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Yucca Mountain Site Characterization Project

Summary Evaluation of Yucca Mountain Surface Transects with Implications for Downhole Sampling

S. A. McKenna, C. A. Rautman

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Summary Evaluation of Yucca Mountain Surface Transects with Implications for Downhole Sampling

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Abstract

The results of previously completed vertical outcrop sampling transects are summarized with respect to planning downhole sampling. The summary includes statistical descriptions and descriptions of the spatial variability of the sampled parameters. Descriptions are made on each individual transect, each thermal/mechanical unit and each previously defined geohydrologic unit. Correlations between parameters indicate that saturated hydraulic conductivity is not globally correlated to porosity. The correlation between porosity and saturated hydraulic conductivity is both spatially and lithologically dependent. Currently, there are not enough saturated hydraulic conductivity and sorptivity data to define relationships between these properties and porosity on a unit by unit basis. Also, the Prow Pass member of the Crater Flat Tuff and stratigraphically lower units have gone essentially unsampled in these outcrop transects. The vertical correlation length for hydrologic properties is not constant across the area of the transects. The average sample spacing within the transects ranges from 1.25 to 2.1 meters. It appears that, with the exception of the Topopah Spring member units, a comparable sample spacing will give adequate results in the downhole sampling campaign even with the nonstationarity of the vertical correlation. The properties within the thermal/mechanical units and geohydrologic units of the Topopah Spring member appear to have a spatial correlation range less than or equal to the current sample spacing within these units. For the downhole sampling, a sample spacing of less than 1.0 meters may be necessary within these units.

This work was supported by the U.S. Department of Energy under contract DE-AC04-94AL85000, WBS element 1.2.3.2.2.2.1, Work Agreement 0014. This work falls under SCP Activities 8.3.1.4.3.1.1 and 8.3.1.2.2.3.1.

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Introduction

The unsaturated zone at Yucca Mountain, Nevada (Figure 1) is being considered as the potential location of a national, high-level nuclear waste repository. Studies of the volcanic tuffs in the unsaturated zone are being pursued with the goals of characterizing the spatial variability of rock properties and determining the lithologic control on rock properties. The final result of these studies will be the development of three-dimensional rock property models for Yucca Mountain. These three-dimensional models will be used as input to hydrologic flow models, for design calculations and for performance assessment calculations.

The three-dimensional rock property models will be based on information obtained from approximately 25 boreholes drilled into the subsurface of Yucca Mountain and the surrounding area. The data obtained from the drill holes will be augmented with data obtained from outcrops on and in the vicinity of Yucca Mountain. A large amount of rock property data has already been obtained from these outcrops and this information is serving as a guide in planning the drilling operations. This report summarizes the outcrop surveys and results obtained up to May 1994 and discusses the implications for the drilling plan as derived from the outcrop (transect) studies. The scope of this report does not include analysis of horizontal transects for design of systematic sampling in the ESF.

Both stochastic and deterministic components to the distribution of rock properties have been observed during the collection of data in the surface transects. This report is a summary evaluation of surface transects with implications for down-hole sampling. A specific question which needs to be addressed is whether or not the proposed drilling plan will adequately characterize both the deterministic and stochastic components of the rock properties at the site.

Methods

Field Sampling

A total of eight outcrop sampling transects have been completed in the vicinity of the potential repository. The majority of the samples were obtained in the spring and summer of 1991, with additional sampling in 1992. One of the eight transects is composed of a series of vertical transects along a 1.4 km horizontal section in the Shardy Base microstratigraphic unit (Rautman, et al., 1993). The objective of this report is to assess the implications of the outcrop transects for drill-hole sampling. Therefore, this report will focuses on analysis of the five vertical transects shown in Figure 1.

Core samples were collected in the field from the outcrops using a portable, gasoline powered drill. The recovered samples have a diameter of 2.5 cm and range in length from 3 to 7 cm. Samples were placed into bags and given an identification number in the field.

Laboratory Methods

Porosity, bulk density and particle density were determined for all samples. These three rock properties were calculated twice for most samples using a slightly different technique each time. Initially, the samples were saturated with carbon dioxide gas. The use of this water soluble gas guards against pockets of air being trapped in the pore spaces during analyses. These samples were then dried in an oven in which the relative humidity was controlled at 45 percent and the temperature was kept at 60° C. The high humidity and low temperature, relative to traditional techniques, preserves the water present in the clays and other hydrated minerals (Bush and Jenkins, 1970). Porosity, bulk density and particle density were then calculated using volume-displacement techniques. The densities and porosities were calculated again for each sample after oven drying at 105° C (the traditional technique).

Sorptivity and saturated hydraulic conductivity were also calculated on a subset of the samples. Sorptivity is determined by allowing the samples to resaturate after drying them in the relative humidity controlled oven. The samples were weighed periodically during the rewetting. The equation $I = St^{0.5}$ (where I is imbibition, S is sorptivity and t is time in seconds) is used to calculate sorptivity (Philip, 1957). Sorptivity is determined as the slope of a line fit through the data plotted in the I, $t^{0.5}$ space (Talsma and Parlange, 1972)

Saturated hydraulic conductivity is calculated on the samples after they have been resaturated during the sorptivity tests. For these measurements, the core samples were encased in heat shrink tubing and a steady-state, constant head flow system was set up across the sample. Darcy's law was used to calculate the saturated hydraulic conductivity. By applying pressure head, it was possible to create a head differential of 60m across the samples if necessary.

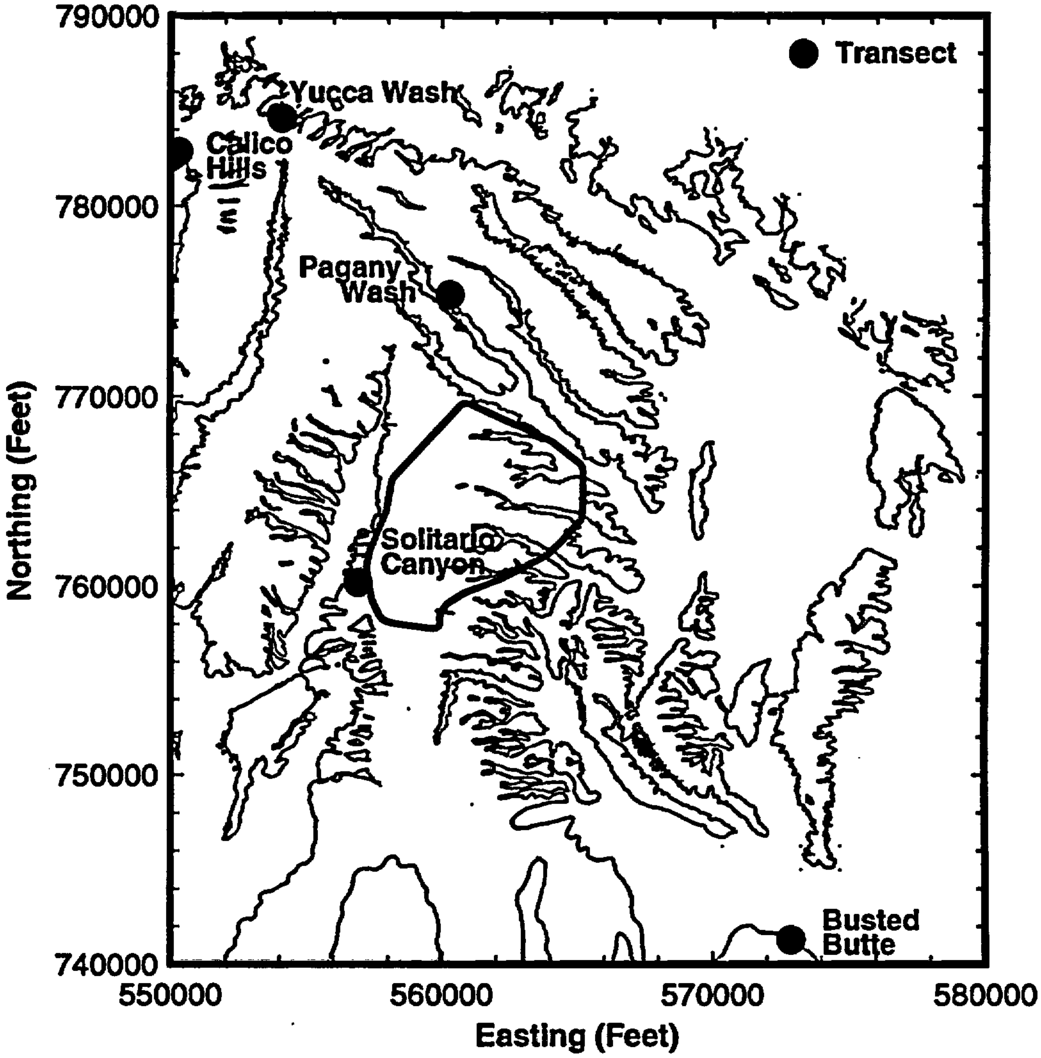

Figure 1. Map showing locations of the vertical transects and the boundary of the proposed repository (solid black line). The bedrock alluvium contact is shown for reference. Northing and Easting are in Nevada State Plane coordinates (After Flint, et al., in review).

Summary of Previous Work

The transect studies have so far been informally broken into two groups: a detailed study of the shardy base microstratigraphic unit of the Tiva Canyon Member of the Paintbrush Tuff and a second set of seven vertical and horizontal transects which cover the major lithologic units within the unsaturated zone at Yucca Mountain.

A total of 306 samples collected along 26 short, vertical transects were collected in a detailed study of the shardy base microstratigraphic unit of the Tiva Canyon Member. The horizontal range covered by these vertical transects is approximately 1.4 km in the north-south direction, and 10 to 17 samples were obtained on each vertical transect. Disposition of the core samples is given in detail in Rautman et al. (1993). The shardy base microstratigraphic unit was singled out for detailed study because it embodies the first major lithologic change below the present topography and above the repository block (Rautman, et al., pers. comm.[1]). This distinct lithologic change may have significant hydrologic impact on vertical infiltration of water. Also, the shardy base microstratigraphic unit is well exposed on the west side of Yucca Mountain. A further description of the sampling in the shardy base microstratigraphic unit is given by Rautman and others (pers. comm.).

Variography on the shardy base data is reported in Rautman and et al. (1993). The correlation lengths (variogram ranges) for porosity in the vertical direction are approximately 0.4 of the stratigraphic thickness of the unit. The vertical correlation length for saturated hydraulic conductivity is similar. In the horizontal direction, the correlation lengths for porosity and saturated hydraulic conductivity are approximately 90 meters after trend removal. For the upper ashflow subunit of the shardy base, the horizontal correlation lengths for the same properties are approximately 400 meters. The shardy base transects and the correlations between properties within the shardy base unit are not repeated here, but are summarized at the end of this report. For details on the shardy base microstratigraphic unit, the reader is referred to Istok, et al. (1994); Rautman, et al. (1993); Rautman, et al. (pers. comm.).

[1] Rautman, C.A., L.E. Flint and A.L. Flint, (in review), Physical and Hydrologic Properties of Outcrop Samples From a Nonwelded to Welded Tuff Transition, Yucca Mountain, Nevada, U.S. Geological Survey, Water Resources Investigations Report 95-4061.

Three horizontal and five vertical transects have been completed that cover the major lithologic units within the unsaturated zone at Yucca Mountain. These eight transects and the samples obtained from them are described in detail by Flint and others (pers. comm.[2]). The transect names and lithologic descriptions are given in Table 1 and the relative positions of the transects are shown on the stratigraphic column in Figure 2. The positions of the five vertical transects, which are the focus of this report, are shown in Figure 1. The Abandoned Wash transect and the Dune Wash transects as mentioned by Rautman and Flint (1992) are not in this study; these two transects were taken in a previous study on the Topopah Spring caprock.

Transect	Length (m)	Number of Samples	Lithologic Description
Solitario Canyon (vertical)	315	169	Upper cliff zone of the Tiva Canyon Member to the lower lithophysal zone of the Topopah Spring Member
Busted Butte (vertical)	135	102	Nonwelded tuff of the Topopah Spring Member to the basal vitrophyre
Yucca Wash (vertical)	290	139	Caprock of the Tiva Canyon Member through the Calico Hills
Pagany Wash (vertical)	25	20	Caprock of the Tiva Canyon Member to the upper lithophysal zone
Calico Hills (vertical)	102	66	Calico Hills to Prow Pass Member
Yucca Crest (horizontal)	5030	45	Upper cliff zone of the Tiva Canyon Member
Shardy Base (horizontal)	701	65	Nonwelded base of the Tiva Canyon Member
Topopah Spring Caprock (horizontal)	1823	50	Vitric caprock of the Topopah Spring Member

Table 1. Description of eight transects (after Flint et al., pers. comm.).

Of the eight transects in the database, three (caprock of Topopah Spring Member, Shardy Base and Yucca Crest) are horizontal transects, while the other five are vertical transects. From these eight transects, a total of 656 measurements of porosity have been obtained. The majority of these measurements were made after drying the samples in a humidity controlled oven.

[2] Flint, L.E., A.L. Flint and C.A. Rautman, (in review), Physical and Hydrologic Properties of Rock Outcrop Samples at Yucca Mountain, Nevada, U.S. Geological Survey, Open File Report 95-280.

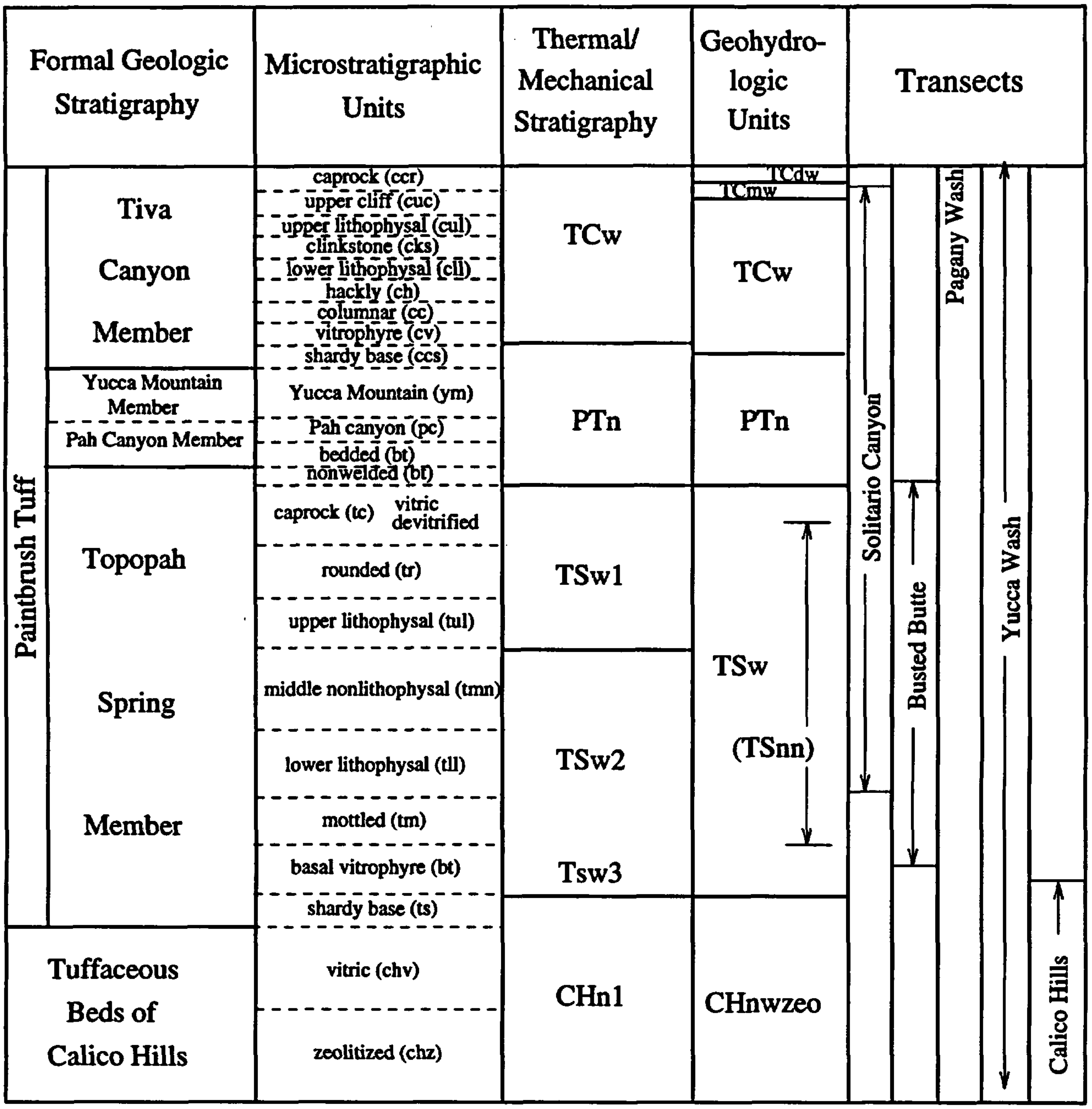

Figure 2. Conceptual stratigraphic section also showing the relative positions of the five vertical transects discussed in this report (after Rautman, et al., pers. comm. and Flint et al., pers. comm.).

Initial variography on the data collected in these eight transects is provided by Rautman and Flint (1992). Horizontal variogram ranges for porosity for the zeolitic tuffs of the Calico Hills is 900 meters. Vertical variogram ranges for porosity in the Paintbrush tuffs, vary from a low of 10 meters (for the nonwelded, PTn) to a high of 61 meters for the welded Topopah Spring units. Variogram calculation and modeling has also been previously completed by Rautman (1991) on data from a separate vertical Calico Hills transect and data from nine boreholes. Results of these calculations show a vertical range of 244 meters (800 feet) for the entire vertical transect and a vertical range of 61 meters (200 feet) for the Calico Hills nonwelded unit within the vertical transect.

Statistical Summary and Relationships

A tabulation of the available data used in this study is given in Flint, et al. (pers. comm.). Also shown in Flint, et al. (pers. comm.) are plots of porosity versus distance along the transect for each of the five vertical transects. Previous work (Rautman et al., 1993) has shown correlations between hydrologic property values and stratigraphic elevation. Other work (Flint et al., pers. comm.; Rautman et al., pers. comm.) have described correlations between several hydrologic parameters. In general, these studies have shown that many bulk and hydrologic properties can be estimated from knowledge of porosity at the same location, albeit with varying levels of accuracy. These relationships are further investigated in this report and augmented with additional relations. The subsets of the transect data allow for the data to be examined in terms of thermal/mechanical units and geohydrologic units (Figure 2). Correlations between properties specific to these units are required for the three-dimensional rock property model of Yucca Mountain. The data from the horizontal transects are not used in the regression relations presented here because of the bias these transects give to the single unit in which they were conducted

Vertical Transects

Several properties in the transect sampling are relatively sparsely sampled (i.e., saturated hydraulic conductivity and sorptivity). For these properties it may not be possible to develop relationships with other properties on a unit by unit basis for the thermal/mechanical and geohydrologic units due to the limited amounts of data. On the other hand, for properties with large amounts of data, it may be possible to define meaningful relationships between properties on a "global" basis. For these two reasons, the relationships between properties sampled on all vertical transects are examined.

The most sparsely sampled property in the vertical transects is sorptivity. A total of 48 sorptivity measurements have been made. The relationships between sorptivity and several other properties are shown in Figure 3. As can be seen in Figure 3, significant relationships between sorptivity, porosity, the log of saturated hydraulic conductivity and bulk density exist. The results of the regression calculations shown in Figure 3 are exhibited in Table 2.

X Variable	Y Variable	n	Regression Equation	R^2
Porosity (%)	Log Sorptivity	48	$Y= 5.00x10^{-4}X^2 +7.60x10^{-2} X - 6.136$	0.869
Log K_{sat}	Log Sorptivity	48	$Y = 2.78x10^{-1}X - 2.412$	0.732
Bulk Density	Log Sorptivity	48	$Y = -1.734X - 1.560$	0.816

Table 2. Results of regression calculations between log sorptivity and other properties.

The next most sparsely sampled property in the vertical transects is saturated hydraulic conductivity. A total of 162 saturated hydraulic conductivity measurements are available from the vertical transects. Several regression relationships between saturated hydraulic conductivity and porosity have been developed previously (Flint, et al., pers. comm). These relationships were developed from the data available on two separate transects: Yucca Wash and Solitario Canyon. Flint et al. (pers. comm.) found that the relationship between porosity and saturated hydraulic conductivity in the two transects was stronger for subsets of the transect relative to the transect as a whole. In general, vitric samples exhibit a weaker relationship between these two properties, due to microfracturing, than do welded and non-welded samples. Zeolitized samples from the Calico Hills unit also demonstrate a weak relationship between porosity and saturated hydraulic conductivity due to the development of zeolites in the pore spaces (Flint, et al., pers. comm.).

In this study, the relationship between saturated hydraulic conductivity and bulk density and porosity is initially investigated on data obtained from all vertical transects. These relationships are shown in Figure 4, and the results of calculating regression equations between the parameters are displayed in Table 3. It is noted that the

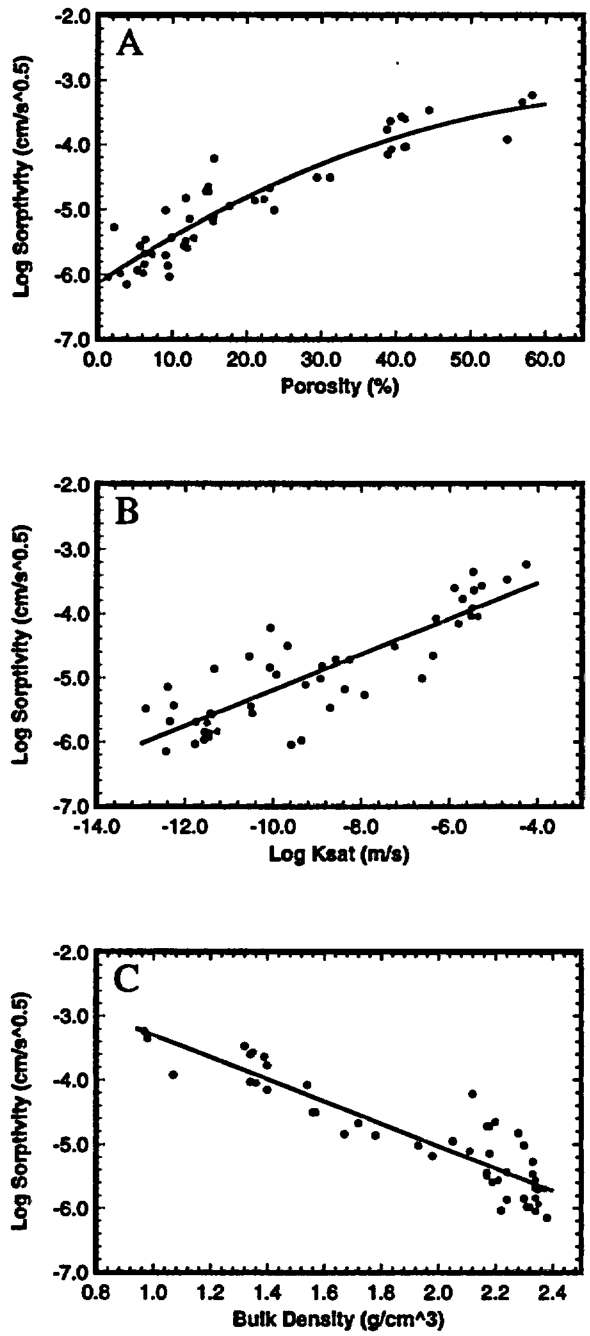

Figure 3. Plots of correlations between log sorptivity and other properties on the vertical transect data. The equations for the regression lines are given in Table 2.

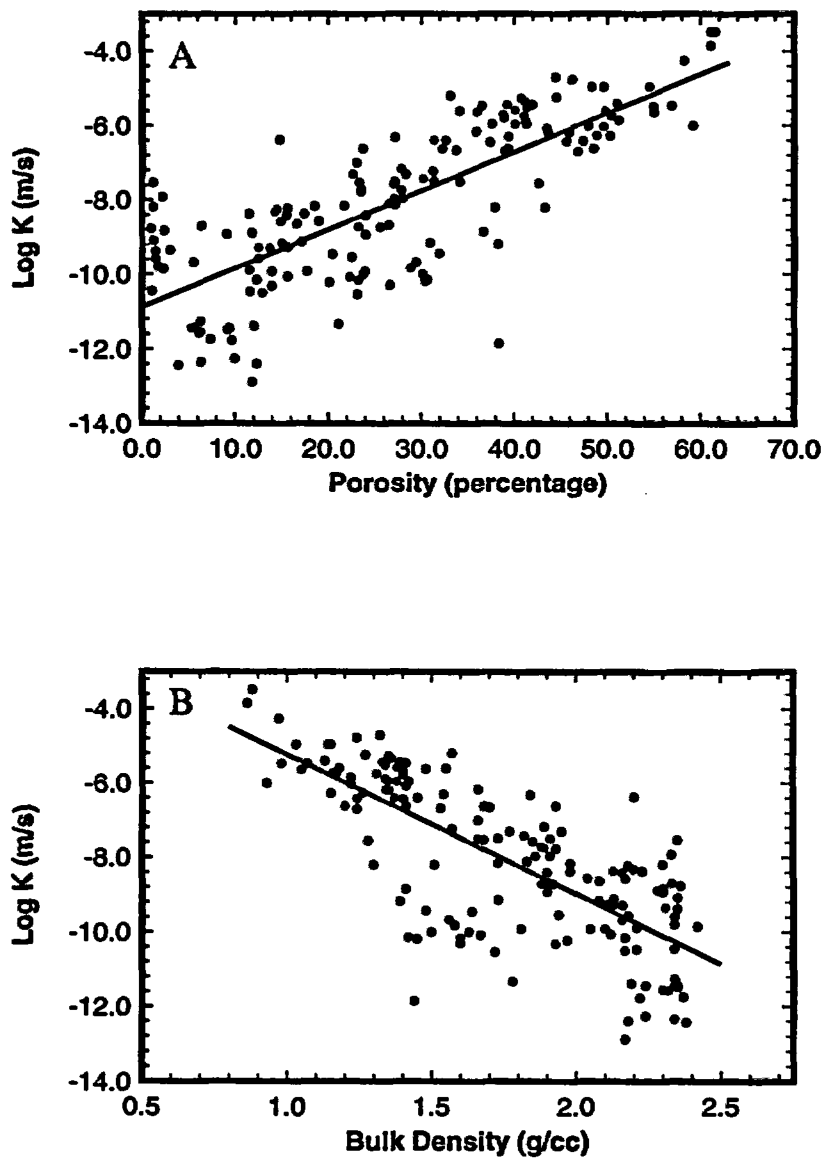

Figure 4. Plots of correlations between log saturated hydraulic conductivity, porosity and bulk density for all the vertical transects.

"global" relationships between saturated hydraulic conductivity , bulk density and porosity are fairly weak (coefficients of determination, r^2, less than 0.65).

X Variable	Y Variable	n	Regression Equation	R^2
Porosity (%)	Log K_{sat}	162	$Y = 1.044 \times 10^{-1}X - 10.888$	0.616
Bulk Density	Log K_{sat}	162	$Y = -3.744X - 1.493$	0.562

Table 3. Results of regression calculations for log saturated hydraulic conductivity and other properties.

Flint et al. (pers. comm.) developed regression equations between porosity and the log of saturated hydraulic conductivity for both the Yucca Wash and the Solitario Canyon vertical transects. These equations were developed using only the welded and non-welded samples (i.e., the vitric and the Calico Hills samples were disregarded). These two regression equations are given in Table 4. As can be seen in Table 4, the correlations between saturated hydraulic conductivity and porosity are fairly strong within these subsets of the data.

X Variable	Y Variable	n	Regression Equation	R^2
Solitario Canyon Transect Porosity (%)	Log K_{sat}	36	$Y = -13.9 + 33.1X - 30.8X^2$	0.90
Yucca Wash Transect Porosity (%)	Log K_{sat}	88	$Y = -11.9 + 18.1X - 10.7X^2$	0.77

Table 4. Results of transect regression calculations from Flint et al. (pers. comm.).

Porosity, bulk density, and particle density were measured for all samples from the vertical transects. Relationships between these properties are examined here. The regression results shown in Tables 2, 3 and 4 above used the values of porosity and bulk density as determined through drying the samples in an oven with a controlled relative humidity. This technique does not remove water from the clay minerals in the rocks and therefore is felt to be more accurate than the traditional method of drying the samples in a 105° C oven. The relationship between these two methods is checked on the 496 measurements of porosity, bulk density and particle density available in the vertical transects. These relationships are shown in Figure 5. Regression relationships for these data are not calculated, but the 1:1 relationship line is shown in each plot (Figure 5).

From Figure 5(A), it appears as though the 105° C oven does dry out the clay minerals which significantly increases porosity in the samples relative to the controlled relative humidity oven. All data points lie on, or above,

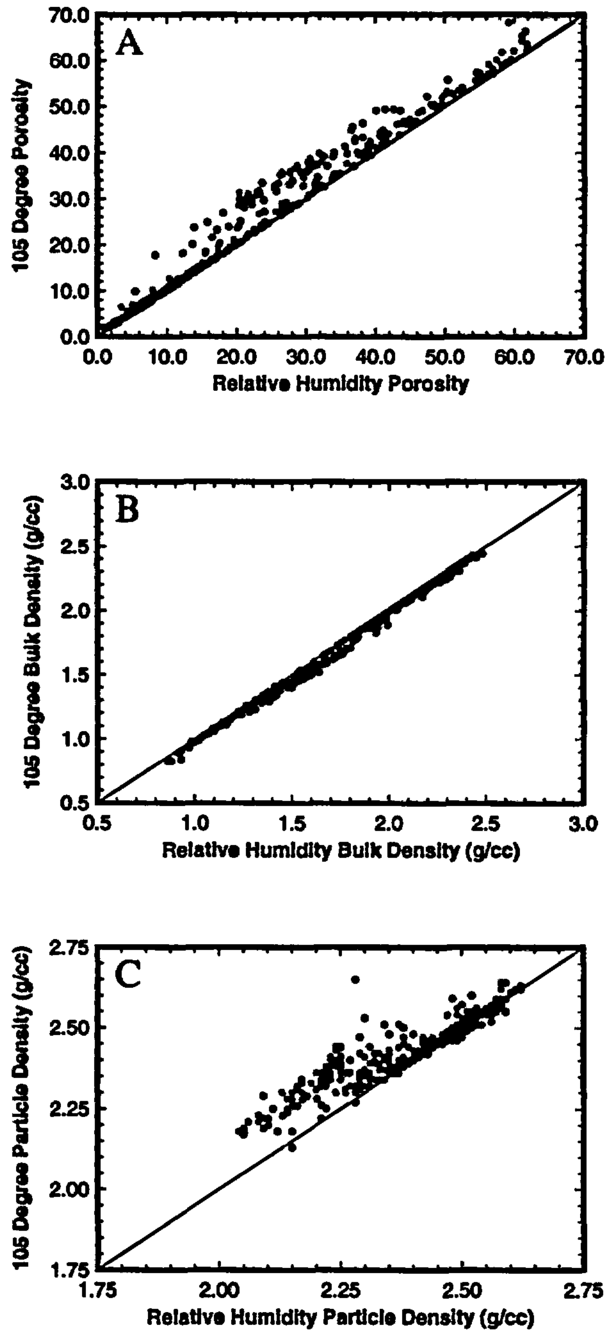

Figure 5. Comparisons of properties determined by drying in a relative humidity controlled oven and in a 105 degree C oven. The 1:1 lines are shown for reference.

the 1:1 line. This increase in porosity due to the higher temperature drying is most pronounced in samples with greater than 15 percent porosity and the increase can be as large as 10 percent (Figure 5(A)). The changes in bulk density are what would be expected given the differences in porosity between the two techniques (Figure 5(B)). As the water is driven out of the clay minerals there is a decrease in bulk density. The relationship between particle density as calculated in the humidity controlled oven versus the 105° C oven is shown in Figure 5(C). The particle density relationship is not as straight forward as the porosity and bulk density relationships. Generally, samples with particle densities above 2.35 g/cc cluster on the 1:1 line, while those generally below 2.35 g/cc lie above the 1:1 line. It appears as though the scatter of points about the 1:1 line for samples above 2.35 g/cc can be attributed to measurement error, while those below 2.35 g/cc undergo a fundamental shift in particle density.

The relationship between porosity and bulk density (both determined through the controlled humidity technique) is shown in Figure 6. The regression relationship calculated between porosity and bulk density is shown in Table 5.

X Variable	Y Variable	n	Regression Equation	R^2
Porosity (%)	Bulk Density	496	$Y = -2.672 \times 10^{-2} X + 2.475$	0.952

Table 5. Results of regression calculation between porosity and bulk density on all vertical transects.

Correlations between particle density and any other property are non-existent in the subsets of the data examined above. This lack of a relationship is not surprising among the strictly hydrologic properties (saturated hydraulic conductivity and sorptivity); however, it is plausible for a relationship to exist between particle density and porosity and/or bulk density in welded tuffs. The degree of welding and compaction during deposition of the flow unit may effect the density of the individual grains, as well as the overall density of the stratigraphic unit. Certainly some process has produced the range of particle densities (approximately 2.1 to 2.6 g/cc) observed in the welded tuffs.

Thermal/Mechanical Units

The thermal/mechanical units have been defined based on porosity and grain density which, can be correlated to thermal, mechanical and hydrological properties (Nimick, et al., 1984). The classification of

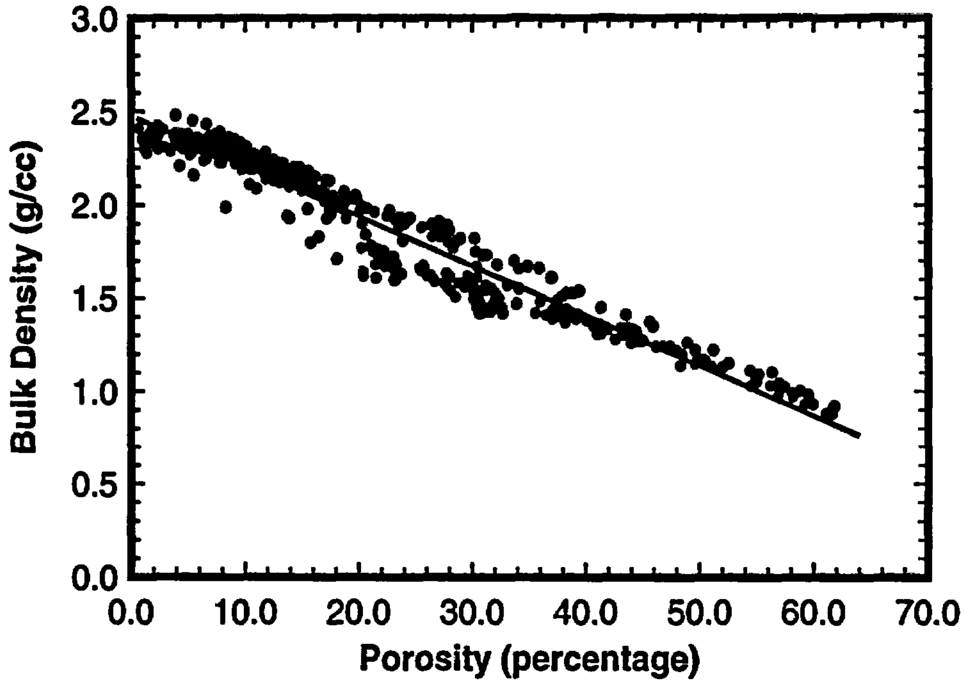

Figure 6. Relationship between bulk density and porosity on all vertical transects. Results of the regression calculation are shown in Table 5.

thermal/mechanical units is the basis of the three-dimensional model of Yucca Mountain developed by Ortiz, et al. (1985). Summary statistics from the five transects grouped in terms of thermal/mechanical units are shown in Table 6.

From Table 6, it can be seen that the welded units have the lowest mean porosity values and the non-welded units have the highest. Conversely, bulk density is highest in the welded units and lowest in the non-welded units. Particle density shows no correlation with welding. The highest values of saturated hydraulic conductivity and sorptivity are found in the Paintbrush Tuff, non-welded thermal/mechanical unit (PTn). The Prow Pass thermal/mechanical unit (PP) has only two data points and therefore is not examined in this report.

Flow Unit	Porosity (%) percentage	Bulk Density (g/cm^3)	Particle Density (g/cm^3)	n	Log K_{sat} (m/s)	n	Log Sorptivity ($m/s^{0.5}$)	n
Tiva Canyon welded	13.5	2.16	2.50	99	-9.18	38	-5.60	14
Paintbrush Tuff nonwelded	34.3	1.57	2.38	117	-6.81	89	-3.90	14
Topopah Spring welded #1	11.4	2.21	2.49	80	-9.65	11	-5.11	10
Topopah Spring welded #2	8.2	2.30	2.50	72	-11.73	4	-5.59	4
Topopah Spring welded #3	3.0	2.32	2.39	18	-9.89	6	-6.04	1
Calico Hills nonwelded zeolitized	33.0	1.54	2.31	62	-10.10	10	-4.72	4
Prow Pass	25.0	1.92	2.55	2	—	—	—	—

Table 6. Mean values of parameters for the thermal/mechanical units.

The relationships between properties within each of the geohydrologic units are also examined. There are not enough sorptivity measurements to warrant the examination of these data on a unit by unit basis. It is only possible to examine the saturated hydraulic conductivity/porosity relationship on two of the thermal/mechanical units (PTn and TCw) (Figure 7) due to the shortage of saturated hydraulic conductivity measurements. The results of the regression calculations for these relationships are given in Table 7. The results show only a weak relationship (coefficient of determination less than 0.60) between porosity and saturated hydraulic conductivity in these two

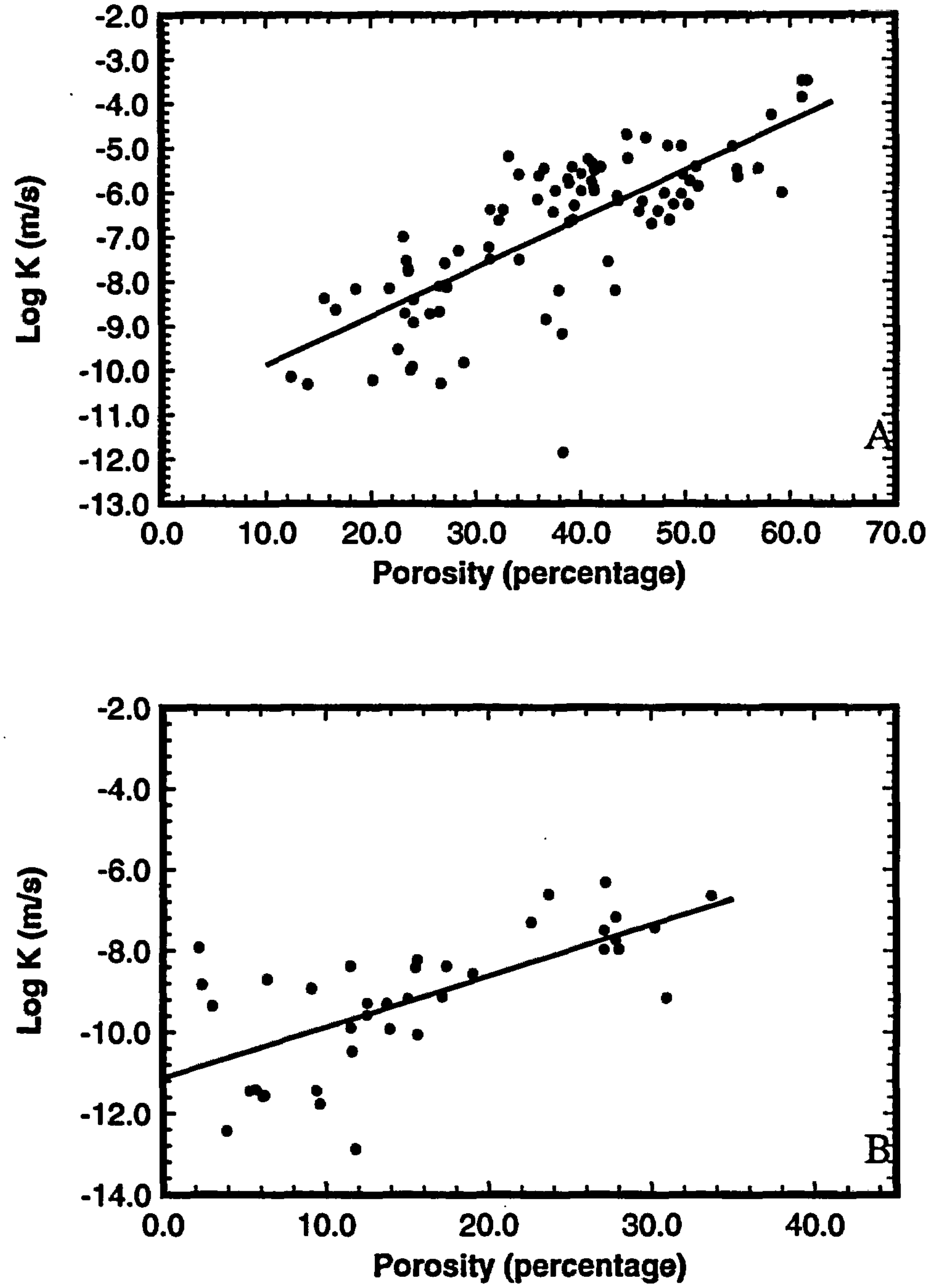

Figure 7. Relationship between porosity and log saturated hydraulic conductivity in the thermal mechanical units PTn (A) and TCw (B). Results of the regression calculations are shown in Table 7.

thermal/mechanical units.

X Variable	Y Variable	n	Regression Equation	R^2
PTn Porosity (%)	PTn Log K_{sat}	89	Y = 1.096X - 10.973	0.579
TCw Porosity (%)	TCw Log K_{sat}	38	Y = 1.256X - 11.128	0.459

Table 7. Results of regression calculations for porosity and saturated hydraulic conductivity in two thermal/mechanical units.

Geohydrologic Units

Geohydrologic units are defined based on their hydrologic properties rather than lithologic description (Flint, et al., pers. comm.). Generally, it is the degree of welding in the tuffs that controls the hydrologic properties and unit designation. The average bulk and hydrologic properties of the geohydrologic units are shown in Table 8.

Flow Unit	Geohydrologic Unit	Porosity (%)	Bulk Density (g/cm^3)	Particle Density (g/cm^3)	n	Log K_{sat} (m/s)	n	Log Sorptivity ($m/s^{0.5}$)	n
Tiva Canyon									
	densely welded caprock (TCdwc)	12	2.23	2.54	27	-9.96	6	-5.01	1
	moderately welded (TCmw)	25	1.92	2.56	56	-8.29	71	-5.01	1
	welded (TCw)	9	2.25	2.47	64	-11.10	62	-5.74	11
Paintbrush Tuff									
	nonwelded (PTn)	41	1.42	2.42	129	-6.24	201	-4.0	15
Topopah Spring									
	welded (TSw)	8	2.28	2.48	240	-10.59	96	-5.35	16
	welded, no vitric caprock or vitrophyre (TSnn)	11	2.24	2.50	163	-10.59	80	-5.33	14
Calico Hills									
	nonwelded zeolitic (CHnwzeo)	33	1.54	2.31	62	-9.85	12	-4.72	4
Prow Pass									
	nonwelded (PPnw)	25	1.92	2.55	2	---	---	---	---

Table 8. Mean values of parameters for the Geohydrologic Units (After Flint et al., pers. comm.)

Table 8 demonstrates some of the same large-scale trends seen in the thermal/mechanical unit groupings (Table 6). Generally, the welded units have lower porosity and higher bulk density than do the nonwelded or the moderately welded units. The Paintbrush Tuff, nonwelded geohydrologic unit has the highest saturated hydraulic conductivity and sorptivity.

Most of the geohydrologic units do not have a large amount of saturated hydraulic conductivity data, and those that do (PTn, TCdw and TCmw) do not show a strong relationship between porosity and saturated hydraulic conductivity. Only the Tiva Canyon, moderately welded unit (TCmw) exhibits a relationship. The relationship between porosity and saturated hydraulic conductivity for the TCmw geohydrologic unit is shown in Figure 8, and the results of the regression calculation are shown in Table 9.

X Variable	Y Variable	n	Regression Equation	R^2
Porosity (%)	Log K_{sat}	13	$Y = 3.069x10^{-1}X - 14.072$	0.599

Table 9. Results of regression calculation on porosity and log saturated hydraulic conductivity in the Tiva Canyon Moderately welded (TCmw) geohydrologic unit.

Variography

In addition to summarizing previous work accomplished on the outcrop transects, this report provides estimates of spatial correlation of the parameters measured in the outcrop study through the calculation of variograms. Variograms have been calculated previously on several of the transects (Rautman and Flint, 1992) as well as on a combination of several boreholes (Rautman, 1991).

In this report, spatial correlation of rock properties is investigated within the same groupings as were the traditional statistical parameters: transects, thermal/mechanical units and geohydrologic units. Due to the paucity of the data within some units, it is not possible to calculate the variograms for all of the thermal/mechanical and geohydrologic units. Variograms are calculated on porosity and, when possible, on saturated hydraulic conductivity. The saturated hydraulic conductivity data set has been augmented for variogram calculations by employing the regression equations developed by Flint et al. (pers. comm.) (Table 4, this report). This augmentation provides saturated hydraulic conductivity values on the welded and non-welded units in the Solitario Canyon and Yucca Wash transects. There are not enough sorptivity data to calculate variograms on this parameter. The

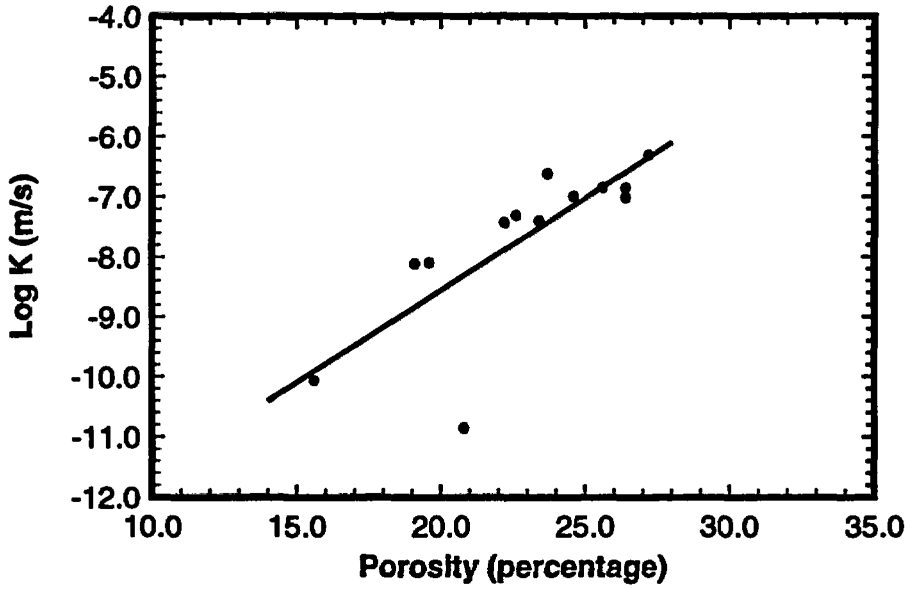

Figure 8. Relationship between porosity and log saturated hydraulic conductivity in the Tiva Canyon moderately welded Geohydrologic Unit. Results of the regression calculation are shown in Table 9.

general strong correlation between porosity and bulk density results in the estimates of spatial correlation for porosity being similar to those for bulk density.

A modification made to the data sets concerns the ultimate goal of the variogram calculations, which is to guide the downhole sampling strategy. In general, the estimated value for a geologic/hydrologic property is given by:

$$z(x) = \mu + V_r + V_s + V_a$$

The estimated value of the property at location x is given as z(x). This estimate can be defined as the mean of the sample distribution (μ) plus variability derived from three sources. V_r is the regional variability of the property being sampled, V_s is the variability of the property which exists across the sample site (e.g., two porosity samples taken at the same location along the transect) and V_a is the variability due to the analytical technique. For mapping purposes, it is desirable to have the regional variability be much larger than the sample and analytical variability.

Variability of hydrologic and bulk properties in these data sets due to analytic error is considered to be small for all parameters with the possible exception of saturated hydraulic conductivity. The level of analytic variability was checked by replicate samples that were run through the analytical equipment used to determine the property values in these data sets prior to analyzing the data. With respect to the regional variability and the site variability, the analytical variability is considered negligible.

Approximately five percent of the sample locations in the vertical transects were sampled twice. Two core plugs were drilled out of the outcrop next to each other (generally within 30cm of each other) and analyses were conducted on each core. These duplicate samples allow a comparison of the sample location variability to the regional variability for each of the parameters. Only if the regional variability is greater than the site (sample) variability is the concept of a property map or a correlation length valid.

The portions of the total variability attributed to sample location versus regional variability can be determined through an analysis of variance (ANOVA). An ANOVA is a method of testing the differences in means and variances between different groups or sources of samples (Davis, 1986). For the problem at hand, a "two-way"

ANOVA is necessary. This analysis tests two hypotheses simultaneously: that the values from the same sample location are the same and that the values from the different sample locations are the same.

A two-way ANOVA was carried out on a total of 27 porosity samples. The results are shown below in Table 10. From Table 10, it is apparent that the variation between sample locations is much larger than the variation within sample locations. The mean squares value calculated on the variation within sample locations is less than 0.2 percent of the regional (between sample locations) mean squares. The within-sample location variability is negligible compared to the regional variability.

The goal of this portion of the study is to determine the regional (between sample locations) spatial correlation. For this reason, the site variability has been smoothed in the variogram calculations. This smoothing was accomplished by reducing the two sample values at any one location on the transect to a single value. This smoothing was done by simply averaging the two values, except in the cases where one sample had a measured value of saturated hydraulic conductivity and the other sample's conductivity was estimated or non-existent. In these cases, the sample with the measured value of saturated hydraulic conductivity was retained for the variogram calculations. Due to the relatively small amount of variability within the sample sites, the variogram calculations with and without the averaging at sample locations are essentially identical.

Source of Variation	Sum of Squares	degrees of freedom	Mean Squares	F statistic
Within Sample Location	1.156	1	1.16	0.27
Between Sample Location	19,804.3	26	761.70	178.55
Error	110.9	26	4.27	
Total	19916.4	53		

Table 10. Results of ANOVA calculation.

Transect Data

Of the eight transects reported in Flint et al. (pers. comm.), five of them are vertical transects and three of them are horizontal. The vertical transects cut across multiple thermal/mechanical and geohydrologic units while the horizontal transects remain within single thermal/mechanical and geohydrologic units. Variograms are calculated on the full vertical transects with the thought that it may be possible to generate an average, or composite, vertical variogram which can adequately describe the vertical correlation of rock properties within a given thermal/mechanical or geohydrologic unit. Such variograms could be useful when geostatistically modeling hydrologic/bulk properties of the repository block as a single entity. The utility of a single composite vertical variogram can be tested by comparing this composite variogram with the variograms constructed on the thermal/mechanical and geohydrologic units.

Variograms are calculated by using the GSLIB (Deutsch and Journel, 1992) software package. All variograms are calculated with the standard variogram equation, given as:

$$\gamma(h) = \frac{1}{2n}\sum_{i=1}^{n}(z(x_i) - z(x_i + h))^2$$

The variogram value is defined as a function of the separation distance, or lag spacing, between samples (h). The number of data per lag spacing are defined as n and z is the property value at location x. The calculated variograms and their corresponding models for the vertical transects are shown in Figures 9 and 10. The results of fitting models to the experimental variograms for the five vertical transects are summarized in Table 11. For the transect porosity variograms, the number of pairs per lag averaged from 250-550 depending on the transect.

Transect	Model Type	Nugget ($\%^2$)	Sill ($\%^2$)	Range (m)
Solitario Canyon	Spherical	10.0	285.0	23.0
Busted Butte	Spherical	13.5	7.0	16.0
Yucca Wash	Spherical	0.0	370.0	90.0
Pagany Wash	Gaussian	2.0	88.0	8.0
Calico Hills	Spherical	9.0	32.4	34.0

Table 11. Variogram parameters for models fit to vertical transect porosity data.

The variogram ranges displayed in Table 11 can be compared to the vertical variogram ranges calculated by Rautman (1991). The ranges calculated by Rautman (1991) were based mainly on drill-hole data across multiple stratigraphic units. These calculations may be similar to the ranges calculated across the vertical transects in this study. Rautman (1991) found that generally 1/3 to 1/2 of the total amount of variability (gamma) could be described as a nugget effect. This high nugget effect is somewhat attributable to the aggregation of multiple

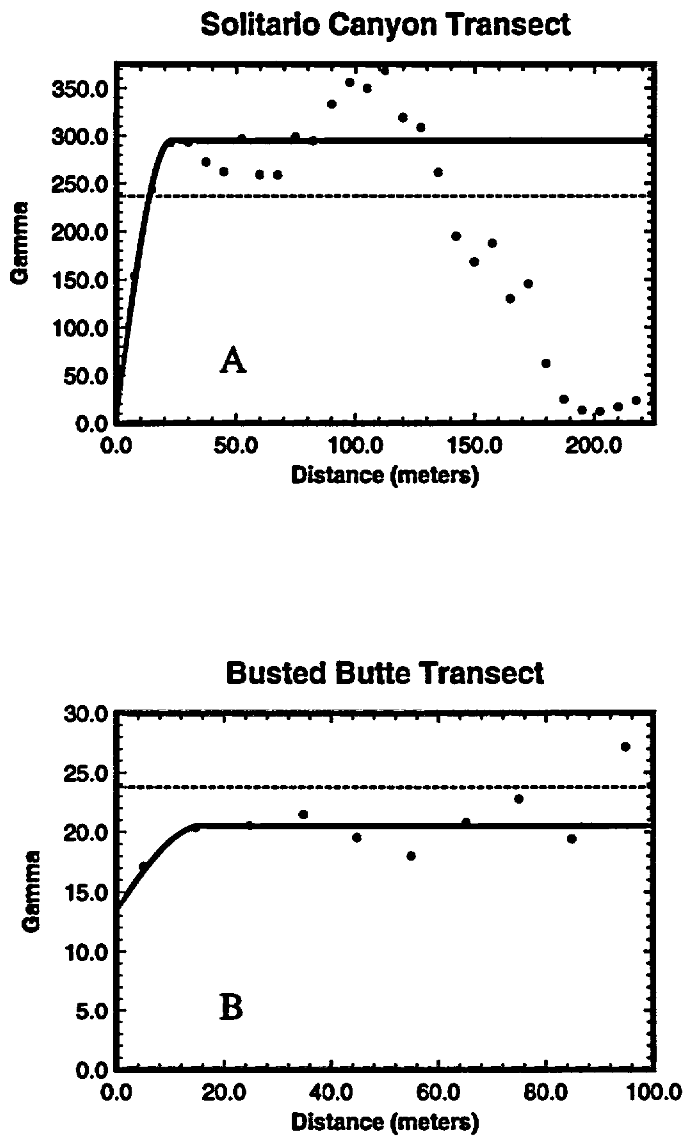

Figure 9. Modeled porosity variograms for the vertical Solitario Canyon (A) and the Busted Butte (B) transects. The horizontal dashed lines denote sample variance.

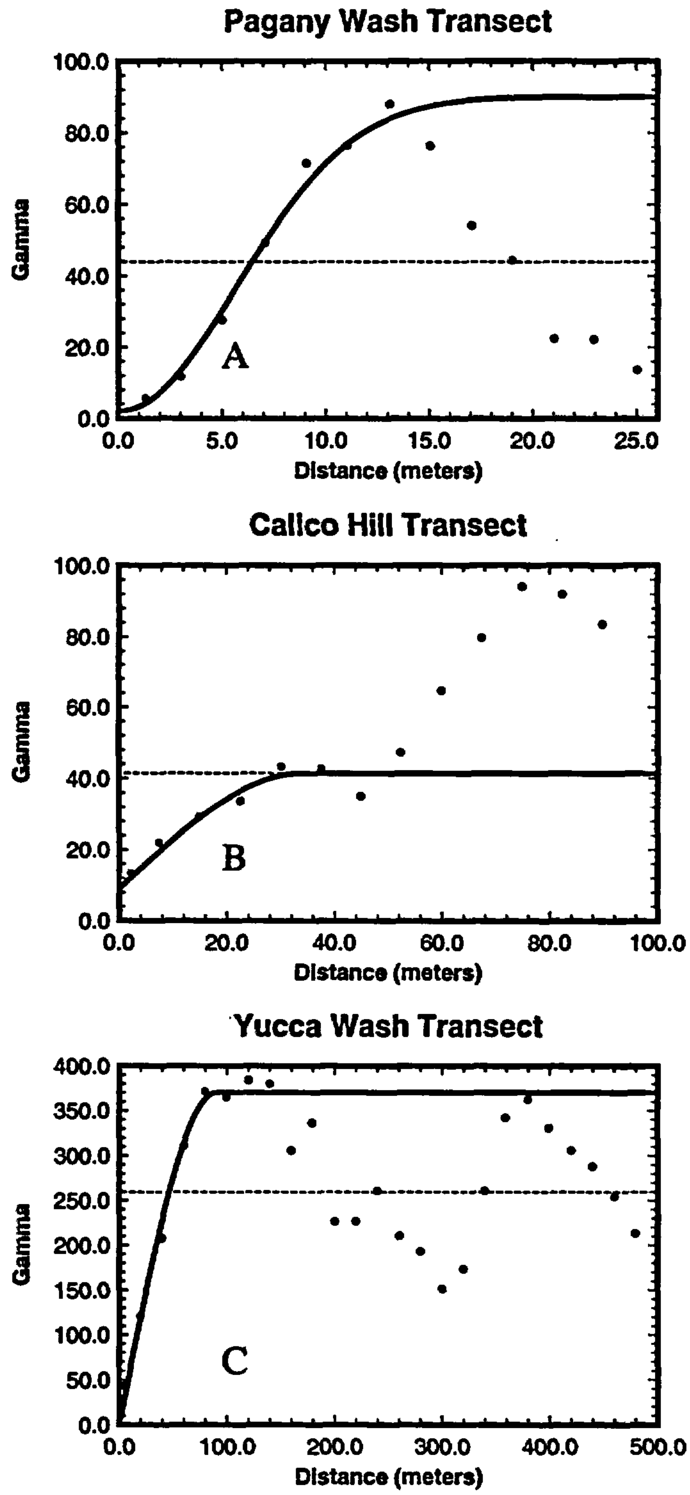

Figure 10. Modeled porosity variograms for the vertical Pagany Wash (A), Calico Hills (B) and the Yucca Wash (C) transects. The horizontal, dashed lines indicate the sample variance.

laboratory analyses into a single data set. In the current study, only the Busted Butte and Calico Hills transects display a significant nugget effect in the composite variograms. The ranges of the composite variograms in this study are between 8.0 and 90.0 meters (Table 11). In general, these ranges are considerably less than the range of the composite, vertical variogram calculated by Rautman (1991) which was 800 feet (244 meters). Refer to Figure 2 to determine the proportions of each stratigraphic unit within each transect.

By using the regression calculations from Flint et al. (pers. comm.) given in Table 4 of this report, it is possible to generate variograms of saturated hydraulic conductivity for the Solitario Canyon and Yucca Wash transects. These variograms are shown with the models fit to them in Figure 11. The results of the model fitting procedure are shown in Table 12. In the Solitario Canyon transect variogram, the average number of pairs per lag is 600 and in the Yucca Wash variogram calculation it is 350. Since the saturated hydraulic conductivity values were derived from a regression relationship with porosity, it is not surprising, that the saturated hydraulic conductivity variograms are very similar to the porosity variograms.

Transect	Model Type	Nugget $(m/s)^2$	Sill $(m/s)^2$	Range (m)
Solitario Canyon	Spherical	1.80	4.85	39.0
Yucca Wash	Spherical	0.00	8.50	88.0

Table 12. Variogram parameters for the models fit to the log saturated hydraulic conductivity transect data.

In order to calculate vertical variograms on rock properties within the thermal/mechanical and geohydrologic units and use all the available information, it is necessary to modify the data files. The vertical outcrop transects represent one-dimensional sampling profiles. It is desirable to use the data from all available transects when calculating variograms on properties within the thermal/mechanical and geohydrologic units. The traditional method of doing this is to calculate the vertical variograms with a wide bandwidth in the horizontal direction (perpendicular to the vertical search direction). However, in this study, the sample locations are given relative to distance away from the transect starting location. Furthermore, the transect starting locations are not, at the present time, located with adequate precision to allow calculation of a composite vertical variogram in the traditional manner.

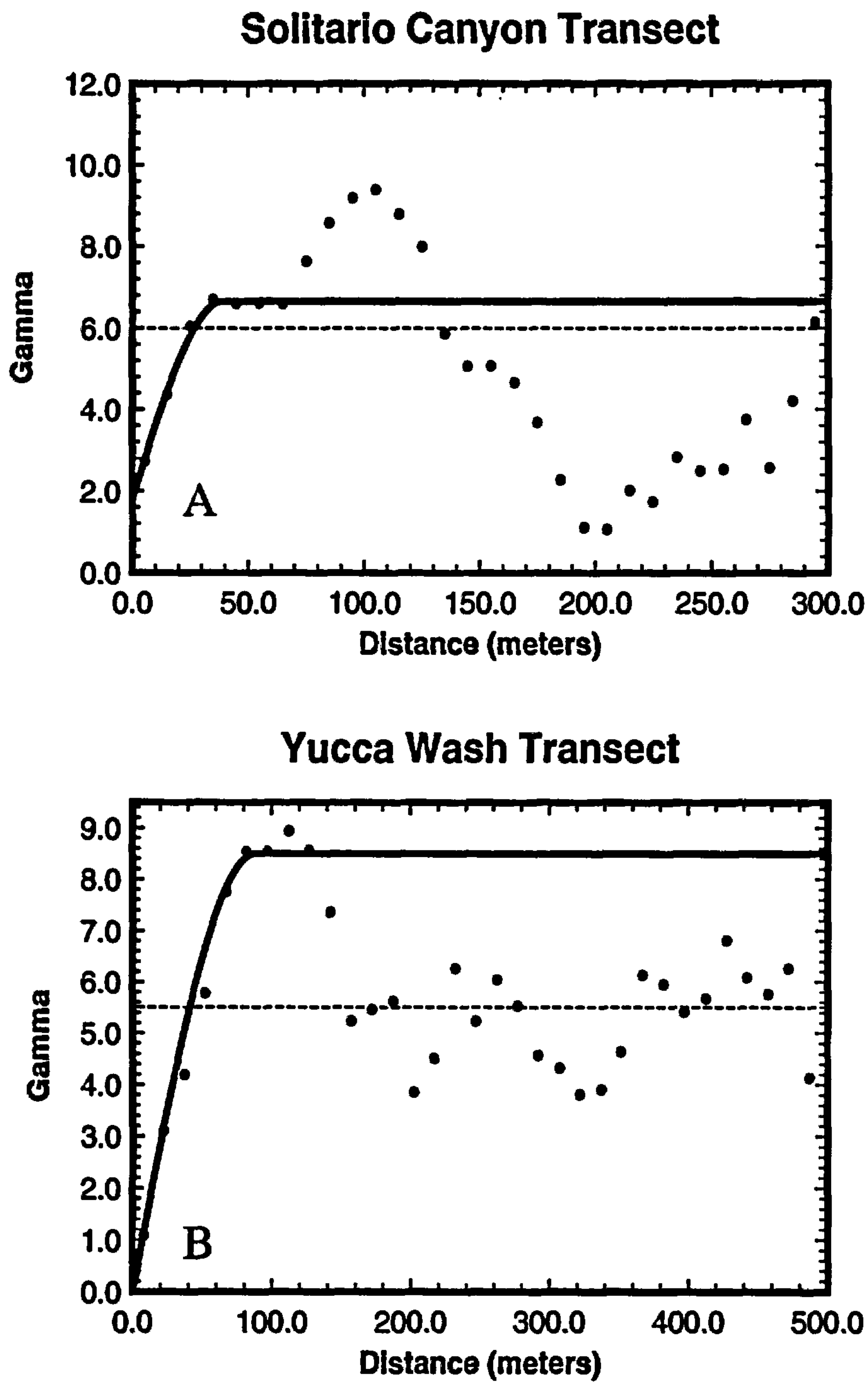

Figure 11. Modeled log saturated hydraulic conductivity variograms for the vertical Solitario Canyon (A) and the Yucca Wash (B) transects. The horizontal dashed lines denote the sample variance.

A less conventional way around the problem of incorporating data from isolated vertical transects was used in the variogram calculations in this study. All portions of each transect covering the unit of interest (thermal/mechanical or geohydrologic) are put together into a single data set. These data sets are created by putting together the various transect segments using the same X and Y coordinates for each and separating the segments in the Z direction by using an artificially large vertical spacing between segments.

For example, the Calico Hills non-welded, zeolitized, geohydrologic unit may be sampled in three separate vertical transects with the maximum distance between samples within any one of the transects being 100 meters. These three segments are combined into a single transect by giving every sample the same X and Y coordinates and making sure the Z coordinates are such that the three segments are separated by a distance much larger than 100m (generally 5000 meters). Through this manipulation, each segment contributes to the calculation of the overall spatial variability at lag distances less than 100m. By disregarding the artificial spatial correlation at distances greater than 5000 meters in the variogram calculation, there is no "cross-talk" between the transect segments. This technique was used in the calculation of the vertical variograms within each of the thermal/mechanical and geohydrologic units.

Thermal/Mechanical Units

Porosity variograms are calculated on all of the thermal/mechanical units, with the exception of TSw3 (the basal vitrophyre) in which there is an inadequate amount of data. The results of these calculations and the subsequent model fitting are shown in Table 13. The average number of pairs per lag in the thermal/mechanical unit variograms calculations ranges from 150 to 200 depending on the unit .The modeled variograms are shown in Figures 12 and 13.

The pure nugget effect variogram for TSw2 (Figure 13) is uncommon. This effect suggests that either the porosity values are randomly distributed within each transect segment, or the range of spatial correlation is below the sample spacing within this unit. Graphical examination of the porosity values with respect to distance does show a fairly random effect. Also, the data set which was used to calculate this variogram contains data from three different vertical transects. The nature of the spatial correlation, or lack thereof, differs between transect segments.

Thermal /Mechanical Unit	Model Type	Nugget ($\%^2$)	Sill ($\%^2$)	Range (m)
TCw	Spherical (structure 1)	0.0	27.0	12.0
	Spherical (structure 2)	N/A	14	60.0
PTn	Spherical	40.0	412.0	135.0
TSw1	Spherical (structure 1)	7.0	6.0	13.0
	Gaussian (structure 2)	N/A	20.0	70.0
TSw2	None	Pure Nugget Effect Variogram (no model fit)		
CHn	Spherical	10.0	30.5	30.0

Table 13. Results of porosity variogram modeling on the thermal/mechanical units

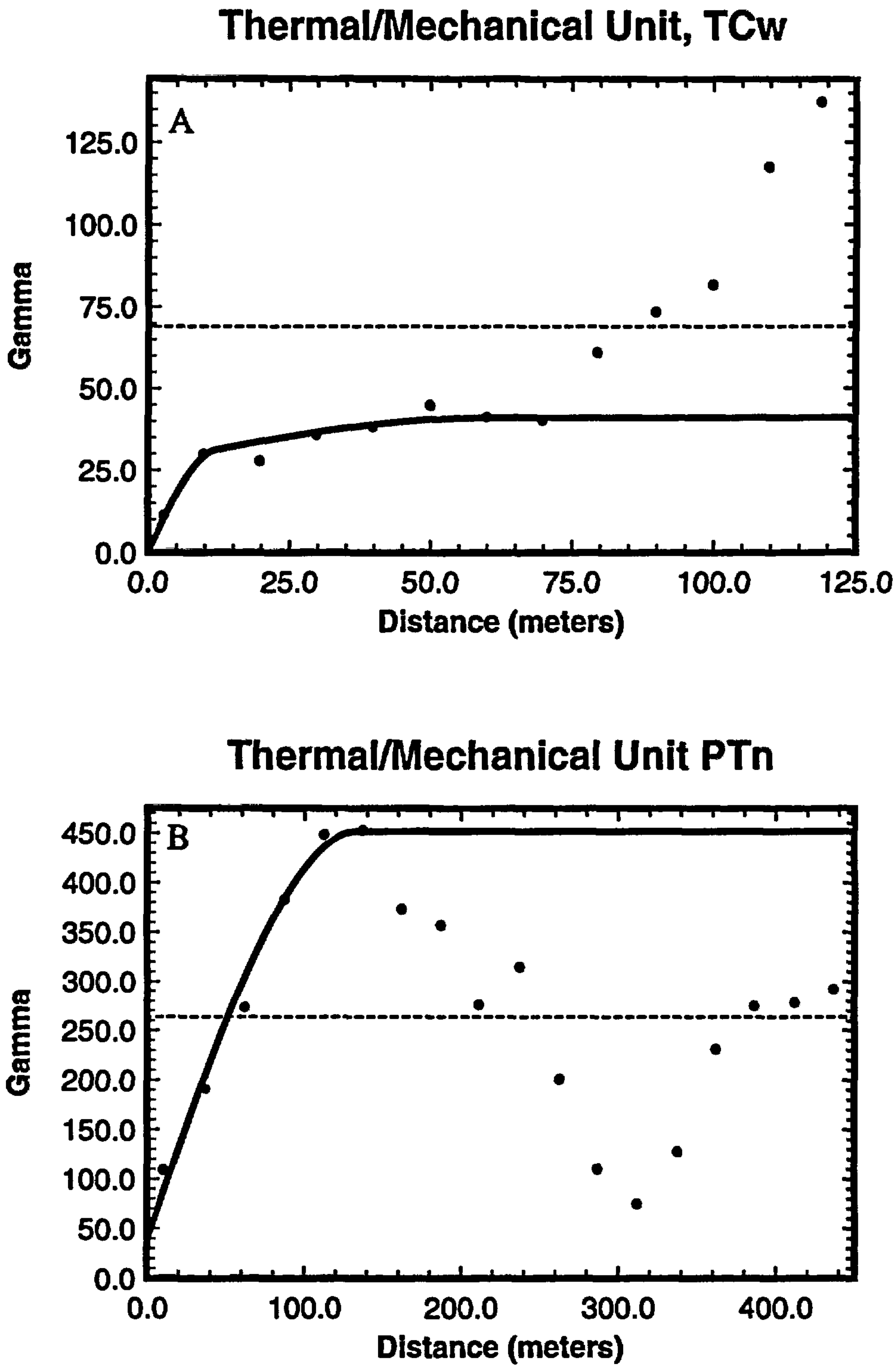

Figure 12. Modeled porosity variograms for the thermal/mechanical units TCw (A) and PTn (B). The dashed horizontal lines indicate sample variance.

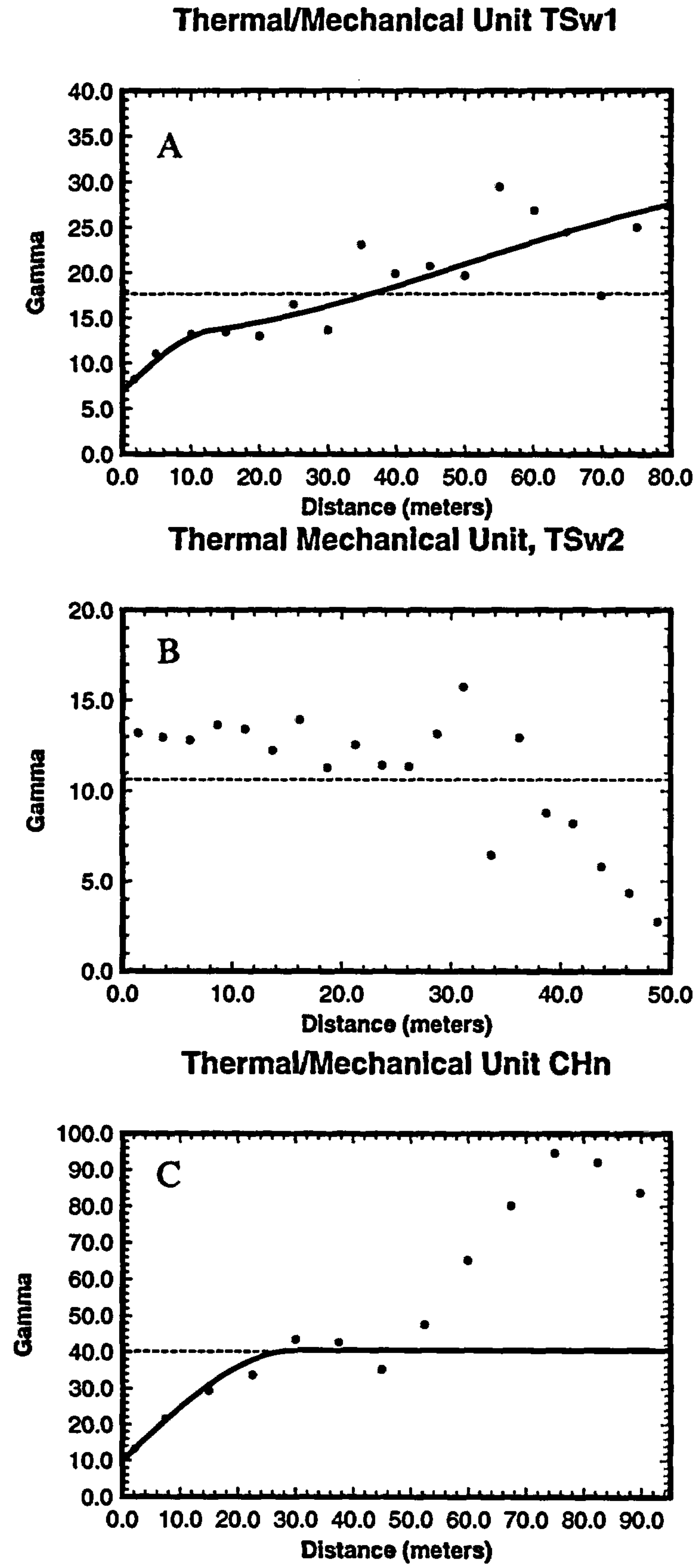

Figure 13. Modeled porosity variograms for the thermal/mechanical units TSw1 (A), TSw2 (B) and CHn (C). The dashed horizontal lines indicate sample variance.

Geohydrologic Units

Variogram calculations are also carried out for the geohydrologic units as defined by Flint et al. (pers. comm.). The results of the variogram calculations and model fitting are shown in Table 14 and the corresponding plots are shown in Figures 14 and 15. The average number of pairs per lag in the geohydrologic unit variograms ranges from 150-500. The most significant nugget effects are in the Topopah Spring units (TSw and TSnn). These also seem to be the units with the highest possibility of a trend in the data. Results of the variogram fitting on the geohydrologic units are consistent with the results of calculating and modeling the variograms in the thermal/mechanical units.

Geohydrological Unit	Model Type	Nugget	Sill	Range (m)
TCw	Spherical	3.2	10.0	33.0
PTn	Spherical	0.0	128.0	11.0
TSw	Spherical	8.0	8.0	10.0
TSw (2nd nest)	Gaussian	N/A	5.0	65.0
TSnn	Spherical	11.0	6.0	82.0
CHnwzeo	Spherical	9.0	26.0	38.0

Table 14. Variogram parameters for models fit to the geohydrologic units.

Summary

Prior to summarizing the work presented in this report, a summary of the detailed investigation of the shardy base microstratigraphic unit is provided.

Shardy Base Microstratigraphic Unit

Results of the many vertical transects completed in the shardy base microstratigraphic unit of the Tiva Canyon Member have been reported previously (Istok et al., 1994; Rautman et al., pers. comm.; and Rautman et al., 1993). The shardy base microstratigraphic unit is generally nine to twelve meters thick in the study area.

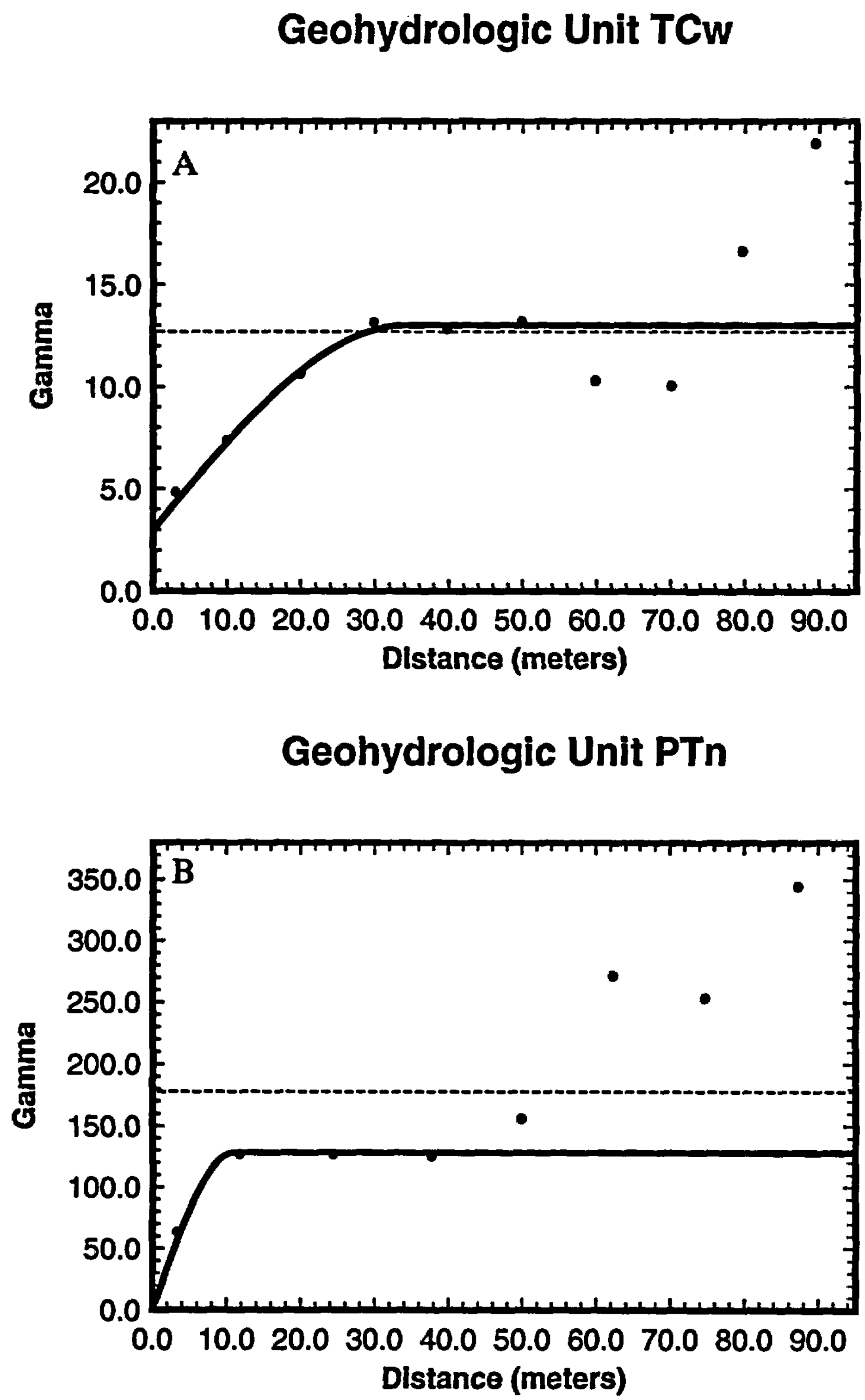

Figure 14. Modeled porosity variograms for the geohydrologic units TCweld (A) and PTnon (B). The horizontal, dashed lines indicate the sample variance.

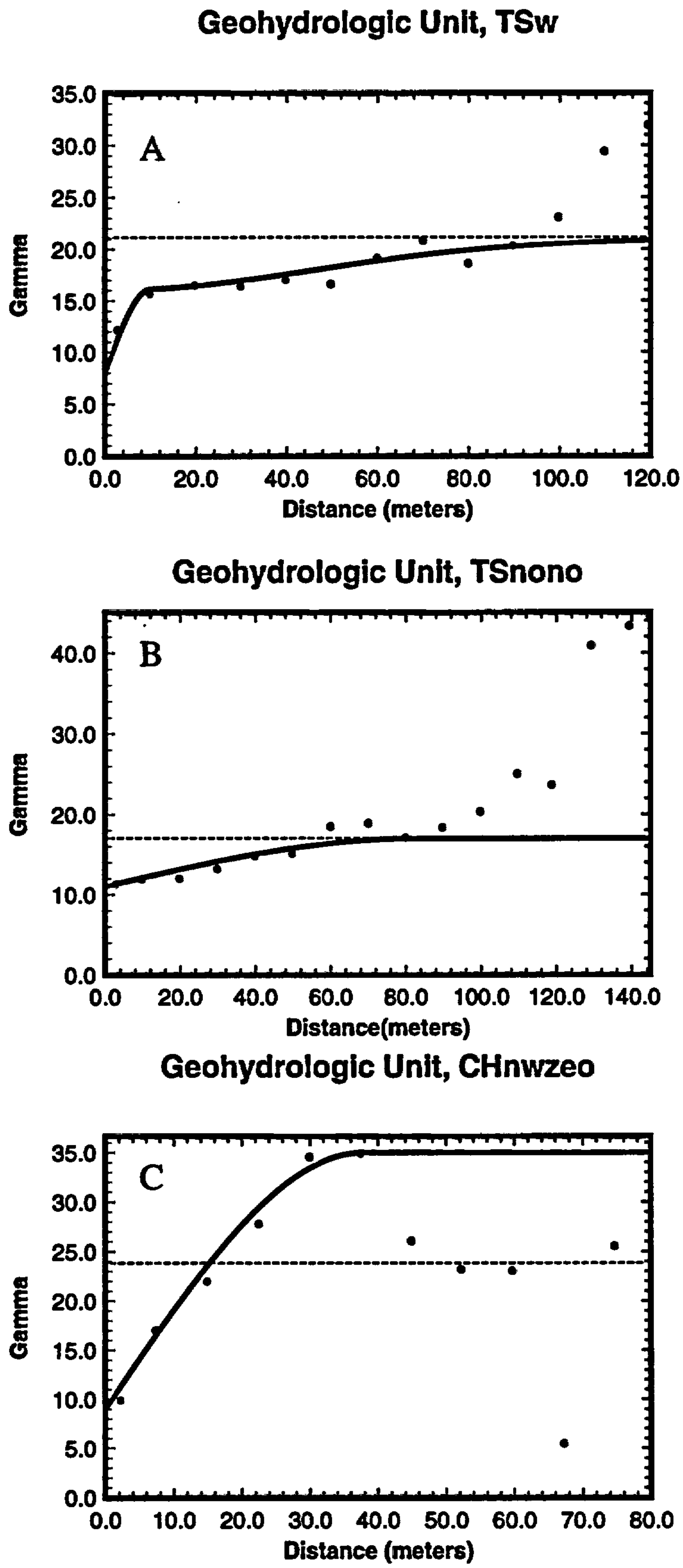

Figure 15. Modeled porosity variograms for the geohydrologic units TSw(A), TSnn (B) and CHnwzeo (C). The horizontal dashed lines indicate sample variance.

Within this thickness, there are three distinct rock types in the shardy base: a high porosity, basal, air-fall pumice, a lower porosity, non-welded ash flow, and an upper ash flow which grades from non-welded to densely welded as elevation increases. By examining porosity against stratigraphic elevation within the shardy base microstratigraphic unit, a simple regression model can be developed to infer porosity from stratigraphic elevation. Significant relationships between porosity, the log of saturated hydraulic conductivity and the log of sorptivity are also demonstrated (Istok et al., 1994; Rautman et al., pers. comm.).By employing the regression model between stratigraphic elevation and porosity in the shardy base microstratigraphic unit, the trend in the porosity data was removed. Removal of deterministic trends is necessary for variogram calculation as the variogram equations assume stationarity of the data. These detrended data were then used to compute vertical variograms. The variogram range determined on these detrended data is approximately 0.25 to 0.3 of the stratigraphic thickness. Using the average stratigraphic thicknesses given above, this range value is roughly 2 to 4 meters. This range value appears to remain stationary across the length of the section which was examined (approximately 1.4 kilometers). From the work on the shardy base microstratigraphic unit, two important results in terms of the down-hole sampling plan are apparent: vertical spatial correlation ranges can exist which are less than the thickness of a microstratigraphic unit and vertical trends can exist within a microstratigraphic unit. When compared to the results of the large-scale vertical transects examined in the current report, these results imply that with high resolution sampling it may be possible to define trends and spatial correlation on a microstratigraphic-unit-by-microstratigraphic-unit basis.

Current Report

The regression relationships for the data set composed of the five vertical transects indicate that, on a global scale, it is possible to predict bulk density from porosity with a high amount of confidence. This could save laboratory effort by requiring only a determination of porosity to provide values for both porosity and bulk density. However, these two properties are determined during the same laboratory procedure, and the effort to calculate both is not much greater than what is needed to calculate just one of them. It also appears possible to infer a sorptivity value from a calculation of porosity across all the transects. This relationship should be checked further by increasing the size of the sorptivity data base. Currently there are only 48 measurements of sorptivity. Prediction of sorptivity from porosity could save time by eliminating the need to run sorptivity tests.

Saturated hydraulic conductivity is not correlated very strongly with any other properties across the set of all transects. As shown in Flint et al. (pers. comm.), the relationship between saturated hydraulic conductivity and porosity is dependent on location (varies from one transect to another) as well as lithology. The regression relations for saturated hydraulic conductivity and porosity developed by Flint et al. (pers. comm.) work well for welded and nonwelded samples within the two transects which had enough hydraulic conductivity data. However, these relationships were shown to be non-stationary and it will require more saturated hydraulic conductivity data to define the variability of these relationships across the site. Relationships between porosity and saturated hydraulic conductivity within the vitric, non-welded clays and the zeolitized portions of the lithology are not defined. It may be possible to define these relations through a larger data set of saturated hydraulic conductivity values, on the other hand, these two properties may just be poorly correlated within these units.

The lack of defined relationships between saturated hydraulic conductivity and porosity within the thermal/mechanical and the geohydrologic units points out the significance of the regression relationships between these two variables as defined on the Solitario Canyon and Yucca Wash transects. These transects show a strong relationship between saturated hydraulic conductivity and porosity even though they are calculated on a composite of several units. The use of these transect regressions to infer values of saturated hydraulic conductivity from measurements of porosity appears reasonable if it is done within the welded and non-welded portions of the units. This was the approach intended by Rautman and Robey (1994).

The lack of saturated hydraulic conductivity and sorptivity data precludes the examination of meaningful relationships between these parameters and porosity on a thermal/mechanical or geohydrological unit basis. It is currently only possible to look at regressions of saturated hydraulic conductivity and porosity in two of the thermal/mechanical units and one geohydrologic unit. Also, the relationships developed in these three units are only weakly defined. Due to the lack of data, it is not possible to determine whether or not these relationships vary across the site area.

The determination of meaningful regression relationships between porosity and sorptivity, as well as, porosity and saturated hydraulic conductivity, is hampered by a lack of sufficient quantity of data. An estimate of how many more samples are necessary to determine these relationships can be obtained from the central limit theorem. The central limit theorem is a basic assumption behind statistical hypothesis testing and regression calculations. The central limit theorem states that as sets of random samples are taken from any population, the mean values of those sample sets will tend to be normally distributed (Davis, 1986). The rule of thumb for the sample size necessary to invoke the central limit theorem when the distribution of the population is unknown is at least 30 samples. The rule of thumb suggests that each set of samples believed to be obtained from a distinct population (e.g., each thermal /mechanical or geohydrologic unit) should contain at least 30 samples. This condition is not met for any of the thermal/mechanical or geohydrologic unit sorptivity data sets. The saturated hydraulic conductivity data sets for the units PTn and TCw are the only thermal/mechanical unit data sets that do contain more than 30 samples. Enough samples have been collected in the majority of the thermal/mechanical and geohydrologic units to overcome the data deficiencies (see Tables 7 and 8). These samples now need to be tested for sorptivity and saturated hydraulic conductivity.

The full transect porosity variograms calculated in this report (Table 11) have smaller nuggets and shorter ranges compared to the composite variograms calculated by Rautman (1991). Each of the porosity transect variograms calculated in this report are calculated on a single transect, where Rautman's (1991) were calculated as the composite of sampling in nine boreholes. Combining all nine boreholes increases variability (higher nugget) by incorporating different portions of the stratigraphy together. Also, the longer variogram ranges in Rautman (1991) may be due to a secondary structure that is on the order of stratigraphic thickness which was reinforced by compositing the nine boreholes. The definition of vertical spatial correlation ranges that are less than the thickness of stratigraphic units could have important implications for performance assessment calculations that have previously assumed a single, randomly drawn, value for each stratigraphic unit.

Variograms calculated on the thermal/mechanical and the geohydrological units (Tables 13 and 14), demonstrate slightly longer average ranges relative to the full transect variograms. These variogram calculations also show behavior that requires description by nested models. The thermal/mechanical and geohydrologic unit variograms for the units within the Topopah Spring Member are modeled with relatively large nugget values and several of these variograms indicate the presence of a trend in the data. The trend behavior showing up in the Topopah Spring Member variograms is most likely caused by the gradual decrease in porosity from the rounded (tr) microstratigraphic unit to the basal vitrophyre (bt) microstratigraphic unit. The cause of this trend has been ascribed to changes in magma chemistry through the eruptive sequence which formed the Topopah Spring Member (Rautman and Flint, 1992). The porosity variogram for the Thermal/Mechanical Unit TCw also exhibits the effect of a trend at large lag spacings. This behavior is due to a decrease in porosity through the Tiva Canyon Member. This trend in porosity is strongest in the Solitario Canyon Transect.

Implications for Down-Hole Sampling

The current average sample spacing from the transects can be compared with the calculated variogram ranges and used as a guide for the down-hole sample spacing. The average spacings from the five vertical transects are given in Table 15. These values are simply determined by dividing the total length of each transect by the total number of samples within that transect. These average sample spacing values are compared to the variogram ranges calculated on the vertical transects.

Transect	Average Sample Spacing (meters)	Variogram Range (meters)	Percentage of Range accounted for by average spacing
Solitario Canyon	1.86	23.0	8.1
Busted Butte	1.32	16.0	8.3
Yucca Wash	2.09	90.0	2.3
Pagany Wash	1.25	8.0	15.6
Calico Hills	1.55	34.0	4.6

Table 15. Comparison of average sample spacing on the vertical transects to the variogram ranges

If the compilations of the variogram ranges for the transects, the thermal/mechanical units and the geohydrologic units are examined, an average range can be determined for each set of variograms. This average is calculated by using the first range in those variograms fit with nested models. The smallest average range is that calculated for the set of transect variograms (approximately 30m). This result is not surprising since the transect variograms are calculated over a combination of thermal/mechanical and geohydrologic units (i.e., they incorporate more variability). The sample spacings from the vertical transects have been adequate to define the spatial correlation across these transects. There appears to be no reason why these sample spacings (generally 1.3 to 2.1 meters) cannot be used in the down-hole sampling. At this point, this sample spacing should be achievable given the various demands on core coming out of the Systematic Drilling Program borings.

Based on the variograms calculated for the Topopah Spring units defined by the thermal/mechanical (TSw1 and TSw2) and geohydrologic (TSw and TSnn) divisions, it appears that some random factor, or a deterministic factor with a very short range of correlation, is controlling the distribution of spatial properties. Also, it is possible that a deterministic vertical trend is exerting some influence on the spatial distribution of properties within these units. An example of a possible trend in this units would be the relation between stratigraphic elevation and porosity observed by Rautman et al. (1993) in the shardy base microstratigraphic unit. Shorter sample spacings within the Topopah Spring units may be able to define the true range of spatial correlation within these units during the down-hole drilling campaign.

Previous work has suggested that a sample spacing of 85 percent of the variogram range should be considered "sparse" (Yfantis et al., 1987). This value has been suggested as a maximum sample spacing for Yucca Mountain drill-holes in previous work (Rautman, 1991). Certainly the maximum sample spacing should be significantly less than the range of spatial correlation. As seen in Table 14, the average sample spacing on the vertical transects ranges from approximately 2 to 15 percent of the variogram range in the different transects.

In general, the more data, the better the site characterization. However, resources for down-hole sampling are not unlimited, and it may be necessary, at some point, to decrease the number of samples obtained due to budgetary constraints. If this becomes the case, it would be possible to increase the sample spacing towards the sparse sampling limit of 85 percent of the range. Another option in the down-hole sampling campaign would be to derive a proxy for samples of porosity and/or other parameters by using the borehole geophysical data which will be collected on site. A strong correlation between a geophysical response and bulk/hydrologic properties would allow estimation of those properties between sample locations and may allow fewer samples to be collected. An advantage of sampling with borehole geophysical techniques is that they provide continuous sampling coverage within the borehole. A disadvantage of applying borehole geophysics at the Yucca Mountain site to determine porosity is the large volume of unsaturated material that needs to be characterized. The prime borehole geophysical technique for determining porosity is a sonic tool. Sonic tools need to be acoustically coupled to the subsurface medium and this generally requires saturated conditions.

The variogram calculations and model fitting within the thermal/mechanical and geohydrologic units did not always result in well-formed variograms. Several of these variograms show large nugget effects or a well defined initial range followed by the calculated points monotonically increasing with greater lag spacings (indicative of a possible trend in the sample data). Detrending of the data sets for recalculation of the variograms is not straightforward due to the use of two or three segments, each from a different transect within the variogram calculation. In most cases, it was possible to define a trend on one or two of the segments but not all of them. Additionally, if a trend was identified in a data set, it only applied to one segment.

Detrending the data sets towards the calculation of more well-defined variograms was not possible. For those variograms which are not well-defined, it is concluded that a separate variogram would have to be calculated for each thermal/mechanical unit and geohydrologic unit at each transect location. However, this effort at detrending identifies an important characteristic of the sample data collected on these vertical transects, that is the spatial correlation lengths of the properties are not stationary across the site. The reason for this nonstationarity is most likely due to the factors controlling the deposition of the tuffs. Furthermore, the presence of trends within the vertical data is most likely the result of deterministic processes controlling the nature of the property distribution. An example of this type of deterministic control is the differences in cooling history of the tuffs within the shardy base microstratigraphic unit as examined by (Rautman et al., 1993).

Conclusions

Currently there are not enough saturated hydraulic conductivity data nor sorptivity data to adequately define relationships between these two parameters and porosity. The available data do show a possible global relationship between porosity and sorptivity. The available saturated hydraulic conductivity data show that the relationship between porosity and saturated hydraulic conductivity can be defined for the welded and non-welded units, although this relationship is non-stationary. Relations between porosity and saturated hydraulic conductivity in the zeolitized, vitric and clay units are not observed with the present data set.

The average sample spacing used in the vertical outcrop transects appears to be adequate for the downhole sampling program, with the exception of the Topopah Spring units which may require a shorter sample spacing. Results of variogram calculations on the transects, as well as on the thermal/mechanical units and the geohydrologic units, indicate that vertical spatial correlation lengths are not stationary across the site. Strong vertical tends in hydrologic properties can exist on the microstratigraphic unit scale as evidenced in the shardy base microstratigraphic unit.

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