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ANALYSIS OF THE POTENTIAL FOR UNSATURATED FLOW WITHIN THE EVAPORITE AQUITARD, DEAF SMITH COUNTY SITE, PALO DURO BASIN

Numerical Evaluation of Conceptual Models
Subtask 3.5
Mini-Performance Assessment Report #1

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1.0 INTRODUCTION

1.1 General Statement of the Problem

Generalized conceptual models of the hydrogeologic system in the Palo Duro Basin assume that there are three major hydrostratigraphic units: 1) an upper fresh-water aquifer comprised of the Ogallala formation and Dockum Group, 2) an evaporite and shale aquitard, which includes the repository horizon, and 3) a deep-basin brine aquifer (DOE, 1986). In the generalized conceptual model, vertical downward flow is presumed to occur from the Ogallala-Dockum aquifer across the evaporite aquitard to the deep-basin brine aquifer. In some conceptual models, there is also presumed to be a small horizontal component to flow within the aquitard. Thus, the evaporite aquitard has been viewed as an avenue for radionuclide transport to the accessible environment, both horizontally via interbeds within the aquitard and vertically to the deep-basin brine aquifer and then horizontally.

All conceptual models proposed thus far have presumed that flow occurs under fully saturated conditions everywhere within the flow system. The evaporite aquitard consists of moderately thick strata which may have rather large contrasts in permeability between adjacent layers. This contrast in permeability may be sufficient to create perched and unsaturated zones within parts of the aquitard, depending upon the thicknesses of impeding layers and the head of water above the impeding layer.

1.2 Relevance to the NRC Waste Management Program

DOE General Guidelines for the Recommendation of Sites for Nuclear Waste Repositories, 10 CFR 960, indicates that in order for the site to qualify for characterization, the pre-emplacement ground-water travel time to the accessible environment must exceed 1000 years. NRC and EPA regulatory requirements (40 CFR 191, 10 CFR 60) for license approval list maximum allowable cumulative quantities of radionuclides which could be released to the accessible environment over a 10,000 year period. This mass flux is controlled to a great extent by ground-water travel time. Numerical and analytical models are used to calculate ground-water travel time. However, the travel time is a function of rock pore space saturation.

The degree of saturation affects travel time calculations in many ways. Two of these are through the permeability and effective porosity, or, more appropriately for unsaturated conditions, effective moisture content. Unsaturated conditions can also affect parameters such as thermal conductivity in analyses of solute transport due to heating of water and rock near the repository. The existence of unsaturated conditions may provide an extra margin of safety to the site, with respect to impact of radionuclide transport travel time to the accessible environment. That is, neglecting unsaturated flow may be conservative and lead to faster travel time; however, we believe the analyses of flow and transport should not be based on an invalid framework for the conceptual model.

Numerical models which are restricted to considering only saturated conditions may lead to inaccurate predictions which guide the development of conceptual models of the performance of the system during pre-emplacement or post-closure conditions. For example, under saturated conditions within the evaporite aquitard, lateral transport through the relatively permeable carbonate interbeds is one of the more likely pathways to the accessible environment (Andrews et al, 1985). If unsaturated conditions occur beneath a contact between a flow-impeding salt layer and an underlying carbonate interbed, then there may actually be virtually no lateral flow within this zone to the accessible environment due to pressure gradients.

We believe that the occurrence of unsaturated conditions is also relevant to site characterization plans. If unsaturated conditions are predicted to occur, then field tests should be designed to characterize this phase and integrate it into a revised conceptual model of the hydrogeologic system.

1.3 Relationship to Other Subtasks, Analyses and Documents

Our subtask 3.4 report on Conceptual Model Evaluation first pointed out the lack of consideration given to the possibility for unsaturated flow within the evaporite aquitard (Stephens and Assoc., 1986; p.71). We believe that the degree of saturation is fundamental to describing the framework of the hydrogeologic setting for the repository. This mini-performance assessment is a first-step toward quantifying the need to consider unsaturated flow in conceptual model development and in the future, more sophisticated performance assessments using numerical models, for example. If required, much more detailed analyses would be included in future investigations within the scope of subtask 3.5.

The motivation for this mini-performance assessment is prompted in part by published statements in DOE documents. For example, Orr (1984) suggests that one explanation for underpressuring of the deep basin brine aquifer is lack of continuity within the hydrostatic Ogallala-Dockum aquifer. If there is a lack of hydraulic continuity, this implies that stresses to the upper and lower aquifers will not propogate across the evaporite aquitard either because the aquitard is impermeable or because the pore space is only partially saturated at some horizon within the aquitard. In another example, it is stated in the Environmental Assessment (DOE, 1986; p. 3-143) that because the evaporite aquitard lies below the water table aquifer, the evaporite aquitard can be assumed to be saturated. This statement is not supported by calculations or field measurements.

2.0 OBJECTIVE

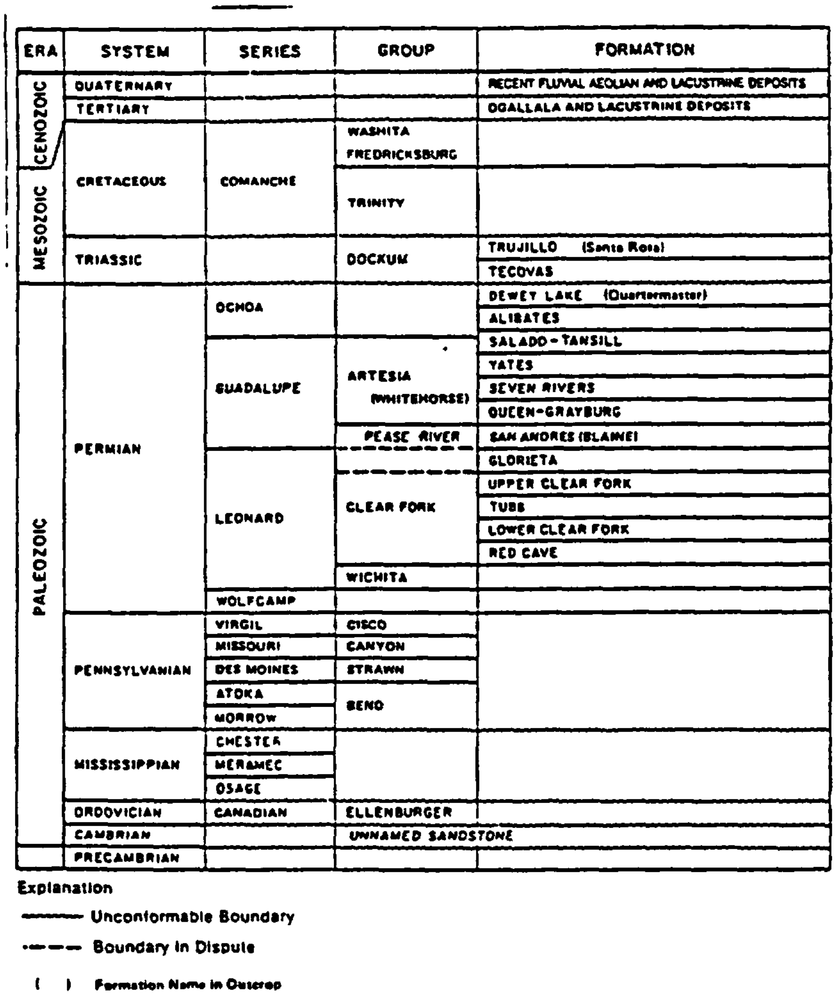
Under what conditions may unsaturated flow occur in a stratified multi-aquifer system? Are conditions present in the Palo Duro Basin which are likely to cause unsaturated flow within the evaporite aquitard?

These objectives address a fundamental aspect of characterizing the hydrogeologic framework within which ground-water flow and radionuclide transport occur.

3.0 GENERAL APPROACH

3.1 Hydrogeologic Setting

The Palo Duro Basin, a sub-basin of the Permian Basin, is underlain by a thick, extensive layer of bedded salt. This salt bed is a potential site for a high level waste repository. Clastic and carbonate sediments of early Permian age and order fill the deepest part of the basin. Much of the mid- and late-Permian period is represented by evaporite deposits. Clastic rocks dominate the stratigraphic sequence after the Permian time (Figure 1 and 2). A more detailed cross-section of the stratigraphic units above the San Andres formation is shown in figure 3. Table 1 gives a brief description of



ERA	SYSTEM	SERIES	GROUP	FORMATION
CENOZOIC	QUATERNARY			RECENT FLUVIAL AEOLIAN AND LACUSTRINE DEPOSITS
	TERTIARY			OGALLALA AND LACUSTRINE DEPOSITS
MESOZOIC	CRETACEOUS	COMANCHE	WASHITA FREDRICKSBURG	
			TRINITY	
	TRIASSIC		DOCKUM	TRUJILLO (Santa Rosa)
				TECOVAS
PALEOZOIC	PERMIAN	OCHOA		DEWEY LAKE (Quartermaster)
				ALIBATES
		GUADALUPE	ARTESIA (WHITEHORSE)	SALADO-TANSILL
				YATES
				SEVEN RIVERS
				QUEEN-GRAYBURG
			PEASE RIVER	SAN ANDRES (BLAINE)
		LEONARD		GLORIETA
			CLEAR FORK	UPPER CLEAR FORK
				TUBB
				LOWER CLEAR FORK
				RED CAVE
			WICHITA	
		WOLFCAMP		
	PENNSYLVANIAN	VIRGIL	CISCO	
		MISSOURI	CANYON	
		DES MOINES	STRAWN	
		ATOKA	BEND	
		MORROW		
	MISSISSIPPIAN	CHESTER		
		MERAMEC		
		OSAGE		
	ORDOVICIAN	CANADIAN	ELLENBURGER	
	CAMBRIAN		UNNAMED SANDSTONE	
	PRECAMBRIAN			

Explanation

——— Unconformable Boundary

-—-— Boundary In Dispute

( ) Formation Name in Outcrop

Figure 1. Stratigraphic Column of the Palo Duro Basin (DOE, 1986)

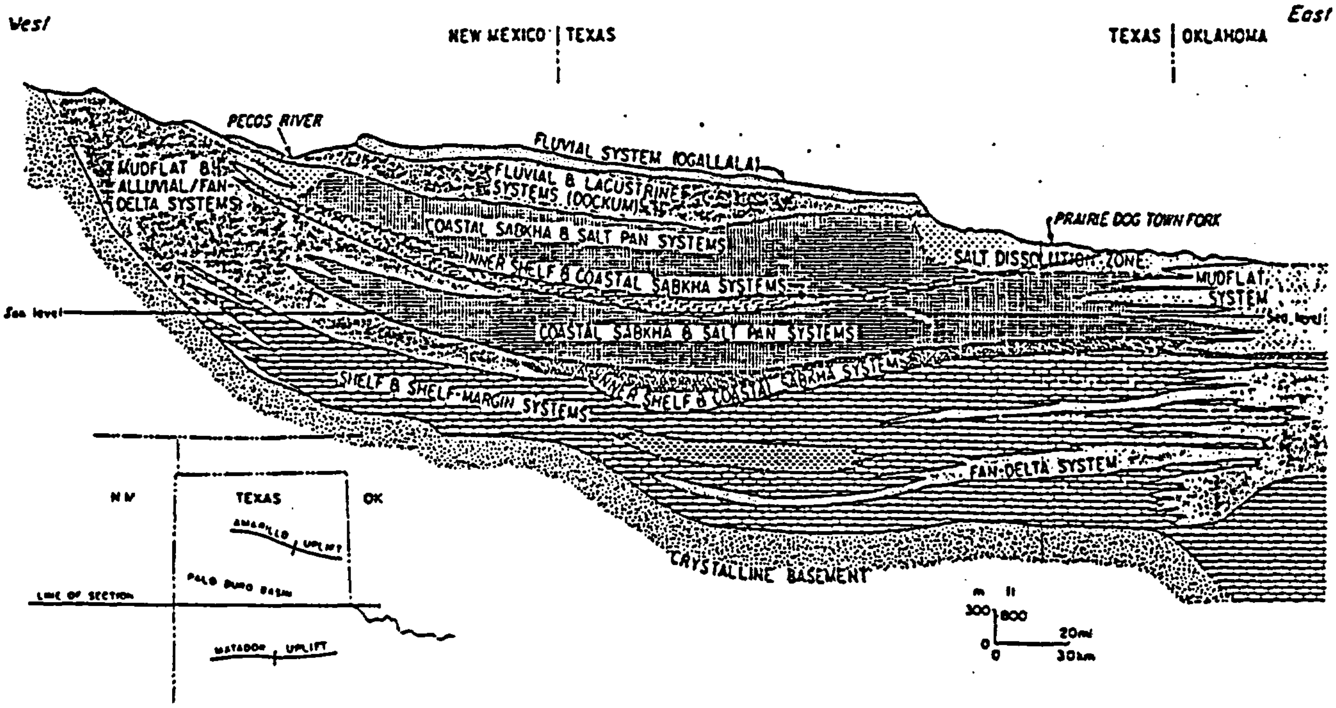
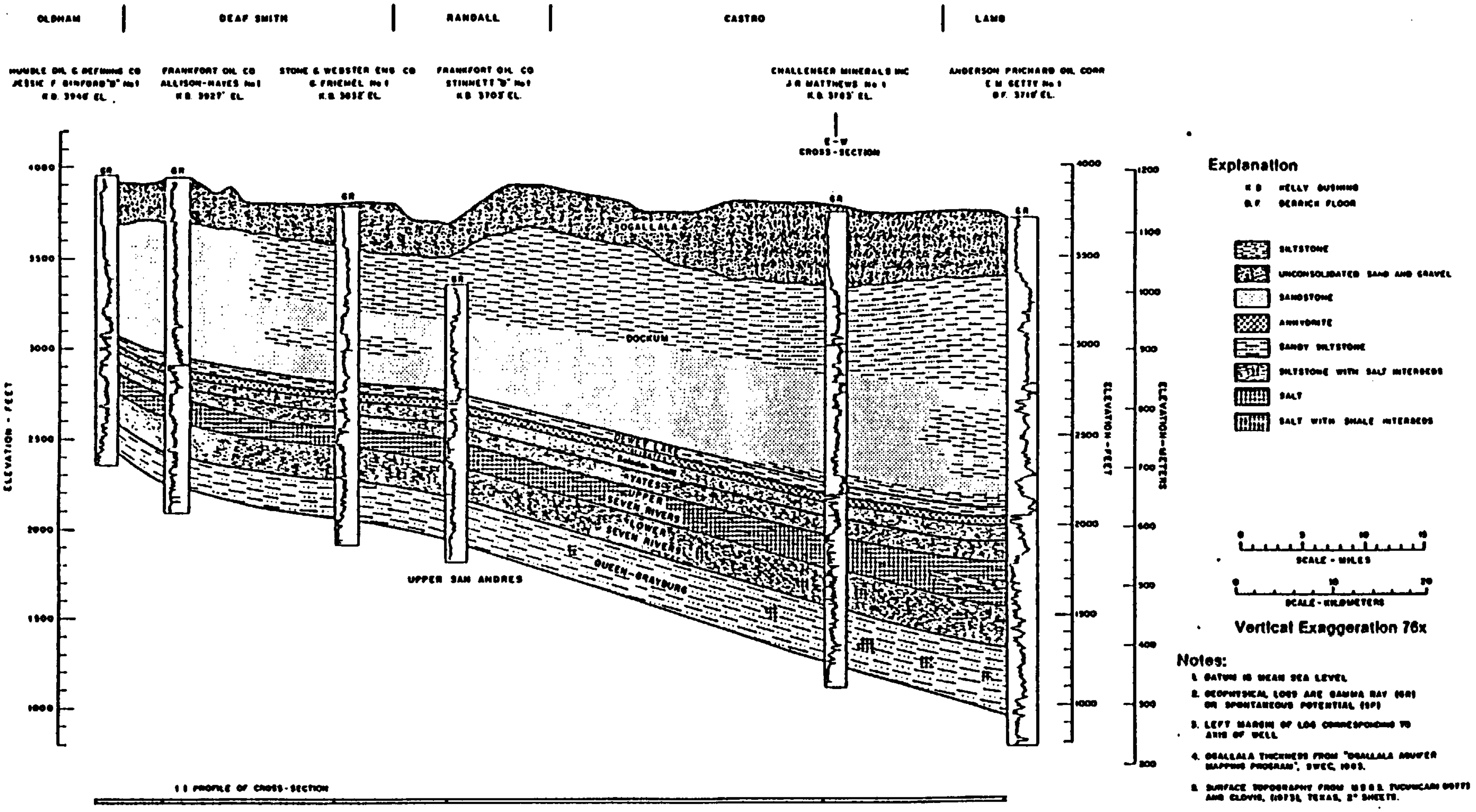


Figure 2. Cross-Section of General Depositional Environment in Palo Duro Basin (SWEC, 1983)



Notes:

1. DATUM IS MEAN SEA LEVEL
2. GEOPHYSICAL LOGS ARE GAMMA RAY (GR) OR SPONTANEOUS POTENTIAL (SP)
3. LEFT MARGIN OF LOG CORRESPONDING TO AXIS OF WELL
4. OGALLALA THICKNESS FROM "OGALLALA AQUIFER MAPPING PROGRAM", SWEC, 1983.
5. SURFACE TOPOGRAPHY FROM U.S.G.S. TUCUMCARI (1977) AND CLOVIS, (1973), TEXAS, 2° SHEETS.

Figure 3. North-South Geologic Cross-Section, Ogallala Through Queen-Greyburg (DOE, 1986)

Table 1. Estimated Stratigraphy at the Deaf Smith County Site (After DOE, 1986)

Geologic Unit	Elevation of Top from MSL (ft.)		Thickness (ft.)		Lithology
Ogallala Formation	4,033	2	340	25	Reddish-tan claystone and sandstone unconsolidated to soft; fine subrounded to round grains.
Dockum	3,693	25	621	50	Red-brown sandy Group siltstone with layers of claystone and sandstone, grading to conglomerate.
Dewey Lake Formation	3,072	75	74	20	Red-brown siltstone and claystone.
Alibate Formation	2,998	150	32	5	Light green to white dolomite with siltstone.
Salado-Tansill Formation	2,966	150	67	5	Red-brown siltstone with some gypsum and anhydrite.
Yates Formation	2,899	150	65	5	Red-brown siltstone and very fine sandstone.
Upper Seven Rivers Formation	2,834	150	130	15	Interbedded gray anhydrite and red-brown claystone/siltstone, salt with some siltstone/claystone and anhydrite.
Lower Seven Rivers Formation	2,704	150	194	5	Red-brown siltstone with minor anhydrite.
Queen-Grayburg Formation	2,510	150	180	10	Red-brown siltstone and sandstone.

Table 1 (continued).

Geologic Unit	Elevation of Top from MSL (ft.)		Thickness (ft.)		Lithology
Upper San Andres Formation	2,330	150	474	10	Salt with varying amounts of red-brown mudstone impurities, occasional anhydrite and dolomite layers. Mostly anhydrite with interbeds of dolomite and siltstone at the base.
Lower San Andres Unit 5	1,856	150	194	10	Upper section alternating beds of salt with some red-brown mudstone impurities and bluish gray anhydrite; lower section alternating beds of bluish gray anhydrite and grayish brown dolomite.
Lower San Andres Unit 4	1,662	150	250	5	Salt with varying amounts of red-brown mudstone. Mainly dolomite and limestone with anhydrite beds at the base.
Lower San Andres Unit 3	1,412	150	120	5	Clear to white salt with a 30-foot-thick layer of gray-brown anhydritic dolomite and limestone at the base.
Lower San Andres Unit 2	1,292	150	71	5	Upper section salt with red-brown siltstone impurities; lower section light to medium gray dolomite with occasional interbeds of salt.

Table 1 (continued).

Geologic Unit	Elevation of Top from MSL (ft.)		Thickness (ft.)		Lithology
Lower San Andres Unit 1	Absent		Absent		
Glorieta Formation	1,221	150	610	10	Thick salt sequence with varying quantities of red-brown siltstone impurities, occasional sandstone.
Upper Clear Fork Formation	611	150	495	10	Mainly salt with some beds of red-brown siltstone, light tan dolomite and white anhydrite; sequence of white anhydrite, red-brown siltstone and light tan dolomite at the base.
Tubb Formation	116	200	212	25	Red-brown siltstone and fine sandstone with some anhydrite and salt.
Lower Clear Fork Formation	-96	200	294	25	Alternating beds of red brown siltstone, clear to white salt, and white anhydrite.
Red Cave Formation	-390	200	543	20	Red shale with some siltstone and anhydrite.
Wichita Group	-933	250	330	20	Upper section interbedded anhydrite and red shale with some medium olive-gray dolomite; lower section olive gray argillaceous dolomite with anhydrite

Table 1 (continued).

Geologic Unit	Elevation of Top from MSL (ft.)		Thickness (ft.)		Lithology
Wolfcamp Series	-1,263	350	1,245	50	Upper section thick sequence of olive-gray dolomite (210 ft); middle section limestone varying in color from olive gray-tan to dark gray (310 ft); lower section dark gray to black argillite (725 ft).
Pennsylvanian System, Upper Section	-2,508	350	309	50	Alternating shale and tan limestone grading downward into a thick sequence of medium gray shale.
Pennsylvanian System, Carbonate Section	-2,817	400	550	75	Limestone and black shale.
Pennsylvanian System, Granite Wash Section	-3,367	450	683	100	Arkose with thin interbeds of shale and limestone.
Precambrian Basement	-4,050	500	--		Rhyolite

the units and their thickness beneath the Deaf Smith County Site. The closest DOE well to the Deaf Smith County Site is the J. Friemel well, located about 3 miles south of the southeastern corner of the 9-mile square site area. A geologic profile and geophysical log of this well are provided in Figure 4. The level of geologic detail presented increases in comparing the sequence in Figures 1 through 4. There are clearly rather significant lithologic variations within mapped geologic units.

Ground water occurs in the Ogallala formation which is extensively used for water supply in the Palo Duro Basin. Sandstones within the underlying Dockum Group also yield water to wells. Some conceptual models of the hydrogeologic system consider the Ogallala and Dockum as a single water-bearing unit called Hydrostratigraphic Unit A (HSU A) (Figure 1). Ground water generally flows eastward and southeast in the Ogallala aquifer. In the Dockum, the direction of flow is less well known, owing to lack of data and discontinuity of sandstone facies. Recharge to the Ogallala is by areal precipitation, and recharge to the Dockum occurs by leakage from the Ogallala. The hydraulic head in the Dockum near the site is approximately 400 feet less than that in the Ogallala. This large difference in head and the occurrence of low-permeable siltstone within the Dockum suggest that the hydraulic connection between the two units is relatively

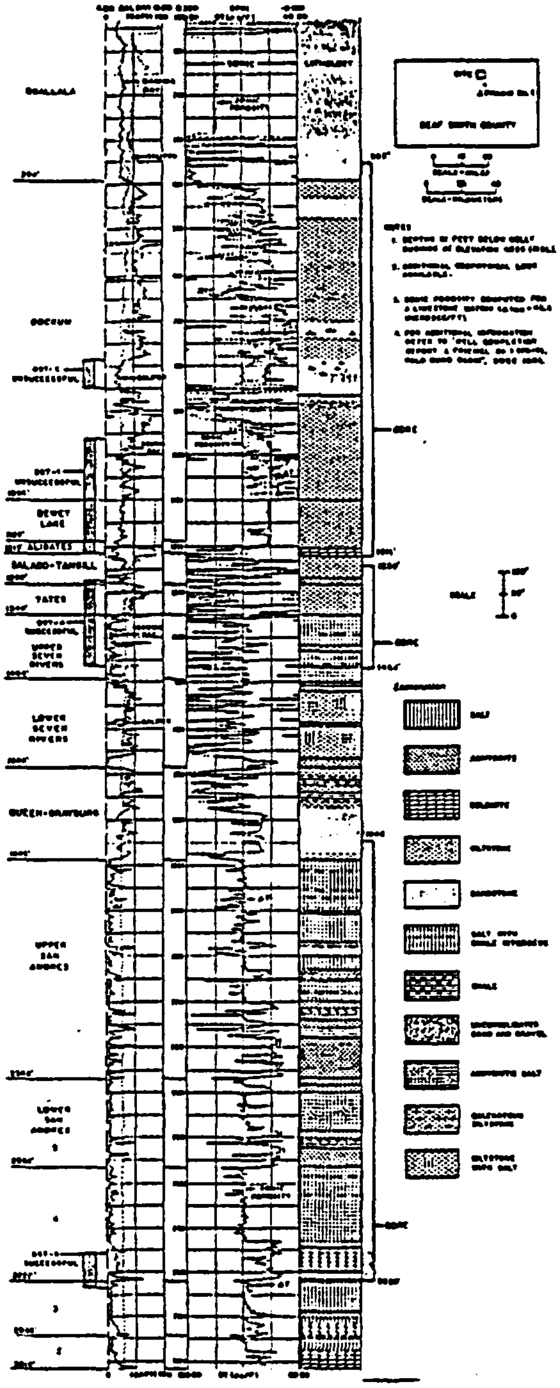


Figure 4. Geologic Profile at J. Friemel Well, Ogallala Through Lower San Andres (DOE, 1986)

poor near the site. The average permeability of the Ogallala has been estimated to range from about 5.7 to 12.3 darcy (DOE, 1986, p.3-139). No reliable permeability data are available for the Dockum Group siltstone facies; however, numerical model studies by Senger et al (1985) found that the vertical permeability of the Ogallala had to be about 10^4 times greater than the Dockum to simulate the observed head difference between the two units (Table 2).

The stratigraphic interbeds between the Dewey Lake formation and the Wichita group comprise a shale and evaporite aquitard which is referred to as HSU B in the simple conceptual models (DOE, 1986) (Figure 1). There is insufficient data to characterize ground-water movement within HSU B; however, it is inferred that the groundwater flow direction is predominantly downward, based on the hydraulic head difference across the aquitard. Some of the numerical models predict that there is also a minor horizontal flow component in HSU B, for example, Senger et al (1985). There are few permeability values for the aquitard. Tests in a carbonate interbed (lower San Andres Unit 4) indicate a median permeability of 0.25 millidarcy. Generic values for shale permeability may range from 10^{-5} to 10^{-1} millidarcy, and salt permeability may range from about 7×10^{-4} to 3×10^{-2} millidarcy (Table 2).

Table 2. Summary of Permeability Data

Unit	Permeability (millidarcy)	Reference
Ogallala	5.7 to 12.3 x 10^3	DOE, 1986
Dockum	1 (est.)	Senger et al, 1985
carbonate interbed	0.25	DOE, 1986
shale	10^{-5} to 10^{-1}	DOE, 1986
salt	7 x 10^{-4} to 3 x 10^{-2}	DOE, 1986

HSU B is underlain by relatively permeable carbonate and clastic sedimentary rocks which are referred to as HSU C (DOE, 1986) (Figure 1). This unit contains brine in most of the basin. Near the site the hydraulic head in the Wolfcamp dolomite in the upper part of HSU C is approximately 1350 feet lower than that in the Dockum Group (DOE, 1986; pp. 3-141, 3-147). Recharge is believed to occur mostly in outcrop areas in New Mexico and by leakage from the overlying shale and evaporite aquitard, HSU B. The groundwater flow direction is to the northeast in HSU C.

3.2 Concepts Used for Analysis

In near-surface processes such as infiltration of irrigation water, it is not uncommon for perched water tables to develop above a low-permeable layer which impedes infiltration. The hydrogeologic setting previously described can be summarized as one in which there is a zone of relatively high-permeable water-bearing units (HSU A) overlying a zone of low-permeable shales and evaporites (HSU B). This mini-performance assessment addresses the possibility that the permeability contrast between layers within HSU B, is sufficient to create local zones of unsaturated conditions.

A very simplified approach is utilized herein as a first step. We assume that one-dimensional, vertical flow occurs from a permeable water-bearing unit across a low-permeable aquitard and into an underlying thick, relatively permeable unit. The degree of saturation of the lower permeable unit depends mostly upon its permeability, the permeability and thickness of the aquitard, and the head of water acting above the aquitard. We will identify combinations of key parameters which lead to unsaturated conditions and determine whether the possibility for unsaturated conditions could potentially occur near the site.

4.0 TECHNICAL APPROACH

4.1 Statement of Problem

An analytical procedure will be utilized to predict the occurrence of the transaction from saturated to unsaturated conditions in a layered porous medium under pre-emplacement conditions.

Consider a three-layered sequence, as shown in Figure 5. The upper layer is highly permeable compared to the flow-impeding middle layer or aquitard. The layer beneath the aquitard is thick and more permeable than the aquitard. A head of water acts above the aquitard, and there is a water table within the lower layer. Steady flow is vertically downward. Because the permeability of the upper layer is much greater than that of the aquitard, the head loss in the upper aquifer is assumed to be negligible. Thus, static equilibrium is assumed in the upper layer and the pressure head at the base of this layer equals the saturated thickness.

In general, provided that the lower layer is sufficiently thick and the water table within it is sufficiently deep, unsaturated flow may occur beneath the aquitard if the rate of deep pecolation through the aquitard exceeds the hydraulic conductivity of the underlying layer.

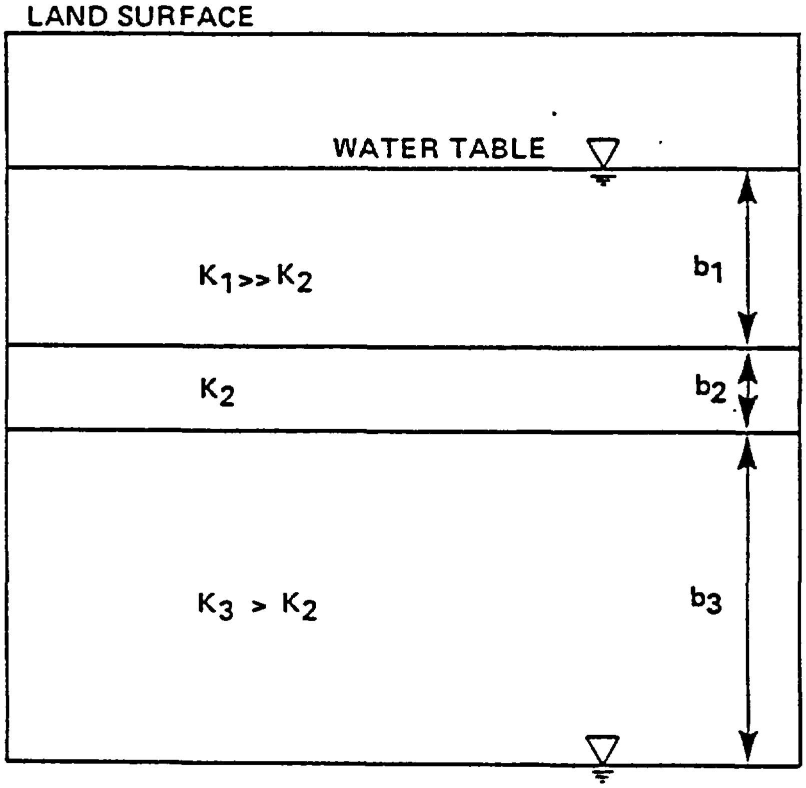


Figure 5. Schematic Diagram of Three-Layer System

4.2 Solution Technique

An unsaturated zone will develop beneath the aquitard if

$$b_1 < b_2 \, (k_3/k_2 - 1) \qquad (1)$$

where b and k denote layer thickness and saturated permeability, respectively, with subscripts referring to layers in Figure 5 (Zaslavsky 1964). Details of the derivation are given in the Appendix.

4.3 Assumptions

In deriving equation 1, the following assumptions were employed:

- one-dimensional, steady flow occurs vertically downward due to pressure and gravity gradients,
- isothermal conditions,
- constant fluid density,
- each layer is homogeneous,
- flow is due only to matrix permeability and rock permeability is unaffected by fracturing.
- a continuous air-phase can exist beneath the aquitard,
- the fluid pressure above the aquitard remains constant,
- the depth of the water table beneath the aquitard is constant and is much greater than the negative of the air entry pressure head of the lower layer,

- the effect of capillarity on flux across the aquitard is negligible

4.4 Application of Solution

The solution will be used to predict the head of water above the aquitard which is necessary to create unsaturated conditions in the underlying layer. The analysis will employ a sensitivity approach using different aquitard thicknesses and various permeability ratios between the aquitard and underlying layer.

One may then use available hydrogeologic data from the Deaf Smith County site area to determine whether unsaturated conditions could exist.

5.0 ANALYSES

Equation 1 was used to predict the maximum or critical values of pressure head above the aquitard, b_1^c, which would preserve unsaturated conditions in rock beneath the aquitard. The results of this sensitivity analysis are given in Table 2 and are graphed in Figure 6. A sample calculation is provided below for the following conditions:

$b_2 = 20$ feet

$k_3/k_2 = 10$

From equation 1, let $b_2(k_3/k_2 - 1) = b_1^c$, then $b_1^c = 20(9) = 180$ feet. If the observed pressure head, or saturated thickness, above the aquitard, b_1, is less than the critical depth b_1^c, then there is potential for unsaturated flow to occur; otherwise, the zone beneath the aquitard will be saturated.

From Figure 6 one can see that for a fixed aquitard thickness, b_2, the pressure required to saturate the rock beneath the aquitard increases as the permeability ratio k_3/k_2 increases. Also, for a fixed permeability ratio, the head of water required to saturate rock beneath the aquitard increases as the aquitard thickness increases.

As further examples, suppose the observed pressure head, b_1, above an aquitard is 100 feet. Then, a 1-foot thick aquitard could cause unsaturated conditions if k_3/k_2 is greater than about 99; a 20-foot thick aquitard could induce unsaturated

Table 3. Values of Maximum Head of Water, in Feet, Allowed for Developing a Transition from Saturated to Unsaturated Conditions Beneath an Impeding Layer of Thickness b_2 for Varying Ratios of Permeability of the Lower Aquifer, k_3, to that in the Impeding Layer, k_2.

	k_3/k_2			
b_2	5	10	10^2	10^3
0.1	0.4	0.9	9.9	99
0.25	1	2.2	25	249
1.0	4	9	99	999
3.0	12	27	297	3×10^3
20.0	80	180	2.0×10^3	2×10^4
74.0	296	666	7.3×10^3	7.4×10^4
100	400	900	9.9×10^3	1.0×10^5

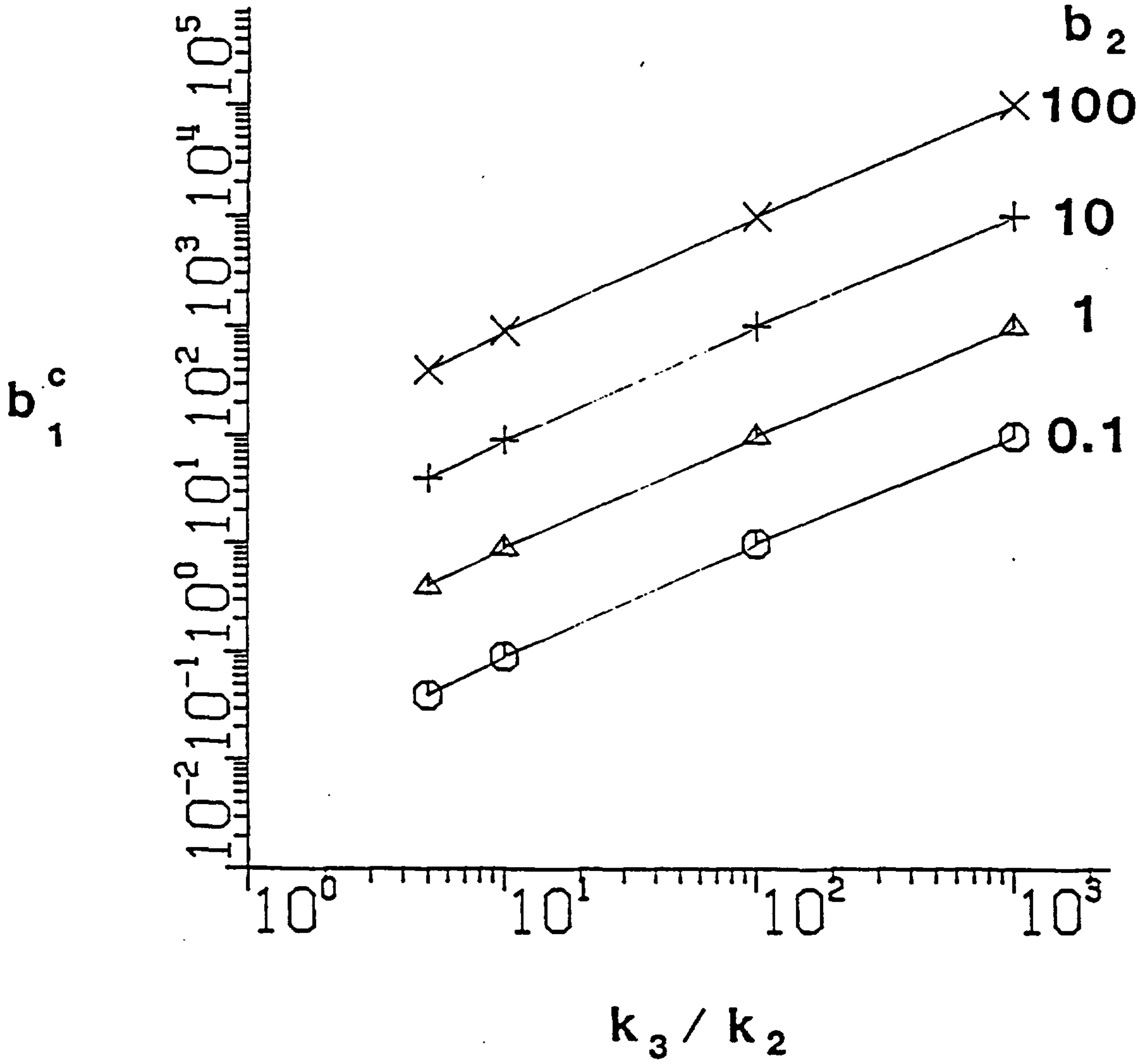


Figure 6. Calculated Maximum Pressure Head Above the Aquitard Necessary to Preserve Unsaturated Conditions.

conditions if k_3/k_2 exceeds 6. Also, for the same observed pressure head, if the permeability ratio is known to be 100, then unsaturated flow may be expected if the aquitard thickness exceeds 1 foot.

6.0 RESULTS

Available hydrogeologic information from the Palo Duro Basin is used in this section to ascertain whether present conditions are favorable for the presence of unsaturated flow relatively pemeable zones within the shale-evaporite aquitard. Site data needs include hydraulic head and layer thicknesses and saturated permeability. There are regional hydraulic head data available for the Ogallala and Dockum water-bearing units in HSU A, and the Wolfcamp and Pennsylvanian water-bearing units in HSU C. (DOE, 1986; pp. 3-57, 3-50, 3-62). Layer thicknesses are obtained from geophysical logs (Figure 4) and stratigraphic and lithologic interpretations (Table 1). There are no permeability measurements within the shale-evaporite aquitard, except for a drill stem test in the San Andres cycle 4 dolomite. Permeability data are therefore based mostly on generic information for representative lithologic units and professional judgement (Table 3).

In the site vicinity, the hydraulic head in the Ogallala is approximately 3,750 feet, whereas that in the underlying Dockum sandstone facies is about 3,350 feet above mean sea level. (DOE, 1986; pp. 3-141,142). The difference in head is probably due to the presence of low-permeable siltstone facies in the Dockum (Figures 3 and 4).

The lower formation in the Dockum Group, the Tecovas, and the underlying Dewey Lake formation are dominately siltstone, although the Dewey Lake appears to be less permeable owing to the presence of claystone. This was apparent in outcrops we observed in Palo Duro Canyon. The thickness of the Dewey Lake formation is about 74 feet. The Dewey Lake is underlain by the Alibates formation, a unit which is approximately 32 feet thick and comprised mostly of dolomite. To implement the analysis we will assume that the Alibates formation has a permeability which is greater than that in the siltstone and also that a zero pressure surface is located at the base of the Alibates. The head in the Dockum Group sandstone is assumed to be applied uniformly across the top of the Dewey Lake formation, which allows for vertical flow across the Dewey Lake formation into the Alibates. The Dockum-Dewey Lake contact is at an elevation of approximately 3,072 feet (Table 1); therefore, the head of water which apparently acts above the Dewey Lake formation at the site is approximately 278 feet (3,350-3,072 feet).

Because so little is known about the permeability of the units, we will use equation 1 to calculate the permeability ratio necessary for developing a transition from saturated to unsaturated conditions. The aquitard (Dewey Lake formation) thickness is assusmed to be 74 feet, and the head above the impeding layer is assumed to be 278 feet. The permeability ratio is calculated to be 4.38. That is, if the saturated permeability of the Alibates is at least 4.38 times greater than that in the Dewey Lake, then there is potential for unsaturated flow within the Alibates. This minimum permeability contrast between a siltstone/claystone and dolomite appears to be quite small and therefore not unexpected to exist, given the highly variable nature of the geologic materials.

There are insufficient hydraulic head and permeability data available for additional meaningful analyses. However, as a hypothetical example using Figure 6, if the aquitard is only 1 foot thick and the head above the aquitard is 100 feet, the permeability ratio required to develop the potential for unsaturated conditions in the lower layer must be greater than approximately 100.

7.0 CONCLUSIONS

Results of a preliminary and simple analysis of available hydrogeologic data indicate that there is potential for unsaturated flow conditions to occur within the shale-evaporite aquitard. Thin low-permeable layers overlying thick layers of relatively higher permeability are favorable conditions for unsaturated flow to occur in a one-dimensional vertical flow field.

8.0 DISCUSSION

The presence of unsaturated flow has been shown to be possible in theory, based on a very simplified analysis. These preliminary findings, if substantiated by subsequent detailed analyses, suggest that during site characterization activities, insitu hydraulic head data should be collected within the most permeable zones of the shale and evaporite aquitard to demonstrate that saturated flow, in fact, does occur throughout the system. Thin low-permeable layers overlying relatively thick more permeable layers should be identified during site characterization studies as a potential area for unsaturated conditions to occur. The scale of testing should be small enough to resolve differences in layer thicknesses which may be as small as about one foot, depending upon the permeability of the layers. Conventional drill stem testing could be used to demonstrate that positive pressures and hence saturated conditions exist, but this test cannot determine whether unsaturated conditions occur.

At this time, we do not believe that there is sufficient information to indicate unsaturated flow conditions are actually present to such an extent that all previous hydrogeologic analyses based on saturated flow in the aquitard should be completely dismissed. There are possible explanations for why saturated flow could occur in places where the simplified analysis suggests that unsaturated flow is present. For example, in the three-layer model of Figure 5, the permeable layer beneath the aquitard may be recharged near its outcrop area rather than by leakage from above. Local permeable fracture zones within the aquitard unit could "short-circuit" the impeding layer and fill the permeable unit below. Lateral discontinuities or facies changes within the aquitard could achieve a similar result. The permeable layer beneath the aquitard may in turn be underlain by a very low permeable unit which inhibits downward movement to such an extent that the permeable layer about it becomes saturated.

Our analysis suggests that there is no basis to conclude that the shale and evaporite is saturated, simply because the overlying hydrostratigraphic unit is saturated, as indicated by DOE (1986; 3-143). The degree of saturation may be variable in a highly heterogeneous, stratified system dominated by vertical flow components. We believe that our analysis demonstrates a need for a numerical simulation of a more complicated geologic cross-section which accounts for variably saturated conditions. The code UNSAT II would be appropriate for such analyses. When lateral flow components, lateral discontinuities in permeability, and multiple layers are taken into consideration, there may be no reason to expect unsaturated flow conditions. However, none of the regional numerical models applied to date have taken into consideration the possibility for variable saturation. In subsequent analyses, we will evaluate the potential for unsaturated flow in a multi-layer subset of the system, and if the results so indicate, we will extend the analysis to the regional scale to aid in interpreting sources of ground-water recharge and pre-emplacememt travel times so that we can develop a consistent and reliable framework for numerical model predictions.

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APPENDIX A

The derivation below follows from Zaslavsky (1964). Assume a steady flow condition occurs in the three-layer system described by Figure 5. According to Darcy's equation, if we neglect heat loss in layer 1 the flux through the entire system is:

$$q = \frac{b_1 + b_2 + b_3}{\frac{b_2}{k_2} + \frac{b_3}{k_3}} \qquad (A.1)$$

if there is an unsaturated condition which develops, the pressure head beneath the aquitard must be less than zero, and it must also be less than the air-entry pressure head, P_a. (The air-entry pressure head is that head at which air begins to enter a saturated porous medium during drainage.) The flux across the aquitard can then be described by:

$$q^1 = \frac{b_1 + b_2 - P_a}{b_2/k_2} \qquad (A.2)$$

Owing to the effect of capillarity on the hydraulic gradient across the aquitard, Flux q^1 is greater than q described by equation (A.1). Therefore, for unsaturated flow to occur:

$$b_1 < b_2 \,(k_3/k_2 - 1) + P_a \,(k_3 b_2/k_2 b_3 + 1) \qquad (A.3)$$

If we neglect capillary effects, $P_a = 0$; then equation (A.3) reduces to

$$b_1 < b_2 (k_3/k_2 - 1) \quad (A.4)$$

The second term on the right-hand side of equation (A.3) is negligible when $b_3 >> b_2$ or when $b_3 >> |P_a|$. Values of P_a are not likely to exceed 2 to 3 meters in fine-grained rocks.

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July 31, 1986

Nuclear Waste Consultants, Inc.
8341 S. Sangre de Cristo Road
Littleton, CO, 80127

Attn: Mark Logsdon, Project Manager

Re: Numerical Evaluation of Conceptual Models Report,
Subtask 3.5

Dear Mr. Logsdon:

Daniel B. Stephens and Associates, Inc. submit the attached as the initial report for Subtask 3.5, Numerical Evaluation of Conceptual Models.

Topics considered for analysis included those identified in our previous report on Conceptual Model Evaluation, Subtask 3.4. Several other planning activities also were utilized to develop a list of topics for numerical analysis. For example, the DBS team along with representatives from Nuclear Waste Consultants, Mr. Mark Logsdon and Mr. Adrian Brown, visited the Palo Duro site vicinity on July 1-3, 1986 and discussed various topics for analysis and their significance to the NRC's Waste Management Program. Some of the earliest planning took place at the meeting with the NRC technical staff in Silver Spring, April 1986. An additional perspective was derived from the conference on hydrodynamics of deep sedimentary basins attended in May by Dr. Fred Phillips of our team. And finally, selected analyses on salt, previously prepared by Golder and Associates, were reviewed.

There are five mini-performance assessment reports submitted for fulfillment of this contract deliverable.

1. Analysis of the potential for unsaturated flow within the evaporite aquitard, Deaf Smith County site, Palo Duro basin.

2. Transport in salt by vertical porous media flow.

3. Transport through interbeds within HSU B by horizontal porous media flow.

4. Transport in the Wolfcamp by horizontal porous media flow.

5. Analysis of the potential for geothermally-induced ground-water convection within the evaporite aquitard, Deaf Smith County site, Palo Duro basin.

Mini-reports 1 and 5 were selected based on their importance to understanding the framework of the conceptual models, whereas topics 2 through 4 are related to travel time sensitivity to basic hydrologic parameters. These analyses were also rather quick to perform and could be presented in time to meet the report deadline. More complex and time consuming analyses will be submitted as updates to this subtask, at least semi-annually.

Topics of mini-reports currently or soon to be in progress may include:

1. use of SWIFT II to determine effect of fractures and anisotropy on ground-water flow paths and velocities, e.g. due to ground-water convection driven by buoyancy forces.

2. use of Chlorine-36 for ground-water dating as an independent method of determining flow velocities given flow paths.

3. relative importance of diffusion of radionuclides vs. advection for varying permeability.

4. magnitude and timing of hydraulic head changes at the proposed repository location due to increased precipitation and ponding in the recharge area of the lower aquifer in New Mexico.

5. use of noble-gas isotope data to obtain residence times and flow paths.

6. fluid density effects due to salinity and/or thermal effects, e.g. buoyancy forces induced by radiogenic heat from the repository.

7. stochastic analyses to evaluate the sensitivity of the conceptual models to heterogeneity.

8. analysis of the significance of unsaturated flow on regional and local scale flow.

Other potential analyses are suggested in the Conceptual Model Evaluation report (Subtask 3.4, DBS team, 1986). The initial and subsequent analyses numerically evaluate the conceptual models using two approaches:

1) through the NRC regulations using the assumed conceptual model;

2) through the conceptualized hydrogeologic framework to determine which processes are important with respect to NRC regulations.

If you have any questions with regard to this work, please do not hesitate to call.

Yours truly,
Daniel B. Stephens & Associates, Inc.

Jeffrie D. Minier

Jeffrie D. Minier
Project Manager
JDM/esj