Assessment of Effectiveness of Geologic Isolation Systems

A Technology Demonstration: Geostatistical and Hydrologic Analysis of Salt Areas

September 1982

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EXECUTIVE SUMMARY

The Office of Nuclear Waste Isolation (ONWI) requested Pacific Northwest Laboratory (PNL) to: 1) use geostatistical analyses to evaluate the 'adequacy' of hydrologic data from three salt regions, each of which contains a potential nuclear waste repository site; and 2) demonstrate a methodology that allows quantification of the value of additional data collection. The three regions examined are the Paradox Basin in Utah, the Permian Basin in Texas, and the Mississippi Study Area. Additional and new data became available to ONWI during and following these analyses; therefore, this report must be considered a methodology demonstration rather than a preliminary assessment for any salt site. However, the methodology demonstrated here would apply as illustrated had the complete data sets been available.

A combination of geostatistical and hydrologic analyses was used for this demonstration. Geostatistical analyses provided an optimal estimate of the potentiometric surface from the available data, a measure of the uncertainty of that estimate, and a means for selecting and evaluating the location of future data. The hydrologic analyses included the calculation of transmissivities, flow paths, travel times, and ground-water flow rates from hypothetical repository sites. Simulation techniques were used to evaluate the effect of optimally located future data on the potentiometric surface, flow lines, travel times, and flow rates. Data availability, quality, quantity, and conformance with model assumptions differed in each of the salt areas. Report highlights for the three locations are given below.

PARADOX BASIN

In the evaluation of the upper and lower hydrostratigraphic units of the Paradox Basin, geostatistical analyses showed that the potentiometric surface of the upper unit can be estimated with an error of less than 700 ft within the area encompassed by the data. This figure is based on a data set of 46 points. Thirty-one of these are spring measurements and some may represent perched water, which may not be connected with the regional aquifer. This may partially explain the high error for this unit.

Because the lower hydrostratigraphic unit provides the hypothetical outflow of a repository breach to the biosphere under the assumed conditions, both geostatistical and hydrologic analyses were performed for this unit. The conclusions of the analyses are:

- The potentiometric surface of the lower hydrostratigraphic unit is moderately well known, with estimation errors of less than 300 ft. This is greater than the expected measurement error. Additional potentiometric data to be obtained from a well in Cottonwood Canyon will most effectively improve the information contained in the data base because of the well's location in an area of currently high uncertainty.
- The flow rate of ground water in the lower unit from a hypothetical repository location (Lavender Canyon), under both nominal^(a) and simulated^(b) cases, is quite low at less than 40 gpm (gallons per minute).
- The variations of the curves for travel time and ground-water flow rate define the uncertainties associated with the current potentiometric data base. The magnitudes of the flow rates and their uncertainties, in comparison to the surface-water flow rate of the Colorado River near the hypothetical repository site, may be inconsequential.
- The estimation error of the potentiometric surface results in flow rates varying by an average factor of 1.1 for steady-state ground-water flow, and by an average factor of 1.6 for a hypothetical 1000-year repository breach.

This study was limited in scope and did not address other uncertainties that could affect travel times and flow rates. These additional parameters are porosity, permeability, aquifer thickness, sorption, diffusion, and fluid density.

(a) 'Nominal' refers to the surface derived from the data and the conceptual model.

(b) 'Simulated' refers to the geostatistically adjusted surface based on hypothetical new well location data.

MISSISSIPPI STUDY AREA

In the Mississippi Study Area, the water-table surface can be estimated with estimation errors between 20 and 50 ft within the area containing the data. The analysis of the deeper aquifers showed the necessity of using a three-dimensional geostatistical and hydrologic analysis. Three-dimensional geostatistical surface estimates were completed and preliminary velocity calculations showed that water density variations are important considerations if directions of ground-water flow from the salt domes are to be predicted realistically. A three-dimensional hydrologic analysis, however, was beyond the scope of the study.

PERMIAN BASIN

For the Permian Basin in Texas, ONWI requested PNL to evaluate the Wolfcampian aquifer. Preliminary geostatistical analyses were performed on the first set of data that was provided by the Texas Bureau of Economic Geology (TBEG). A review of the analyses at ONWI demonstrated a high degree of uncertainty, and additional data were provided by TBEG. Preliminary hydrologic analysis performed on the second data set indicated that either grouped erroneous measurements exist in the data set, or that the Wolfcampian aquifer is in hydraulic connection with other units. Hydrologic modeling in two dimensions was not attempted under these circumstances. Preliminary geostatistical analysis indicated that no correlation existed among the data; this implies that the data are effectively random. These results were discussed with TBEG, who then provided a third data set to PNL. Time and funding constraints did not allow analysis of the third data set.

Because of the substantial differences between the combined first and second data sets compared to the third data set, PNL considers that reporting any results on the first and second data sets would be misleading and inappropriate.

The experience of working with data from salt areas, which are considered to be potential geologic waste repository sites and which are undergoing hydrogeologic characterization, led to two general conclusions and recommendations:

- Geostatistical and hydrologic analyses should be integrated with the field work as soon as possible after data collection begins. This would allow additional characterization data to be collected while the study is in progress, creating a more cost-effective data base.
- Methods to couple data uncertainties through the calculation of flow rates and travel times should be defined and used. This will allow a quantification of all uncertainties affecting flow, and will identify areas where new data will provide the most useful information. That is, determining new data locations would reduce the data uncertainty in light of total repository performance.

CONTENTS

ACKNOWLEDGMENTS	iii
EXECUTIVE SUMMARY	v
INTRODUCTION	1
CONCLUSIONS AND RECOMMENDATIONS	5
PARADOX BASIN	7
HYDROGEOLOGIC CONCEPTUAL MODEL	7
GEOSTATISTICAL ANALYSIS--UPPER HYDROSTRATIGRAPHIC UNIT	13
Potentiometric Surface Estimation	14
Estimation Errors	14
Identification of Anomalous Data	14
Location of Future Data	17
GEOSTATISTICAL ANALYSIS--LOWER HYDROSTRATIGRAPHIC UNIT	17
Potentiometric Surface Estimation	18
Estimation Errors	18
Identification of Anomalous Data	18
Reduction in Variance Analysis.	21
HYDROLOGIC ANALYSIS	23
Potentiometric Surface Adjustment	23
Hypothetical Repository Siting	25
Ground-Water Flow in Lower Hydrostratigraphic Unit.	25
Reduction in Variance--Location of Future Data	27
Flow Analysis	27
Aquifer Evaluation	35
SIMULATION OF ADDITIONAL DATA	38

Assessment of Effectiveness of Geologic
Isolation Systems

A TECHNOLOGY DEMONSTRATION:
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ANALYSIS OF SALT AREAS

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Potential Surface	40
Spatial Transmissivity	41
Aquifer Evaluation	41
Lavender Canyon Evaluation	44
CONCLUSIONS	45
MISSISSIPPI STUDY AREA	47
CONCEPTUAL MODEL	47
GEOSTATISTICAL ANALYSES OF THE TOP OF THE FRESH-WATER POTENTIOMETRIC SURFACE	48
Potentiometric Surface Estimation	53
Estimation Errors	53
Identification of Anomalous Data	54
Analysis of the Location of Future Data	54
GEOSTATISTICAL AND HYDROLOGIC ANALYSES OF THE DEEP AQUIFERS	59
CONCLUSIONS	64
PERMIAN BASIN	65
REFERENCES.	67
APPENDIX A – GEOSTATISTICAL THEORY	A.1
APPENDIX B – INVERSE METHOD TO CALCULATE TRANSMISSIVITY	B.1
APPENDIX C – PARADOX BASIN SIMULATION RESULTS	C.1
APPENDIX D – THREE-DIMENSIONAL FLOW EQUATIONS	D.1

FIGURES

1	Paradox Basin Study Area	8
2	Generalized Composite Stratigraphic Column for the Paradox Basin	9
3	Potentiometric Surface of the Upper Stratigraphic Unit of the the Paradox Basin	11
4	Potentiometric Surface of the Lower Hydrostratigraphic Unit of the Paradox Basin	12
5	Geostatistically Estimated Potentiometric Surface of the Upper Hydrostratigraphic Unit of the Paradox Basin	15
6	Estimated Error Map for the Upper Hydrostratigraphic Unit of the Paradox Basin	16
7	Geostatistically Estimated Potentiometric Surface of the Lower Hydrostratigraphic Unit of the Paradox Basin	19
8	Estimated Error Map for the Lower Hydrostratigraphic Unit of the Paradox Basin	20
9	Percent Reduction in Variance Map of the Lower Hydrostratigraphic Unit of the Paradox Basin	22
10	Geostatistically Estimated Potentiometric Surface of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Nominal Case	24
11	Location Map of Wells and Hypothetical Repository Site Used in the Paradox Basin Hydrologic Analysis	26
12	Percent Reduction in Variance Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Nominal Case	28
13	Hydrologic Model Boundary Used in the Paradox Basin Flow Analysis	30
14	The Subregion Hydrologic Model Boundary Used in the Paradox Basin Flow Analysis	31
15	Smoothed Subregion Potentiometric Surface for the Lower Hydrostratigraphic Unit of the Paradox Basin	32
16	Flow Net Used in the Transmissivity Calculation for the Paradox Basin Flow Analysis	33

17	Flow Net Showing Calculated Transmissivities (ft ² /day) at the Center of Each Flow Net Element	34
18	Transmissivity Map for the Lower Hydrostratigraphic Unit of the Paradox Basin	36
19	Streamtubes Showing the Path of Ground Water Flowing from the Lavender Canyon Hypothetical Respository	37
20	Arrival Time Curve for the Lavender Canyon Hypothetical Respository	39
21	Summary Arrival Time Curve for the Lavender Canyon Hypothetical Respository	43
22	An Example of a Geohydrologic Response Function	44
23	Geohydrologic Response Function Curve for the 1000-Year Period for the Lavender Canyon Hypothetical Respository	45
24	Mississippi Study Area	49
25	Mississippi Study Area Stratigraphic Column	51
26	Geostatistically Estimated Top of Fresh-Water Surface.	52
27	Potentiometric Map of Top of Fresh-Water Surface.	55
28	Estimation Errors for Top of Fresh-Water Surface	57
29	Percent Reduction in Variance for the Top of Fresh-Water Surface	58
30	Vertical Cross-Section of Estimated Pressure Surface Through Richton and Cypress Creek Domes	61
31	Vertical Cross-Section of Estimated Density Surface Through Richton and Cypress Creek Domes	62
B.1	Streamtubes and Streamtube Elements Showing the Relationship of the Variables Used in the Transmissivity Calculation	B.2
C.1	Geostatistically Estimated Potentiometric Surface for the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (High) – Well B (High)	C.3
C.2	Transmissivity Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (High) and Well B (High).	C.4

C.3	Streamtubes from the Lavender Canyon Hypothetical Repository for the Case: Well A (High) – Well B (High)	C.5
C.4	Arrival Time Curve for the Lavender Canyon Hypothetical Repository for the Case: Well A (High) – Well B (High)	C.6
C.5	Geostatistically Estimated Potentiometric Surface for the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (High) – Well B (Low)	C.8
C.6	Transmissivity Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (High) – Well B (Low)	C.9
C.7	Streamtubes from the Lavender Canyon Hypothetical Repository for the Case: Well A (High) – Well B (Low)	C.10
C.8	Arrival Time Curve for the Lavender Canyon Hypothetical Repository for the Case: Well A (High) – Well B (Low)	C.11
C.9	Geostatistically Estimated Potentiometric Surface for the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (Low) – Well B (High)	C.13
C.10	Transmissivity Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (Low) – Well B (High)	C.14
C.11	Streamtubes from the Lavender Canyon Hypothetical Repository for the Case: Well A (Low) – Well B (High)	C.15
C.12	Arrival Time Curve for the Lavender Canyon Hypothetical Repository for the Case: Well A (Low) – Well B (High)	C.16
C.13	Geostatistically Estimated Potentiometric Surface for the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (Low) – Well B (Low)	C.18
C.14	Transmissivity Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (Low) – Well B (Low)	C.19
C.15	Streamtubes from the Lavender Canyon Hypothetical Repository for the Case: Well A (Low) – Well B (Low)	C.20
C.16	Arrival Time Curve for the Lavender Canyon Hypothetical Repository for the Case: Well A (Low) – Well B (Low)	C.21

TABLES

1	Arrival Time Data for the Lavender Canyon Hypothetical Repository Site	39
2	Geostatistical Potential Estimates for Hypothetical Well Locations in Paradox Basin	40
3	Vertical Component of Force for Selected Elevations on a Transect Through Richton and Cypress Creek Domes.	63
C.1	Arrival Time Data for the Lavender Canyon Hypothetical Repository Site for the Case: Well A (High) and Well B (High).	C.6
C.2	Arrival Time Data for the Lavender Canyon Hypothetical Repository Site for the Case: Well A (High) and Well B (Low)	C.11
C.3	Arrival Time Data for the Lavender Canyon Hypothetical Repository Site for the Case: Well A (Low) and Well B (High).	C.16
C.4	Arrival Time Data for the Lavender Canyon Hypothetical Repository Site for the Case: Well A (Low) and Well B (Low)	C.21
D.1	Well No. 11 Water Level Data	D.2

INTRODUCTION

The Office of Nuclear Waste Isolation (ONWI) requested Pacific Northwest Laboratory (PNL) to: 1) use geostatistical analyses to evaluate the "adequacy" of hydrologic data from three salt regions, each of which contains a potential nuclear waste repository site; and 2) demonstrate a methodology that allows quantification of the value of additional data collection. The three regions examined are the Paradox Basin in Utah, the Mississippi Study Area in Mississippi, and the Permian Basin in Texas. The original purpose of the work was to provide technical information to aid a decision concerning which of the three regions should be further evaluated. The decision was to be made by the end of CY-81, but has been postponed for another year.

This study demonstrates how geostatistical and hydrologic analyses can be used to determine whether the available regional data bases allow accurate evaluation of ground-water flow from a hypothetical nuclear waste repository. The study also indicates where more data, if required. Essential data in a hydrologic investigation are hydraulic head or potential, permeability, porosity, and aquifer geometry. From discrete measurements, a spatial distribution of these parameters can be inferred. The question of whether the available discrete measurements are adequate to define their spatial distribution really asks if enough wells have been drilled to adequately characterize the hydrologic system. The scope of this study is limited to geostatistical evaluation of hydrologic potentials, and the resulting implications for ground-water flow.

Geostatistical analyses are objective techniques that provide an optimal estimate of the potentiometric surface from the available data, a measure of the uncertainty of that estimate, and a means for selecting and evaluating the location of future data. Because an evaluation of the 'adequate characterization' of hydrologic data is not a specific enough objective with which to work, two operational questions determining 'adequate characterization' are appropriate here:

- Can the surface in all areas within the region of interest be estimated with an estimation error approaching the measurement error of

one data point? The error incurred in estimating a surface from discrete data points contains both a measurement error and a spatial estimate (interpolation) error. When the estimation error of the surface approaches the measurement error, additional data provide little additional knowledge of the surface.

- Will the addition of new potentiometric data change the computed values of ground-water flow rates and travel times significantly? The potentiometric surface is not the end product of a hydrologic characterization, but it is used to estimate the real parameters of interest: If a repository failure occurs, where will the ground water that has been in contact with the repository go; what is the minimum travel time to the biosphere; and what will the ground-water outflow quantity be? Conceivably, when the data are adequate, changes in the potentiometric surface caused by the addition of new data may cause little change in the flow lines, travel times, or quantity of outflow.

Based on the above definitions of 'adequate characterization', PNL's demonstration evaluation of the hydrologic data at the three salt regions is twofold:

- geostatistical analysis—to provide an estimate of the potentiometric surface with the resulting estimation uncertainties
- hydrologic analysis—to assess the effect of changes in the potentiometric surface on the estimated transmissivity, flow lines, travel times, and ground-water flow rates.

Geostatistical models are based on the assumption that the surface can be described by a deterministic component, which is estimated by a local polynomial structure, and by fluctuation, which in turn has a spatial component and can be described by an autocovariance function. For a brief description of the geostatistical theory, see Appendix A. The geostatistical analysis of the potentiometric surface produces the best representation of the surface based on the available data. The result of the geostatistical analysis is the optimal characterization of the surface (given the geostatistical model) in

the form of estimates on a regular grid. These are conveniently represented as a contour map of the surface. Because it is a statistical method, it also produces the estimation error associated with the surface. At each grid point where the surface is estimated, an estimation error is incurred. This estimation error is a function of the locations of the data used to estimate the surface and the geostatistical model.

Based on the estimated surface and the estimation error, geostatistical analyses can be used to identify anomalous data. An extremely valuable by-product of a geostatistical analysis is the identification of data points that deviate significantly from the model. These statistical analyses efficiently detect incorrect data such as transcription errors and (for hydrologic applications) data that are not part of the flow system under study. For example, geostatistical analyses have identified wells located in zones of perched water at the Hanford Site (Doctor 1979). Geostatistical analyses can be used to evaluate the effect of future data on the surface. Again, because the analyses are statistical, producing an estimation error, they allow us to analyze the effect of additional data without actually obtaining them. This helps us select the location of future data, as does cultural, hydrologic, and geologic criteria.

The purpose of the hydrologic modeling is to examine the effects of changes in the potentiometric surface on the final results of a hydrogeologic site characterization. The hydrologic modeling reported here is therefore a sophisticated form of sensitivity analysis on potentiometric head, and not a detailed examination of all facets of the flow system. The model is as detailed as the data base allows at the present time.

Hydrologic analyses examine the individual data bases in two major stages: through an examination of the flow field from known data and through a re-examination based on simulated data. First, the flow system is analyzed based on the present data base. This analysis uses the potentiometric surface as determined from geostatistics, and determines the flow system from the hypothetical repository. The spatial transmissivity for the area is determined by solution of the inverse problem using known boundary conditions. An average regional porosity value and aquifer thickness are used to calculate ground-

water flow quantities and travel times. The modeling of ground-water flow from a hypothetical repository location is summarized by geohydrologic response functions (Nelson 1981). Geohydrologic response functions allow an examination of the flow front arriving at a line of evaluation, and hence reflect all known hydraulic factors of the flow system.

The second major stage of the hydrologic analysis involves using simulations of additional potentiometric data and an analysis of the resulting changes to the geohydrologic response functions. The expected data extremes are estimated for each proposed additional well site by the use of geostatistics. Knowing the expected range of potentiometric values at a new data location allows the flow evaluation to be repeated, using the expected high and low values. That is, for each geostatistically expected extreme value of potential, a new potentiometric surface, a new spatial transmissivity, new pathlines, and new geohydrologic response functions are generated.

Through comparison of the nominal (known data) and simulated geohydrologic response functions, advantages of additional data collection can be determined. If the geohydrologic response functions for the various conditions are superimposed, the hydrology is considered sufficiently well known, and the data base adequate. If the geohydrologic response functions, including their uncertainties, demonstrate that expected extreme conditions violate the minimum criteria for travel time or flow quantity, additional data must be collected to confirm or refute such prohibitive conditions.

Each salt region is discussed in a separate section in this document. The geostatistical and hydrologic analyses described above have been completed for the Paradox Basin. The complete two-dimensional hydrologic analysis described above is not appropriate for the Mississippi Study Area because the vertical ground-water flow and fluid density variations require three-dimensional analysis. The analyses of the Permian Basin were terminated because of the time delays in receiving a complete data set.

CONCLUSIONS AND RECOMMENDATIONS

Working with hydrologic data from salt areas that are considered to be potential geologic waste repository sites, and that are in the process of hydrogeologic characterization, led to two general conclusions and recommendations:

- Geostatistical and hydrologic analyses should be integrated with the field work as soon as possible after data collection begins. This would allow additional characterization data to be collected while the study is in progress, creating a more cost-effective data base.
- Methods to couple data uncertainties through the calculation of flow rates and travel times should be defined and used. This will allow a quantification of all uncertainties affecting flow, and will identify areas where new data will provide the most useful information. That is, determining new data locations would reduce the data uncertainty in light of total repository performance.

Geostatistical and hydrologic analyses can help guide the field work by identifying deficiencies in the data as soon as possible. The geostatistics can also be used to help select the best locations for additional data.

The only uncertainties dealt with in this study were the uncertainties in the potentiometric surface. They were used to evaluate the precision of the estimated surface itself. However, uncertainties exist in the aquifer thickness, fluid density, rock permeability, and porosity data as well; permeability data are inherently more variable than potentiometric data. The variability in the permeability data may affect the results of hydrologic modeling more than variability in the potentiometric data. The method used in this report to calculate transmissivities is susceptible to uncertainties in the potential surface, its gradient, and flow net geometry. Inverse methods are being developed to minimize these effects (Arnold 1981).

Methods must be developed to carry the data uncertainties through all stages in the hydrologic analysis process to the final calculation of travel times and flow rates. Some work has been done in this area. Devary and

Doctor (1981) developed a method to combine the estimation errors for the potential and hydraulic conductivity surfaces to estimate an error for the resulting pore velocity. Oster and Gibbs (1981) are developing a method to calculate the variance of contaminant concentrations in the transport equation from estimates of the velocity variances.

PARADOX BASIN

The Paradox Basin is located in southeast Utah and southwestern Colorado. For this report, the Paradox Basin Study Area (henceforth referred to as the Paradox Basin) is restricted to Utah (see Figure 1). Of particular interest is the area defined by the zero isopleth of the Pennsylvanian salt beds. This area encompasses 10,000 square miles of the Canyon Lands section of the Colorado Plateau physiographic province. The climate is semiarid and rainfall averages 9 to 12 in./year (Hunt 1967). Figure 1 shows the western boundary of the salt deposit, which is commonly referred to as the "zero salt line."

The Paradox Basin contains Precambrian to Cenozoic strata. Figure 2 presents the composite stratigraphic column for the area. The upper Paleozoic formations, which include the bedded salt deposits, are the concern of this study. During the Mississippian period, the region was covered by a broad, shallow sea and deposits of limestone and dolomite formed. Later in the middle-Pennsylvanian period, the Paradox Basin began to subside, forming a depositional trough. The sea was intermittently landlocked during the subsidence, causing periodic evaporation of the water body. The resulting Paradox Formation in the central portion of the basin contains over 5000 ft of bedded salt and shale representing 29 cycles of inland sea formation and evaporation. The Paradox Formation would be the host medium for a potential repository. Permian sandstones and shales up to 2000 ft thick overlie the Paradox Formation.

HYDROGEOLOGIC CONCEPTUAL MODEL

A basic understanding of an aquifer flow system is expressed in the hydrogeologic conceptual model. The hydrogeologic data for the Paradox Basin indicate that a minimum of three hydrostratigraphic units exist. A hydrostratigraphic unit consists of a formation (or series of formations) with considerable lateral extent that composes a reasonably distinct hydrologic system.

The upper hydrostratigraphic unit of the Paradox Basin contains all of the strata above the Paradox Formation and contains 2600 to 4000 ft of

FIGURE 1. Paradox Basin Study Area (After Thackston et al. 1981)

Erathem	System	Rock Unit
CENOZOIC	Quaternary	Alluvial, Eolian and Glacial Deposits
	Tertiary	Igneous Rock
MESOZOIC	Cretaceous	Mesaverde Group
		Mancos Shale
		Dakota Sandstone
		Cedar Mt Formation Burro Canyon Formation
	Jurassic	Morrison Formation
		Bluff Sandstone
		Summerville Formation ?
		Curtis Formation ?
		Entrada Sandstone
	Triassic	Carmel Formation
		Navajo Sandstone
		Kayenta Formation
		Wingate Sandstone
		Chinle Formation
		Moenkopi Formation
PALEOZOIC	Permian	White Rim (De Chelly) Sandstone
		Organ Rock Shale
		Cedar Mesa Sandstone
		Elephant Canyon Formation
	Pennsylvanian	Honaker Trail Formation
		Paradox Formation
		Pinkerton Trail Formation
		Molas Formation
	Mississippian	Redwall Limestone (west side)
		Leadville Limestone (east side)
		Ouray Limestone
	Devonian	Upper Elbert Member
		Elbert Formation
		McCracken Sandstone Member
	Cambrian	Aneth Formation
		Lynch Dolomite ?
		Muav Limestone
		Bright Angel Shale
		Ignacio Formation (quartzite)
Pre-Paleozoic	Pre-Cambrian	Basement Complex of Igneous and Metamorphic Rock

FIGURE 2. Generalized Composite Stratigraphic Column for the Paradox Basin (After Thackston et al. 1981)

sandstone, siltstone, limestone, and red shale. The upper Honaker Trail and Cutler Group Formations are grouped together under this definition.

The middle hydrostratigraphic unit consists of the lower Honaker Trail and Paradox Formations. The unit is over 5000 ft thick at the center of the basin. The middle hydrostratigraphic unit contains evaporitic salt beds, interlayered with beds of shale.

The lower hydrostratigraphic unit consists of all sedimentary formations below the Paradox Formation. Formations included are the Pennsylvanian Pinkerton Trail and Molas; the Mississippian Leadville Limestone; the Devonian Ouray Limestone, Elbert Dolomite, McCracken Sandstone; and the Cambrian Lynch Dolomite and Muav Limestone. The vertical extent of the lower hydrostratigraphic unit is uncertain because of the sparse data at these depths. This unit is at least 2200 ft thick in the area of the Paradox Basin (Mallory 1972).

Potentiometric water levels, expressed in fresh-water equivalents, have been determined for each hydrostratigraphic unit. These data were collected over a number of years in the course of private exploration and are not synoptic data. The potentials of the upper hydrostratigraphic unit (see Figure 3) have relatively higher levels and general flow directions away from topographic highs. In the middle hydrostratigraphic unit, the potentiometric levels demonstrate no discernible pattern. This is consistent with other hydrologic evidence that indicates that salt beds restrict fluid migration and can form isolated geopressurized pockets of brine (Baar 1977). The lower hydrostratigraphic unit, shown in Figure 4, has a relatively lower potentiometric level. The regional flow direction is to the south and west. Data concerning groundwater density as affected by salinity variations were not available for this study and could alter flow direction projections.

In summary, the Paradox Basin flow system consists of an upper hydrostratigraphic unit that receives recharge from surface sources, a nearly impermeable middle hydrostratigraphic unit, and a lower hydrostratigraphic unit that is recharged at discrete locations. A generalized flow direction to the south and west characterizes the Paradox Basin (Thackston et al. 1981).

FIGURE 3. Potentiometric Surface of Upper Stratigraphic Unit of the the Paradox Basin (After Thackston et al. 1981)

FIGURE 4. Potentiometric Surface of the Lower Hydrostratigraphic Unit of the Paradox Basin (After Thackston et al. 1981)

GEOSTATISTICAL ANALYSIS—UPPER HYDROSTRATIGRAPHIC UNIT

The specific request from ONWI concerning the Paradox Basin was for PNL to evaluate the potentiometric surfaces for both the upper and lower hydrostratigraphic units.

A total of 46 data points were given to us by Woodward-Clyde Consultants on large-scale maps that represented the potentiometric surface (in feet above sea level) of the upper hydrostratigraphic unit (Thackston et al. 1981). The area covered by the data was about 1.5° longitude and 2.0° latitude. Thirty-one of the data points were spring elevations. Two of the spring measurements were very close, differing by 0.0003° latitude; because they had the same head value, one of the points was dropped from the analysis as a redundant datum. The data were scattered in a somewhat cross-shaped pattern, with the exception of one spring measurement outside the zero salt line, south of the confluence of the Dolores and Colorado Rivers. A well measurement of 3771 ft (southwest of the town of Blanding) was not included in the study at the suggestion of Woodward-Clyde personnel. The range in head measurements over the upper hydrostratigraphic unit is 4800 ft.

The components of the geostatistical analyses are the range over which data are taken to estimate the surface at a particular location, the local behavior of the surface in terms of a polynomial approximation (drift), and the spatial covariance of the data about the drift. The geostatistical estimation code BLUEPACK 3-D (Delfiner et al. 1979) was used to analyze the data. Between 8 and 16 data points, representing one to two data points per 45° sector surrounding the location of interest, were used to estimate the surface at that location. For the upper surface, the average data range for the estimation of locations within the data set was 0.9°, which is rather large, as the horizontal dimension of the study area is only 1.5°.

Similar to many of the hydrologic surfaces that have been modeled at PNL, the drift is a linear function of the data. The covariance function is more data-set dependent, and in this case, the model that best fit the data was a linear covariance with a constant term:

$$K(|h|) = 40,000 \delta - 2,500,000.0 |h| \quad (1)$$

where δ is the Kronecker δ function^(a) and $|h|$ is the regular Euclidean distance measure. A constant term of 40,000 corresponds to a measurement error of ± 200 ft. The mean deviation of the estimated head value from the actual value was -14.0 ft with a mean square deviation of 201,582 ft². In terms of evaluating the model, these quantities were smaller than those for any of the other models tested.

Potentiometric Surface Estimation

The potentiometric surface of the upper hydrostratigraphic unit that was generated from grid point estimates produced from this model is shown in Figure 5. The geostatistically estimated surface appears to show the same general character as the contour map (Figure 3) given in Thackston et al. (1981). The elongated potentiometric mound that is north of Highway 46, near Monticello, is not present in the geostatistically estimated map. This mound is inferred based on geologic knowledge and is not included in the head data on which the geostatistical analyses were based.

Estimation Errors

The contour map of the estimation errors of the potentiometric surface is shown in Figure 6. In the cross-shaped region where the data are located, the estimation errors are less than or equal to 700 ft. Outside this area, the errors increase steeply to the map boundaries. Within the central area containing the data, the estimation errors range from 300 to 600 ft. This seems rather large, but the measurement error for estimating the head from the pressure measurements, using the methods employed by the oil companies that obtained the data, is ± 100 ft. For the spring measurements, the elevations are taken as the value of the nearest isopleth (200-ft intervals) of topographical maps of the region.

Identification of Anomalous Data

The geostatistical analysis did not identify any data points that had an estimated potential value differing from the actual value by over 2.5 times

(a) Kronecker δ function is defined to be 1 if $h = 0$, otherwise it is defined to be 0.

FIGURE 5. Geostatistically Estimated Potentiometric Surface of the Upper Hydrostratigraphic Unit of the Paradox Basin

FIGURE 6. Estimated Error Map for the Upper Hydrostratigraphic Unit of the Paradox Basin

its estimation error. Such data are defined as anomalous. However, one data point (boxed in Figure 5) did differ by 2.4 times the estimation error. This data point, which differs from adjacent measurements by 1000 ft, is a spring measurement at the top of the Abajo Mountain Range. This would appear to be a discontinuity in the potential surface, which is anomalous. After the analyses were completed, PNL was informed that the springs are thought by ONWI to be perched water zones. However, published data (Thackston et al. 1981) consider the springs to be part of the upper potentiometric surface. The other somewhat anomalous data point (boxed in Figure 5) is one of a pair of close wells at about latitude 38.4° north and longitude 110.25° west, whose head measurements differs by nearly 800 ft. These anomalous data should be investigated.

Location of Future Data

The analysis to evaluate the effect of new wells was completed under the assumption that all of the data were from the same aquifer. In view of the possible perched conditions of some of the spring measurements, reporting those results would be inappropriate. The information on the spring data was received too late for a re-analysis of the data for this report.

GEOSTATISTICAL ANALYSIS--LOWER HYDROSTRATIGRAPHIC UNIT

The potentiometric surface of the lower hydrostratigraphic unit was estimated from 74 data points, all of which are well measurements. Although there are more data points for this unit than were available for the upper unit, the pattern of the data distribution is less uniform (Figure 4). Most of the data are concentrated in oil and gas fields stretching from the Lisbon Valley to the San Rafael River. Two widely separated data points occur in the Abajo Mountains, with a swath of data north of the San Juan River.

The head values for the lower hydrostratigraphic unit ranged from 3200 to 5800 ft above sea level, showing considerably less variation than was observed for the upper hydrostratigraphic unit. The average range of the data used to estimate the points of the potential surface was 0.6° . Like the upper hydrostratigraphic unit, the drift was linear. The covariance function that best fit the data was linear with a constant term:

$$K(|h|) = 8,966.0 \delta - 250,000.0 |h| \quad (2)$$

The covariance function is more data-dependent than the order of the drift. The constant term of 8,966 approximately corresponds to a measurement error of ± 100 ft. The mean deviation was -27.5 ft and the mean squared deviation was 119,038.6 ft².

Potentiometric Surface Estimation

The geostatistically estimated surface contour map is shown in Figure 7. The map is similar to the one shown in Figure 4. One exception is that in Figure 4, the Abajo Mountains are contained in one closed contour instead of two. Because only two well measurements exist in the Abajos, a dip occurs between the two values in the geostatistically estimated surface.

Estimation Errors

The geostatistical error map is given in Figure 8. As with the error map of the potential surface of the upper hydrostratigraphic unit, the area containing data is clearly visible. This area is bounded by the 300-ft isopleth line. Estimation errors within the area of the data range from about 130 to 300 ft. The estimation errors in oil field areas are often less than 150 ft, which approaches the measurement error.

The smaller estimation errors for the lower hydrologic surface are a result of the larger data set, 74 data points, as compared to 45 for the upper unit. The smaller errors are also a function of the smaller local discontinuities in the lower unit and of the difference in the upper vs lower unit data ranges.

Identification of Anomalous Data

Five data points were identified as anomalous data by the analysis and are boxed in Figure 7. The two isolated wells in the Abajo Mountains were declared anomalous primarily because they are much higher than the data south of the mountains. If there were more data in the mountains, these data would probably not be declared anomalous. The three other anomalous data points are from pairs or groups of closely spaced points. The head values of these data points differ substantially from adjacent measurements. One of the pairs is

9090 Fig 7

FIGURE 7. Geostatistically Estimated Potentiometric Surface of the Lower Hydrostratigraphic Unit of the Paradox Basin

FIGURE 8. Estimated Error Map for the Lower Hydrostratigraphic Unit of the Paradox Basin

south of the Abajos and differs from the nearest measurements by 400 ft. The other two anomalous data points occur along rivers. The data point on the Green River differs from the nearest measurement by 500 ft. The data point on the Dirty Devil River differs from its nearest neighbor by 400 ft.

Reduction in Variance Analysis

A major decision in field exploration work concerns where to drill additional wells. Several reasons for obtaining data exist: to characterize a hydrologic system, to improve the knowledge of the stratigraphy of a region, or to investigate geochemical and geophysical properties.

One goal of this work was to suggest locations for drilling new wells to improve the knowledge of the potentiometric surface of the region. As stated earlier, the geostatistical analysis provides a method for evaluating the effect of new data on the precision of the estimated surface before the data are actually taken. This provides the possibility of substantial savings, as the cost of drilling a single well with extensive geologic, hydrologic, geophysical, and geochemical measurements is several million dollars. An analysis of hydrologic data will not provide locations for data that will improve the knowledge of the stratigraphy. To facilitate geologic and hydrologic data collection, stratigraphic data should be analyzed and a map of a coupled potentiometric-stratigraphic reduction in variance should be produced. The reason for drilling a new well is to better define the entire flow system, not just the potentiometric surface.

Four siting constraints were used in the selection of locations for additional characterization wells. First, the collection of additional hydrologic data should be in the area of greatest interest, that is, the area adjacent to and down the potentiometric gradient from the hypothetical repositories. Second, well siting must avoid national parks, national monuments, and wilderness areas, where legal access to drill exploratory wells is denied. Third, the location must be topographically accessible. This constraint excludes steep slopes, mesa tops, and areas where the terrain is too rugged for even primitive roads. Fourth, geostatistics should be used to select locations that produce the greatest percent reduction in variance of the potentiometric surface of interest.

The geostatistical criterion of where to place a new well is based on the principle of reducing the variance of the overall mean value estimate of the surface. This global criterion is used instead of the location where the geostatistical error, which is a measure of the local variance of the surface, is the largest. In this manner, locations are selected which will minimize the variance of the entire surface.

The percent reduction in variance contour map is shown in Figure 9 for a rectangular subregion (longitude $110^{\circ}19'$ to $109^{\circ}09'$ west, latitude $37^{\circ}25'$ to $38^{\circ}31'$ north), which is described in detail in the Hydrologic Analysis

FIGURE 9. Percent Reduction in Variance Map of the Lower Hydrostratigraphic Unit of the Paradox Basin

Section. The most advantageous location for a new well appears to be near latitude 37°54' north, longitude 109°57' west, which would produce a variance reduction of over 28%. We do not recommend using these results to help select a new well location, but have included them in the report for completeness. Instead, for the hydrologic analysis, a reduction in variance analysis, assuming a more realistic regional potential that was adjusted for stratigraphy and topography, was used. A description of that analysis is given in the Reduction in Variance--Location of Future Data Section below.

HYDROLOGIC ANALYSIS

The hydrologic analysis combines geostatistical and hydrologic modeling. To examine the effects of geostatistically estimated changes in the potentiometric surface on the aquifer evaluation (flow rates and flow quantities away from the hypothetical repository), we used hydrologic modeling. The modeling of ground-water flow was bounded by the two locations of prime interest, the hypothetical repository site and the Colorado River.

Potentiometric Surface Adjustment

The potentiometric surface produced by the geostatistical analysis was based solely on well measurements. The surface does not take into account the increase of fracture permeability under the Colorado River. Major river systems that cut deep canyons produce isostatic rebound along their course. The rebound of the lower rock units is due to the removal of weight of surficial rock by erosion. The isostatic rebound causes fracturing of lower rock units as they expand and uplift. Therefore, we slightly altered the potentiometric surface by adjusting contours at the Colorado River to reflect the assumed increased fracture permeability. The adjusted potentiometric surface (as shown in Figure 10) agrees more closely with the surface produced by Thackston et al. (1981) shown in Figure 4. Statistical analysis demonstrated that the adjusted and unadjusted surfaces were not significantly different. The adjusted potentiometric surface is referred to as the nominal case in this report.

Hypothetical Repository Siting

Lavender Canyon (see Figure 11), was chosen for the hypothetical waste repository site. The site selection was based on a suggestion from ONWI. An additional criterion was that no known factor precluded repository placement at this location. The four siting constraints used to locate additional well locations were applied to the hypothetical repository location.

Ground-Water Flow in Lower Hydrostratigraphic Unit

The lower hydrostratigraphic unit was chosen as the zone for data evaluation. This decision was based on the hydraulic head relationship between the upper (higher head) and lower (lower head) hydrostratigraphic units. In the event that a large-scale vertical fault formed at the repository location (cutting through all three hydrostratigraphic units), fracture permeability could possibly provide an avenue for fluid migration from the upper unit into the lower unit. Also, human intrusion, such as by an exploration well, could affect all of the units. This study examines the more severe case of a fault-induced aquifer interconnection. Therefore, under the hypothetical conditions, the lower hydrostratigraphic unit could receive ground water from the hypothetical repository area. These conditions must be considered highly improbable. In addition, we assumed that the interaquifer flow, if any, initiated by repository breaching is insufficient to alter regional flow paths. Repository shape and fault geometry of vertical flow paths affect the flow in the lower units. For this study, a hypothetical repository is assumed to have a length of 8200 ft and to be oriented parallel to equipotentials in the lower hydrostratigraphic unit.

To judge the sensitivity of the hydrologic model to changes in the potentiometric surface, a down-gradient location is chosen as a line of evaluation. This line is usually set at the first location where ground water is known to be discharged into surface water and hence enters the biosphere. In the Paradox Basin study area there is no known ground-water discharge location from the lower hydrostratigraphic unit that is down gradient from the hypothetical repository sites. Therefore, the Colorado River was used as a convenient line of evaluation. This does not imply a connection between the lower hydrostratigraphic unit and the surface water.

FIGURE 11. Location Map of Wells and Hypothetical Repository Site Used in the Paradox Basin Hydrologic Analysis

Reduction in Variance—Location of Future Data

The percent reduction in variance contour map for the nominal case is shown in Figure 12. Compared to Figure 9, the main peak (now reduced to about 20%) is steeper and has moved south to latitude $37^{\circ} 42'$ north, southwest of the Canyonlands National Park. A local maximum of about 16 has appeared near the eastern boundary of the park.

The two peaks suggest that two additional data points may materially improve the precision of the estimated potentiometric surface. Therefore, two locations for wells were chosen as close to the peaks in Figure 12 as possible, while staying outside the park boundary and in areas accessible to drilling rigs.

In this manner, locations were obtained that will minimize the variance of the whole surface. The two locations chosen for new potentiometric data collection are: Well A (latitude $38,0129^{\circ}$ north, longitude 109.5899° west), located in Cottonwood Canyon; and Well B (longitude 109.9297° west, latitude $37,9422^{\circ}$ north), located in Gypsum Canyon (see Figure 12).

Flow Analysis

From the conceptual model and available data, a hydrologic model was set up to determine spatial transmissivity, flow paths, and travel times from the hypothetical repository location to the line of evaluation along the Colorado River. The Convective Transport Submodel of the Two-Dimensional Variable Thickness Transient (VTT) Code (Reisenauer 1979) was selected for the hydrological evaluation of the lower aquifer unit of the Paradox Basin. In this evaluation, a horizontal x-y coordinate grid system represents the study area. Model parameters defining the aquifer system were assigned to, and evaluated at, nodes in the center of each grid and were considered representative of the whole grid area.

The following input parameters are required over the region as input to a node-centered grid system of the VTT Convective Transport Code:

- a potential surface
- a transmissivity matrix

FIGURE 12. Percent Reduction in Variance Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Nominal Case

- a porosity distribution
- an aquifer thickness or stratigraphic surfaces for the top and the bottom of the aquifer.

Each of these input parameters, as they pertain to the analysis of the lower hydrostratigraphic unit of the Paradox Basin, is described below.

The large hydrologic region evaluated in this study corresponds to the boundaries of the geostatistically estimated potential surface (Figure 13). The region is divided into an 88-by-125-node grid with a one-mile node spacing. The potential surface was provided by geostatistics; however, because geostatistical estimation tends to distort values near the region's boundary as a result of a lack of data, a subregion was generated within this region. The subregion eliminated anomalous values near the edges of the grid, and saved computer time and space in performing subsequent computations. The subregion, shown in Figure 14, runs from node 17 to node 77 in the x-direction and from node 22 to node 94 in the y-direction of the large region grid and has a node spacing of one mile.

The geostatistically estimated potentiometric surface is shown in Figure 11 for the large region grid. The potential surface was estimated over the one-mile grid system outlined above, and overlayed directly onto the VTT grid. The potential estimates were smoothed by using a five-point interpolation scheme. Smoothing was necessary to generate more realistic streamlines because small deviations in the estimated equipotentials would cause undue distortions when streamlines were calculated. During the smoothing process, the mound centered around node (46,45) in the large region was held at its original potential so that the difference between the estimated and smoothed potential values at any node did not exceed 10 ft in the subregion model area. The smoothed subregion potentiometric surface is shown in Figure 15.

Using the auxiliary program of the VTT code, MXPLT, streamlines were generated in the area of the hypothetical repository. The flow net generated for the smoothed potentiometric subregion is shown in Figure 16. The flow net was densely constructed so that the sides of the flow net elements could be approximated by straight lines. The flow net elements were then digitized to obtain the dimensions of each element, which became an input to the transmissivity calculation. An approximation to the general inverse solution method was used to calculate transmissivities (Arnold 1981). A description of the approximation method as first proposed by Bennett (1962) is given in Appendix B. This approach was used to generate a transmissivity value for every element in the flow net between the hypothetical repository and the line of evaluation, as shown in Figure 17.

FIGURE 14. The Subregion Hydrologic Model Boundary Used in the Paradox Basin Flow Analysis

FIGURE 15. Smoothed Subregion Potentiometric Surface for the Lower Hydrostratigraphic Unit of the Paradox Basin

FIGURE 16. Flow Net Used in the Transmissivity Calculation for the Paradox Basin Flow Analysis

FIGURE 17. Flow Net Showing Calculated Transmissivities (ft²/day) at the Center of Each Flow Net Element. Hatched elements show the starting band of transmissivity values for the inverse calculation.

A critical input to this calculational sequence is a known transmissivity, T_0 , for one element in each streamtube of the flow net. As only one transmissivity data point was available at Gibson Dome No. 1 (GD-1), this value ($53 \text{ ft}^2/\text{day}$) was placed in a band of flow net elements adjacent to GD-1 (see Figure 17). The transmissivity value of $53 \text{ ft}^2/\text{day}$ was calculated by combining reported hydraulic conductivities and stratigraphic thicknesses at Gibson Dome No. 1 and estimated values for the remainder of the hydrostratigraphic unit. The calculated transmissivities range from $42 \text{ ft}^2/\text{day}$ to $150 \text{ ft}^2/\text{day}$, which compare well with the reported average of $60 \text{ ft}^2/\text{day}$ for Paleozoic carbonates in the Colorado Plateau (McComas 1963).

The transmissivity values, as well as the coordinates of the center of each flow net element, were submitted to the geostatistical analysis to transform the data to a regular grid. The data had to be edited to remove the values around the outer edges of the flow field when the transmissivities became very large.

The geostatistical model that best fit the data was a linear drift and a covariance function:

$$K(|h|) = -28640.0 |h| \quad (3)$$

The geostatistically estimated surface over the subregion's one-mile grid is mapped in Figure 18. The estimation errors for the data points were in the range of $15 \text{ ft}^2/\text{day}$ to $25 \text{ ft}^2/\text{day}$. Most of the observed errors were less than 1.5 times the estimation error.

For the other input parameters of the VTT Convective Transport Code, an average porosity value of 0.095 was used in this study, based on McComas' (1963) regional average for Paleozoic carbonate rocks in the Colorado Plateau area, and an average aquifer thickness of 2200 ft was used over the modeled area (Mallory 1972).

Aquifer Evaluation

The VTT Convective Transport Code was used to predict ground-water flow paths to the Colorado River. Figure 19 depicts the ground-water flow paths

110° 19'

109° 09'

38° 31'

37° 25'

FIGURE 18. Transmissivity Map for the Lower Hydrostratigraphic Unit of the Paradox Basin. Transmissivities are in units of ft^2/day ; contour interval is $26.7 \text{ ft}^2/\text{day}$.

FIGURE 19. Streamtubes Showing the Path of Ground Water Flowing from the Lavender Canyon Hypothetical Repository

from the Lavender Canyon site. The VTT Convective Transport Code also was used to calculate travel times from the hypothetical repository site to the line of evaluation along the Colorado River. From these, arrival time curves were developed, which depict the relative cumulative flow as a function of time from an instantaneous pulse at time zero. The relative cumulative flow is defined as the sum of the flow in successive streamtubes that reaches the line of evaluation, divided by the total flow in the streamtubes. Two reference times can be defined to facilitate comparisons of these arrival curves between repository sites. The first is delay time, which is the time between the departure of the first ground water from the repository and its arrival at the line of evaluation. The second is spread time, which is the duration between the arrival of the first ground water at the line of evaluation and the arrival of the last ground water that had been in contact with the repository. The longer the delay time and spread time, the more effective the repository location (Nelson 1981). By comparing arrival time curves for differing sites, their comparative effectiveness can be assessed.

Lavender Canyon Site

Figure 20 is the arrival time curve for the hypothetical Lavender Canyon repository. The leading edge of the front arrives at the southern portion of the line of evaluation at the Colorado River in 50,400 years after the repository breach. The last flow arrives in the northern portion of the line of evaluation 68,000 years after the assumed repository breach. The spread time for the Lavender Canyon site is 17,600 years (see Table 1).

SIMULATION OF ADDITIONAL DATA

The two hypothetical well locations on the lower hydrostratigraphic unit were chosen to be as close as possible to the two high points of the geostatistical variance reduction map based on the nominal case data set, with the other constraints taken into account. Hypothetical Well A (latitude 38.0129° north, longitude 109.5899° west) is located in Cottonwood Canyon, and hypothetical Well B (longitude 109.9297° west, latitude 37.9422° north) is located in Gypsum Canyon (see Figure 12).

FIGURE 20. Arrival Time Curve for the Lavender Canyon Hypothetical Repository

TABLE 1. Arrival Time Data for the Lavender Canyon Hypothetical Repository Site

Stream-Tube Number	Average Ground-Water Arrival Time (yr)	Ground-Water Flow Rate (gpm)	Cumulative Ground-Water Flow Rate (gpm)	Cumulative Flow Rate Divided by Total Flow Rate
	50,425	0.0	0.0	0.00
1	51,009	1.9	1.9	0.09
2	52,533	2.6	4.5	0.21
3	54,452	2.9	7.4	0.35
4	56,064	2.9	10.3	0.48
5	57,878	2.9	13.2	0.62
6	60,500	2.9	16.2	0.75
7	63,856	2.7	18.9	0.88
8	68,034	2.6	21.5	1.00

Total ground-water flow rate = 21.5 gpm

Potential Surface

The expected value of the potentiometric surface was estimated using geostatistics at the two locations. An estimation error was also obtained at each of the two locations. The data locations, the potentiometric values, and the estimation errors are given in Table 2. To study the effect of Wells A and B at these locations, four new data sets were generated, each simulating the effect of different potential values. The potentiometric values for the two hypothetical wells were obtained by adding or subtracting the respective estimation error from each estimated potential. The four data sets are composed of all of the nominal case data plus one of the four combinations:

- High Potential in Well A – High Potential in Well B
- High Potential in Well A – Low Potential in Well B
- Low Potential in Well A – High Potential in Well B
- Low Potential in Well A – Low Potential in Well B.

The hydrologic evaluation used for the nominal potentiometric surface is repeated for four simulated potentiometric surfaces. The simulated potentiometric surfaces are based on expected data extremes at locations of large variances; hence, the simulations bracket the full range of expected hydrologic flow conditions. The results of the geostatistical and hydrologic flow analysis for these four simulated cases are given in Appendix C.

When the new data sets were fit with the existing geostatistical model [see Equation (2)], the estimated potentiometric surface changed among the four cases. The potentiometric surfaces are shown in Appendix C, Figures C.1, C.5, C.9, and C.13.

TABLE 2. Geostatistical Potential Estimates for Hypothetical Well Locations in Paradox Basin

Well	Location		Potential ft	Estimation Error (ft)
	Latitude North	Longitude West		
A	38.0129°	109.5899°	4623	+212
B	37.9422°	109.9297°	4380	+242

Spatial Transmissivity

The spatial transmissivity was recomputed for each of the four simulated surfaces by means of flow net generation, parameter estimation, and geostatistics. Geostatistical models were estimated separately for each case. Although the best order of the drift was linear like the one for the nominal case, the choice of a covariance function was not as obvious. The criteria used to select the best covariance model gave inconsistent results for each case. A constant covariance was finally chosen because it was the only one that produced consistent results for one criterion. The best constant covariance model for each case is given below:

<u>Case</u>	<u>Well A</u>	<u>Well B</u>	<u>Covariance Model</u>
Paradox HH	High	High	$K(h) = 746.3s$
Paradox HL	High	Low	$K(h) = 427.8s$
Paradox LH	Low	High	$K(h) = 105.4s$
Paradox LL	Low	Low	$K(h) = 106.8s$

The covariance functions had the lowest variance for the simulation in which Well A is low. Conversely, they had the highest variance for the simulations in which Well A was high. This suggests that Well A has the most influence on the estimate of the transmissivity surface. The transmissivity maps for the four simulated cases are given in Appendix C, Figures C.2, C.6, C.10, and C.14.

Aquifer Evaluation

To examine the hypothetical repository site, the flow paths and travel times were calculated for each of the four simulated potentiometric surfaces. Flow paths from the Lavender Canyon site for the four cases are shown in Figures C.3, C.7, C.11, and C.15, in Appendix C. The simulated changes to the potentiometric surface cause a shift in flow paths to the south for the Paradox HL and Paradox HH cases. The flow paths changed the least for the Paradox LL and caused a northern shift for the Paradox LH case. The Paradox LH flow paths pass through an area of very low potentiometric gradient adjacent to a groundwater divide.

Arrival time curves for the four simulated surfaces for the Lavender Canyon hypothetical repository are shown in Appendix C in Figures C.4, C.8, C.12, and C.16. Tables C.1 through C.4 in Appendix C give the travel times and flow rates associated with each of these curves. The earliest arrival of the flow front from a hypothetical repository to the line of evaluation occurs for the Paradox HL potentiometric surface, at 34,900 years after the repository breach.

The combined arrival time curves, based on nominal and simulated potentiometric surfaces are shown for Lavender Canyon in Figure 21. The format of these arrival time curves is somewhat different from previous figures. The y axis now represents the cumulative flow rate rather than the cumulative flow/total flow. This change allows the flow rate, as well as travel time changes, for the various conditions to be examined.

A comparison of peak discharge rates was made for two scenarios. In the first scenario, the assumed fault remains open, thus supplying a steady stream of ground water to the lower hydrostratigraphic unit. The peak discharge of water that had been in contact with the repository is shown at the top of each curve in Figure 21.

In the second scenario, the geologic isolation medium closes 1000 years after the fault formation. The 1000-year period is used because it enables a more realistic comparison between the four simulated cases and the nominal case. The 1000-year period is based on a probable elimination of fault-induced fracture permeability caused by salt flow under lithostatic pressure. The limited time period reduces the peak discharge rate to the line of evaluation of water that had been in contact with the repository. Time-limited peak flow rates are not necessarily comparable with steady-state flow rates. Peak flow rates can be represented by geohydrologic response functions. An example of a time-limited geohydrologic response function is shown in Figure 22 for the readers convenience. The flow rate of the ground water reaching the line of evaluation at the Colorado River from the first pulse of ground water entering the lower hydrostratigraphic unit is represented by the first curve in each of the five cases in Figure 23. The second parallel curve represents the last pulse of ground water flowing into the lower hydrostratigraphic unit before

FIGURE 21. Summary Arrival Time Curve for the Lavender Canyon Hypothetical Repository

salt flowage seals the hydraulic connection between the hydrostratigraphic units. The flow rate for the 1000-year period was calculated for the nominal potential surface and was then used to calculate the period of each of the other four cases. Thus, the same quantity of ground-water flow (represented by the shaded areas in Figure 23) would occur during the 1000-year period. Taking the difference between these two curves at all times yields the distribution of outflow rate into the line of evaluation in relation to the arrival time at that location (represented by the dashed lines in Figure 23). Accordingly, the peak ground-water flow rate is significantly reduced and is shown at the top of each dashed curve.

FIGURE 22. An Example of a Geohydrologic Response Function

Lavender Canyon Evaluation

The Lavender Canyon summary arrival curves are given in Figure 21. The Lavender Canyon site also has streamlines pass through an area of low gradient for the Paradox LH simulation, producing a delay time of 71,000 years. The Paradox HL simulation yielded the shortest delay time of 37,000 years. The delay times of the simulated cases are up to 21,000 years greater than (+141%) to 15,000 years less than (-69%) the nominal case. Flow rates vary from 16.0 gpm greater than, to 12.5 gpm less than, the value of 21.5 gpm calculated from the nominal data. The geohydrologic response function curves for the 1000-year period at Lavender Canyon are given in Figure 23. The peak flow rates vary from 10.5 gpm (Paradox HL) to 1.0 gpm (Paradox LH). The nominal case has a peak discharge of 2.7 gpm. The Lavender Canyon arrival curves show a lack of superimposition of the simulated results on the nominal case.

FIGURE 23. Geohydrologic Response Function Curve for the 1000-Year Breach for the Lavender Canyon Hypothetical Repository

CONCLUSIONS

The simulated potentiometric surfaces were generated such that they reflect the range of expected variations in that surface. The geohydrologic response function curves graphically demonstrate the uncertainty that can be expected in flow analysis, based on the nominal-case data base. Hence, the following conclusions can be made:

- The flow rate of ground water that is assumed to have been in contact with the Lavender Canyon hypothetical repository, under both nominal and simulated cases, is quite low at less than 40 gpm.
- The variations of the geohydrologic response curves define the uncertainty associated with the current potentiometric data base. The magnitude of these uncertainties in comparison to the flow of the entire ground-water system and the flow of surface water in the Colorado River may be inconsequential.

- The perturbation in the potentiometric surface caused by simulated data results in outflow rates varying by an average factor of 1.2 for a permanently open fault fracture, and an average factor of 1.6 for a 1000-year breach.
- The potentiometric surface of the lower hydrostratigraphic unit in Paradox Basin is moderately well known. Additional potentiometric data at Well A will yield the most significant improvement to the data base. This is evidenced by both the differences in the covariance functions and by the Paradox HL and Paradox LH simulations, which form the bounding response curves from the Lavender Canyon site.

MISSISSIPPI STUDY AREA

The Mississippi Study Area is located in southeastern Mississippi and encompasses 1440 square miles of the East Gulf Coastal Plain (see Figure 24). The area consists of gently rolling hills and mature river valleys developed on Cenozoic sedimentary deposits. The climate is humid and the area averages 60 inches of rainfall per year (Hunt 1967).

The Mississippi Study Area is situated within the southeastern portion of the Mississippi Salt Basin. The basin contains sedimentary deposits of the upper Jurassic through Tertiary Periods (see Figure 25). The deposits were formed from cyclic marine transgressions and regressions. In the southern portion of the study area, the sedimentary deposits have a thickness of over 27,000 ft. At the base of the sedimentary sequence lies the Louann Salt, an evaporite deposit that ranges up to 5000 ft thick. The Louann Salt has flowed under lithostatic pressure and density differences to form piercement salt domes. Salt domes in the study area have penetrated the sediments and are within 2000 ft of the land surface. Faulting in the study area is associated with salt movement and sediment compaction.

CONCEPTUAL MODEL

A basic understanding of an aquifer flow system is expressed in the conceptual model. Hydrogeologic data for the Mississippi study area indicate a single regional flow system, bounded by the relatively impervious Midway Group at its base and by the water table at the top. Permeability variations caused by changes in lithology can form localized ground-water flow restrictions. The Cockfield, Cook Mountain, and Sparta Formations are generally of low permeability. No geologic unit, however, forms a regional barrier to water movement. Aquifer heterogeneities are wide-spread and no spatial trends have been identified.

In general, rainfall in the northern portion of the Gulf Coastal Plains recharges the aquifer. Water movement is regionally to the south. The magnitude of density variations within the aquifer, however, negates the use of water levels for the determination of flow directions. Therefore, no

accurate description of the regional flow regime exists for the study area at this time. Fresh-water aquifers overlay saline aquifers. The fresh-water aquifer is unconfined and shows local recharge along topographic highs.

ONWI requested an evaluation of the top and the base of fresh-water potentiometric surfaces near the Richton Dome. The request to analyze the base of fresh water, which has little hydrologic significance, was a result of draft regulatory criteria at that time. These draft criteria were later deleted, removing the need for a surface analysis; in view of certain hydrologic considerations (to be explained later), the elevation of the base of fresh water was not analyzed. Instead, the need for a three-dimensional geostatistical and hydrologic analysis to adequately characterize the regional hydrology of the salt domes was identified, outlined, and partially completed.

GEOSTATISTICAL ANALYSES OF THE TOP OF THE FRESH-WATER POTENTIOMETRIC SURFACE

The data provided by Law Engineering and Testing Company (LETCO 1980) consisted of 186 water table measurements collected over approximately 30 years. The head values range from 190 to 388 ft above sea level over a rectangular study area of 1.1° longitude and 0.43° latitude. Richton and Cypress Creek Domes are in the eastern part of the study area. The data distribution over the study area was fairly uniform (see Figure 26).

Because of the density of data points, the average neighborhood from which data were used to estimate points of the surface was 0.2°. This is a much smaller range than was required for the Paradox potentiometric surfaces. The best representation of the drift for the geostatistical model of the surface was a linear drift, which is consistent with the other potentiometric surfaces analyzed to date.

The best model for the covariance function was

$$K(|h|) = 93.31 \delta - 38420.0 |h| + 35680.0 |h|^3 \quad (4)$$

This model is more complex than the covariance models used for the Paradox Basin because of the smaller study area and a larger data set. When there are

FIGURE 24. Mississippi Study Area (After LETCo 1980)

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TIME PERIOD	SERIES	GROUP OR STAGE	FORMATION	AGE MYBP	REGIONAL CORRELATION	LITHOLOGY
CENOZOIC	RECENT		ALLUVIUM		0-125	Quartz sands, chert and quartz gravels, and silty clays
	PLEISTOCENE		TERACE DEPOSITS		0-50	Fine to coarse grained quartz sands with some gravel and clay lenses.
	PLIO-PLISTOCENE		CITRONELLE		150 ±	Silty, clayey sands grading into basal gravel beds.
	PLIO-PLISTOCENE		PACAGOULA/HATTISBURG	1.8	130 to 330	Interbedded gravelly sands, sands, silty clays, and lignites.
	PLIO-PLISTOCENE		CATAHOULA		Up to 1,000	Silt, clays, fine to medium grained sands, gravels, lignites, and a marker Heterostegina zone (Tatum limestone member).
	MIOCENE		PAYNES	22.5	5-23	Glauconitic marls interbedded with sandstones, clays, and silty limestones.
			HAMMUCK CHICKA SAWHAY		30	Argillaceous to sandy limestones interbedded with clays and marls.
			BUCATUNNA		50-215	Clayey sandstones or sandy marls interbedded with lignitic, calcareous clays.
	OLIGOCENE	VICKSBURG	VICKSBURG LIMESTONES			Limestones with associated bentonites, clay shales, and clays.
			FOREST HILL		55-150	Sandy to silty carbonaceous clays and partially indurated fossiliferous marls.
			RED BLUFF		Up to 500	Variably limy, glauconitic, sandy and silty clays with basal chalky limestones (Ocala facies).
	OLIGOCENE	JACKSON	YAZOO	38	Up to 45	Glauconitic, partially indurated and sometimes sandy marls.
			MOODYS BRANCH	42	25-215	Limestones, sand streaked, lignite-bearing clays and silt.
			COCKFIELD		115-235	Loosely cemented, porous carbonate sands, glauconitic clay shales, and calcarenitic limestones.
	Eocene	CLAI-BORNE	COOK MOUNTAIN	44.5	90-625	Slightly porous, chalky limestones, well cemented calcarenitic limestones interbedded with glauconitic clay shales. Locally sandy.
			KOSCIUSKO (SPARTA)	48		Interbedded glauconitic clay shales, chalks, and chalky limestones.
			ZILPHA		90-200	Clay shales containing chalk or marl lenses in the lower half.
MESOZOIC	7	WILCOX	WINONA			Glauconitic and limy siltstones and claystones interbedded with clay shales.
			TALLAHATTA		49-90	Crossbedded sands, containing sandy shales and lignitic clays.
			UNDIFF.	50	2,250-3,200	Silty, lignitic shales, interbedded with silt, sands, lignitic siltstones, and fine to medium grained sandstones.
	PALEOCENE	MIDWAY	PORTERS CREEK	53.5	650-1,050	Shales interbedded with thin lignite beds, silt, siltstones, and very fine to fine grained argillaceous sandstones.
			CLAYTON		10-25	Sandy, glauconitic marls, marly chalks, or calcareous clays.
			UNDIFF.	65	925-1,500	Sandy to very argillaceous to pure chalks containing bentonite traces and fissile shales.
	GULFIAN	TUSCALOOSA	EUTAW		92	Fissile, slightly sandy or calcareous, lignitic shales, very fine to fine grained sandstones, and calcareous siltstones.
			UPPER TUSCALOOSA		300-900	Fissile shales, mudstones, and fine to medium grained, glauconitic, porous sandstones.
			MIDDLE TUSCALOOSA		620-1,160	Interbedded carbonaceous shales, mudstones, siltstones, and thin, fine grained sandstones with a basal chalk or chalky limestone unit.
	COMANCHEAN	T	LOWER TUSCALOOSA	100	575-1,150	Fissile shales, calcareous and glauconitic sandstones and siltstones with a basal massive, fine to coarse grained, conglomeritic sandstone unit.
			WASHITA		1,000-1,880	Micaceous shales alternating with mudstones, nodular limestones, fine to medium grained, lignitic, calcareous or silty sandstones.
			WASHITA-FREDERICKSBURG	104	1,000-1,450	Shales, silty mudstones, fine to medium grained, silty, carbonaceous sandstones, and pseudo oolitic, sometimes sandy, limestones.
	COAHUILAN	NUEVO LEON	PALUXY		200-1,000	Fissile shales, lignitic mudstones, and fine to coarse grained, argillaceous, carbonaceous gravel-bearing sandstones.
			MOORINGS-PORT		160-240	Limy shales alternating with mudstones, silty, fine grained sandstones, and pseudo-oolitic anhydrite-bearing limestones.
			FERRY LAKE		750 ±	Shales alternating with oolitic limestones and white anhydrite.
JURASSIC	UPPER	LOUARK	RODESSA/PINE ISLAND UNDIFF.	113	300	Thin anhydrite stringer overlying shales, very fine to fine grained, calcareous sandstones and siltstones, and pseudo oolitic limestones.
			SLIGO		1,800-2,650 ±	Sulphureous shales interbedded with fine to medium grained, argillaceous sandstones, and occasionally, nodular limestones.
			HOSSTON	136	2,000-2,900 ±	Very fine to coarse grained, calcareous sandstones, sandy carbonaceous shales, and sandy, lignitic mudstones.
	LOWER	LOUANN	COTTON VALLEY	143		Fine to medium grained, silty and calcareous sandstones alternating with mudstones and shales.
			HAYNESVILLE BUCKNER		1,500-3,450 ±	Dense, lithographic limestones, dolomitic carbonates, and anhydrite.
CRETACEOUS	UPPER	LOUARK	SMACKOVER			Dense, oolitic limestones, finely crystalline limestones, dolomitic limestones, and dolomites.
			NORPHLET			Sandy shales and poorly sorted shaly sandstones.
TERTIARY	LOWER	LOUANN	LOUANN SALT		n-5,000 ±	Coarsely crystalline white halite containing anhydrite inclusions.

FIGURE 25. Mississippi Study Area Stratigraphic Column (After LETCo 1980)

FIGURE 26. Geostatistically Estimated Top of Fresh-Water Surface

more data, more details of the surface can be resolved, and the covariance structure becomes more complex. The constant term of 93.31 ft^2 is much smaller than the one for the Paradox Basin lower hydrostratigraphic unit, which reflects the smaller data range.

Potentiometric Surface Estimation

The geostatistically estimated surface is shown in Figure 26. The contour interval is 50 ft. Figure 26 shows the major features of the surface given in the LETCo report (Figure 27). Specifically:

- The 250- and 200-ft equipotential lines trending northwest to southeast near Hattiesburg in the LETCo map are evident in the geostatistically estimated map.
- The two high points west and southwest of Hattiesburg are visible on the geostatistically estimated map.
- The detail around Lampton Dome on the geostatistically estimated map agrees quite well with the LETCo map.
- The dipping in the southeast corner of the LETCo map is apparent in the geostatistically estimated map.

However, in the area around Richton and Cypress Creek Domes, less agreement is evident between the two maps. The shape of the 150-ft isopleth in Figure 26 is similar to the 100-ft isopleth in Figure 27: three lobes are open to the south. The 150-ft isopleth in Figure 27 is open to the north and is perhaps based on data not available for this analysis. Well values of 150 ft and less above the dome are not consistent with the 200-ft contour above the dome in the LETCo report. A 200-ft lobe would have to be very narrow, unless its existence is based on additional topographic information that was not available for the geostatistical analysis.

Estimation Errors

The map of the estimation errors incurred in fitting the top of fresh-water surface is given in Figure 28. The contour interval is 25 ft; the area containing the data is bounded by a 50-ft contour line. Estimation errors ranged from 20 to 50 ft within the study area. The estimation errors in the

immediate vicinity of Richton Dome are all less than 40 ft. A realistic measurement error for the wells in this region would be 30 ft. If so, the measurement variance constitutes half of the estimation variance; this suggests that the surface is fairly well known.

Identificaton of Anomalous Data

Compared to the other potentiometric surfaces analyzed, more data for this surface were identified as deviating significantly from the geostatistical model prediction. Eleven well measurements were identified as anomalous (boxed in Figure 26). They are data points that differ from their close neighbors by over 200 ft. A cluster of such data is located at the western edge of the study area. The rest of the anomalous data are located directly to the west of Richton Dome near Hattiesburg, with the exception of one anomalous data point east of the dome. These data should be investigated, particularly with respect to the age of the readings, as pumping for commercial and domestic use could have significantly changed the water table over the years.

Analysis of the Location of Future Data

Analyses were performed to identify where new wells should be placed to improve the knowledge of the surface. The contour map of the percent reduction in variance analysis based on 66 data points is shown in Figure 29. Putting a new well in the study area would achieve a reduction in variance of less than 2%. A new well in the area immediately surrounding Richton Dome would reduce the variance of the mean value of the surface by less than 0.10%. This confirms the evidence of the estimation errors around Richton Dome based on the entire data set: putting any more wells near Richton Dome to improve knowledge of the fresh-water surface would have little effect. Such a conclusion should not be accepted, however, without a thorough evaluation of the available data applicability. The above data were not reviewed with the geologic program manager at LETCo.

This analysis should not be taken as a strict justification for not drilling any wells near Richton Dome. Reasons for drilling other than to define the fresh-water surface near Richton Dome would be: to investigate the hydrology of the lower strata, the salt dissolution areas, the stratigraphy, and the geochemical and geophysical characteristics.

FIGURE 27. Potentiometric Map of Top of Fresh Water Surface (After LETCo 1980)

FIGURE 28. Estimation Errors for Top of Fresh-Water Surface

FIGURE 29. Percent Reduction in Variance for the Top of Fresh-Water Surface

GEOSTATISTICAL AND HYDROLOGIC ANALYSES OF THE DEEP AQUIFERS

The data obtained from LETCo included elevation, measured head, and fresh water equivalent head at various depths from eleven wells (see Figure 24). To compute the saline density (ρ) from the measured head and fresh water equivalent, the following formula was used:

$$\text{saline density} = (\text{density fresh} \times \text{length fresh-water column} / \text{length saline-water column}) \quad (\text{Walton 1970}) \quad (5)$$

The pressure (p) is given by

$$p = (\text{length of fresh-water column}) \times (\text{gravitational constant}) \times (\text{fresh-water density}) \quad (6)$$

Examination of the saline densities indicated that the more generalized form of Darcy's Law must be used for a meaningful hydrologic analysis. Appendix D demonstrates this conclusion and outlines the three-dimensional version of Darcy's Law described in Hubbert (1956). The BLUEPACK 3-D Code was used to estimate pressure and ($1/\text{density}$) on a three-dimensional grid [denoted by (x_1, x_2, x_3)] over the study region. The dimensions of the grid are 1.5 miles x 1.5 miles x 0.1 miles in the east-west, north-south, and vertical directions, respectively.

Both the pressure and ($1/\text{density}$) were geostatistically estimated on a three-dimensional grid. For the pressure data, the best geostatistical model in three dimensions was found to be a trilinear drift, and the power function covariance:

$$K [d(X,Y)] = -1971 \times d(X,Y)^{1.925} \quad (7)$$

where $d(X,Y) = [(x_1 - y_1)^2 + (x_2 - y_2)^2 + 2000 (x_3 - y_3)^2]^{1/2}$. The multiplier 2000 for the vertical distance represents the anisotropy in the vertical dimension of the covariance or variogram function.

The estimation errors for the pressure and density were not calculated because the work was terminated (for reasons discussed later in this report).

A three-dimensional irregular surface is not easily represented in two-dimensions. A layered representation would require cross-sections in all three dimensions and would be difficult to visualize. The main areas of interest are Richton and Cypress Creek Domes; therefore, a single two-dimensional representation of the three-dimensional pressure surface through Richton and Cypress Domes is given in Figure 30. The pressure increases vertically, as expected. Cypress Creek Dome is indicated by a small rise in the pressure surface, starting at -2100 ft. Richton Dome is not as apparent.

For the (1/density) data, the best geostatistical model was found to be a trilinear drift and the power function covariance:

$$K [d'(X,Y)] = -295 \times d'(X,Y)^{0.54} \quad (8)$$

where $d'(X,Y) = [(x_1 - y_1)^2 + (x_2 - y_2)^2 + 2500 (x_3 - y_3)^2]^{1/2}$

The cross-section of the (1/density) surface is given in Figure 31. The cross-section was located (see Figure 27) to examine the density variations adjacent to Richton, Glazier, (not shown on LetCo map---located approximately midway between Richton and Cypress Creek Domes, along Thompson Creek) and Cypress Creek Salt Domes. Density values observed in the study area range from 0.9982 g/cm³ for fresh water to 1.0765 g/cm³ for saline water. The density variations are a function of total dissolved solids, temperature, and hydrostatic head. High density water ($\rho > 1.05$ g/cm³) is found nearer to land surface in the southern portion of the cross-section. There is a rapid change in density at about latitude 31°13' north, which is supported by data from Wells 2 and 3. The change suggests that there is some effect associated with Cypress Creek Dome.

Examination of Figures 30 and 31 reveals that the pressure and density surfaces are not colinear (see Appendix D). This evidence, along with the variable density, demonstrates the necessity of a three-dimensional treatment of the flow field.

FIGURE 30. Vertical Cross-Section of Estimated Pressure Surface Through Richton and Cyress Creek Domes. Unit is Pascals. Cross-section location shown in Figure 24.

FIGURE 31. Vertical Cross-Section of Estimated Density Surface Through Richton and Cyress Creek Domes. Unit is Pascals. Cross-section location shown in Figure 24.

The force field E from Equation (D.2—Appendix D) was calculated from the geostatistical estimates of $(1/\text{density})$ and of pressure on the three-dimensional grid. A three-dimensional streamline code, based on the International Mathematical and Statistical Libraries (IMSL 1979) Runge-Kutta differential equation solver routine DVERK, was developed to calculate travel paths from the force field [Equation (D.10)]. Table 3 shows the vertical component of the force field e_3 (see Appendix D) for elevations from -1056 to -3168 ft for six points along the transect. In the half of the transect near Richton Dome, e_3 is positive. This indicates that the movement of water is upward; however, the density measurements suggest that there is fresh-water recharge from above. South of Cypress Creek Dome the flow of water appears to be generally downward, and north of Cypress Creek Dome, the trend is upward. No stratigraphic features have been correlated with these results.

For that reason and because of inadequate hydraulic conductivity information, travel times for particles along streamlines [Equation (D.11)] were not calculated. A three-dimensional "back-calculation" of hydraulic conductivities using inverse methods similar to those employed in the two-dimensional Paradox Basin analysis is necessary before travel times can be calculated. These calculations were not included in the original scope of work and budget and time constraints did not allow their addition.

TABLE 3. Vertical Component of Force for Selected Elevations on a Transect Through Richton and Cypress Creek Domes (m/sec^2) (Location of transect shown in Figure 24, Longitude is 89° west)

Elevation (ft)	Latitude ($^\circ$ north)					
	31.078	31.142	31.206	31.270	21.334	31.400
-1056	-0.3089 ^(a)	0.3416	0.4827	0.3982	0.6943	0.8437
-1584	0.1170	0.7574	0.7666	0.2098	0.1727	0.4418
-2112	0.4047	0.5996	0.9523	0.3212	0.0057	0.1727
-2640	0.4697	0.1077	0.6367	0.4975	0.3583	0.3490
-3168	0.2841	-0.1892	0.2284	0.5996	0.5810	0.4975

(a) Negative force indicates downward flow

CONCLUSIONS

The main conclusions of the Mississippi Salt Dome data analysis are that the top of fresh-water surface is adequately described by the geostatistical analysis and that a three-dimensional flow analysis is absolutely necessary to accurately characterize this variable-density ground-water flow system. Analysis of vertical force revealed significant vertical flow components: the fluid density variations dictate that Equation (D.1) must be used to determine whether the vertical flow component is up or down at a particular repository depth.

More complete data and a three-dimensional flow analysis are needed to accurately characterize the streamlines and travel times to the biosphere from the Richton Dome (or from any other hypothetical repository location) in the Mississippi Study Area, and must include: 1) three-dimensional "back-calculations" of hydraulic conductivities to be used in Equation (D.11) for travel times, and 2) a coupling of additional fresh-water head data (above the salt-water/fresh-water interface) to the existing data so that the streamline may be traced to the biosphere. This is necessary because at proposed repository depths (~2000 ft) vertical flow is evident.

PERMIAN BASIN

The data for the Permian Basin salt area were obtained from the Texas Bureau of Economic Geology (TBEG--Austin, Texas). PNL received the first set of data consisting of 91 well head measurements on August 12, 1981. The geostatistical analyses were presented to ONWI on September 29, 1981. ONWI believed that the analyses showed an unacceptable level of variation in the data, and subsequently obtained from TBEG a second data set consisting of 11 head measurements in which a greater level of confidence could be placed. This set was received by PNL on October 16, 1981. On January 20, 1982, PNL presented the geostatistical and hydrologic analyses on an edited version of data sets 1 and 2 to TBEG and ONWI. The preliminary geostatistical analysis indicated that negligible covariance was evident among the data points and that the data set was effectively random. Preliminary hydrologic analysis indicated that either grouped erroneous measurements exist in the data set, or the Wolfcampian aquifer is in hydraulic connection with other units. Two-dimensional ground-water modeling was not attempted under these circumstances. The meeting of January 20 resulted in a third data set given to PNL by TBEG.

Because of substantial differences between the combined first and second data sets as compared to the third data set, PNL believes that reporting any results on the first and second data sets would be misleading and inappropriate. Time and funding constraints did not allow further analysis of TBEG data.

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APPENDIX A

GEOSTATISTICAL THEORY

APPENDIX A

GEOSTATISTICAL THEORY

The following is a brief description of the theory behind the geostatistical analyses described in this report. For more detail, see Doctor (1979), Devary and Doctor (1981), and Ripley (1981).

Let $z(X)$ be the value of a continuous surface at location $X = (x_1, x_2, x_3)$ in a three-dimensional set. $z(X)$ is assumed to be the realization of a stochastic process. Given that $z(X)$ is observed at discrete locations $X_1, X_2, \dots, X_n$, the geostatistical (kriging) estimate of z at an unobserved point X_0 is the linear combination of observed data

$$z^*(X_0) = \sum_{i=1}^n \lambda_i z(X_i) \quad (A.1)$$

such that:

- (1) $E[z^*(X_0) - z(X_0)] = 0$
- (2) $E([z(X_0) - z^*(X_0)]^2)$ is minimal.

(E denotes the probabilistic expectation operator.) This means that $z^*(X_0)$ is an unbiased and minimum variance estimator of $z(X_0)$. To determine $z^*(X_0)$, which involves calculating the kriging weights $\{\lambda_i\}$, it is necessary to characterize the drift (mean-value) function, and the covariance or variogram functions of $z(X)$. Specifically, for each X and Y within the neighborhood of a point X_0 , the order of the drift

$$E[z(X)] = m(X) = \sum_{\ell} a_{\ell} f^{\ell}(X) \quad (A.2)$$

where $\{a_{\ell}\}$ are unknown constants and $\{f^{\ell}(X)\}$ are monomial functions of some finite order, and the covariance function

$$K(|X - Y|) = E([z(X) - m(X)][z(Y) - m(Y)]) \quad (A.3)$$

or the variogram function

$$\frac{E[z(X) - z(Y)]^2}{2} \quad (A.4)$$

must be known or estimated from the data.

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APPENDIX B

INVERSE METHOD TO CALCULATE TRANSMISSIVITY

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INVERSE METHOD TO CALCULATE TRANSMISSIVITY

The inverse transmissivity calculation is based on Darcy's Law of ground-water flow. By Darcy's Law, the instantaneous flow rate (Q) for the jth element of the ith streamtube of the flow net (see Figure B.1) is:

$$Q_{i,j} = T_{i,j} \frac{[h_1 - h_2]}{L_{i,j}} W_{i,j} \quad (B.1)$$

where

Q = flow rate (ft/day)

T = transmissivity (ft²/day)

L = length (ft)

W = width (ft)

h = head (ft)

j = streamtube element number

i = streamtube number in the flow net.

The flow net is constructed such that $\Delta h = h_1 - h_2$ is constant down each streamtube. If T_0 is the known starting transmissivity value for the j_0 element of the ith streamtube, then:

$$Q_{i,j_0} = T_0 \left[\frac{\Delta h}{L_{i,j_0}} \right] W_{i,j_0} \quad (B.2)$$

Because flow down the streamtube is constant

$$Q_{i,j} = Q_{i,j_0} \quad (B.3)$$

FIGURE B.1. Streamtubes and Streamtube Elements Showing the Relationship of the Variables Used in the Transmissivity Calculation

Substituting Equations (B.1) and (B.2) in Equation (B.3) yields:

$$T_{i,j} \left[\frac{\Delta h}{L_{i,j}} \right] W_{i,j} = T_{i,j_0} \left[\frac{\Delta h}{L_{i,j_0}} \right] W_{i,j_0} \quad (B.4)$$

defining $C_{i_0} = T_{i,j_0} [W_{i,j_0}/L_{i,j_0}]$, substituting into Equation (B.4) and solving for $T_{i,j}$:

$$T_{i,j} = C_{i_0} \left[\frac{L_{i,j}}{W_{i,j}} \right]$$

where C_{i_0} is constant for each element in streamtube i .

The assumptions underlying the construction of the flow net are:

- The flow net is constructed sufficiently dense so that the sides of the flow net elements can be approximated by straight lines (see dashed lines in Figure B.1).
- The calculated transmissivity ($T_{i,j}$), is an average value for the flow net element and is representative of the transmissivity at the center of the flow net element (see Figure B.1).

APPENDIX C

PARADOX BASIN SIMULATION RESULTS

APPENDIX C

PARADOX BASIN SIMULATION RESULTS

Appendix C is divided into four sections, one for the results of each of the following simulated cases:

- Well A (high potential) – Well B (high potential)
- Well A (high potential) – Well B (low potential)
- Well A (low potential) – Well (high potential)
- Well A (low potential) – Well B (low potential)

Each of these sections includes the following figures and tables:

- geostatistically estimated potential surface
- calculated transmissivity map
- Lavender Canyon hypothetical repository streamtubes
- Lavender Canyon arrival time curve
- table of arrival time data for the Lavender Canyon hypothetical repository.

RESULTS OF THE SIMULATED CASE:
WELL A (HIGH POTENTIAL) – WELL B (HIGH POTENTIAL)

FIGURE C.2. Transmissivity Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (High) and Well B (High) Transmissivities are in Units of ft^2/day ; Contour Interval is $26.7 \text{ ft}^2/\text{day}$

FIGURE C.3. Streamtubes from the Lavender Canyon Hypothetical Repository for the Case: Well A (High) - Well B (High)

FIGURE C.4. Arrival Time Curve for the Lavender Canyon Hypothetical Repository for the Case: Well A (High) - Well B (High)

TABLE C.1. Arrival Time Data for the Lavender Canyon Hypothetical Repository Site for the Case: Well A (High) and Well B (High)

Stream-tube Number	Average Ground-Water Arrival Time (yr)	Ground-Water Flow Rate (gpm)	Cumulative Ground-Water Flow Rate (gpm)	Cumulative Flow Rate Divided by Total Flow Rate
	36751	0.0	0.0	0.00
1	37356	4.4	4.4	0.12
2	38398	3.3	7.8	0.21
3	39500	4.8	12.6	0.34
4	41076	5.0	17.7	0.47
5	43377	5.2	22.9	0.61
6	46732	4.5	27.4	0.73
7	51869	5.1	32.6	0.87
8	56023	4.9	37.5	1.00

Total ground-water flow rate = 37.5 gpm

RESULTS OF THE SIMULATED CASE:
WELL A (HIGH POTENTIAL) – WELL B (LOW POTENTIAL)

110° 19'

109° 09'

38° 31'

FIGURE C.6. Transmissivity Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (High) – Well B (Low)
Transmissivities are in Units of ft^2/day ; Contour Interval is $26.7 \text{ ft}^2/\text{day}$

FIGURE C.7. Streamtubes from the Lavender Canyon Hypothetical Repository for the Case: Well A (High) – Well B (Low)

FIGURE C.8. Arrival Time Curve for the Lavender Canyon Hypothetical Repository for the Case: Well A (High) - Well B (Low)

TABLE C.2. Arrival Time Data for the Lavender Canyon Hypothetical Repository Site for the Case: Well A (High) and Well B (Low)

Stream-tube Number	Average Ground-Water Arrival Time (yr)	Ground-Water Flow Rate (gpm)	Cumulative Ground-Water Flow Rate (gpm)	Cumulative Flow Rate Divided by Total Flow Rate
	34945	0.0	0.0	0.0
1	35129	3.8	3.8	0.1
2	35508	3.6	7.4	0.2
3	35736	4.3	11.8	0.3
4	35865	3.0	14.8	0.4
5	36225	3.1	18.0	0.5
6	36570	3.2	21.3	0.5
7	36902	3.4	24.7	0.6
8	37495	3.5	28.3	0.7
9	38276	3.6	32.0	0.8
10	39069	3.8	35.8	1.0

Total ground-water flow rate = 35.8 gpm

RESULTS OF THE SIMULATED CASE:
WELL A (LOW POTENTIAL) - WELL B (HIGH POTENTIAL)

FIGURE C.9. Geostatistically Estimated Potentiometric Surface for the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (Low) – Well B (High)

110° 19'

109° 09'

38° 31'

37° 25'

FIGURE C.10. Transmissivity Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (Low) - Well B (High) Transmissivities are in Units of ft^2/day ; Contour Interval is $26.7 \text{ ft}^2/\text{day}$

FIGURE C.11. Streamtubes from the Lavender Canyon Hypothetical Repository for the Case: Well A (Low) - Well B (High)

FIGURE C.12. Arrival Time Curve for the Lavender Canyon Hypothetical Repository for the Case: Well A (Low) - Well B (High)

TABLE C.3. Arrival Time Data for the Lavender Canyon Hypothetical Repository Site for the Case: Well A (Low) and Well B (High)

Stream- tube Number	Average Ground-Water Arrival Time (yr)	Ground-Water Flow Rate (gpm)	Cumulative Ground-Water Flow Rate (gpm)	Cumulative Flow Rate Divided by Total Flow Rate
	71143	0.0	0.0	0.00
1	72119	0.5	0.5	0.07
2	84171	1.7	2.3	0.26
3	98299	1.7	4.0	0.45
4	111809	1.6	5.7	0.64
5	136960	1.6	7.4	0.82
6	159629	1.6	9.0	1.00

Total ground-water flow rate = 9.0 gpm

RESULTS OF THE SIMULATED CASE:
WELL A (LOW POTENTIAL) - WELL B (LOW POTENTIAL)

FIGURE C.13. Geostatistically Estimated Potentiometric Surface for the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (Low) – Well B (Low)

110° 19'

109° 09'

38° 31'

SCALE

37° 25'

FIGURE C.14. Transmissivity Map of the Lower Hydrostratigraphic Unit of the Paradox Basin for the Case: Well A (Low) - Well B (Low)
Transmissivities are in Units of ft^2/day ; Contour Interval is $26.7 \text{ ft}^2/\text{day}$

FIGURE C.15. Streamtubes from the Lavender Canyon Hypothetical Repository for the Case: Well A (Low) - Well B (Low)

FIGURE C.16. Arrival Time Curve for the Lavender Canyon Hypothetical Repository for the Case: Well A (Low) - Well B (Low)

TABLE C.4. Arrival Time Data for the Lavender Canyon Hypothetical Repository Site for the Case: Well A (Low) and Well B (Low)

Stream- tube Number	Average Ground-Water Arrival Time (yr)	Ground-Water Flow Rate (gpm)	Cumulative Ground-Water Flow Rate (gpm)	Cumulative Flow Rate Divided by Total Flow Rate
	55941	0.0	0.0	0.00
1	56195	0.5	0.5	0.06
2	57685	1.1	1.6	0.18
3	60875	1.2	2.9	0.31
4	63956	1.1	4.0	0.43
5	66859	1.1	5.1	0.55
6	69816	1.0	6.2	0.65
7	74185	1.1	7.3	0.78
8	80949	1.0	8.4	0.89
9	87234	1.0	9.5	1.00

Total ground-water flow rate = 9.5 gpm

APPENDIX D

THREE-DIMENSIONAL FLOW EQUATIONS

APPENDIX D

THREE-DIMENSIONAL FLOW EQUATIONS

Examination of the saline densities for the Mississippi Study Area indicated a range of 0.964 g/cm^3 to 1.076 g/cm^3 as computed from LETCo data.

When fluid density is variable, modeling of ground-water flow requires that the more generalized form of Darcy's Law be used (Hubbert 1956):

$$E = g - (1/\rho) \vec{\nabla} P \quad (D.1)$$

where

E = force per unit mass

g = gravitational field

ρ = density

P = pressure

$\vec{\nabla}$ = del or gradient operator

For cases of fresh water (constant density) this is usually shortened to:

$$E = -\vec{\nabla} \Phi \quad (D.2)$$

where

$\Phi = gh$ = work required to lift a unit mass of water from datum (sea level) to h .

The force per unit mass (E) can be derived from the water level potential when (E) is irrotational, which is determined by the curl of (E) equal to 0:

$$\text{curl } E = \text{curl } [g - (1/\rho) \vec{\nabla} P] \quad (D.3)$$

$$= \vec{\nabla} \times g - \vec{\nabla} \times [(1/\rho) \vec{\nabla} P] \quad (D.4)$$

$$\text{If } g \text{ is a constant, then } \vec{\nabla} \times g = 0, \text{ and } \text{curl } E = \vec{\nabla} \times (1/\rho) \vec{\nabla} P, \quad (D.5)$$

so that

$$\text{curl } E = 0 \text{ when } -\vec{\nabla} \times (1/\rho) \vec{\nabla} P = 0 \quad (D.6)$$

Therefore, for the field to be irrotational, either $-\nabla(1/\rho) = 0$ (constant fluid density), or $\nabla P = 0$ (constant fluid pressure) or the surfaces of equal density and equal pressure are collinear. None of the above conditions are met in the Mississippi Study Area. Hence there is no potential of E that can be derived solely from the water-level elevations.

An example is provided to illustrate the magnitude of error associated with assuming that water levels in the Mississippi Study Area are potentials. Data from Well No. 11 at $31^{\circ} 20.6'$ latitude, $88^{\circ} 59.8'$ longitude is used to calculate the force per unit mass at the -4029 ft elevation.

TABLE D.1. Well No. 11 Water Level Data

<u>Elevation (ft)</u>	<u>Saline Head (ft)</u>	<u>Fresh-Water Head (ft)</u>	<u>Density g/cm³</u>
-4029	93	322	1.0556
-2339	216	234	1.007

An examination of equivalent fresh-water heads indicates a higher head at depth. If we incorrectly assume that this represents a potential, then, Equation (D.2) (in the vertical dimension only for simplicity) yields:

$$E = (9.79434 \text{ m/sec}^2) (0.05207) \quad (\text{D.7})$$

$$E = 0.510 \text{ m/sec}^2$$

which is an upwards force. If we incorrectly assume that the saline heads are a potential, then Equation (D.2), again in the vertical, yields:

$$E = (9.79434 \text{ m/sec}^2) (-0.07278) \quad (\text{D.8})$$

$$E = -0.7128 \text{ m/sec}^2$$

which is a downward force.

The correct form of Darcy's Law for this flow system is Equation (D.1) and the vertical component of force is:

$$E = (9.79434 \text{ m/sec}^2) - \frac{1}{1055.6 \text{ kg/m}^3} (10310 \text{ N/M}^2) \quad (\text{D.9})$$

$$E = -0.02738 \text{ m/sec}^2$$

which is a downward force. Comparison of the results in Equations (D.7), (D.8), and (D.9) indicates the error associated with not using the generalized form of Darcy's Law in variable density ground water.

Given the more general case of variable density, a force field $E = (e_1, e_2, e_3)$ and an isotropic hydraulic conductivity σ , then the streamlines for ground-water flow, through a particular point $X^* = (x_1^*, x_2^*, x_3^*)$ in the aquifer, are given by the following system of linear ordinary differential equations (the streamline characteristic equations):

$$\begin{aligned} \frac{dx_1}{ds} &= e_1 & \text{where } x_1(0) &= x_1^* \\ \frac{dx_2}{ds} &= e_2 & \text{where } x_2(0) &= x_2^* \\ \frac{dx_3}{ds} &= e_3 & \text{where } x_3(0) &= x_3^* \end{aligned} \quad (\text{D.10})$$

The travel times along pathlines are calculated by incorporating the hydraulic conductivities and effective porosities, θ , into the pathline characteristic equations

$$\begin{aligned}
 \frac{dx_1}{dt} &= \frac{\sigma}{\theta} e_1 & x_1(t_0) &= x_1^* \\
 \frac{dx_2}{dt} &= \frac{\sigma}{\theta} e_2 & x_2(t_0) &= x_2^* \\
 \frac{dx_3}{dt} &= \frac{\sigma}{\theta} e_3 & x_3(t_0) &= x_3^*
 \end{aligned}
 \tag{D.11}$$

where

t = time.

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Hubbert, M. K. 1956. "Darcy's Law and the Field Equations of the Flow of Underground Fluids." Journal of Petroleum Hydrology.

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