DOE/ER/60843--1

MATHEMATICAL AND GEOLOGICAL APPROACHES TO
MINIMIZING THE DATA REQUIREMENTS FOR STATISTICAL
ANALYSIS OF HYDRAULIC CONDUCTIVITY DISTRIBUTIONS

Project Number DE-FG04-89ER60843
August, 1990

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Submitted to the
U.S. Department of Energy
Office of Health and Environmental Research
Office of Energy Research

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SUMMARY TECHNICAL PROGRESS REPORT

This report constitutes a technical summary of progress on the 'Mathematical and Geological Approaches to Minimizing the Data Requirements for Statistical Analysis of Hydraulic Conductivity Distributions' project for the 12-month period extending from June 1, 1989 to June 1, 1990. More detailed information on each of the research activities can be found in the appendix.

Research conducted on the aquifer characterization project during the 12-month period includes items (1), (2), and (3) of Phase I and item (1) of Phase II, as described in the original proposal of July, 1988. In addition, research related to item (4) of Phase I has been initiated. Since both Phase I and Phase II extend beyond the initial 12-month period into years 2 and 3, these items are considered to be ongoing research activities. The following research was completed during the previous year:

- 1) Refinement of air-permeameter design, calibration of the permeameter with respect to laboratory constant-head permeameter tests on core samples of fluvial sediments, and statistical analysis of permeameter measurement error [Item (1), Phase I].
- 2) Collection of air-flow-rate data measured at the facies scale [Item (2), Phase I].
- 3) Mapping of depositional facies at an outcrop located west of Bosque, New Mexico [Item (3), Phase I].
- 4) Delineation of "permeability facies" from mapped depositional facies and geostatistical analysis of air-flow-rate data observed at the facies scale [Item (1), Phase II].
- 5) Evaluation of threshold-crossing theory as a means of inferring the correlation structure of permeability from morphological characteristics of the sedimentary deposits [Item (4), Phase I].

Refinement of Permeameter Design, Permeameter Calibration, and Statistical Analysis of Permeameter Measurement Error

Permeameter Design. In order to obtain a sufficient number of permeability measurements, a portable air minipermeameter was developed. Although the air permeameter is similar in principle to a device developed by Goggin and others at the University of Texas (UT) at Austin (1988a, 1988b), it follows a completely different design that results in a much more portable instrument. Since the Sierra Ladrones Formation deposits consist primarily of highly permeable unconsolidated material, it is necessary to apply a very small, yet accurately measurable pressure. Our new permeameter is accurate over the appropriate pressure range, but is only a fraction of the size and weight of the UT apparatus. The basis for the gravity-driven piston design was adapted from Heller

(1988). More detailed discussion of the permeameter design and operation has been included in the appendix.

Permeameter Calibration. Calibration of the air-permeameter has focused on comparing the intrinsic permeability measured with a laboratory constant-head water permeameter to permeability values calculated from air-flow-rate data using analytic equations. Results of the calibration are presented in the appendix. As the calibration process continues, problems inherent to the measurement of gas permeability, such as slippage at low pressures and non-Darcy behavior at high pressures, will need to be addressed (Katz et al., 1959). Numerical simulation of air-flow rates observed in both core and outcrop sediment samples will aid in the calibration effort by explicitly relating observed air-flow rates to intrinsic permeability.

Analysis of Permeameter Measurement Error. An analysis of variance (ANOVA) was performed on a set of logarithmic air-flow rates measured at 25 different locations to determine if variation of flow rates observed at these different locations could be attributed to permeameter measurement error rather than to actual variation in the properties of the sampled geologic material. The data set was comprised of 25 groups of data, each of which contained 2 or 3 replicate logarithmic air-flow-rate measurements observed at the same location. The variance of measurements within each group was compared to the variance of measurements between groups in an effort to determine whether the total variance of the logarithmic data set could be explained as the result of true variation in geologic materials or might instead be caused by an inability of the permeameter to replicate measurements. Dominance of within-group variance with respect to between-group variance would suggest that the flow-rate variance was largely due to variance inherent to the permeameter, while dominance of between-group variance would imply that changes in the flow rates from location to location are related to changes in the geology of the outcrop rather than to any instrument limitations. Results of the ANOVA indicate that the air-permeameter is a reliable device for measuring true variations in the permeability of geologic materials, and are presented in the appendix.

Collection of Air-Flow-Rate Data at the Facies Scale

No *a priori* sampling strategy was employed during collection of permeameter measurements. Rather, the approach has been to allow the observations to dictate further sampling strategy, thereby addressing the questions of interest as the study progresses. The primary purpose for collecting the air-flow-rate data is two-fold: first, to serve as the foundation for geologic interpretation and secondly, to permit calculation of geostatistical parameters on the basis of permeability measurements and to compare them to parameters inferred from the geologic record. A detailed description of the methodology used to locate and sample air-flow rates in the sedimentary deposits is presented in the appendix.

Mapping of Depositional Facies

Initial reconnaissance work at outcrops of the Sierra Ladrones Formation revealed that lithologic facies in the northern part of the study area west of Belen, New Mexico

were laterally continuous on the scale of tens of meters to a few kilometers. Similar packages of sediments were observed in both the north and south areas of the field site. Generally, these packages fine upward from coarse sand and gravel to soils and clays. As such, they are believed to represent major cycles of sedimentation. Some are dominated by stacked channels of gravel and coarse sand while others exhibit an abundance of laterally continuous paleosols and overbank material. In an effort to tie the sediments together from north to south, three such packages were noted and mapped on an enlarged topographic map. It is believed that these packages of sediments will aid in the interpretation of the large scale depositional environment. Further interpretation of the depositional environment is included in the appendix.

Delineation of "Permeability Facies" and Geostatistical Analysis of Air-Flow-Rate Data Observed at the Facies Scale

Two facies-scale studies of permeability distributions were conducted at the Sierra Ladrones Formation field site. In addition, a numerical experiment was performed in an effort to evaluate the statistical structure of the aquifer heterogeneity. Probability distributions of grain sizes were also derived using grain sizes observed in the study area. Results of geostatistical analyses of these data sets are presented in the appendix.

Histogram and Variogram Analysis. The most significant implication of the histogram analysis of the air-flow-rate data observed at the facies scale is that, in the deposits studied thus far, the distribution of air-flow rate as a surrogate to permeability approximates a lognormal distribution. The assumption that geologic variables are lognormally distributed has been made time and time again in studies of stochastic hydrology, but in most cases has not yet received proper field validation. Further work is necessary to see if this underlying probability distribution holds true for element- and formation-scale heterogeneities as well.

The second implication of the statistical analysis of the data is that observed and quantifiable geologic features such as cross-bedding, lateral and vertical changes in lithofacies, and changes in grain size appear to be strongly related to statistical parameters estimated on the basis of air-flow-rate data. Specifically, correlation scales estimated from variograms derived from "hard" flow-rate data obtained at the facies scale agree closely with the average dimensions of lithologic facies observed in outcrop. While some geostatisticians might deem this result trivial, it verifies a critically important hypothesis that will enable us to estimate spatial statistical parameters from geologic observations with relatively little "hard" data. Moreover, the derivation of admissible variograms from observed and mean permeability values suggests that permeability can, in fact, be described by some kind of intrinsic random field, and that the correlation structure of heterogeneity can be adequately described by the permeability variogram. This particular property of the random permeability field will greatly facilitate further geostatistical analysis.

Results of the variogram analysis to date appear to substantiate the hypothesis that there exists a quantifiable relationship between observed geologic structure and the statistical parameters of permeability fields. It has been shown that geostatistical parameters

such as correlation scale agree well with those that can be inferred from geologic observations. The extent of the agreement has yet to be determined rigorously. However, it is felt that the practice of studying geologic features in parallel with structural statistics of air-flow-rate data is warranted and necessary for realistic and practical characterization of aquifer heterogeneities.

Distribution Studies. In addition to studying the distributions of each sample set as a whole population, distributional analysis has also been carried out based on grain-size classes within sample sets. Distributional analysis of principal grain-size class data observed during the facies-scale permeability studies reveals that each class follows an approximately lognormal distribution and exhibits distinctively different means.

While delineating permeability according to grain size is common in the hydrologic sciences (Carmen, 1939; Freeze and Cherry, 1979; Milne-Home and Schwartz, 1989), investigation of the distributions of permeability according to grain-size classification may contribute additional proxy information in the estimation of permeability in natural geologic material. One of our primary goals is to develop methods of supplementing "hard" permeability measurements with "soft" geologic information. Grain size is an example of "soft" information that may be used in conjunction with indicator kriging to incorporate additional information into the geostatistical assessment of aquifer heterogeneity. As discussed in the appendix, it may also be possible to define and remove trends in the air-flow-rate data using grain size as proxy information.

Evaluation of Threshold-Crossing Theory

One of the primary objectives of the aquifer characterization study is the incorporation of "soft" geologic information into a mathematical framework for characterizing the spatial correlation structure of permeability in fluvial deposits. As discussed in the project proposal, threshold-crossing theory represents a systematic methodology for translating such qualitative information into a geostatistical framework that is inherently quantitative in nature. One of the many implications of threshold-crossing theory is that the correlation scale of a stationary random field at a particular spatial scale can be inferred from the gross morphology of that field. In a geologic context, the dimensions of mappable features in a stationary field at a given spatial scale, along with the variability of the properties of those features, will describe the correlation structure of the underlying random geologic process. Theoretical and numerical analyses of correlation scale as a function of the morphological characteristics of a random field have been included in the appendix.

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ANTICIPATED RESEARCH ACTIVITIES FOR 1991

It is expected that research conducted during 1991 will focus on continuation of research activities outlined in the original project proposal. These activities will involve permeameter calibration [Phase I: Item (1)], collection of air-flow-rate data at the facies scale [Phase I: Item (2)], mapping of depositional and "permeability" facies at selected outcrops [Phase I: Item (3) and Phase II: Item(1)], geostatistical analysis of facies-scale air-flow-rate data [Phase II: Item (1)], and evaluation of threshold-crossing theory [Phase I: Item (4)]. Further geostatistical analysis of air-flow-rate data will emphasize comparison of geostatistical parameters estimated from conventional variogram analysis to those calculated according to threshold-crossing theory, as discussed in item (1), Phase II of the original proposal. Geostatistical analysis will also include characterization of permeability distributions within sedimentary facies proposed in item(2), Phase I. Extension of threshold-crossing theory to locally-averaged, high-order, and non-Gaussian fields will also be implemented in keeping with the goals of item(4), Phase I. In addition, mapping and permeability testing of geologic units at intermediate- and element- scales will be initiated during the upcoming year. Finally, a systematic means of relating the sedimentary deposits of interest to statistical models will be developed in accordance with item (2), Phase II. This particular aspect of the study will help to resolve the issue of how the hierarchy of spatial dimensions of geologic entities relates to the anticipated hierarchical form of the nested permeability correlation structure.

In addition to the activities discussed above, we hope that further research will help to address problems that were encountered during the initial 12-month period of the aquifer characterization study. Problems incidental to the originally-proposed study that have significant implications with respect to the success of the aquifer characterization project include constraints on measuring permeabilities of clays and gravels and difficulties in the conceptualization of a quantitative framework based on spatial scale in the presence of geologic structures that defy classification based on scale. The development of a rigorous methodology for incorporating "soft" geologic information into this quantitative framework will also be a critical issue during 1991. Following is a brief discussion of recommended approaches for resolving these problems and issues:

Measurement of Clay and Gravel Permeabilities

Since extreme-value units play a key role in the determination of contaminant migration pathways, alternate methods of estimating the permeabilities of clay and gravel units need to be developed. A number of alternative methods of measuring clay and gravel permeability are under consideration. It may be sufficient to map out the spatial extent of extreme-value permeability deposits and incorporate that "soft" information into the analysis, particularly if they are characterized by much larger or smaller permeabilities than adjacent or overlying deposits. It may also be possible to correlate the compaction variables of the low-permeability clay to a permeability value (Harrop-Williams, 1985). If this approach can be validated on the specific clays of interest, then clay permeability may be estimated in the field from quick consolidation experiments. Another possibility

is to perform actual clay permeability tests in the field. A device described by Olson (1966) allows rapid measurement of clay permeability by observing the pressure response to a given influx of fluid. The problem of obtaining saturated clay samples in the field is still the major factor limiting the utility of such a device.

In a similar manner, it may be possible to draw an empirical correlation between type of deposit and permeability for gravels based on field permeameter tests. It is most likely that these field tests would require a large volume permeameter to ensure that a sufficient volume of gravel be sampled. The envisioned permeameter consists of a cylindrical water tank, approximately 1 meter in diameter, 0.5 meter in height, and open at the top. With the tank approximately two-thirds full, a 1-liter cylindrical sample of gravel screened at the bottom and open at the top is inserted so that there is approximately 1 cm difference between the water level in the tank and the water level in the sample cylinder. Once the system reaches steady state, the difference in head and the flow rate through the sample can be measured. The permeability can then be estimated based on Darcy's equation.

Conceptualization of a Hierarchical Scheme for Relating Geologic and Correlation Scales

A second difficulty encountered during the past year relates to the hierarchical permeability correlation structure made apparent during the intermediate scale numerical experiment. The development of a method for relating the progression of scales of sedimentary structures to the anticipated nested hierarchy of correlation scales will be critical to the successful characterization of fluvial-aquifer heterogeneity. Such a methodology may prove to be elusive because lithofacies and architectural elements, in general, transcend spatial scales. The current problem facing the quantification of such a hierarchical scheme is defining a suitable methodology to incorporate and study the spatial statistics of a system that defies a classification scheme based simply on spatial scale. Meaningful geological and geostatistical characterization at all scales will be pursued following the concepts of parameter averaging.

Development of a Methodology for Incorporating "Soft" Information into a Quantitative Framework

Finally, the problem of incorporating qualitative observations into what is essentially a quantitative methodology must be resolved. One possibility for incorporating "soft" grain size information into the statistical analysis is to use the distribution of permeability based on grain size to supplement "hard" permeability data taken from a region. Using an indicator approach, it is possible to incorporate prior information such as cumulative distribution functions into the estimation of permeability (Journel, 1989). Another possibility may be to incorporate geologic information on the spatial distribution of grain sizes in a deposit in order to better estimate the behavior of the mean. The estimated mean could then be used to remove trends from the permeability data, thereby maintaining an intrinsic permeability field and justifying the assumption of second-order stationarity essential to variogram analysis. Knowledge of the spatial distribution of permeability for a given grain size may enable us to delineate between a trend in the mean

and random fluctuation about the mean. Say, for instance, a variogram estimate is desired for a fining-upward sequence as we encountered in the facies-scale permeability study. The observed spatial distribution of grain sizes in the deposit would enhance our understanding the spatial distribution of the mean and constitute a physical justification for using a fitted trend model. Further study of how permeability is related to grain size, as well as the degree to which grain size and spatial patterns of grain size in sedimentary deposits reflect spatial permeability trends, may enhance our ability to incorporate proxy information into statistical analysis of hydraulic conductivity distributions.

In summary, further research activities during 1991 will be devoted to all research items pursuant to completion of Phases I and II of the original proposal. It is also intended that research not anticipated in the original proposal focus on 1) developing methods of obtaining field permeability measurements or estimates for gravels and clays, 2) addressing the question of how the geostatistics of nested structures and the rather evasive hierarchy of sedimentary bedding surfaces are interrelated, and 3) conducting experiments with various proxy structural estimators to determine the best method for removing trends and for optimizing the amount of available data.

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Appendix: Detailed Technical Progress Report

1.0 Refinement of Permeameter Design, Permeameter Calibration, and Statistical Analysis of Permeameter Measurement Error

A1.1 Permeameter Design. Figure A1 presents the basic design of the air-minipermeameter developed for the aquifer assessment study. A Becton-Dickenson® 100cc ground glass syringe was ground further with fine grit corundum to provide a fairly frictionless contact while maintaining an adequate seal between the piston and the syringe casing. The flow rate is obtained by automatic electric timing of the displacement of a known volume with a stopwatch, a set of photoresistors, and lamps. The tip seal is the part of the apparatus that governs the flow geometry at the permeameter/outcrop interface. The UT tip-seal design was modified so that the same flow geometry could be obtained on unconsolidated samples. The modification entails an increase in the outer diameter of the tip seal in order to provide structural stability when applied to an unconsolidated outcrop.

It has been noted in the literature (Journal and Alabert, 1988) that ground water flow depends greatly on the spatial distribution and interconnection of the extreme-value gravel and clay permeability units. Because of the problems associated with clay dessication and inadequate sampling volume in measuring gravel permeability, sampling of these extreme-value sediments remains a major stumbling block for experimental hydrologists. In order to measure the permeability of the clay and gravel units, new permeameter designs will have to be developed, or at least a methodology adopted that will enable estimation of the permeability of extreme-value deposits within a specified degree of certainty.

A1.2 Permeameter Calibration. Calibration results are shown in Figure A2. Large differences in volumes being sampled may be partially responsible for the absence of a one-to-one relationship between $\ln(k_w)$ and $\ln(k_a)$. The air-permeameter has a radius of investigation on the order of one centimeter, and thus samples approximately a 1cc. volume. However, the ring samples used for the constant-head tests are 5 centimeters in diameter and 5 centimeters in length, a volume of approximately 100cc. A one-to-one correlation of permeability measured from two such vastly different volumes should not be expected. While the calibration thus far has not resulted in a robust relationship between permeability derived from the constant head apparatus and air-permeability, the estimated correlation coefficient of 0.86 is encouraging. Simulation of air-flow-rate response using numerical models will aid in the calibration of air-flow rate with respect to permeability.

A1.3 Analysis of Permeameter Measurement Error. Table A1 shows the results of the analysis of variance. The mean square within groups, or the 'average' variation within groups (MSW), was estimated to be equal to 0.006, while the 'average' variation between groups (MSB) was calculated to be 1.183. The F-value, determined as the ratio MSB/MSW, was equal to 171.45, indicating that between-group variance was more than 2 orders of magnitude greater than within-group variance and likely not due to permeameter error. Since this value is much larger than the F-statistic of 1.79 estimated at a significance level of 5%, the null hypothesis that the means of the 25 groups of logarithmic flow rates are equal was rejected. Thus, variance of the data can not be related to random fluctuations in the response of the permeameter, but can be attributed to true variation in

1: 100cc syringe	7: circuit board switch
2: lamps (#222)	8: stopwatch switch
3: circuit board	9: stopwatch reset
4: photoresistors	10: battery pack
5: stopwatch	(4 'c' cells)
6: lamp switch	11: outlet to tip seal

1: #6 rubber stopper	2
2: foam rubber	
3: 1/8" o.d. grommet	3

Figure A1. Schematic diagram of air permeameter.

Figure A2. Comparison of log-permeabilities derived from air permeameter (k_a) and constant-head device (k_w).

Table A1.
Results of ANOVA for 25 groups of logarithmic air-flow-rate data.

Source of Variation	Sum of Squares (SS)	Degrees of Freedom (df)	Mean Square (MS)
Between Groups	28.39	24	1.183
Within Groups	0.25	42	0.006
Total	28.65	66	0.434

the nature of the sampled geologic materials. The results of the ANOVA confirm that the air permeameter is a reliable means of characterizing the structure of permeability variations in the Sierra Ladrones Formation fluvial deposits.

A2.0 Collection of Air-Flow-Rate Data at the Facies Scale

Spatially located permeability data are necessary for statistical analysis and interpretation of the depositional environment. The methodology developed for obtaining spatially located permeability is still in its infancy. It has resulted from a rather substantial set of constraints and it should be noted that the method described here is somewhat site specific.

At this stage of the research, we have chosen to neglect effects of diagenesis, such as cementation. Colluvial cover of the uncemented portion is highly variable, but generally only a few inches need be removed before uncemented, undisturbed deposits are encountered. The preparation of a permeability measurement site had two primary objectives: 1) to remove colluvial cover to expose undisturbed sediment, and 2) to obtain sampling locations that can be located efficiently.

The method of locating permeability measurement locations was based on a survey that establishes control points on the ridge. Outcrops were prepared for permeameter sampling by locally digging away the colluvial cover to obtain a vertical face of undisturbed deposit measuring approximately 3 meters by 1 meter. The outcrop was then photographed so that the location of permeability measurements could be recorded. The photograph of the prepared surface, including a scale, served as a base map on which the location of measurements were recorded. The sampling locations marked on the photograph were then digitized to obtain a set of "local" coordinates. Also digitized from the photograph were the surveyed control points.

The control points on the photograph allowed transformation of the "local" coordinates into the "global" coordinates of the study area. A similar type of locating scheme was employed to supplement the digout type study. In some locations, small surfaces measuring 15 centimeters by 15 centimeters were prepared and the permeability measurements were performed on a grid of known dimensions. Similarly, these "local" coordinates were then transformed into the "global" system. Figure A3 diagrammatically illustrates the permeability collection scheme. Two facies-scale sets of air-flow-rate data have been collected and are discussed in greater detail in section 4.0.

A3.0 Mapping of Depositional Facies

A large-scale reconnaissance effort conducted at the field site shown in Figure A4 indicated that major changes in depositional style occur at certain stratigraphic levels. A package of sediments was chosen to be the initial focus of the facies-scale mapping west of Bosque, New Mexico. The base of the current package under study is a gravelly channel deposit which lies unconformably on what is possibly an alluvial fan deposit. The upper contact is another large unconformity in which a series of stacked channels cut into the sediments under study. The package under study is approximately 25 meters thick at

Figure A3. Diagrammatic sketch of method used to locate permeability measurements.

Figure A4. Location of field site.

the location of OUTCROP1. OUTCROP1 trends approximately N35E, has an average slope of approximately 45 degrees, and a lateral dimension of approximately 60 meters.

The facies-scale mapping exercise was initiated in order to begin to define the architectural elements of this particular package. The goal of the facies-scale mapping was to define in detail some of the gross geologic features that were apparent from initial reconnaissance of the area. Mapping exercises began with a traditional survey with theodolite and rod. Prepared outcrops for permeability measurements were also surveyed. The survey data were then reduced and translated to a two-dimensional representation of the outcrop being studied. The second phase consisted of a more detailed geologic mapping of the outcrop. The surveyed points were supplemented with field sketches of the facies relationships. The field sketches were then transferred to a base map containing the control points. Clearly, a certain degree of spatial accuracy was forfeited at this scale so that an interpretive level of geologic detail could be incorporated into the study. It was important, however, that there be a geologic and hydrologic basis for definition of architectural elements at larger scales.

Miall's (1978) classification scheme shown in Table A2 was used as a basis for the classification of observed lithofacies. Lithofacies Smb, Sfl, and Sm were added to Miall's (1978) classification to include facies observed at OUTCROP1. Facies Smb consists of crudely crossbedded sand, sand size clay clasts, and armored mud balls. The basal contact of the Smb facies is commonly erosional. The facies Sfl is a fining upward sand facies. The genesis of the Sfl facies is uncertain, but it may represent proximal floodplain deposits. The third addition to Miall's (1978) classification is the facies Sm. The Sm facies is a massive sand in which most or all sedimentary structures have been destroyed. This facies is interpreted as an immature soil. A facies map of OUTCROP1 is presented in the attached plate.

Paleosol facies occur commonly in the study area. The soils preserved in the Sierra Ladrones Formation may be very useful in the delineation of major depositional cycles for two reasons. First, they indicate a long hiatus in fluvial deposition and may thus serve as an indicator of relative quiescence. Second, their general character of being very laterally continuous may make it possible to use the soils as a type of marker bed for the mapping of larger scale features. When studying the sedimentology of fluvial systems over distances on the order of kilometers, the paleosols provide a means to correlate different cycles of sedimentation (Allen, 1974). The correlation of these cycles of sedimentation is vital to the reconstruction of a depositional environment.

Four elements have been defined based on the facies observed at OUTCROP1 and are summarized in Table A3. The channel elements can be broken into two types, but more elements may be necessary as the study progresses. Additionally, it is likely that the definitions of the four elements observed thus far will be modified as more information is collected regarding their genetic origin. The two distinct types of channel elements preserved in the study area of OUTCROP1 include one that is generally dominated by clean fine-to-coarse grained sandy and gravelly facies, and a second element dominated by sand and sand size clay clasts. The former can be interpreted as the result

Table A2. Lithofacies observed in OUTCROP1 study.

Facies Code	Lithofacies	Sedimentary structure	Interpretation
Gms	massive, matrix supported gravel	none	debris flow deposit
Gm	massive or crudely bedded gravel	horizontal bedding, imbrication	longitudinal bars, lag deposits, sieve deposits
Gt	gravel stratified	trough crossbeds	minor channel fills
St	sand, medium to v. coarse, may be pebbly	solitary (theta) or grouped (pi) trough crossbeds	dunes (lower flow regime)
Sp	sand, medium to v. coarse may be pebbly	solitary (alpha) or grouped (omikron) planar crossbeds	linguoid, transverse bars, sand waves (lower flow regime)
Sr	sand, v. fine to coarse	ripple marks of all types	ripples (lower flow regime)
Sh	sand, v. fine to v. coarse, may be pebbly	horizontal lamination parting or streaming lineation	planar bed flow (l. and u. flow regime)
Sl	sand, fine	low angle ($< 10^\circ$) crossbeds	scour fill
Smb	erosional scours with mud balls	crude crossbedding	scour fill
Sfl	sand, v. coarse to fine	fining upward sand sequence	proximal floodplain
Sm	sand, v. fine to v. coarse, may be pebbly	none	immature soil
Sgm	sand, fine to v. coarse, pebbly	none	slumped bank ?
Fl	sand, silt, mud	fine lamination, very small ripples	overbank or waning flow deposits
Fsc	silt, mud	laminated to massive	overbank deposits
Fm	mud, silt	massive, desiccation cracks	drape deposits
Fr	silt, mud	rootlets	overbank
P	carbonate	pedogenic features	soil

Table A3. Architectural elements of OUTCROP1.

Element code	Lithofacies present	Description/ Comments
CH-I	Gm, Gt, Sp, St, Sl, Sgm	Channel element consists dominately of gravelly and coarse sand facies. Much of the element is covered by colluvium and will require further study elsewhere.
CH-II	Gms, St, Sp, Sfl, Sh, Sl, Smb, Fl, Fm, Fsc	Sand and sand size clay clasts dominate with local lag gravel deposits.
P	P, Sm, Fsc	Soils and stacked soils
OF	Fr, Fm, Fsc, P	Overbank fines

of a large, distal, braided, or meandering stream environment. The latter element is dominated by a much finer scale heterogeneity. Small-scale (0.1–1 m) scour fill structures, which suggest a tributary scale channel, have also been observed. The common occurrence of sand-size clay clasts and armored mud balls indicates that hardened mud drapes were ripped up, broken into sand size clasts, redeposited, and buried in a relatively short distance within the tributary channel. The occurrence of clay clasts and mud balls suggests that the channel was ephemeral in nature, since conditions of high fluvial energy would have likely been required to erode the mud drapes.

The overbank fine elements (OF) are composed of several distinct overbank deposits. Some of the elements contain weakly to moderately developed, stage I of McGrath and Hawley (1987), soil horizons. The paleosol elements (P) consist of soil horizons that are generally Stage I–II. Reconstruction of the depositional environment entails interpreting the relationships and extents of the elements mapped. The paleosol elements will be used as a basis for that interpretation.

The observed architectural elements and the models of Allen (1974) enable an interpretation of the depositional environment. It is hypothesized that the deposits of at least two types of channels are preserved in the study area. The occurrence of overbank fines and paleosols between these channel deposits indicate migration of the channel away from its previous position. It is not clear whether the deposits represent an environment in which two distinct types of channels coexisted throughout the depositional history, or one in which the channel character changed in time.

The sediments observed in the Sierra Ladrões Formation appear to reflect depositional environments ranging from high-energy channel deposits to low-energy overbank deposits. Thus, the deposits can be considered to represent a spectrum of the types of heterogeneities typically encountered in alluvial aquifer systems, and the overall approach used to characterize the Sierra Ladrões Formation can be assumed widely applicable to such aquifers. Continued mapping and interpretation of the architectural elements will

be necessary to further determine the depositional environment of this area. The geologic interpretation and reconstruction of a depositional environment is crucial to the description and prediction of lithologic distributions and, ultimately, to the characterization of aquifer heterogeneity.

4.0 Delineation of "Permeability Facies" and Geostatistical Analysis of Air-Flow-Rate Data Observed at the Facies Scale

Three air-flow-rate data sets have been analyzed using geostatistical methods. The first two facies-scale data sets consist of air-flow-rate data measured with the permeameter at small outcrops located at the field site. Analysis of the distribution and structural statistics have been conducted for each separate facies-scale data sets. The third data set, which was generated during a numerical experiment using estimated mean permeabilities, resulted from an effort to study the structural statistics of the intermediate-scale heterogeneity. Mean permeability was estimated from the literature based primarily on grain size and assigned to each facies, and variograms were derived from the estimated mean permeability data.

A4.1 Permeability study 1 (PS1). The location referred to as PS1 is located at the field site west of Bosque. The prepared outcrop is approximately 2 meters wide and 0.5 meters high. The outcrop appears to be a channel bar deposit dominated by a horizontally laminated coarse sand deposit. On top of what appears to be the major bar form, a variety of lithofacies are present. Horizontally-laminated fine to medium sands including magnetite and/or illmenite are interbedded with clay drapes, trough cross-laminated sands and ripple-laminated sands. This upper third of the outcrop is interpreted as representing a period of decreased, periodic flow. Two bioturbated zones which destroy the lateral continuity of the primary deposits were also observed and mapped. Each of the disturbed zones terminate upward at different stratigraphic locations, indicating at least two periods of relative quiescence. The prepared outcrop represents a small percentage of the overall deposit. That is, the deposit has a larger vertical and a much larger lateral extent than the sample space dimensions. Two-hundred and seventy-seven (277) measurements of air flow rate were obtained from PS1.

A histogram of the PS1 flow-rate data indicates a skewed-right distribution. After performing a natural logarithm transform of the original data, the logarithmic data appear to be normally distributed. Structural analysis via directional variogram estimation was also performed on the logarithmic data set. The horizontal variogram is presented in Figure A5. The number of data pairs are also shown on the variogram for each estimated covariance. An exponential variogram model with a slight nugget was used to fit the experimental variogram shown in Figure A5. The resulting fitted model is:

$$\gamma(\xi) = 0.04 + 0.27[1 - e^{(-|\xi|/40)}] \quad (1)$$

The nugget of 0.04 is approximately one order of magnitude larger than the mean square error within groups (MSW) estimated from the analysis of variance. Therefore, it may be partially attributed to measurement error associated with use of the air permeameter. The

Figure A5. Fitted horizontal variogram of logarithmic PS1 air-flow-rate data. Number of pairs in variogram calculation shown next to each estimate. (N = 277)

range of approximately 40 cm appears to correspond to the approximate average separation of the bioturbation zones. However, it will be necessary to conduct many more studies of similar nature to better understand the geologic foundation behind the correlation statistics. An experimental vertical variogram was not derived due to inadequate vertical sample dimension and an insufficient number of data pairs for many lag distances.

A4.2 Permeability study 2 (PS2). The second outcrop studied (PS2) is located west of Bosque in the lower channel element (type CH-I). PS2 is approximately 1.5 meters wide and 0.5 meter high. The outcrop can be characterized as a high energy channel deposit with crudely stratified to cross-stratified pebbly gravel interbedded with low angle cross-laminated and trough cross laminated fine to coarse sand. A zone of ripple laminated sand, representing a decrease in flow energy, occurs at the top of the outcrop.

Unlike the PS1 data set, the PS2 data represents approximately 80 percent of a depositional unit. That is, the spatial dimensions of the sample space approach the spatial dimension of the deposit. Eighty-six (86) measurements of air flow rate were obtained from PS2. Again, histogram analysis of the original data indicates a skewed-right distribution. When a natural logarithm transform was applied, an apparently normal distribution resulted.

Directional variogram analysis was performed on the logarithmic PS2 data in order to estimate the correlation structure. The horizontal variogram estimate is shown in Figure A6. Truncation of the variogram for lags greater than approximately 85 centimeters, or half of the sample space dimension, results in what appears to be either an exponential or "bell-shaped" (sometimes referred to Gaussian) variogram. Functionally, the

fitted variograms are given by :

$$\text{Exponential model: } \gamma(\xi) = 1.24[1 - e^{(-|\xi|/60)}] \quad (2a)$$

“Bell-shaped” (Gaussian) model:

$$\gamma(\xi) = 0.07 + 0.90[1 - e^{-(|\xi|/45)^2}] \quad (2b)$$

As in the case for PS1, the nugget in the “bell-shaped” model for PS2 is one order of magnitude larger than the mean square error within groups and can be considered partly the result of measurement error associated with use of the air permeameter. The correlation lengths of 45 and 60 centimeters both appear to correspond with the average horizontal dimension of the gravelly facies. Again, a vertical variogram was not estimated due to insufficient sample space dimension and data.

Geologic observations indicate the possibility of a trend in the mean in the vertical direction for both PS1 and PS2 data. Trend analysis was not considered feasible given the insufficient length of the vertical sample space dimension. However, grain size observations appear to offer the most reliable means of removing trends in the permeability data.

A4.3 Intermediate-Scale Permeability Studies

In addition to the two facies-scale permeability studies, a study was conducted to estimate the spatial statistics of permeability at a larger scale by maintaining the lithofacies distinction as a basis of analysis. The study entailed performance of a numer-

Figure A6. Fitted horizontal variogram of logarithmic PS2 air-flow-rate data. Number of pairs in variogram estimation shown next to each estimate. (N = 86)

ical experiment that helped to characterize the spatial distribution of mean lithofacies permeability. The utility in such an experiment lies in the ability to obtain large numbers of "measurements" so that a reliable structural analysis can be performed. This experiment is not intended to replace geostatistical analysis using actual measured values, but rather to help direct the investigation and give a preview of what one may expect to see at the larger scale.

The lithofacies observed at OUTCROP1 and shown in the attached plate were broken into four classes based on lithology and approximate permeability. The permeability estimates of Freeze and Cherry (1979) were used to estimate log-permeability of the observed lithologies. Although the resulting experimental variograms were not based on observed air-flow-rate measurements or permeability, they do reflect the overall correlation structure of the permeability field at the intermediate scale. The experimental horizontal and vertical directional variograms are presented in Figures A7 and A8. It was found that both directional variograms exhibit a hole effect, which reflects a positive correlation at some finite distance.

The shape of the horizontal variogram, while exhibiting a slight hole effect, conforms to the properties of an exponential model. After Journel and Huijbregts (1978), the model for the horizontal variogram is based on the product of the exponential and cosine covariance functions. A nested structure is also apparent in the horizontal variogram. This is described mathematically by appending an additional variogram model to the original one for all lags greater than the break at a lag of 17.5 meters. The resulting model is:

$$\gamma(\xi) = \begin{cases} \gamma_1(\xi) & \text{for } \xi < 17.5 \text{ meters} \\ \gamma_2(\xi) & \text{for } \xi \geq 17.5 \text{ meters} \end{cases} \quad (3)$$

$$\begin{aligned} \text{where } \gamma_1(\xi) &= 1.5[1 - e^{-\xi/3.3} \cos(0.3\xi)] \\ \gamma_2(\xi) &= \gamma_1 + 0.7\gamma_1(\xi - 17.5) \end{aligned}$$

The results of the horizontal variogram analysis also indicate that the statistical structure of permeability in natural geologic material reflects a well-defined nested hierarchy of scales. Thus, it may be possible to characterize each geologic entity as a separate geostatistically-homogeneous region. As discussed previously, removal of permeability trends using grain size information would permit the assumption of an intrinsic random field to be made even in the presence of permeability trends.

The vertical variogram shown in Figure A8 appears to be strongly periodic. As such, a trigonometric function was used to model the vertical variogram. The fitted function is: The wavelength of the variogram model is 2π (6.28) meters, which appears to correspond to the average repeatability of the facies in the vertical dimension.

$$\gamma(\xi) = \begin{cases} a|\xi| & \text{for } \xi < 2.45 \text{ meters} \\ 2.5 + 0.65\cos(\pi + \xi) & \text{for } \xi \geq 2.45 \text{ meters} \end{cases} \quad (4)$$

Figure A7. Fitted horizontal variogram estimate of intermediate scale study.

Figure A8. Fitted vertical variogram estimate of intermediate scale study.

A5.0 Evaluation of Threshold-Crossing Theory

A5.1 Correlation Scale as a Function of Excursion Length: Continuous Case. Philips and Wilson (1989) proposed that “soft” geologic information related to permeability of geologic materials be incorporated into a geostatistical framework using threshold-crossing theory developed by Vanmarcke (1983). Assuming a continuous, zero-mean, weakly stationary, Gaussian (normally-distributed) permeability random field and a “bell-shaped” autocovariance function, the expected value of the length of excursion above the mean permeability in the i th dimension parallel to the principal direction of permeability $E(l_i)$ was shown to be a linear function of the correlation scale λ_i in the i th dimension as follows:

$$E(l_i) = \sqrt{2\pi}\lambda_i \quad (5)$$

Figure A9 shows the theoretical linear relation between expected excursion length and correlation scale for the case of a “bell-shaped” covariance function. Also shown are average excursion lengths predicted from one-dimensional fields generated using the fast Fourier transform method for scales of 1, 2, 3, 5, and 10 spatial units and a variance of 1.

Figure A9. Theoretical and simulated relation between correlation scale and expected or average excursion length.

Expression (5) permits the estimation of correlation scale for a Gaussian, stationary, logarithmic permeability field described by a “bell-shaped” covariance function and characterized by a morphology that can be loosely delineated according to observable macroscopic geologic properties. Along with the variance of the field, the correlation

scale completely describes the stochastic nature of a weakly-stationary logarithmic permeability field. Air-flow-rate data collected at PS1 and PS2, however, suggest that the covariance may be described equally as well by an exponential function as it can by a "bell-shaped" function. In an effort to determine the influence of an exponential permeability covariance function on correlation scales estimated from threshold-crossing theory, a covariance function similar to the exponential function was used to derive a new expression describing the relation between expected excursion length above the mean and the correlation scale. In order to force the exponential covariance to be mean-squared differentiable at the origin such that the variance of the derivative of the field be finite and threshold-crossing theory applicable, the function was constructed to be "bell-shaped" at lags close to zero and exponential at points further from the origin. Thus, for all practical purposes, the hybrid function behaves similarly to the exponential covariance function and will henceforth be referred to as the modified exponential covariance function. The modified exponential covariance function, along with the "bell-shaped" and exponential covariance functions, are presented in Figure A10 for the case of variance and correlation scale equal to 1. As can be seen in the inset of Figure A10, the modified exponential function is mean-squared differentiable at the origin.

Figure A10. Exponential, "bell-shaped", and modified exponential covariance function.

Figure A9 shows the theoretical and simulated relationships between the expected or average excursion length and correlation scale for the case of the modified exponential covariance function. It is evident that, for a given estimate of average excursion length above the mean, adoption of the exponential covariance function will generate a correlation scale that is approximately 4 times larger than would be estimated on the basis of a "bell-shaped" covariance. The reduced continuity associated with the exponential covariance was anticipated because the exponential covariance decays much more rapidly with increasing separation distance than the "bell-shaped" covariance, giving rise to fields in which morphological features are less spatially interconnected. It is clear that the correlation scale estimated on the basis of threshold-crossing theory using the observed morphology of the permeability field may be quite sensitive to the form of the covariance function assumed. Accurate estimation of the correlation scale is essential if the correlation structure of the field is to be maintained during predictive phases of the study. It is hoped that collection of additional air-flow-rate data will help to better define the appropriate form of the covariance functions typical of fluvial deposits at all spatial scales of interest.

A5.2 Correlation Scale as a Function of Averaging Length: Discrete Case

While threshold-crossing theory as applied to continuous fields has significant utility with respect to characterizing the correlation structure of the Sierra Ladrone Formation permeability field, the lack of continuous geologic exposure in portions of the study area will somewhat constrain the applicability of continuum theory to the problem of defining the correlation structure of the fluvial deposits. In the absence of continuous mappable features, it will be necessary to interpolate or "average" the observable morphology of the field to regions where little or no geologic information is available. Moreover, the manner in which facies are grouped, which effectively amounts to averaging of aquifer properties, is expected to have a significant impact on the perceived correlation structure of the permeability field. Under such conditions, the effect of spatial averaging on both variance and correlation scale of the logarithmic permeability field will be of great concern.

In order to assess the impacts of spatial averaging extent on these geostatistical parameters, a numerical experiment was conducted. The experiment involved generation of a two-dimensional grid of square cells, each of unit area. Using a Monte Carlo approach, these square cells can randomly be assigned values of 0 or 1 on the basis of a uniform probability density function. An example of the resulting "checkerboard" pattern, which represents a field of discrete, uncorrelated random variables, is shown in Figure A11. A new discrete averaged random field was generated by calculating weighted averages of the cell values over a square block of specified dimension L that was displaced at discrete intervals over the original uncorrelated field. These weighted averages were assigned to the point located at the center of the averaging block to define the new field. Boundary effects were avoided by performing the averaging over a subset of cells interior to the original grid. To the extent that L is a smoothing operator, it can be viewed as a surrogate to expected excursion length, with larger, more "smoothing" values of L corresponding to larger average excursion lengths. As the spatial scale of interest increases this smoothing effect will be the natural consequence of the process of grouping facies into

Figure A11. Example of “checkerboard” field of uncorrelated random variables.

facies assemblages and assemblages into architectural elements. The numerical experiment amounts to an extension of threshold-crossing theory to a discrete random field with minimal *a priori* assumptions regarding the form of the underlying covariance structure.

Figure A12 illustrates the effect of such averaging on experimental covariances using square blocks ranging in dimension from 0.05 to 3 units. The covariances have been normalized to a variance of 1.0. Note that these are exact theoretical results and are not based on a Monte Carlo approach. Unlike the original field, the averaged fields are second-order stationary, as evidenced by the fact that covariances approach zero at large separation distances and that the variance of each field is finite. Stationarity is, in fact, characteristic of fields derived from moving averages of uncorrelated fields. It is exactly such an averaging mechanism typical of most geologic phenomena that lends correlation structure to the local randomness of fields generated by natural physical processes. As expected, larger blocks of averaging produce longer correlation scales and more “bell-shaped” behavior due to the greater extent of overlap between averaging domains for larger block dimensions, giving rise to a greater degree of correlation between points centered in the blocks and a smoother, more connected field.

Figure A13 shows the effect of block size L on both the correlation scale and the variance of the random field generated by the moving average procedure. The variance decreases with increasing L due to the smoothing effect of increasing block size, as a greater number of cells are included in the block average and block properties become progressively more homogeneous. In the limiting case for which block size L is equal to the dimension of the grid, the averaged domain is physically homogeneous and the variance approaches zero. Like the continuous case, the correlation scale increases approxi-

Figure A12. Experimental covariance functions generated by various values of averaging block dimension (L).

Figure A13. Correlation scale and variance as a function of L .

mately linearly with respect to the averaging dimension L (surrogate to excursion length) for values of L greater than or equal to the cell size of 1. For values of L less than 1, the correlation scale is somewhat insensitive to the averaging dimension because changes in the dimensions of the averaging block do not have a pronounced smoothing effect on the field when the averaging blocks are of smaller dimension than the unit cells. As the spatial scale of interest and the extent of spatial averaging increases, the correlation scale will increase without bound.

The effect of averaging dimension L on spatial correlation scale and variance has significant implications for characterizing the permeability field of the Sierra Ladrone Formation deposits. Results of the numerical experiment suggest that correlation scale, in particular, will depend on the degree of spatial averaging of geologic information as progressively larger packages of sediments are lumped into statistically-homogeneous groups. Continued experimentation with both observed and artificially-constructed permeability fields will serve to quantify the sensitivity of geostatistical parameters and generated random fields to spatial averaging extent.

SW

NE

Facies Map of Outcrop-1