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Hydrogeology • Mineral Resources Waste Management • Geological Engineering • Mine Hydrology

April 23, 1986
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Communication No. 47

Mr. Jeff Pohle
Division of Waste Management
Mail Stop 623-SS
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

RE: SALT

Dear Jeff:

I am enclosing a copy of the following document reviews.

1. Andrews, R.W., Kelley, V.A., McNeish, J.A., LaVenue, A.M., Campbell, J.E., November 1985, Travel Path/Travel Time Uncertainties at Salt Sites Proposed for High Level Waste Repositories. INTERA Technologies, Inc., Austin, TX, ONWI/E512-02900/TR-36.

2. Orr, E.D., 1984, Investigation of Underpressuring in the Deep-Basin Brine Aquifer, Palo Duro Basin, Using Pressure/Depth Profiles. Texas Bureau of Economic Geology, Austin, TX, OF-WTWI-1984-6.

3. Thompson, B.M., Campbell, J.E., and Longsine, D.E., November 1985, PTRACK A Particle Tracking Program for Evaluating Travel Path/Travel Time Uncertainties. INTERA Technologies, Inc., Austin, TX, ONWI/E512-02900/CD-27.

Please contact me if you have any questions.

Sincerely,

Gerry

Gerry V. Winter

GVW:sl

enclosures

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WMGT DOCUMENT REVIEW SHEET

FILE #:

ONWI #: ONWI/E512-02900/TR-36, (410-20G-03B)

DOCUMENT: Travel Path/Travel Time Uncertainties at Salt Sites Proposed for High Level Waste Repositories. R.W. Andrews, V.A. Kelley, J.A. McNeish, A.M. LaVenue, J.E. Campbell, INTERA Technologies, Inc., Austin, Texas, November 1985.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: April 21, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E Williams

The objective of the report under review is to model and predict probabilistically groundwater travel paths and travel times from the edge of the disturbed zone to the accessible environment for the proposed waste repository sites in three general geologic environments of salt. Specifically, the report contains information about seven salt sites, but only three are considered in this review: 1) the Deaf Smith County site in the Palo Duro Basin of Texas (bedded salt), 2) the Davis Canyon site in the Paradox Basin of Utah (bedded salt), and 3) Richton dome site in Mississippi (salt dome). The report implies that the results from these three studies can be extended to nearby or similar salt sites.

A two-dimensional simulation model is used in the travel path/time analysis. Porous-media flow is the assumed mechanism of groundwater flow, but several analyses also are conducted for fracture-zone related flow. The character of predicted travel paths is highly dependent on the vertical gradients and the permeabilities assigned to the geologic units. The predicted travel times for a salt dome are significantly greater than those for the bedded salt sites. This greater travel time is a direct result of the low permeability assigned to salt and the fact that interbeds (dolomite, sandstone, siltstone), which are more permeable than salt, are absent in salt domes. The horizontal travel time for the bedded sites is controlled primarily by the horizontal flux through the non salt interbeds; consequently,

travel times are highly dependent on the horizontal gradients and permeabilities of the interbeds.

Sensitivity analyses based on scatter plots (input parameters versus output variable), partial rank correlation coefficients, and step-wise regression analysis are conducted on the simulation output. Critical input parameters are identified and suggestions made for future modeling and field data collection.

BRIEF SUMMARY OF DOCUMENT:

A. Conceptual Model:

Hydrostratigraphy at each of the three sites simulated is inferred from limited information and data. Information from a "representative" drill (test) hole is used to create a two-dimensional model for the bedded salt sites, wherein horizontal isotropy is assumed to a distance of 5 km from the expected disturbed zone. Hydrogeologic properties in the layers (geologic units) are considered globally stationary over the 5-km distance. That is, a given parameter in a layer has the same probability distribution everywhere in the study area. Consequently, spatial heterogeneities in the horizontal direction are ignored, and the probability of their occurrence is not incorporated into the model. Also, a horizontal to vertical permeability anisotropy of 10 to 1 has been assumed for each lithology (layer) except for salt. Salt is assumed to be isotropic.

The report assumes that only horizontal, porous-media flow (one dimensional travel path) will occur in the salt domes. Therefore, only horizontal hydraulic conductivity, effective porosity of salt, and the horizontal hydraulic gradient are required for estimating travel time from the disturbed zone to the edge of the salt dome. The report states that "Each of these data is uncertain" (p. 201).

Two types of groundwater flow are considered for the bedded salt sites. In the first case, flow is treated as porous-media flow, the most likely situation according to recommendations made by an "expert panel of hydrogeologists." In the second case, potential effects of fracture zones and fracture-dominated flow are investigated by using maps of digitized representations of surface lineaments. Each lineament is assumed conservatively to be a fracture zone that is vertically continuous through the entire geologic sequence under study. In calculating the groundwater travel time for fracture flow, the porous-media effective porosity for a given layer is reduced by a factor of 100 to yield a fractured-media effective porosity. This assumption causes the interstitial velocity in the fracture zone to be 100 times larger than the velocity in the non-fractured portion of a given layer.

B. Parameter Estimation:

The two-dimensional computer model PTRACK simulates potential groundwater flow paths and determines the 5-km (net) travel time. The model requires inputs of the probability distributions for the following parameters:

1. pressure (head) at three elevations in the geologic sequence,

2. horizontal permeability of each layer,

3. effective porosity of each layer,

4. TDS (total dissolved solids) of each layer,

5. horizontal hydraulic gradient of each layer,

6. distance from disturbed zone to a major fracture zone (only for the case of assumed fracture-dominated flow).

These estimates are obtained from regional hydrogeologic data (mostly from petroleum exploration sources), from hydraulic and geophysical data collected from the DOE-OCRWM well closest to the potential repository site, from laboratory tests of cores obtained from the OCRWM wells, from subjective and judgmental interpretations of all the above, and from generic information provided by studies in similar geologic settings.

Due to the paucity of data, the types of probability distributions have been assigned subjectively in most cases, based upon published results for similar geologic materials. The exception consists of histogram plots of permeability data from some of the geologic layers. The types of input distributions are assigned as follows:

1. pressure (head)--normal distribution,

2. permeability--lognormal distribution,

3. effective porosity--normal distribution,

4. TDS--triangular distribution,

5. horizontal gradient--triangular distribution,

6. distance from disturbed zone to fracture zone(for the case of assumed fracture dominated flow)--"empirical" distribution

obtained from a simulation model that determines random distances to lineament traces (fracture zones) in the down-gradient direction.

Professional judgment and subject-matter knowledge are relied upon heavily in selecting these input distributions and their appropriate statistical parameters such as mean and standard deviation. Appendices in the document contain copies of memos from Stone and Webster Engineering Corp. (Deaf Smith site contractor) and from Woodward-Clyde Consultants (Davis Canyon site contractor) that describe their best estimate of mean values and standard deviations or ranges of the input variables. Unfortunately, except for a few actual data listings no information is provided by the contractors on sample size (number of observations) and what criteria were used in assigning a range or accuracy level to test results.

C. Simulation:

The goal of the simulation study using the PTRACK ("particle tracking") computer code is to predict potential groundwater travel paths and travel times over distances of 1 to 5 km. The simulation procedure uses Latin hypercube sampling rather random Monte Carlo sampling of the probability distributions of input parameters. Except for specific correlation studies of the Deaf Smith County site, the selected hydrogeologic parameters for a given run are assumed to be independent of each other and constant over the distance of interest. A given simulation consists of 1,000 passes (runs), the results of which are presented as 1) a table showing the distribution (percentage) of geologic layers where water particles exit a 1, 2, 3, 4, or 5-km window, and 2) a histogram and a complementary cdf (cumulative distribution function) of groundwater travel time across a 1 or 5-km window (or to the edge of the dome for the Richton site). The simulated travel time values essentially have a lognormal distribution for all three salt sites.

Simulations that account for fracture flow are conducted for the bedded salt sites (case two, as mentioned previously). The prime input is a map of ground surface lineaments. Each of these mapped features is assumed to represent a fracture zone that vertically intersects all geologic layers under consideration. An areal, random sampling scheme (1,000 iterations) provides an estimated distribution of distance from the disturbed zone to a fracture zone. This objective is accomplished by generating a random spatial point ("repository") and then searching in a 180-degree arc in the down-gradient direction to find the nearest fracture zone. As expected, the output travel times for fracture flow have more values at lower ranges than those for porous flow.

The sensitivity of particle-exit layer and travel time to the various input parameters is investigated by analyzing the samplings and results of the simulations. Scatterplots of individual variables versus travel time and of particle exit elevation versus travel time provide a means of visibly identifying the strength of a relationship between the input and output variables. Partial correlation coefficients also are calculated and used to evaluate sensitivity. The parameter ranks are used in the calculations rather than the actual parameter values. The rank transformation has the effect of linearizing the relationship between the two differently-scaled variables (input and output) so that the partial rank correlation coefficient provides a more accurate indication of the dependence between the two variables. Forward-selection stepwise regression also is applied to the rank-transformed values as a third method of evaluating sensitivity. Results of the sensitivity analyses for the bedded salt sites generally show that the input hydrogeologic properties that most influence travel time for porous flow are the permeabilities of interbed layers nearest the disturbed zone. For fracture flow, an equally important variable is the distance a particle travels from the disturbed zone before it intersects a fracture zone. Head values and horizontal gradient also may be important under different assumptions for the input parameter distributions of hydrogeologic properties.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

This document is important to the NRC Waste Management Program because it presents the DOE's current thinking on the estimation of travel times at the bedded salt sites and at the salt dome sites. The methodology described herein is new to the salt program based on the information provided to the NRC to date. In addition, this methodology differs significantly from the methodology employed at the BWIP site. A consistent approach toward estimating travel time stochastically among the sites is not apparent, based on our reviews of documents from all the sites. A comparison of the approach used in the report under review with that described in the NRC's draft technical position paper is not practical because the subject position paper is undergoing revision. The last draft of the NRC technical position paper that we have seen offered essentially no guidance on the type of procedure used in the report under review.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The conceptual model and the simplifying assumptions used in the PTRACK simulations contain several issues that must be considered when interpreting results of the simulations. For the case of porous-media flow, heterogeneity of geologic and hydrogeologic properties within layers is ignored in any given pass (run), or iteration, of the simulation. All properties are assumed constant in the geologic formations over the horizontal distance of concern (1 to 5 km). For the next and subsequent simulation passes (runs), a new set of properties is selected randomly and considered constant over that same horizontal distance. Local zones of hydraulic connectiveness (such as lithologic lenses, stringers, fractures or bedding planes) are ignored. For the case of fracture-dominated flow, simplifying assumptions are made on the geometry and character of fracture zones over the study area. The input probability distributions of hydrogeologic parameters should reflect the large-scale character (values) of the application of the parameters; typically this is not the case for the PTRACK input.

This report highlights a critical issue in probabilistic modeling. Without external, independent verification of modeling results, considerable suspicion of the validity of the results arises if the sampling scale (used to determine input distributions of the hydrogeologic variables) is different from the modeling scale for a heterogeneous medium. This is especially important if the scale of the heterogeneities exceeds the scale of the testing procedures from which the distribution of values was derived. All to often the scale of the field testing (sampling) is smaller than the modeling scale. Some of these difficulties could be alleviated by dividing the modeled area into discrete zones (elements) that have dimensions similar to the testing scale. Ideally, for a given simulation pass (run), values of input hydrogeologic parameters can be simulated for every element so that they have the proper probability distribution, spatial correlation, and intercorrelation (with each other). However, the PTRACK study is representative of many hydrogeologic investigations wherein very few data usually are available that can provide reliable estimates of probability distributions of input parameters and of spatial correlation and intercorrelation relationships. Under these circumstances, in order to conduct a simulation, the information supplied by limited field data obtained at the scale of the model must be augmented by laboratory data (obtained from small-scale samples) and by subject-matter knowledge and professional judgment. The PTRACK study has relied on this procedure to construct ranges and probability distributions of the input hydrogeologic parameters (Appendices B-F in the report). In some instances, the estimates are presented with no back-up information on how they were obtained, no information on the number of data available (sample size), no information on the method of data collection (testing), and no information on the reliability or confidence interval of the measurements or estimates. Subjective guesses (such as plus or minus 25-percent) need to be justified in some manner.

Without this kind of documentation there is no rational way to evaluate or defend the hydrogeologic parameter inputs. For example, the authors seem to place more confidence in laboratory-obtained porosity values than in resistivity-derived porosity values (p. 25-26). Considering the amount of subjective judgment used to construct hydrogeologic parameter distributions, Bayesian analysis techniques should prove useful in the probabilistic estimation of parameter distributions and in updating them as new sample data are obtained. These methods provide a mechanism for combining "hard" information (data) with "soft" information (subject-matter knowledge and professional judgment) to produce reasonable estimates of parameter distributions.

There are several key limitations of the PTRACK simulation procedure that may have a strong influence on the calculated travel times. The horizontal permeability in all non-salt beds is assumed to be 10 times the vertical permeability. This ratio is constant for every simulation and every interbed. This ratio is critical because, as the model shows, permeability is the key influence on travel time at the salt sites. The horizontal hydraulic gradients are very small and the effective porosity distributions cover a short range for most layers (range usually spans less than 10 percent, and rarely exceeds 25 percent). Consequently permeability is the critical variable. The ability of the model to accept vertical gradient estimates at only three elevations is another limitation. This issue is especially critical if formation pressures change appreciably over vertical distance, such as the case at the Davis Canyon site. At this site simulated travel paths are downward if the Ismay Formation pressures are used in the model but they are upward if the Honaker Trail Formation pressures are used (p. 135-137). In general, if the pressure distributions at the three selected elevations overlap each other and are sampled independently during simulation passes, then some of the simulated travel paths would be directed upward and some would be directed downward. This observation may represent correctly the uncertainty in the conceptual model and in field conditions, but it does not seem realistic. Obviously, formation pressures (and the resulting vertical gradient) have to be measured and estimated with considerable reliability if the PTRACK-simulated travel paths are to be considered representative of reality.

Section 2.3.4 (p. 56-73) of the report describes how parameter correlations are incorporated in the PTRACK analysis for the Deaf Smith bedded salt site. The simulations that include parameter correlations (among interbed permeabilities, among interbed horizontal gradients, and among permeability and horizontal gradient) consist of only 100 passes, or trials. The authors state that 100 trials are sufficient to indicate the relative importance of correlations (p. 56), but no statistical evidence or sensitivity tests are conducted to verify this assertion.

Several repeated simulations of 100 passes, using the same input except for a different initial random "seed", would show how stable the simulation results are. The size of confidence intervals estimated for the output (travel time) would be identified also. Without this kind of information, it is difficult to conclude whether travel times estimated by the correlation-input model are significantly different from previously calculated values (i.e., the new set of results may be different from the previous set but well within the statistical error bounds for 100 trials).

The so-called treatment of permeability spatial correlation (p. 69-72) for the Palo Duro Basin lacks substance and is essentially meaningless in a real, physical sense. The authors improperly define (or model) spatial correlation, at least in the manner used in modern geostatistics and regionalized-variable analysis. The authors of the report under review effectively define the correlation distance as the distance over which constant hydrogeologic parameters are assumed for a given simulation pass. Thus, if their "correlation distance" is 500 m over a study distance of 5 km, then 10 equal sized cells (or blocks) are considered in the simulation, with a unique random sampling of input distributions for each cell. Conceivably, this approach could generate a low permeability value in one cell and a much larger value (perhaps orders of magnitude larger) in an adjacent cell. In a geostatistical framework, this condition corresponds to independence between cells, or lack of spatial correlation between cells. Spatial correlation within a cell may exist, but it has to be studied and evaluated by using data from a sampling scale much smaller than the cell.

The character of the current PTRACK model does not allow for the incorporation of spatially correlated hydrogeologic parameters because layer parameters are assumed constant over considerable distances. If a hydrogeologic property is assumed constant over an area then it <u>is not</u> assumed to be highly correlated. A parameter that is constant over an area has no spatial variance, whereas a highly correlated parameter has some variance and a long range of influence. This range is estimated from variogram or autocorrelation plots. Spatial correlation, variation, and trend actually are scale-dependent properties, and proper modeling of them in engineering investigations is necessarily reliant on careful regard of sampling (testing) scale and modeling scale. There are much better ways of dealing with spatial correlation than those used by the authors. They claim "there are no data with which one could define an appropriate spatial correlation distance for hydrogeologic properties in the Palo Duro Basin" (p. 69). Yet extensive variogram and kriging estimation has been conducted by the University of Texas/Bureau of Economic Geology on head values in several different geologic formations. The type of "correlation distance" sought by the authors, as they have defined it, is impossible to estimate on a usable scale and it is not realistic or practical anyway. Perhaps what they are really after is the size of hydrogeologic heterogeneities that significantly influence groundwater flow in an area of interest.

The sensitivity analyses applied to determine the relative importance of input parameters on travel time rely on input to and output from the simulation model PTRACK. Consequently, the results obtained from such analyses are necessarily tied to the model and its assumptions and capabilities. The authors recognize this fact (p. 101), but offer no advice or guidance on how to confirm their results. Other possible scenarios of geologic conditions and hydrogeologic properties should be used in PTRACK simulations. More importantly, results of the sensitivity analyses (i.e., identification of parameters most influential on travel time estimates) should be verified by alternate PTRACK modeling assumptions, alternate models altogether, and professional judgment.

The use of stepwise regression in the parameter-influence studies seems to add little to the knowledge gained from the partial rank correlation coefficients (PRCC's), because the order in which variables are added in the steps is determined by partial correlations (p. 75, 91, 189). Consequently, the two methods are not independent, and their results by definition will be similar in that the same variables will be identified to have the greatest influence on travel time. Descriptions of the stepwise regression procedure and the tables that summarize the results (p. 89-90, for example) apparently indicate <u>forward selection</u>, a simplified form of stepwise regression. This procedure does not consider the effect that adding a variable at the current step has on variables added at previous steps. In other words, the variable selection procedure is based on the principle that variables are added sequentially to the model until there are no remaining candidate variables that produce a significant increase in the regression sum of squares (as evaluated by a general F-test). Forward selection omits the partial F-test for deleting variables from the model that have been added at earlier steps.

<u>EDITORIAL COMMENTS</u>:

Page 19, second paragraph. The last sentence should read "The practical minimum and maximum values in the log-normal distribution ..." The insertion of the word practical is required because the theoretical true minimum and maximum of the normal distribution are minus and plus infinity, respectively.

Page 30, fourth paragraph. The word define or defined should be replace with the word estimate or estimated.

Pages 36 and 37, Figure 2A. It would be helpful to label the major stratigraphic units on the figures.

Page 43, final sentence. The authors discuss the probable travel paths. The reader should remember that these travel paths are restricted by the selected assumptions and by the conceptual model that they have selected for use. Other travel paths may be defensible.

Page 44, Table 2-2 and other, similar tables through the rest of the report. It would be useful if the data entries in these tables showed three significant figures rather than the two significant figures that are presented.

Page 70. The top line of text. The word correlated should be replaced with the word constant. In the first paragraph on the same page the words underpredict and overpredict should be replaced with underestimate and overestimate, respectively.

Page 72, third paragraph from bottom. The following sentence should be added at the end of this paragraph: The sampling distribution of the mean of a random variable always has less variance than that of the random variable itself.

Page 74, top line on page. The phrases "various input parameters" and "the predicted results" should be interchanged so that the sentence reads: Several different approaches may be used to define the sensitivity of the predicted results to the various input parameters. This change is needed because results are sensitive to input not vice-versa.

Pages 87-89. Somewhere during this discussion on standardized regression analysis, the authors should present the regression model or at least a general form of the regression model they are using.

Page 201, Section 5.2. The second sentence in this paragraph should read: Each of these parameters is uncertain.

Page 210. The top paragraph, final sentence. The phrase "bedded salt layers have no effect" should be changed to "the bedded salt layers have little effect..."

WMGT DOCUMENT REVIEW SHEET

FILE #:

TEXAS BUREAU OF ECONOMIC GEOLOGY REPORT #: OF-WTWI-1984-6

DOCUMENT: Orr, E.D., 1984, Investigation of Underpressuring in the Deep-Basin Brine Aquifer, Palo Duro Basin, Using Pressure/Depth Profiles.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: April 22, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

The report under review analyzes problems in use of pressure vs depth relationships including terminology confusion, pressure vs depth data quality, and the effects of hydrologic setting and data distribution on pressure vs depth plot interpretation. This analysis is applied to pressure vs depth relationships for the deep-basin brine aquifer in the Palo Duro Basin of Texas. Research methodology involved the division of the basin into seventeen "homogeneous" subareas and the application of a model to data from each subarea to reduce error in determination of aquifer pressure conditions. Results indicate that the aquifer is underpressured in the southwest, central and eastern part of the basin, is hydrostatically pressured along a zone associated with known salt dissolution, and overpressured in the northwest part of the basin.

Problems with the study include assumptions of linearity of structural and topographic gradients in each subarea, subarea definition, data quality, and data distribution. Potentially significant changes in the conceptual model of groundwater flow are also presented in the discussion.

BRIEF SUMMARY OF DOCUMENT:

The report under review presents the results of a study of pressure vs depth data from the so-called "deep-basin brine aquifer" of the Palo Duro Basin of Texas. The hypothesis expressed in the report is that pressure vs depth data will provide information on the potential for vertical fluid movement within the aquifer which ultimately can effect travel time calculations. The objectives of the report (p. 3) are:

> "(1) to document and characterize underpressured conditions in the confined Deep-Basin Brine Aquifer using pressure-depth data, (2) to investigate the difficulties associated with the interpretation of pressure-depth data from confined aquifers, (3) to refine the observed pressure-depth relationships by evaluating the effects of possible sources of pressure-depth variation, such as data quality and hydrologic setting, (4) to document and aerially delineate any varying potentials for vertical flow (cross-formational flow) within the Deep-Basin Brine Aquifer, and finally (5) to identify the hydrologic causes of varying nonhydrostatic conditions."

The report is divided into two principal sections. The first section discusses the interpretation of pressure vs depth data from confined aquifers and some of the potential problems associated with these interpretations. Problems discussed in the report include confusion of terminology, the effects of hydrologic setting and data distribution on pressure vs depth plot interpretation, and pressure vs depth data quality.

A computer program was developed to model pressure, depth and head data for an imaginary confined aquifer in an effort to examine the effects of hydrologic setting on pressure vs depth relationships. Several different cases were simulated. The model assumed a hydrostatic gradient of 0.466 and (p. 7) that "hydrostatic conditions of parallel flow" exist in the aquifer. Least square regressions were plotted on pressure vs depth diagrams for each different simulation. Model results show that if topography, aquifer structure or potentiometric surfaces (p. 7) "vary significantly within an area, the plot and regression line of pressure-depth data from several wells may give a false representation of pressure-depth conditions." The major conclusions of this modeling effort are that topography, aquifer structure and potentiometric surface can affect pressure vs depth diagrams and produce erroneous conclusions regarding actual aquifer pressure vs depth conditions.

The report suggests that because of the potential problems associated with pressure-depth data modeling be done to evaluate the extraneous effects before attempting to draw conclusions regarding hydrogeologic conditions from the data. Modeling would be done for "a given hydrogeologic setting assuming parallel flow, and then comparing the plotted results to the field data" (p. 9).

The second section of the report under review discusses the deep-basin brine aquifer and the analysis of pressure vs depth data derived from this aquifer. The deep-basin brine aquifer is composed of (p. 10) "the Wolfcamp Aquifer, Pennsylvanian Carbonate and Granite Wash Aquifers, and Lower Paleozoic Carbonate and Sandstone Aquifers." The deep-basin brine aquifer is overlain by the evaporite aquitard which, in turn, is overlain by the Ogallala-Dockum aquifers. The vertical pressure distribution in the Ogallala-Dockum aquifers is said to be hydrostatic. The deep-basin brine aquifer is said to be underpressured. The marked difference in potentiometric surface elevation of the Ogallala-Dockum and deep-basin brine aquifers is seen as creating potential for downward flow between the two aquifers. Potentiometric surface elevation differences between the two units are greatest in the northwestern part of the Palo Duro Basin and least in the southeastern part. The paper portrays the deep-basin brine aquifer as being even more underpressured than indicated by these differences "because the potentiometric surfaces were constructed using equivalent fresh water heads; computed heads based on density of brines would be lower" (p. 11).

The analytical process first involved determination of the hydrostatic line for the deep-basin brine aquifer. Using an average total dissolved solids (TDS) value of 132,000 ppm, a gradient of 0.466 was determined. Then the 466 DST data were evaluated and any values which fell below a gradient of 0.2 were discarded automatically. The paper presents no explanation as to why the value of 0.2 was chosen except to state that (p. 13) this "cutoff subjectively culled 'invalid' DST measurements reflected by unreasonably low values of pressure and/or total recovery." The data were also ranked into classes based on similarity of initial and final shut-in pressure readings. Finally, the Palo Duro Basin was divided into seventeen "homogeneous" subareas based on hydrogeology, topographic and structural similarities, and a "pressure vs depth" diagram was produced for the deep-basin brine aquifer from each of these subareas. Variations in structural trend were approximated by assuming linear structural gradients for each of the seventeen subareas as determined from a structure contour map of the top of the Wolfcamp Series. Through the use of modeling, factors which affect pressure vs depth values such as depth, surface elevation, and structure of the deep-basin brine aquifer were identified. By eliminating these variables the authors believe that a more accurate picture of the actual degree of underpressuring for each subarea was obtained.

Results of this analysis indicate that vertical flow may not be universal within the Palo Duro Basin. The report suggests that the possibility for downward cross-formation flow is present in the southwest, central and extreme eastern part of the Palo Duro

Basin. An arcuate zone of horizontal flow may exist that is roughly coincident with the current limits of salt dissolution within the basin. A zone of upward flow may exist in the north and northwest part of the Palo Duro Basin.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

Transport by groundwater is the most probable method of contaminant movement if release from a repository should occur. For this reason efforts to define both the direction and rate of groundwater movement in proximity to a proposed repository site are of critical interest to the site characterization process. This report provides insight into possible groundwater flow paths; therefore it is of major importance in the licensing process.

PROBLEMS, DEFICIENCIES, OR LIMITATIONS OF REPORT:

The report under review constitutes an attempt to define more accurately pressure vs depth relationships in the deep-basin brine aquifer. In any such attempt a certain number of assumptions are needed in order to reduce the number of variables. One of the assumptions in this study involves the definition and use of subareas of the Palo Duro Basin. The basin was divided into seventeen separate "homogeneous" subareas because of the large variation in the total population of data. The effects of topography and structure on pressure vs depth evaluation were used in this process, as explained before. Pressure vs depth regression plots were produced for each subarea. The "homogeneous" subareas were defined by superimposing a contour map of the top of the Wolfcamp Series on a map of surface topography of the Palo Duro Basin. Crude quadrilateral areas were produced because the trends of the two contour maps were nearly perpendicular in many locations. The subareas then were defined as these quadrilateral areas bounded by the two sets of contour lines. The assumption connected with this selection process is that within each "homogeneous" subarea neither topography nor structure varies significantly. This assumption itself may not be valid; however, the problem is compounded by the fact that a variable contour interval was used for contouring both surfaces. Non-constant contour intervals were chosen (p. 16) "(1) to facilitate the most even data distribution possible and (2) to display the most separate trends in the plotted pressure-depth data." This decision may seriously bias resulting pressure vs depth diagrams for two reasons. First, the assumption of linear structural and topographic gradients and the decision to define subareas using a non-constant contour interval may bias seriously the resulting pressure vs depth diagrams. The assumption of linear topographic and structural gradients neglects variation in these gradients which is surely present in virtually every subarea. Depending upon the magnitude of this variation it could alter significantly the position of the modeled regression lines and affect conclusions regarding pressure conditions.

Second, significant variation in pressure vs depth diagrams seems even more probable when it is recognized that the "homogeneous" subareas are produced by variable contour intervals. As previously indicated, one of the reasons for using a non-constant contour interval was to insure that subareas could be created that had an adequate number of data points. This means that the subareas were defined less on the similarity of topographic and structural conditions than on the overall distribution of data. Such a rationale of subarea definition tends to contradict the intended purpose for creation of the subareas and makes the assumption of linearity of topographic and structural gradients within each subarea even more questionable.

Certain assumptions also have been made about the reliability of the DST data. The data have been grouped into three classes based on the shut-in pressure values. It is evident from the regression diagrams of each of the three data groups that considerable differences exist among them. The calculated gradient for the Class A data group is 0.403, while gradients for Class B and C groups are 0.423 and 0.354 respectively. The report states (p. 16) that in some areas sufficient Class A data exist to be used exclusively in the preparation of pressure-depth diagrams. In other locations it was necessary to include data of Classes B and C. Given the differences in regression characteristics of each data class it may not be completely valid to interpret underpressured conditions using different data sets. Comparison of conditions from one area to another may be subject to question.

Despite attempts in the report under review to define and clarify the meaning of underpressuring, confusion is still present in parts of the discussion. On page 2 the statement is made that the deep-basin brine aquifer "is underpressured with respect to fresh-water hydrostatic conditions in the overlying Ogallala and Dockum aquifers." The discussion in this sentence is linked to a following sentence which uses potentiometric data presented in figure 3 of the report as evidence for the possibility of downward flow between the Ogallala-Dockum aquifers and the deep-basin brine aquifer. The result of this discussion is a degree of confusion about the relationship of pressure and fluid potential or head. Fluid potential is measured relative to a particular datum and includes not only pressure but an elevation component as well. For this reason vertical pressure and fluid potential gradients are not equivalent. Pressure and head gradients are analogous only in the horizontal plane. Thus, to use vertical differences in fluid potential as an indication of pressure gradient in these aquifers is incorrect.

A problem also is associated with data distribution. Despite attempts to create subareas with relatively equal amounts of data, several of the subareas contain relatively few data points. Pressure vs depth diagrams for subarea D contains only fifteen data points; the diagram for subarea E contains fewer than ten. Considering the relatively low number of data points and the fact that data were derived from a combination of all data classes, the regression lines generated from these data may not be realistic. Consequently the resulting conclusions regarding the nature of underpressured conditions in these areas may be of limited value.

The conceptual model of groundwater flow within the Palo Duro Basin presented in this report differs from conceptual models presented in previous reports. Figure 9 of the report under review presents an illustration of a two-dimensional cross-sectional groundwater model of the basin. The source of this model is unclear. The report under review references a report by Senger contained in the yearly progress report for 1983 (Gustavson and others, 1983). Examination of this progress report reveals no such article. The progress report does contain an article by Senger and Fogg (1983) which presents results of two-dimensional modeling; however, the conceptual model and the results therefrom as presented by Senger and Fogg differ markedly from those presented in the report under review. In the report under review model results suggest that virtually no recharge reaches the deep-basin brine aquifer from the assumed recharge area associated with the Pecos River in New Mexico. Instead model flow lines suggest that virtually all recharge occurring in that area is discharged to the Pecos River. This conclusion differs markedly from that presented in Senger and Fogg whose model suggests a substantial amount of recharge to the deep-basin brine aquifer from this area. The model results presented in the report under review are suggested as a possible explanation for underpressuring in the deep-basin brine aquifer. It is interesting to note in the related discussion on page 11 that the evaporite <u>aquitard</u> is referred to as the evaporite <u>aquiclude</u>. The implication is that the deep-basin brine aquifer is completely isolated from near-surface flow systems by the presence of the aquiclude and the nature of recharge to the flow system at the western side of the basin.

<u>REFERENCES CITED</u>:

Gustavson, T.C., Kreitler, C.W., Bassett, R.L., Budnik, R.T., Ruppel, S.C., Baumgardner, R.W., Jr., Caran, S.C., Collins, E.W., Dutton, A.R., Dutton, S.P., Fisher, R.S., Fogg, G.E., Hovorka, S.D., Kolker, A., McGookey, D.A., Orr, E.D., Roberts, M.P., Senger, R.K., Smith, Dale A., and Smith, D. Anderson, 1983, Geology and Geohydrology of the Palo Duro Basin, Texas Panhandle. Texas Bureau of Economic Geology, Geological Circular 83-4, 156 p.

Orr, E.D., and Kreitler, C.W., 1985, Interpretation of Pressure-Depth Data from Confined Underpressured Aquifers Exemplified By the Deep Basin Brine Aquifer, Palo Duro Basin, Texas. Water Resources Research, vol. 21, no. 4, p. 533-544.

Senger, R.K., and Fogg, G.E., 1983, Regional Modeling of Ground-Water Flow in the Palo Duro Basin, Texas Panhandle <u>in</u> Geology and Geohydrology of the Palo Duro Basin, Texas Panhandle. Texas Bureau of Economic Geology, Geological Circular 83-4, p. 109-115.

WMGT DOCUMENT REVIEW SHEET

FILE #:

ONWI #: ONWI/E512-02900/CD-27, (410-20G-02C):

DOCUMENT: PTRACK A Particle Tracking Program for Evaluating Travel Path/Travel Time Uncertainties. B.M. Thompson, J.E. Campbell and D.E. Longsine, INTERA Technologies, Inc., 6850 Austin Center Blvd, Suite 300, Austin, Texas 78731, November 1985.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: April 21, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

PTRACK is a computer program which simulates the path of a radionuclide particle released from a nuclear waste repository into a groundwater flow system in a two-dimensional stratified geologic medium. The program calculates the time required for a particle to travel from the release point at the edge of the disturbed zone to a specified horizontal or vertical boundary (the accessible environment). The hydrogeologic properties input into the program can be derived from known values or as random variables sampled from probability distributions. PTRACK assigns a value for each parameter in each run and tracks a particle for this "realization" in the system. Repeated trials reflect the effects of parameter variations on travel paths/travel times to be quantified. Partial correlation coefficients among dependent variables and independent variables can be calculated also. The paper under review presents little discussion of the amount of data required to define the input distributions for the various physical parameters.

A sampling code (LHS) must be used with the program. This code is not described in the documentation. There appears to be an inconsistency in that the program states that no vertical movement is allowed in the top or bottom layer. However, later in the report the movement of particles to the accessible environment through the upper and lower layers is discussed. There also appears to be a problem with mass balance in that mass balance for dissolved salt is not satisfied. The mass balance of liquid also is questionable.

BRIEF SUMMARY OF DOCUMENT:

PTRACK is designed to aid in the evaluation of variations of predicted travel time in bedded geologic settings surrounding a potential nuclear waste repository. The requirements for use of the code are:

1) A detailed knowledge of the hydrogeology of the site under investigation, including an understanding of the variability of system parameters and data sufficient to quantify the variability.

2) A general understanding of Monte Carlo and/or Latin Hypercube techniques and access to a suitable sampling code required for the use us such techniques.

3) An understanding of the solution strategy used in PTRACK and the data required to perform analyses. An understanding of how to interpret and use the results which the code provides also is required.

4) An awareness of the capabilities, assumptions and limitations of the code.

The mathematics of the code are quite simple. At least two head measurements are required. The code calculates the environmental head at any desired point by use of an equation from Lusczynski (1961). By application of Darcy's Law the hydraulic gradient and the velocity in any hydrostratigraphic unit can be calculated given the hydraulic conductivity and effective porosity. The calculation starts with a particle at specified location. The time required for the particle to move horizontally to a vertical boundary or vertically to a horizontal boundary then is calculated. The shortest travel time is selected and the coordinates for that point are calculated. If the particle has reached a horizontal boundary, in other words another layer with different hydrogeologic properties, the vertical and horizontal gradient in that unit are used to determine the particle's next position. The track of the particle is calculated until the particle reaches the accessible environment.

The process is repeated for another particle. It should be noted that the conductivity and porosity selected in each step is a sample from the distribution of these parameters for a particular hydrostratigraphic unit. Thus, particles released from the same position will not follow the same path unless the same values of hydraulic conductivity and porosity are selected at each step. The authors do not state how much data are necessary to define a probability frequency distribution properly for any of the hydrogeologic properties. This seems to be a weak point of the analysis; the report seems to assume that these probability distributions simply will be available.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

Assumption 7 (p. 17) states that flow is assumed to be horizontal with no vertical component in the uppermost or lowermost hydrostratigraphic layers of the system. If a particle enters these layers it is assumed to continue horizontally to the accessible environment which would lead one to conclude that a particle could not exit through the upper or lower layers. This assumption seems to be contradicted later in the report. On page 103 in the program documentation, the variable NUPB is defined as the number of the upper layer interface to be used as the accessible environment. This value is set to 0 if only vertical boundaries are considered as the accessible environment. A variable number also is assigned for the number of the lower layer interface to be used as the accessible environment. These variables do not appear to be consistent with the prior statement that no vertical flow occurs in either the upper or lower boundaries. This concept of no flow in the vertical direction in either the upper or lower layer also appears to preclude the possibility of vertical flow in the interior layers. If each layer is homogeneous in the horizontal direction, then it appears improbable that vertical flow could occur between the layers unless flow occurs through the top or bottom layer. Basically, this issue boils down to a question of whether or not conservation of mass, in the liquid, is satisfied.

The discussion of total dissolved solids (salt content) (Assumption 3, p. 18) states that conservation of mass is not necessarily considered in the conceptual model. It appears to us that this violation of conservation of mass may have an effect on the calculated head values in the various layers.

Verification for the model is provided on page 21 (Verification Tests and Results). Hand calculations agree with the computer output.

A sample problem is solved (p. 23) using a 19 layer case based on data from the J. Friemel #1 well located in Deaf Smith County, Texas. Computer output agrees with hand calculations. In this case a fractured material is used which is simulated by decreasing the effective porosity (multiplying by 0.5); the in-fracture particle velocity is doubled by decreasing the porosity.

The program cannot be field verified at the present time. Documentation of the code appears to be adequate. A nice feature has been incorporated into the program in that considerable checking of input data is required. Error messages point out problems as they occur. The program is written in Fortran 77 for a Harris 800 computer. The code contains enough comments to facilitate checking of the various subroutines.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

This document is important because it outlines a particle tracking program; the program output describes particle pathways and travel times from the edge of the disturbed zone to the accessible environment. The program treats the hydrogeologic properties as random variables.

REFERENCES:

Lusczynski, N.J., 1961, Head and Flow of Groundwater of Variable Density. Journal of Geophysical Research, vol. 66, no. 12, pp. 4247-4256.