively. As with in situ bulk density, the approach will be to use Equation 2.2-8 to estimate the in situ heat capacity rather than to try to obtain samples that preserve the in situ condition of the rock.

Of the parameters in Equation 2.2-8, data for $C_p^{H_2O}$ and C_p^{air} are available in engineering handbooks, data on matrix porosity will be obtained as a part of this study (Section 2.2.5.1.4), and data for fracture porosity, lithophysal-cavity abundance and in situ saturation will be obtained by other studies for the Yucca Mountain Site Characterization Project (discussed in Section 2.3.8). The intent of this portion of the Laboratory Thermal-Properties Study is to obtain the data to calculate the heat capacity of the solid portion of the tuffs (i.e., C_p^{solid}).

The experimental technique selected for use in measuring heat capacities is adiabatic calorimetry. In this method, the amount of electrical power (or heat) required to rise the sample temperature by a given amount is monitored. Under the condition that all power input goes to heating the sample (i.e., none is lost to the surroundings), the heat capacity is obtained as a simple function of sample mass, temperature change, and power input.

For this study each sample [nominal dimensions of 5.1 cm (diameter) and 7.0 cm (length)] will be saturated before testing. The sample will be heated at a constant rate ($\leq 2^\circ\text{C}/\text{min}$) to the maximum temperature (nominally 100°C for Units TCw, PTn, CHn2v, and CHn2z, and 300°C for the other units). At or near the nominal boiling temperature of 100°C , it is anticipated that the heating rate will be reduced to allow the pores of the sample to dehydrate. The optimum rate reduction will be determined during development of test procedures.

Two alternative techniques were considered to perform these measurements. One is a classical technique — drop calorimetry — in which a sample (either a solid or a powder) is heated to a prescribed temperature, then dropped into an essentially adiabatic receiver containing a fluid, the specific heat and

enthalpy of which are well known. The enthalpy of the sample is calculated from the temperature change induced in the fluid by the hot sample. After numerous similar measurements at different initial temperatures have been made, the sample enthalpy is plotted as a function of temperature, and the heat capacity (at constant pressure) is obtained as the slope of the resulting curve. This technique is described in a number of recommended procedures, including ASTM C-351, Lewis and Tandanand (1974), and Shuri et al. (1981).

This technique suffers from several limitations. It is quite time-consuming, and many potential inaccuracies can occur (e.g., radiation loss to surroundings, small temperature changes for small enthalpies). Also, the technique is unsuitable for materials and temperature ranges in which solid-state phase transitions occur, as is expected for silica (SiO_2) polymorphs in Units TSw1 and TSw2 for temperatures above 150°C.

The second alternative technique considered is known as differential scanning calorimetry (DSC). In this method, a sample and a reference material (approximately 5 to 10 mg of each) are heated (or cooled) at a constant rate (1 to 20°C per minute depending on type of sample and desired information) using separate heaters. The temperatures of both materials are monitored using thermocouples, and small amounts of power are applied at intervals to the heater for the unknown sample to continuously adjust the temperature of the sample to be equivalent to that of the reference material. The heat (power in a specific period of time) required to make such adjustments is monitored. Comparison of these data with equivalent data obtained from empty sample pans and from a known material (usually sapphire) allow the heat capacity of the unknown sample to be calculated as a function of temperature. Details of the technique have been summarized in a number of publications, including McNaughton and Mortimer (1975).

The DSC technique is not truly adiabatic, so that some heat loss to the surroundings occurs. More importantly, samples are quite small, and the possibility that samples would be nonrepresentative would always be an issue if this technique were selected.

Heat capacities measured using the adiabatic technique will be bulk heat capacities (i.e., will be composites of the heat capacities of pore fluid and solids). Using the measured values of sample porosity and textbook values for $C_p^{H_2O}$, C_p^{air} , or both, the heat capacities of the solid components as a function of temperature can be calculated.

In addition to the experimental technique, a method for estimating the heat capacity of the solid components is available as well. This method involves the determination of the chemical composition of the solid in terms of oxides (SiO_2 , Al_2O_3 , etc.) followed by calculation of the weighted sum of the heat capacities of the oxides. Solid-state phase transitions and dehydration are included in this estimation process using known enthalpies for the reactions and assuming a temperature range over which each reaction occurs. When

the mass of the reacting substance is also included, an approximation to the heat capacity of the reaction is obtained. This method has been used to obtain preliminary values for the heat capacities of the solid components of Units TSw1, TSw2, and TSw3 (Nimick and Schwartz, 1987), but has yet to be verified for these units using experimental data. If the calculations are shown to provide accurate estimates of heat capacities, then chemical data obtained for other studies for the Yucca Mountain Site Characterization Project [e.g., Study 8.3.1.3.2.1 (Mineralogy, Petrology, and Chemistry of Transport Pathways)] can be used to expand the data base on heat capacity without performing additional measurements.

Another option for determining heat capacity is to measure thermal diffusivity [equal to $K/(\rho_b C_p)$], then calculate C_p from knowledge of K and ρ_b . This approach suffers from one of the same shortcomings as drop calorimetry: the heat capacities pertaining to transitions that occur over a temperature range (e.g., SiO_2 polymorphic transitions or continuous dehydration) cannot be determined because data for K will not be available at numerous closely spaced increments of temperature. Thus, this approach to obtaining C_p data probably will not be used.

As a result of the considerations above, the probable approach to be used for this study is a combination of adiabatic calorimetry and calculations from bulk chemical compositions. Measurements are essential both to provide experimental data and also to provide data by use of which the validity of the calculational method can be examined.

A limitation in the application of either adiabatic calorimetry or the calculational method to clay-rich or zeolitic tuffs is potential inaccuracy in the reproduction of the dehydration behavior of the material (for both methods) and of the heat capacity of the channel water in the zeolites (for the calculation method). Before either method is applied routinely, experiments using both adiabatic calorimetry and thermogravimetric analysis on zeolitic samples will be performed to establish the most appropriate heating and cooling rates, and atmospheric environment to use for calorimetry measurements. Once data from these experiments are available, an evaluation can be made of the various thermodynamic functions proposed for the channel water of the zeolites [e.g., "perlite" water (King et al., 1948), "hydrate" water (Robinson and Haas, 1983)].

2.2.5.3 Thermal Conductivity

The approach to be used to obtain data for the in situ thermal conductivity of the tuffs is the same as outlined earlier for the other thermal properties (Sections 2.2.5.1 and 2.2.5.2) — estimation of appropriate values rather than attempting to preserve in situ saturations. The equation(s) to be used to estimate an in situ value from laboratory-determined data has not been selected but will take the general form

$$K = K(K_s, K_w, K_a, \phi_m, \phi_L, \phi_f, S) \quad (2.2-9)$$

where K_s is the thermal conductivity of the solid material, and K_w and K_a are the thermal conductivities of water and air, respectively, and ϕ_m, ϕ_L, ϕ_f , and S will be obtained from other studies (see Figure 2.2-1).

(Note that fracture porosity is included in Equation 2.2-9. If site-characterization data show fracture porosity to be negligible, the fracture porosity can be excluded from the explicit form of Equation 2.2-9.) The equation(s) will be selected from those described in Section 3.4.5. The equation used for most calculations of in situ thermal conductivity is likely to be the same equation that is selected for use in extrapolation of laboratory-measured thermal conductivities to zero-porosity values. For specific geometries, (e.g., heat flow perpendicular to a planar fracture or elongate lithophysal cavities), different equations may be used that were originally derived for the problem of interest. In addition, a number of in situ measurements of thermal conductivity will be made for other studies (Table 1.0-1) as a part of the overall determination of rock-mass thermal conductivity.

Data for K_w and K_a are available in the published literature. Data for matrix porosity will be obtained for this study (Section 2.2.5.1.4) and data on fracture porosity, in situ saturation and lithophysal-cavity abundance will be obtained by other studies for the Yucca Mountain Site Characterization Project (Section 2.3.8). Thus only the thermal conductivity of the solid components needs to be determined experimentally in this portion of the Laboratory Thermal-Properties Study.

Many experimental methods are available for measuring thermal conductivity. Also, many equations have been proposed for extrapolating measured thermal conductivities at known porosities to the zero-porosity condition (i.e., to obtain the thermal conductivity of the solid components). The alternatives for the experimental methods and the extrapolating equations are discussed separately in the following subsections.

2.2.5.3.1 Alternatives for Experimental Determination of Thermal Conductivity

Many methods of measuring thermal conductivity have been proposed in the published literature; numerous overviews of this broad topic exist in the literature. A brief synopsis of the survey of techniques is given below, followed by a discussion of the techniques being considered for this study.

1. Rod method (steady-state, absolute): axial heat flow through a relatively long rod, suitable for good conductors.

2. Plate or disk method (steady-state, absolute): axial heat flow through a relatively thin disk; suitable for poor conductors and insulators.
3. Divided-rod method (steady-state, comparative): axial heat flow through a series of rods, one of which is the material with unknown conductivity.
4. Plate or disk method (steady-state, comparative): axial heat flow through a series of plates or disks, one of which is the material with unknown conductivity.
5. Cylindrical method (steady-state, absolute): radial heat flow in a cylindrical sample.
6. Spherical method (steady-state, absolute): radial heat flow in a spherical sample.
7. Concentric cylinder method (steady-state; comparative): radial heat flow (in series) through a material of unknown conductivity, then through a reference material.
8. Disk method (steady-state, comparative): radial heat flow into a disk of reference material combined with axial heat flow into and through adjoining disks of material of unknown conductivity.
9. Longitudinal heat flow method (transient, absolute): application of a heat pulse to one end of an isothermal rod or to one face of an isothermal disk or plate.
10. Flash method (rapid transient, absolute): flash of thermal energy applied to one face of a disk by flash tube or laser.
11. Radial heat flow method (transient, absolute): application of heat pulse to the center or to the outer surface of cylinder (heater not a line source).
12. Line heat source/thermal probe method (transient, absolute): application of heat pulse to the center of a cylindrical sample by a heat source that approximates a line heat source in an infinite medium.

As stated by Touloukian et al. (1970, p. 13a), "...no one method is suitable for all the required conditions of measurement." The method that is selected for this study must be suitable for poor conductors.

should be able to accommodate a relatively small-sized sample, and should be as simple and rapid as possible given the other two constraints. In addition, some degree of control of environmental variables other than temperature (e.g., pressure, saturation) may be necessary.

Of the methods listed above, three are under consideration for use in this study. The technique to be used for most of the testing will be the guarded-heat-flow-meter method, a version of Option (2) above. The advantages of the technique are that it is relatively simple, does not require instrumentation of the sample (e.g., thermocouples within the sample), and has a suitable testing range for the thermal conductivities expected for all of the tuff samples. Samples for this testing technique would have nominal diameters of 2 in. (5.1 cm) and nominal thicknesses between 0.5 and 0.75 in. (1.3 and 1.9 cm).

The other two testing techniques that probably will be used on a few samples are a thermal-comparative technique [Option (3) or (4) above] and a guarded-hot-plate technique [a version of Option (2) above]. The comparative technique would be used primarily in the scoping study on the effect of normal stress on the thermal conductivity of fractured samples (Section 2.2.3). Samples used in this technique would have nominal diameters of 2 in. (5.1 cm) and nominal lengths between 0.5 and 1.5 in. (1.3 and 3.8 cm). The guarded-hot-plate technique uses larger samples [nominal diameter of 8 in. (20.3 cm) and nominal thickness between 1 and 2 in. (2.5 and 5.1 cm)] and would have two uses — as the testing technique for the larger samples in the sample-size-effects scoping study (Section 2.2.3) and as the technique for testing samples of Unit TSw1 with a high content of lithophysal cavities (Section 2.2.2.2).

All three of the methods mentioned in the preceding paragraphs use cylindrical samples, which is the general shape that specimens will have when obtained from either core holes or instrumentation holes in the ESF. All three are techniques that have been used successfully on rock samples, and have related ASTM standards (F-433 for the guarded heat flow meter; E-1225 for the comparative method, and C-177 for guarded hot plate). In addition, a detailed examination of the comparative, steady-state disk method has been made as described in Sweet (1986) and Sweet et al. (1986).

Thermal conductivities will be determined for at least two temperatures below 100°C for all samples, and at five temperatures above 100°C for samples from Units TSw1, TSw2, TSw3, CHn1v, CHn1z and from altered TSw3 (the nominal maximum temperature for these units is 300°C). For some randomly selected subset of the samples, measurements will be repeated at identical temperatures during cooling of the sample to evaluate the possibility of hysteresis in thermal conductivity. This evaluation will provide data to test the assumption that thermal conductivities will be the same during the cooling of the rock around waste canisters as they were during heating.

Some experimental data on the thermal conductivity of damp (i.e., partially saturated) porous materials suggest that the effective conductivity will be higher in partially saturated material than in the saturated material at temperatures $\geq 60^{\circ}\text{C}$ (Pratt, 1969). This possibility indicates that an attempt should be made to measure the effective thermal conductivity of tuff samples at known values of intermediate saturation. Pratt (1969) describes a method of interpreting thermal conductivity data obtained by use of a steady-state method [Option (2) above] for partially saturated samples. A scoping study will be performed on saturation effects on thermal conductivity (Section 2.2.3). The results of this study will be used to determine the initial saturation for all routine testing. This initial saturation will be used for all measurements at temperatures below 100°C . Samples then will be oven-dried, the measurements at temperatures below 100°C will be repeated, and the higher-temperature measurements will be performed. Although the oven drying will remove channel water from zeolites, the final state of oven-dried zeolitic samples will be similar to that of the in situ zeolitic material at 105° to 110°C (because of slower heating in situ); measured high-temperature thermal conductivities are expected to be representative of in situ conditions.

Evaluations will be made of the extent to which convection of pore water might be contributing to heat transfer. For any of the methods to be used in this study, comparison of the thermal conductivities obtained with heat flowing against gravity with those obtained with downward heat flow will provide information on the magnitude of convection in the experiments.

2.3 Constraints on Laboratory Thermal-Properties Study

2.3.1 Potential Impact on the Site

The potential impact on the site of the coring of new core holes will be addressed as the various proposals for drilling and coring from the surface are evaluated. The proposals are summarized in Section 8.3.1.4 of the SCP. The potential impacts related to the construction of the ESF on the site are discussed in Section 8.4 of the SCP. No additional impacts on the site are expected as a result of the experiments to be conducted for this study. No additional coring or excavation presently is anticipated to be required beyond that already planned for other studies.

2.3.2 Repository Simulation

The ultimate goal of this study is to characterize the thermal properties of the rocks in the vicinity of the underground facilities. As such, data gathered for this study will be combined with data on lithophysal-cavity abundance, fracture porosity, and in situ saturation state to be collected in other studies (Section 2.3.8) to provide property values appropriate to the scale and apparent variability of the in situ rock mass (see Figure

2.2-1 for a diagram of the process). Thus, within the limitations imposed by the assumptions involved in extrapolating the measured data to the in situ conditions and to the areas from which no samples were obtained, the results of this study will have accounted for the scales (spatial dimensions) and the environmental conditions expected to be experienced by the rock surrounding a repository.

The major assumption constraining this study is that the dominant mechanism of heat transfer from waste canisters in the unsaturated tuffs will be conduction. Examination of the validity of this assumption will be made during the several in situ heater tests planned for the ESF as well as in some of the thermal-conductivity experiments to be conducted in the laboratory. Determination of the validity of the assumption does not affect the measurements to be performed in the laboratory, but might have an influence on the method(s) used to estimate in situ thermal properties from laboratory data (e.g., if convective heat transfer needed to be incorporated in an "effective thermal conductivity" term). The initial strategy for this study is to assume that heat transfer by convection and radiation from waste canisters will be negligible, so that estimation of in situ thermal properties will be a straightforward extension of laboratory measurements. If, as expected, the in situ experiments to be performed for Study 8.3.4.2.4.4 (Engineered Barrier System Field Tests) demonstrate that convection is a significant component of heat transfer from waste canisters, the data from this study will be integrated with the in situ data to provide a more realistic representation of the in situ thermal properties. Laboratory measurements of the steady-state, effective thermal conductivity of partially saturated samples may help in the integration effort.

2.3.3 Required Accuracy and Precision of Thermal Properties

For each thermal property, the accuracy and precision required for use of the data are built into the data requirements expressed by repository-design and performance-assessment personnel through the performance-allocation process. For all experimental techniques considered for use in this study, the achievable accuracy and precision of the experimentally determined values are of much smaller magnitudes than the variation of values caused by heterogeneity between samples. Thus, all constraints imposed by required accuracies and precisions will be accounted for by satisfaction of the data requirements and are included in the estimation of the numbers of samples required to obtain the data (Section 2.2.1).

2.3.4 Limits and Capabilities of Analytical Methods

No analytical models or numerical methods will be used either for designing experiments or for interpreting the thermal-properties data to be obtained for this study. Thus, analytical models and numerical methods impose no constraints on the study.

2.3.5 Time Required Versus Time Available

This study is designed to provide current information on thermal properties whenever such information is requested (e.g., by personnel associated with in situ experiments or by those associated with analysis of the thermal response of the rock to the presence of heat-producing waste) and to provide in a timely manner written summaries of data for use in analyses supporting major deliverables such as the Draft Environmental Impact Statement or the License Application. Thus, time will not be a constraint on the study. However, the timely availability of the samples that are required for this study is a prerequisite to the timely completion of the study.

Part of the basis for planning this study is the existing definition of the thermal/mechanical units. At intervals during data collection, statistical evaluation of thermal-properties data will be performed to evaluate whether the unit divisions are reasonable and defensible. If they are, no changes will be made. If a need for definition of new unit boundaries is indicated, the redefinition will be performed and sampling plans for any remaining core holes will be amended as necessary.

2.3.6 Statistical Relevance of Data

The strategy for sampling and testing of the thermal/mechanical units that is discussed in Section 2.1 is based on satisfying the data requirements of repository design and performance assessment using statistical considerations. As such, the results of the Laboratory Thermal-Properties Study will be directly relevant in the applications for which they are required. Should site characterization be unable to provide thermal-properties data with the required constraints, the data base for thermal properties should still be sufficient to provide a statistical basis for any reevaluation of the design or performance-assessment goals.

2.3.7 Scale of Phenomena

The methods to be used in extrapolating laboratory data on thermal properties to rock-mass values are discussed in various parts of this document. The only potential problem with the extrapolations is the possibility that the in situ experiments will indicate that conduction is not the only significant mechanism of heat transfer, whereas laboratory experiments may not show this possibility. Such a discrepancy will not be a constraint on the methods used to acquire laboratory data, but may affect the extrapolation procedures and the comparison of extrapolated values to data obtained during in situ experiments.

2.3.8 Interrelationships With Other Studies

The experiments planned in the Laboratory Thermal-Properties Study will contribute to a data base that will serve as the primary input for thermal calculations, both for repository design and performance assessment. Data from several other studies (Table 1.0-1) will provide measurements of in situ thermal properties that can be used to evaluate the validity of the methods used to extrapolate laboratory-determined thermal properties to the rock mass. In addition, thermal properties measured in the laboratory on location-specific samples will aid in the interpretation of the in situ experiments listed in Table 1.0-1.

In order to perform the systematic sampling described in Section 2.2, the locations of contacts between thermal/mechanical units must be defined. This definition will be performed as part of Study 8.3.1.4.3.2 (Three-Dimensional Rock Characteristics Models.)

This study will provide estimated values of the rock-mass thermal properties. To do so, some information is required that will not be obtained as part of the study. The abundance of lithophysal cavities in three of the thermal/mechanical units (TCw, TSw1, and TSw2) must be characterized so that the contribution of the cavities to heat capacity and thermal conductivity can be included. Information on the abundance of lithophysal cavities will be gathered as part of the following Studies: 8.3.1.4.2.1 (Characterization of the Vertical and Lateral Distribution of Stratigraphic Units Within the Site Area) and 8.3.1.4.2.2 (Characterization of the Structural Features Within the Site Area).

Second, and more important, information on the in situ saturation of the various units is required. In situ bulk density, heat capacity, and thermal conductivity all are strongly influenced by the saturation state in the pores. Information on in situ saturations will be obtained as part of the following Studies: 8.3.1.2.2.3 (Characterization of Percolation in the Unsaturated Zone-Surface-Based Study) and 8.3.1.2.2.4 (Characterization of Yucca Mountain Percolation in the Unsaturated Zone — ESF Investigations).

The fracture porosities of various units will be estimated based on information on fracture frequency, orientation, spacing and distribution. This information will be obtained as part of several studies, including Studies 8.3.1.2.2.3, 8.3.1.2.2.4, and 8.3.1.4.2.2. The calculated effect of fracture porosity on the thermal properties of the rock mass will be evaluated to determine whether the effect is significant.

If the method of calculating heat capacities from bulk chemical composition (Section 2.2.5.2) proves to be valid for tuffaceous rocks, bulk chemical data to be obtained in Study 8.3.1.3.2.1 (Mineralogy, Petrology, and Chemistry of Transport Pathways) will be used to expand the data base for heat capacity. In addition, Study 8.3.1.3.2.2 (History of Mineralogic and Geochemical Alteration of Yucca Mountain) may provide

information on the dehydration kinetics of glass, zeolites, and clay that may be useful in developing and refining experimental procedures for determination of thermal properties.

Some data on thermal properties will be gathered as ancillary information during work for other studies. Matrix porosity will be determined in Studies 8.3.1.2.2.3, 8.3.1.2.2.4, and 8.3.1.4.2.1. Density data also will be obtained by two of these Studies: 8.3.1.2.2.3 and 8.3.1.4.2.1. Data on thermal conductivity at ambient temperature will be obtained during work for Study 8.3.1.15.2.2.1 (Surface-Based Evaluation of Ambient Thermal Conditions).

The potential effects of radiation on the thermal conductivity of Unit TSw2 will be examined as part of Study 8.3.4.2.4.3 (Mechanical Attributes of the Waste Package Environment). Interpretation of the test results in Study 8.3.4.2.4.3 will require input from this study in the form of thermal-conductivity data on samples that have not been irradiated.

2.3.9 Interrelationships With ESF Construction Activities

A large number of samples for determination of laboratory thermal properties will be taken from core obtained from the MPBX holes planned as part of activities for other studies. The construction schedule for the ESF will determine when the MPBX holes can be placed in the main accesses and drifts, and thus, will constrain the sampling activities for thermal-properties experiments. In addition, tests on large-diameter samples to examine sample-size effects on lithophysae-rich tuff will be constrained by the construction of the upper DBR.

3.0 DESCRIPTION OF LABORATORY THERMAL-PROPERTIES EXPERIMENTS

The Laboratory Thermal-Properties Study Plan is composed of three groups of experiments that collectively are intended to provide most of the data necessary to perform thermal calculations for a repository at Yucca Mountain. Experiments will be performed at testing laboratories that (1) have been determined to possess the technical expertise necessary to obtain quality data for the thermal properties of the tuffs and (2) are able to satisfy all Sandia National Laboratories YMP quality-assurance requirements. The experimental methods that will be used or from which a method will be selected are discussed in Section 2.2.5.

3.1 EXPERIMENT UNCERTAINTY

The uncertainty of determinations of properties is best specified using two quantities: precision and accuracy (also known as bias) (Eisenhart, 1963). Accuracy is defined as the deviation of a determination of a property from the "true" value for the property. In theory, the accuracy is unknowable because the "true" value cannot be determined. In the remainder of this document, accuracy will be used to describe the difference between the mean of the measured values of a property for a standard material and the accepted mean value for that property.

In addition to accuracy, precision must be determined. Precision is the reproducibility of successive determinations of a property. Eisenhart (1963) suggest that a useful index of the precision of a series of measurements made on the same sample is the calculated value of the standard deviation or of the variance. For the work conducted for this study, the standard deviation will be used.

Properties may be determined for standard materials (i.e., materials for which "true" values have been estimated with a degree of accuracy that is assumed to be high) and for rock samples. The accuracy of property determinations for the rock samples will be estimated by replicate determinations of a property for one or more standard materials and comparison of the mean value of the results with the accepted "true" value of the property for the standard(s). Statements about accuracy will include an estimate of the accuracy (the difference between the accepted "true" value and the mean value of the replicate measurements) and the precision (the standard deviation of the replicate measurements).

The precision of property determinations for rock samples also will be estimated by performing replicate measurements on individual rock samples. Because the precision may be a function of rock type as well as of the experimental technique, the precision of a property will be determined for each thermal/mechanical separately. The initial estimates of precision will be made using five replicate property determinations on each of five samples from each thermal/mechanical unit. These precisions will be

indicative of values of multi-operator, single-location measurements (see ASTM E-177 for definitions of these and related terms), so that they will be described as "repeatability" rather than "reproducibility."

The precision with which measurements have been made for each thermal property using standard materials is discussed in Section 3.2.

3.2 Density and Porosity Characterization

As mentioned earlier, data for the in situ bulk densities of the thermal/mechanical units will be obtained by calculation using data on grain density, matrix porosity, lithophysal cavity abundance, in situ saturation state, and potentially fracture porosity. Of these, grain density and matrix porosity will be determined for this study. Previous experience with the tuffs indicates that optimum results for these two properties can be obtained by measuring grain density, saturated bulk density, and dry bulk density. Matrix porosity then is calculated from any two of the three measured properties.

The following subsections address each of these "bulk" properties individually. The number of samples is tied to the summary at the end of Section 2.2.4, with all four properties determined for each sample. The usual sequence of measurement will be saturated bulk density, dry bulk density, and grain density, followed by calculation of matrix porosity. Deviations from, or exceptions to, this general sequence will be addressed in the pertinent subsections. After discussion of the four properties, a synopsis is provided that addresses the range of expected results and analyses of results for calculated values of in situ bulk density.

3.2.1 Saturated Bulk Density

3.2.1.1 Technical Procedures

Appropriate planning documents and Technical Procedures (TPs) (Table 3.2-1) will be prepared for each experiment. The planning documents and TPs will be issued before data are collected for saturated bulk density.

3.2.1.2 Accuracy and Precision

Previous determinations of density by SNL for the Yucca Mountain Site Characterization Project included calibration checks using magnesium and steel. The density of a standard material was required to be within ± 1 percent of the "true" value before the density of rock samples was determined. Thus, saturated bulk densities are expected to be accurate to within ± 1 percent of the experimental value if samples are fully

Table 3.2-1
Technical Procedures* for Measurement of Saturated Bulk Density

TP-057	Procedure for laboratory bulk density measurements
TP-064	Procedure for vacuum saturation of geologic core samples (completed)

*Technical procedures for this work will be standard procedures and will incorporate relevant portions of nationally recognized procedures.

saturated. Failure to achieve full saturation (i.e., if $0.95 \leq S < 1.0$) will add from 0.1 percent (Unit TSw3) to 1.3 percent (Unit PTn) to the value given earlier for bounds on accuracy.

The precision of determinations of saturated bulk density has not been evaluated. Future measurements will include such an evaluation.

3.2.1.3 Range of Expected Results

The range of expected values for the saturated bulk density of the thermal/mechanical units is given in Table 3.2-2. The ranges have been calculated as $\bar{X} \pm 2S$, where \bar{X} and S are based on existing data.

3.2.1.4 Equipment and Design Requirements

The equipment required to perform measurement of saturated bulk density is composed of an apparatus for vacuum-saturation of samples, glass beakers, one or more balances, a temperature-measuring device, and an apparatus that can be used to suspend a sample in water while weighing the sample. This last portion of the equipment is the only portion that can involve significant variability in experiment design, with potential methods of suspension including string, thin wire, fine netting, and small metal pans. The method described in ISRM (1979) suggests a wire basket or perforated container hanging from a thin wire. The actual method used will depend on the equipment used by the testing laboratory that obtains saturated-bulk-density data for this study.

Table 3.2-2
Ranges in Expected Values of Saturated Bulk Density

Unit	Range (10^3kg/m^3)	Existing Measurements
TCw	2.20-2.48	17
PTn	1.31-2.20	5
TSw1	2.19-2.45	40
TSw2	2.28-2.48	53
Altered TSw3	No Data	0
TSw3	2.29-2.39	12
CHn1v	1.61-2.11	4
CHn1z	1.81-2.08	17
CHn2v	1.83-2.06	6
CHn2z	2.23	1

3.2.1.5 Analyses of Measurements

Data obtained for saturated bulk densities will be subjected to the statistical analyses discussed in Section 3.5.

3.2.2 Dry Bulk Density

3.2.2.1 Technical Procedures

Appropriate planning documents and Technical Procedures (TPs) (Table 3.2-3) will be prepared for each experiment. The planning documents and TPs will be issued before data are collected for dry bulk density.

One of the TPs listed below involves oven drying of the samples. As discussed in Section 2.2.5.1.2, two of the thermal/mechanical units (CHn1z and CHn2z) contain significant quantities of zeolites. Analysis indicates that the dry bulk density of zeolitic samples (determined using oven drying) will be systematically low; the magnitude of the error will depend on the duration and temperature of heating and on the quantity and type of zeolites in the sample. A method has not been identified with which the systematic error can be avoided. Therefore, dry bulk density will not be determined experimentally for rocks in which zeolites are an important mineral (volume fractions greater than 0.1). Instead, estimates of dry bulk density will be obtained by calculation using experimental values of grain density and saturated bulk density in the following equation:

$$\rho_{db} = \frac{\rho_g(\rho_{sb} - 1)}{\rho_g - 1} \quad (2.2-5)$$

Table 3.2-3
Technical Procedures* for Measurement of Dry Bulk Density

TP-057	Procedure for laboratory bulk density measurements
TP-065	Procedure for drying geologic core samples to constant weight (completed)

*Technical procedures for this work will be standard procedures and will incorporate relevant portions of nationally recognized procedures.

3.2.2.2 Accuracy and Precision

Previous determinations of density by SNL for the Yucca Mountain Site Characterization Project included calibration checks using magnesium and steel. The density of the standard material was required to be within ± 1 percent of the "true" value before the density of rock samples was determined. Thus values of dry bulk density are expected to be accurate to within ± 1 percent of the experimental value. The accuracy of values calculated for zeolitic samples will be evaluated after the accuracy of experimentally determined grain densities for such samples are determined.

The precision of determinations of dry bulk density has not been evaluated. Future measurements will include such an evaluation.

3.2.2.3 Range of Expected Results

The range of expected values for the dry bulk density of the thermal/mechanical units is given in Table 3.2-4. The ranges have been calculated as $\bar{X} \pm 2S$, where \bar{X} and S are based on existing data.

The values given in Table 3.2-4 for Units CHn1z and CHn2z are based on data obtained using an experimental technique that includes oven drying. Thus, as stated earlier, the dry bulk densities of these units probably are systematically low by an unknown amount.

Table 3.2-4
Ranges in Expected Values of Dry Bulk Density

Unit	Range (10³kg/m³)	Existing Measurements
TCw	2.02-2.45	18
PTn	0.58-2.04	2
TSw1	1.97-2.39	48
TSw2	2.12-2.41	87
Altered TSw3	No Data	0
TSw3	2.23-2.37	10
CHn1v	1.07-1.93	13
CHn1z	1.41-1.83	39
CHn2v	1.41-1.75	2
CHn2z	2.00	1

3.2.2.4 Equipment and Design Requirements

Dry bulk densities will be determined using the same samples used for determination of saturated bulk densities. After a saturated bulk density is determined, each non-zeolitic sample will be oven-dried to constant weight. This weight then will be combined with the sample volume determined during the measurements for saturated bulk density to provide the dry bulk density.

The only additional equipment required for the determination of dry bulk density of non-zeolitic samples is an oven capable of long-term operation at $105^{\circ} \pm 5^{\circ}\text{C}$.

3.2.2.5 Analyses of Measurements

Data obtained for dry bulk densities will be subjected to the statistical analyses discussed in Section 3.5.

3.2.3 Grain Density

3.2.3.1 Technical Procedures

Appropriate planning documents and Technical Procedures (TPs) (Table 3.2-5) will be prepared for each experiment. The planning documents and TPs will be issued before data are collected for grain density.

Table 3.2-5
Technical Procedures* for Measurement of Grain Density

TP-065	Procedure for drying geologic core samples to constant weight (completed)
TBA	Procedure for determination of grain density of non-zeolitic samples
TBA	Procedure for determination of grain density of zeolitic samples

*Technical procedures for this work will be standard procedures and will incorporate relevant portions of nationally recognized procedures.

TBA: Procedure number to be assigned in the future.

The measurement technique used in previous determinations of grain density for the Yucca Mountain Site Characterization Project uses oven drying of powders as an integral part of the procedure. Nationally recognized standard techniques (e.g., ASTM D-854) recommend such drying as well. However, as mentioned in Section 3.2.2.1, drying of samples containing significant quantities of zeolites also is likely to remove water from the zeolites. Thus the grain densities of zeolitic samples are likely to be systematically too high if conventional measurement techniques are used. The magnitude of the error will depend on the intensity and duration of the heating and on the quantity of zeolites in a sample.

Alternative procedures are being evaluated for determination of the grain density of zeolitic samples, as discussed in Section 2.2.5.1.3. The validity of these approaches will be examined during development of the relevant TP. All other aspects of conventional determinations of grain density will remain unchanged.

3.2.3.2 Accuracy and Precision

Previous determinations of grain density by SNL for the Yucca Mountain Site Characterization Project included calibration checks using powdered quartz. The density of the standard material was required to be within ± 1 percent of the "true" value before the grain density of rock samples was determined. Thus, experimental values of grain density are expected to be accurate to within ± 1 percent of the value. The accuracy of values calculated for zeolitic samples will be evaluated after the appropriate experimental data are obtained.

The precision of determinations of grain density has not been evaluated. ASTM D-854 states that single-operator precision in the determination of the specific gravity of cohesionless soils has been found to be 0.021 (water-pycnometer method). If this literature value pertains to tuff samples, the precision of mean values for grain density would range between 0.8 percent (Unit TSw2) and 0.9 percent (Unit CHn1v).

3.2.3.3 Range of Expected Results

The range of expected values for the grain density of the thermal/mechanical units is given in Table 3.2-6. The ranges have been calculated as $\bar{X} \pm 2S$, where \bar{X} and S are based on existing data.

Table 3.2-6
Ranges in Expected Values of Grain Density

Unit	Range (10^3 kg/m^3)	Number of Existing Measurements
TCw	2.43-2.59	24
PTn	2.07-2.67	6
TSw1	2.45-2.62	44
TSw2	2.48-2.62	76
Altered TSw3	No Data	0
TSw3	2.35-2.41	14
CHn1v	2.24-2.44	18
CHn1z	2.29-2.53	42
CHn2v	2.41-2.59	3
CHn2z	2.30-2.78	5

The ranges given in Table 3.2-6 for Units CHn1z and CHn2z are based on data obtained using oven drying as part of the measurement technique. As described earlier, a systematic error probably was introduced into the data because of this procedure. Thus the bounds of the ranges for these two units are probably too high.

3.2.3.4 Equipment and Design Requirements

The equipment required for grain-density determinations includes grinding and sieving equipment, calibrated pycnometers, a balance capable of determining masses to 0.001 g, a temperature-measuring device accurate to $\leq 1^\circ\text{C}$, a device for measuring relative humidities up to approximately 90 percent, and an oven capable of long-term operation at 105°C without significant temperature change. Material for grain-density

determinations will be powders obtained by grinding and sieving of the samples used for bulk-density determinations.

3.2.3.5 Analyses of Measurements

Data obtained for grain densities will be subjected to the statistical analyses discussed in Section 3.5.

3.2.4 Matrix Porosity

3.2.4.1 Technical Procedures

Appropriate planning documents and TPs will be issued before the density data are collected that will be used to calculate values for matrix porosity and before any direct measurements of matrix porosity are made. The methods and equations to be used in the calculation or measurement of matrix-porosity values will be defined in these documents.

3.2.4.2 Accuracy and Precision

Because most of the values for matrix porosity will be calculated, the accuracy and precision of matrix porosity usually will be a function of the accuracies and precisions of the densities used in the calculations. In addition, because the calculated values of matrix porosity depend on more than one other property, the accuracy and precision of calculated matrix porosities are a function of the values of these other properties. Thus, no exact values can be given for the accuracy and precision of calculated matrix porosity until density data are obtained.

Although both Lewis and Tandanand (1974) and ISRM (1979) discuss direct measurement of matrix porosity by means of helium displacement, neither reference presents any information on accuracy and precision. Thus, such information will need to be obtained as part of the measurement program.

An estimated uncertainty in a calculated mean value for matrix porosity of each thermal/mechanical unit can be made using existing data for dry bulk density and grain density. Assuming that the mean values for the densities are equivalent to the "true" mean values, and that the existing standard deviations are representative of the precisions of the density values, the mean values of matrix porosity should be definable with an uncertainty (quasi-precision) of approximately 0.01.

3.2.4.3 Range of Expected Results

The range of expected values for the matrix porosity of the thermal/mechanical units is given in Table 3.2-7. The ranges have been calculated as $\bar{X} \pm 2S$, where \bar{X} and S are based on existing data.

Table 3.2-7
Ranges in Expected Values of Matrix Porosity

Unit	Range	Number of Existing Measurements
TCw	0.03-0.19	18
PTn	0.15-0.75	2
TSw1	0.07-0.22	41
TSw2	0.07-0.17	70
Altered TSw3	No Data	0
TSw3	0.01-0.07	10
CHn1v	0.18-0.54	13
CHn1z	0.25-0.41	35
CHn2v	0.30-0.44	2
CHn2z	0.24	1

The ranges given above for Units CHn1z and CHn2z are based on existing matrix-porosity values that have been calculated using data for grain density and dry bulk density that were gathered using oven drying as part of the measurement techniques. As described in Sections 3.2.2.1 and 3.2.3.1, the density data for zeolitic samples probably suffer from systematic errors. Combination of these errors in calculating the matrix porosities of zeolitic samples leads to systematically high values of matrix porosity. The magnitude of the error has yet to be quantified, but the values given above for these two units are probably too high.

3.2.4.4 Equipment and Design Requirements

No equipment is needed for the calculation of matrix porosity. For measurement of matrix porosity, equipment requirements include calibrated pycnometers, a balance capable of determining masses to 0.001 g, a temperature-measuring device accurate to $\leq 1^\circ\text{C}$, a device for measuring relative humidities up to approximately 90 percent, and an oven capable of long-term operation at 105°C without significant temperature change. Material for matrix-porosity determinations will be the same samples on which bulk densities are determined.

3.2.4.5 Analyses of Measurements

Data obtained for matrix porosities will be subjected to the statistical analyses discussed in Section 3.5.

3.2.5 In Situ Bulk Density

3.2.5.1 Technical Procedures

No planning documents or TPs are required for obtaining data on the in situ bulk densities of the different thermal/mechanical units. Data obtained in this study for grain density and matrix porosity will be combined with data from other studies for lithophysal-cavity abundance, in situ saturation, and possibly fracture porosity to calculate in situ bulk density. The calculations will be performed as a part of the data-analysis activities, the culmination of which will be data on in situ bulk densities that will satisfy the requirements of repository design and performance assessment.

3.2.5.2 Accuracy and Precision

Because the values for in situ bulk density will be calculated, the accuracy and precision of in situ bulk density will be a function of the accuracies and precisions of the properties used in the calculations. In addition, because the values of in situ bulk density depend on more than one other property, the accuracy and precision of the bulk densities are a function of the values of these other properties. Thus, no exact values can be calculated for the accuracy and precision of in situ bulk density.

3.2.5.3 Range of Expected Results

The range of expected values for the in situ bulk density of the thermal/mechanical units is given in Table 3.2-8. The ranges have been calculated as $\bar{X} \pm 2S$, where \bar{X} and S are based on existing data. Both \bar{X} and S have been estimated using existing mean values and standard deviation for grain density, matrix porosity, lithophysal cavity abundance, and in situ saturation. The assumption was made, consistent with past practice, that because of the distribution of water content in partially saturated geologic media, the lithophysal cavities are entirely dry.

No data are available with which a mean value and a standard deviation can be estimated for the lithophysal-cavity abundance in Unit TCw. No cavity volume was included in calculating the in situ bulk density of this unit even though cavities are present in situ, so the range given above for Unit TCw

Table 3.2-8
Ranges in Expected Values of In Situ Bulk Density

Unit	Range ^a (10 ³ kg/m ³)	Approximate Range from Geophysical Logs of USW G-4 ^b
TCw	2.14-2.48	1.3-2.4
PTn	1.01-2.15	No Data
TSw1	1.81-2.51	1.8-2.4
TSw2	2.16-2.47	1.2-2.4
Altered TSw3	No Data	No Data
TSw3	2.27-2.38	~2.3
CHn1v	1.56-2.10	1.8-2.3
CHn1z	1.71-2.01	1.5-2.2
CHn2v	1.78-2.04	Absent
CHn2z	1.85-2.28	2.0-2.2

^aCalculated from laboratory data on grain density and porosity and estimated values of lithophysal porosity and in situ saturation.

^bThe values given here are estimated from Spengler and Chornack (1984). Data from rugose portions of core hole have not been included.

probably is too high. If the cavity contents of Units TSw1 and TSw2 were averaged and then used as representative data for Unit TCw, the range would be 1.87×10^3 to 2.60×10^3 kg/m³. The upper end of this tentative range is physically unreasonable; it is the result of the large standard deviation estimated for the lithophysal-cavity abundance.

No values were available for standard deviations of in situ saturation for Units CHn1v and CHn2v. A value of 0.06 was assumed based on values provided in Montazer and Wilson (1984) for the zeolitized equivalents of these units. Neither the validity of the assumption nor the effect on the estimated ranges of in situ bulk density can be evaluated at this time.

Fracture porosity has not been included in the estimated values of in situ bulk density because such porosities are assumed to be negligible. If site-characterization data should indicate that this assumption is wrong, the in situ bulk densities for the units with significant fracture porosity will be lower than the values given above.

3.2.5.4 Equipment and Design Requirements

No equipment is required for the determination of in situ bulk density because all values are to be calculated from other data.

3.2.5.5 Analyses of Measurements

Data obtained for in situ bulk densities will be subjected to the statistical analyses discussed in Section 3.5.

3.3 Heat Capacity

As discussed in Section 2.2.5.2, in situ heat capacity of the tuffs will be calculated from data on the heat capacities of components (solid, liquid, and air), the matrix porosity, lithophysal-cavity abundance, and in situ saturation data. Of these, only the heat capacity of the solid components will actually be determined as a part of this study. The following subsections first address these determinations, then a discussion of applications to the calculation of in situ heat capacities is provided.

3.3.1 Technical Procedures

Appropriate planning documents and Technical Procedures (TPs) (Table 3.3-1) will be prepared for each experiment. The planning documents and TPs will be issued before data are collected for heat capacity.

3.3.2 Accuracy and Precision

Because no heat-capacity experiments have been performed on tuff samples for the Yucca Mountain Site Characterization Project, no data are available with which to assess accuracy and precision. Accuracy will be evaluated using several materials that have accepted values of specific heat. Precision will be obtained by replicate measurements on selected samples from each thermal/mechanical unit. Conceivably, both accuracy and precision could be functions of temperature. This possibility also will be evaluated during the measurements.

Neither accuracy nor precision has been assessed for the method using calculations from bulk chemistry.

Table 3.3-1

Technical Procedures* for Measurement of Heat Capacity of Solid Components

TP-061	Procedure for laboratory sample bulk chemistry determination (completed)
TP-065	Procedure for drying geologic core samples to constant weight (completed)
TP-204	Procedure for measurement of specific heat of geologic samples by adiabatic pulse calorimetry
TBA	Procedure for preparation of zeolitic samples
TBA	Procedure for determination of volatile content by thermogravimetric analysis
TBA	Procedure for determination of heat capacity from bulk chemical analyses

*Technical procedures for this work will be standard procedures and will incorporate relevant portions of nationally recognized procedures.

TBA: Procedure number to be assigned in the future.

3.3.3 Range of Expected Results

Only rough estimates can be made of expected results of specific heat measurements. For devitrified Units (TCw, TSw1, TSw2), values of the heat capacities of solid components estimated from bulk chemical analyses range from 0.8×10^3 to 1.1×10^3 J/kg-K for temperatures ranging from 25° to 327°C (Nimick and Schwartz, 1987). Similar estimates for vitric units (PTn, TSw3, CHn1v, CHn2v) range from 0.8×10^3 to 1.2×10^3 J/kg-K for the same range in temperatures (Nimick and Schwartz, 1987). These values may not be inclusive of the entire range for vitric tuffs because of the potential for relatively large variations in the water content of the glasses in the different vitric units.

Estimates of the specific heat of the solid components of zeolitic tuff (Units CHn1z and CHn2z) using bulk chemistry is more difficult because of the high water content in the zeolites and the uncertainty as to how to treat the water thermodynamically. The estimated range allowing for the possibility that either one of the likely thermodynamic models is correct is 0.9×10^3 to 1.4×10^3 J/kg-K for the temperature range of 25° to 327°C.

3.3.4 Equipment and Design Requirements

Equipment needs include an adiabatic calorimeter, an oven capable of long-term operation at 85° to 105°C, a balance accurate to 0.01 g, and a thermogravimetric analyzer operable to 300°C. This last piece of equipment will allow the results of adiabatic calorimetry for zeolitic samples to be corrected for weight losses experienced during heating of samples. In addition, equipment suitable for a given method of chemical analysis will need to be available if the calculational method is selected.

3.3.5 Analyses of Measurements

Data obtained for the heat capacities of solid components will be subjected to the statistical analyses discussed in Section 3.5.

Once the heat capacities of the solid components have been obtained, in situ heat capacities must be estimated. Equation 2.2-8 will be used for the estimation, together with data on lithophysal-cavity abundance, in situ saturation, and fracture porosity.

Estimates have been made of expected values of in situ heat capacities. Table 3.3-2 summarizes the estimated ranges. These ranges do not include the contribution from fracture porosity because existing data on such porosity are insufficient. Site-characterization data on fracture porosity will be included in future estimates of in situ heat capacities; in situ values for units with significant fracture porosity will be lower than the values given above.

Data obtained for in situ heat capacities will be subjected to the statistical analyses discussed in Section 3.5.

3.4 Thermal Conductivity

As discussed in Section 2.2.5.3, thermal conductivity of the tuffs will be calculated from data on the thermal conductivities of components (solid, liquid, and air), the matrix porosity, lithophysal-cavity abundance, and in situ saturation data. Of these, only the thermal conductivity of the solid components will actually be determined as a part of this study. The following subsections first address these determinations, then a discussion of applications to the calculation of in situ thermal conductivities is provided.

Table 3.3-2
Estimated Ranges in the Values of In Situ Heat Capacity

Unit	Range (10^3 J/kg-K)	Temperature Interval °C
TCw	0.8-0.9	25-99
PTn	0.9-1.1	25-99
TSw1	0.8-0.9	25-99
	0.9-1.0	101-250
TSw2	0.8-0.9	25-99
	0.9-1.1	101-327
Altered TSw3	No Data	25-250
TSw3	0.8-1.0	25-99
	1.0-1.2	101-250
CHn1v	0.9-1.1	25-99
	1.0-1.2	101-200
CHn1z	1.0-1.1	25-99
	1.0-1.1	101-200
CHn2v	0.9-1.1	25-99
CHn2z	1.0-1.1	25-99

Note: Estimates obtained by using data for heat capacities of solid components, water and air as a function of temperature; assuming mean values of matrix porosity, lithophysal-cavity abundance, and saturation; and assuming that all pore water was removed at 100°C.

3.4.1 Technical Procedures

Appropriate planning documents and Technical Procedures (TPs) (Table 3.4-1) will be prepared for each experiment. The planning documents and TPs will be issued before data are collected for thermal conductivity.

3.4.2 Accuracy and Precision

The three experiment techniques to measure thermal conductivity are described in Section 2.2.5.3.1. Most of the techniques by which thermal conductivity can be measured are capable of determining values with accuracies of ± 10 percent or better (Laubitz, 1969; McElroy and Moore, 1969; Pratt, 1969); careful control of the experiment may reduce this to ± 5 percent. The three selected techniques all are expected to be capable of providing data within these limits. However, the accuracies that will be determined for the thermal

Table 3.4-1
Technical Procedures* for Measurement of Thermal Conductivity

TP-064	Procedure for vacuum saturation of geologic core samples (completed)
TP-065	Procedure for drying geologic core samples to constant weight (completed)
TP-202	Procedure for measurement of thermal conductivity of geologic samples by the guarded-heat-flow-meter method (completed)
TP-205	Procedure for measurement of thermal conductivity of geologic samples by the guarded-hot-plate method
TP-206	Procedure for measurement of thermal conductivity of geologic samples by the comparative method (completed)

*Technical procedures for this work will be standard procedures and will incorporate relevant portions of nationally recognized procedures.

conductivities of the solid components will be worse than ± 5 percent because of the need to extrapolate from the measured data.

3.4.3 Range of Expected Results

The thermal conductivities of the solid components of the tuffs will be governed by the thermal conductivities of the major mineral constituents. The following are rough estimates of the expected ranges (at ambient temperature) for the major lithologic types occurring at Yucca Mountain (based on data in Lappin and Nimick, 1985):

Devitrified (Units TCw, TSw1, TSw2):	2.7-3.6 W/m-K (15 samples)
Vitric (Units PTn, TSw3, CHn1v, CHn2v):	1.2-1.7 W/m-K (10 samples)
Zeolitized (Units CHn1z, CHn2z)	1.2-1.7 W/m-K (10 samples).

No temperature dependence has been observed for the thermal conductivities of solid components.

Some samples of Units TCw, PTn, TSw1, and TSw2 may be obtained from rubble in the main accesses and the associated main drifts if sufficient core is not available. It is possible that mining may induce enough microfracturing in this rubble to reduce the apparent thermal conductivities of the solid components below those determined for core samples. This possibility will be evaluated by comparing thermal conductivity values for rubble samples with values measured on core samples. If a significant difference in thermal conductivity is found, data for rubble samples will not be used in analyses.

3.4.4 Equipment and Design Requirements

The equipment required to perform measurements of thermal conductivity include testing apparatus appropriate to the testing techniques described in Section 2.2.5.3.1, an apparatus for vacuum-saturation of samples, length-measuring devices, a balance capable of determining masses to 0.001 g, and an oven capable of long-term operation at 105°C without significant temperature change. Material for thermal-conductivity measurements will be cylinders of different dimensions, depending on which technique is used (see Section 2.2.5.3.1).

3.4.5 Analyses of Measurements

Data obtained for the thermal conductivities of solid components will be subjected to the statistical analyses discussed in Section 3.5.

Once the thermal conductivity of a tuff sample has been measured, the value must be extrapolated to a zero-porosity value using information about the porosity (including matrix porosity and lithophysal-cavity abundance), and potentially the saturation state. Many empirical correlations between thermal conductivity and porosity have been proposed. Eleven of the correlations were compared by Robertson and Peck (1974) using data from samples of basalt. Several of the correlations were found to provide reasonable fits to the experimental data. However, no claim was made that the same correlations could be used successfully for other rock types.

One of the first steps in this study will be to evaluate the alternative correlations for use with tuff samples. In the past, a geometric-mean correlation has been used for analysis of thermal-conductivity data. This correlation is satisfactory for water-saturated rocks, but may give erroneous results when used for dry materials. Thus there is a need for evaluation of the alternative correlations, which are tabulated in Table 3.4-2.

Table 3.4-2. Empirical Correlations Between Thermal Conductivity and Porosity

Correlation	Equation	Reference
Nomenclature: K_c = thermal conductivity of composite (porous) material K_s = thermal conductivity of solid material K_f = thermal conductivity of fluid in pores K_w = thermal conductivity of water		
Two-Phase (Solid + Pores)	$K_c = (1-\phi)K_s + \phi K_f$	
Parallel	$K_c = (1-\phi)K_s + \phi K_f$	(P) Woodside and Messmer (1961)
Series	$\frac{1}{K_c} = \frac{(1-\phi)}{K_s} + \frac{\phi}{K_f}$	(P) Woodside and Messmer (1961)
Mixed Parallel-Series	$K_c = \frac{1}{2} \left[(1-\phi)K_s + \phi K_f + \frac{K_f K_s}{(1-\phi)K_f + \phi K_s} \right]$	(P) Robertson and Peck (1974)
Geometric Mean	$K_c = K_s^{(1-\phi)} K_f^\phi$	(P) Woodside and Messmer (1961)
Rayleigh	$K_c = K_f \left[1 - \frac{3(1-\phi)}{2 + \frac{K_s}{K_f} + (1-\phi) + 0.525(1-\phi)^{10/3} \left(\frac{K_s - 1}{K_f} + \frac{1}{K_f + 1} \right)} \right]$	(P) Rayleigh (1982)
	NA	
	Three-Phase (Solid + Partially-Saturated Pores)	
	$K_c = (1-\phi)K_s + \phi[(1-S)K_s + SK_w]$	(P) Woodside and Messmer (1961)
	$\frac{1}{K_c} = \frac{(1-\phi)}{K_s} + \phi \left[\frac{(1-S)}{K_s} + \frac{S}{K_w} \right]$	(P) Woodside and Messmer (1961)
	$K_c = \frac{1}{2} \left[(1-\phi)K_s + \phi(1-S)K_s + \phi SK_w + \frac{K_s K_w}{(1-\phi)K_s K_w + (1-S)K_s K_w + \phi SK_s K_s} \right]$	(P) Robertson and Peck (1974)
	$K_c = K_s^{(1-\phi)} K_w^{S\phi} K_s^{\phi(1-S)}$	(P) Woodside and Messmer (1961)

K_a = thermal conductivity of air
 K_{vac} = thermal conductivity of porous solid with pores evacuated
 ϕ = porosity, expressed as a volume fraction
 S = saturation, expressed as a volume fraction

Table 3.4-2. Empirical Correlations Between Thermal Conductivity and Porosity (Continued)

Correlation	Two-Phase (Solid + Pores)	Three-Phase (Solid + Partially Saturated Pores)	Reference ¹
Eucken	$K_c = K_s \left[\frac{1-\phi}{1+\frac{\phi}{2}} \right]$	NA	(S) Dell'Amico et al. (1967)
Brailsford & Major #1	$K_c = \frac{1}{4} \left\{ (3\phi - 1)K_f + (2 - 3\phi)K_s \right. \\ \left. \pm \left[\left[(3\phi - 1)K_f + (2 - 3\phi)K_s \right]^2 + 8K_f K_s \right]^{1/2} \right\}$	NA	(P) Brailsford and Major (1964)
Brailsford & Major #2	NA	$K_c = \frac{(1-\phi)K_s + \phi SK_w \left(\frac{3K_s}{2K_s + K_w} \right) + \phi(1-S)K_a \left(\frac{3K_s}{2K_s + K_a} \right)}{(1-\phi) + \phi S \left(\frac{3K_s}{2K_s + K_w} \right) + \phi(1-S) \left(\frac{3K_s}{2K_s + K_a} \right)}$	(P) Brailsford and Major (1964)
Wyllie & Southwick	$K_c = \frac{(1.03 - \phi)K_s K_f}{\left(\frac{0.03}{1.03 - \phi} \right) K_s + \left(\frac{1 - \phi}{1.03 - \phi} \right) K_f} \\ + K_{vac} + (\phi - 0.03)K_f$	NA	(S) Woodside and Messmer (1961)
Asaad	$K_c = K_s^{(1-c\phi)} + K_f^{c\phi}$ (c = 1 is a fitting parameter)	NA	(S) Woodside and Messmer (1961)

Table 3.4-2. Empirical Correlations Between Thermal Conductivity and Porosity (Continued)

Correlation	Two-Phase (Solid + Pores)	Three-Phase (Solid + Partially Saturated Pores)	Reference ¹
Ribaud	$K_c = K_f \phi^{1/3} + K_s (1 - \phi^{2/3})$	NA	(S) Sugawara and Yoshizawa (1961)
Russell	$K_c = K_s \left[\frac{\phi^{2/3} + \frac{K_s}{K_f} (1 - \phi^{2/3})}{\phi^{2/3} - \phi + \frac{K_s}{K_f} (1 - \phi^{2/3} + \phi)} \right]$	NA	(S) Sugawara and Yoshizawa (1961)
Maxwell, solid-continuous	$K_c = K_s \left[\frac{K_f (1 + 2\phi) + 2K_s (1 - \phi)}{K_f (1 - \phi) + K_s (2 + \phi)} \right]$	NA	(S) Woodside and Messmer (1961)
Maxwell, fluid-continuous	$K_c = K_f \left[\frac{2\phi K_f + (3 - 2\phi) K_s}{(3 - \phi) + K_f + \phi K_s} \right]$	NA	(S) Woodside and Messmer (1961)
Sibbit, Dodson & Tester	$K_c = K_s \left[\frac{1 - 2\phi \left(\frac{K_s - K_f}{2K_s + K_f} \right)}{1 + \phi \left(\frac{K_s - K_f}{2K_s + K_f} \right)} \right]$	$K_c = K_s \left[\frac{1 - 2\phi S \left(\frac{K_g - K_w}{2K_g + K_w} \right) - 2\phi(1-S) \left(\frac{K_g - K_a}{2K_g + K_a} \right)}{1 + \phi S \left(\frac{K_g - K_w}{2K_g + K_w} \right) + \phi(1-S) \left(\frac{K_g - K_a}{2K_g + K_a} \right)} \right]$	(P) Sibbit et al. (1979)
Sugara & Yoshizawa	$K_c = K_s + (K_f - K_s) \left[\frac{2^n}{2^n - 1} \left(1 - \frac{1}{(1 + \phi)^n} \right) \right]$ (n > 0 is a fitting parameter)	NA	(P) Sugara and Yoshizawa (1961)

Table 3.4-2. Empirical Correlations Between Thermal Conductivity and Porosity (Concluded)

Correlation	Two-Phase (Solid + Pores)	Three-Phase (Solid + Partially Saturated Pores)	Reference ¹
Quadratic-Parallel	$K_c^{1/2} = (1-\phi)K_s^{1/2} + \phi K_f^{1/2}$	$K_c^{1/2} = (1-\phi)K_s^{1/2} + \phi SK_w^{1/2} + \phi(1-S)K_g^{1/2}$	(P)Robertson and Peck (1974)
Quadratic-Series	$\frac{1}{K_c^{1/2}} = \frac{(1-\phi)}{K_s^{1/2}} + \frac{\phi}{K_f^{1/2}}$	$\frac{1}{K_c^{1/2}} = \frac{(1-\phi)}{K_s^{1/2}} + \frac{\phi}{K_w^{1/2}} + \frac{\phi(1-S)}{K_g^{1/2}}$	(P)Robertson and Peck (1974)
Mixed Quadratic	$K_c = \frac{1}{2} \left\{ \left[(1-\phi)K_s^{1/2} + \phi K_f^{1/2} \right]^2 + \left[\frac{K_s^{1/2} K_f^{1/2}}{(1-\phi)K_f^{1/2} + \phi K_s^{1/2}} \right]^2 \right\}$	$K_c = \frac{1}{2} \left\{ \left[(1-\phi)K_s^{1/2} + \phi SK_w^{1/2} + \phi(1-S)K_g^{1/2} \right]^2 + \left[\frac{K_s^{1/2} K_w^{1/2} K_g^{1/2}}{(1-\phi)K_w^{1/2} K_g^{1/2} + \phi SK_g^{1/2} K_s^{1/2} + \phi(1-S)K_w^{1/2} K_g^{1/2}} \right]^2 \right\}$	(P)Robertson and Peck (1974)
Mixed Maxwell	$K_c = \frac{1}{2} \left\{ K_s \left[\frac{K_f(1+2\phi+2K_s(1-\phi))}{K_f(1-\phi)+K_s(2+\phi)} \right] + K_f \left[\frac{2\phi K_f(3-2\phi)K_s}{(3-\phi)K_f + \phi K_s} \right] \right\}$	NA	(P)Horai and Simons (1969)

¹P = primary reference; S = secondary source.

The constraints that must be met for a correlation to be useful are as follows:

1. A correlation equation must allow for the presence of three components (solid, water, and air), so that reliable estimates of the thermal conductivity of partially saturated tuffs may be obtained.
2. An equation must be applicable over a wide range of porosities (potentially 0.01 to 0.50).
3. An equation must be applicable over the entire range of potential saturation states (0.0 to 1.0).
4. Extrapolation from a measured thermal conductivity using an equation must provide a reasonable value as an estimate of the zero-porosity thermal conductivity.

Only rough estimates can be made of expected ranges for in situ thermal conductivities. The ranges (estimated for a temperature of 25°C) are given in Table 3.4-3. These ranges do not include the contribution from fracture porosity because existing data on such porosity are insufficient. Site-characterization data on fracture porosity will be included in future estimates of in situ thermal conductivities; the in situ values for the units with significant fracture porosity will be lower than the values given above.

Data obtained for in situ thermal conductivities also will be subjected to the statistical analyses discussed in Section 3.5.

3.5 Analysis of Results

Results of experiments performed for this study will be analyzed using several statistical techniques. The general sequence of steps for each property will be as follows:

1. Examine the spatial correlation [(as a function of depth, of distance from the point of origin (e.g., ground surface, collar of core hole, etc.) or of location within a unit] using geostatistical techniques and analyses thereof.
2. Examine the statistical distribution of data gathered at a specific location (i.e., core hole, lateral drift, etc.) for each unit.
3. Calculate parameters appropriate to the statistical distribution of the data from each location for each unit, or of subgroups of data identified at a single location within each unit.

Table 3.4-3
Expected Ranges in the Values of In Situ
Thermal Conductivity

Unit	Range (W/m-K)
TCw	1.4-1.8
PTn	0.5-0.7
TSw1	1.3-1.7
TSw2	1.5-1.9
Altered TSw3	No Data
TSw3	1.0-1.4
CHn1v	0.7-0.9
CHn1z	1.0-1.1
CHn2v	0.7-0.9
CHn2z	1.0-1.1

Note: These ranges have been estimated by assuming mean values for matrix porosity, lithophysal-cavity abundance, and saturation; using the range in thermal conductivities of solid components given in Section 3.4.3; and calculating in situ thermal conductivity using the average of the parallel and series empirical models. (See Table 3.4-2 for definition of these models.)

4. To the extent possible, use analysis-of-variance techniques to evaluate the variability between locations for each unit.
5. When appropriate, perform correlation analysis of properties with each other and with spatial location for each unit.
6. Report the results of these analyses in one or more analysis reports.

Implicit in the listing above is the validity of the current definition of the thermal/mechanical units. At several times during the data-gathering process, data from adjacent units will be examined and compared to evaluate whether the division into thermal/mechanical units is appropriate. One criterion used for an evaluation will be whether the mean values of a given property for two adjacent units are statistically distinguishable at a 95 percent confidence level. Other criteria may be used as well.

The analyses outlined above will be performed on the data resulting from laboratory experiments. In addition, laboratory data will be extrapolated to values pertinent to in situ conditions. Inferences about the spatial variability of rock-mass thermal properties will be made based on the results of analysis of laboratory thermal-properties data as well as on any observed spatial variability in lithophysal-cavity abundance, fracture porosity or in situ saturation.

3.6 Quality Assurance Requirements

All work will be performed in accordance with the Sandia National Laboratories YMP quality assurance requirements. The experiments will be governed by SNL Quality Assurance Grading Report (QAGR) No. 1.2.3.2.7.1.1 which specifies applicable QA criteria.

3.7 Representativeness of Results

On the basis of the statistical considerations included in the sampling strategy (discussed in Section 2.2) and on the plans for analyses of the resulting data, experimental results for laboratory thermal properties are expected to be as representative of the site as necessary for the requirements of repository design and performance assessment.

3.8 Performance Goals and Confidence Levels

The performance goals and confidence levels established by repository design and performance assessment have been included in the design of a sampling strategy. As such, there is a reasonable assurance that the goals will be achieved with the required confidence. The variability of existing data for some of the properties in some of the thermal/mechanical units suggests that a certain number of the performance goals may not be achievable as established (e.g., high confidence that the thermal conductivity of Unit TSw2 will fall within the tolerance limits given by repository design). Should this appear to be the case as data are obtained, consultations will be held with the appropriate Project personnel to reevaluate the performance goals, the confidence levels, or both.

4.0 APPLICATION OF RESULTS

Sections 1.1.1, 1.2.1, and 1.2.2 of this document discuss the manner in which results from the laboratory thermal-properties experiments are to be applied for resolution of regulatory requirements and the Information Needs and Investigations identified by the performance-allocation process. The data from this study will be used to address or help to resolve the Issues and Investigations identified by the Yucca Mountain Site Characterization Project that are listed in Table 4.0-1. Data obtained in the laboratory for thermal properties will be used to estimate rock-mass thermal properties. The data for the rock mass then will be reviewed with respect to values obtained during in situ experiments and an evaluation of the most suitable rock-mass thermal properties will be made. These properties then will be used as input to thermal calculations that are a part of the evaluation of stability, operability, and flexibility of the underground-facility design (Issues 1.11, 2.4, 4.2, and 4.4) and of the evaluation of the waste-package environment (Issues 1.5 and 1.10).

Table 4.0-1

Issues and Investigations Addressed During the
Laboratory Thermal-Properties Study

Issue	Investigation	SCP Section
1.1	Total system performance (data requirements subsumed in Issue 1.11)	8.3.5.13
1.2	Individual protection (data requirements subsumed in Issue 1.11)	8.3.5.14
1.5	Engineered barrier system release rates (data requirements subsumed in Issue 1.10)	8.3.5.10
1.6	Ground-water travel time	8.3.5.12
1.10	Waste-package characteristics (post-closure)	8.3.4.2
1.11	Configuration of underground facilities (post-closure)	8.3.2.2
1.12	Seal characteristics	8.3.3.2
2.2	Worker radiological safety-normal conditions (data requirements subsumed in Issue 2.7)	8.3.5.4
2.4	Waste Retrieval Option (data requirements subsumed in Issue 4.4)	8.3.5.2
2.7	Repository design criteria for radiological safety	8.3.2.3
4.2	Nonradiological Health and Safety (data requirements subsumed in Issue 4.4)	8.3.2.4
4.4	Preclosure design and technical feasibility	8.3.2.5

In addition, the thermal-properties data will contribute to the definition of the disturbed zone (Issue 1.6), to determination of requirements for sealing of underground openings (Issue 1.12), and to determination of radiologic-shielding parameters that contribute to radiologic safety during the operations period (Issues 2.2 and 2.7).

4.1 Resolution of Site Programs

Results of the Laboratory Thermal-Properties Study will provide data to aid in resolving Site Program 8.3.1.15 (Thermal and Mechanical Rock Properties Program). The contribution of the study will be both direct (by determination of thermal properties) and indirect (by contributing to the results of a number of in situ experiments). Also, data from this study will be used in Study 8.3.1.4.3.2 (Three-Dimensional Model of Rock Characteristics) to establish a model of the distribution of thermal properties throughout the volume of rock within the boundary of the underground facilities.

4.2 Resolution of Performance and Design Issues

This study will contribute to the resolution of performance and design Issues by providing data on thermal properties that will be used as input to thermal, thermomechanical, and possibly thermohydrologic calculations. These calculations will in turn aid in resolving those Issues that require such calculations (e.g., 1.6, 1.10, 1.11, and 4.4).

5.0 SCHEDULE AND MILESTONES

5.1 Durations and Interrelationships of Laboratory Thermal-Properties Study Experiments

The work for this study can be divided into three major parts — preliminary scoping studies using existing core or outcrop samples, followed by site-characterization testing in two stages, first using samples from new core holes and then using samples from the ESF. It is anticipated that plans for random sampling of each thermal/mechanical unit would be developed prior to the time that coring of the new holes begins. Sampling then would begin as soon as core from the first randomly selected interval was available for sampling. Sample preparation for "bulk" property measurements are minimal, so experiments would begin very soon after samples were obtained, with thermal-conductivity and heat-capacity experiments beginning shortly thereafter. Sampling and experiments would continue until all preselected intervals had been sampled.

For sampling in the main accesses and drifts, the sequence will be very similar to that described for the new core holes. For sampling to be performed to support determinations of the possible effects of anisotropy, fractures, and lithophysal-cavity content on thermal conductivity, samples will be obtained during appropriate sampling intervals for mechanical-experiment specimens, as described in Study Plan 8.3.1.15.1.3.

5.2 Scheduling Relative to Other Studies

This study interfaces with other studies in two areas. First, data on in situ saturation, lithophysal-cavity abundance, and fracture porosity must be obtained from other Site Programs and Studies before reliable estimates of rock-mass thermal properties can be made. Second, thermal properties will be determined in the laboratory in support of a number of in situ experiments. Interpretation and analysis of these in situ experiments will depend in part on the laboratory data. Samples in support of the in situ experiments will be obtained during experiment set-up in the ESF, and laboratory data should be available before each relevant in situ experiment is completed.

This study exerts no presently identifiable constraints on other YMP studies.

5.3 Schedule and Milestones

The exact schedule for obtaining samples and conducting experiments is dependent upon the scheduling of new core holes, the construction schedule for the ESF, and the level of funding.

6.0 REFERENCES

ASTM (American Society for Testing and Materials)

The following Standard Test Methods have been cited in the text. The dates given in parentheses after the titles indicate the versions used in preparation of this document. ASTM procedures are reviewed periodically, with some reviews resulting in rewriting of one or more of the methods. The most current version will be followed for each type of experiment.

- C-128: Specific Gravity and Absorption of Fine Aggregate (1984)
- C-134: Size and Bulk Density of Refractory Brick and Insulating Firebrick (1984)
- C-135: True Specific Gravity of Refractory Materials by Water Immersion (1966; reapproved 1976)
- C-177: Steady-State Heat Flux Measurements and Thermal Transmission Properties by Means of the Guarded-Hot-Plate Apparatus (1985)
- C-351: Mean Specific Heat of Thermal Insulation (1982)
- C-604: True Specific Gravity of Refractory Materials by Gas-Comparison Pycnometer (1979)
- D-854: Specific Gravity of Soils (1983)
- D-1188: Bulk Specific Gravity and Density of Compacted Bituminous Mixtures Using Paraffin-Coated Specimens (1983)
- D-2320: Specific Gravity of Solid Pitch (Pycnometer Method) (1966; reapproved 1976)
- E-177: Use of the Terms Precision and Accuracy as Applied to Measurement of a Property of a Material (1971; reapproved 1980)
- E-1225: Thermal Conductivity of Solids By Means of The Guarded-Comparator-Longitudinal Heat Flow Technique (1988)
- F-433: Evaluating Thermal Conductivity of Gasket Materials (1977; reapproved 1982)
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