WM S/F
WMHT r/f
CF
REBrowning
HJMiller
MBell
PAltomare
JBunting
JGreeves
PJustus
JERhoderick & r/f
WMHT Staff

WMHT DOCUMENT REVIEW SHEET

FILE: ~~3001.5/413.2~~ 413.2

DOCUMENT: "Hydrology of Sealing a Repository in Saturated Tuff", SAND83-0280, by Lisa A. Mondy of Sandia National Laboratories, Albuquerque, NM, March 1983

REVIEWER: Jay E. Rhoderick JR

DATE REVIEW COMPLETED: 8/18/83

BRIEF SUMMARY OF DOCUMENTS

DATE APPROVED: 8/23/83

The report presents hydrologic modeling studies which were performed to determine the need for and design of drift and shaft seals of nuclear waste repositories. The repository was hypothetically located in the saturated zone of volcanic tuff at Yucca Mountain. Results indicated that observable deviations in the groundwater flow near a repository would occur unless the drifts and shafts were backfilled to a permeability approaching that of the native rock.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

Performance assessment modeling studies will assist DOE in determining the need for and design of borehole and shaft seals. This report identifies changes to flowpaths caused by excavation and sealing of underground openings. It does not identify travel times or consequences caused by changes in the original flow regime. However, this report is a good beginning in understanding the phenomena of flowpaths around underground openings. DOE should extend this study to identify at what point changes to the flow regime will effect repository performance.

ACTION TAKEN:

Copies of the report will be given to J. Buckley, T. Verma, and M. Logsdon.

FOLLOW-UP ACTIVITY:

Results of this study will be compared to other performance assessment results on shaft sealing.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND83-0372

DOCUMENT: Johnstone, J.K., Peters, R.R., and Gnirk, P.F., 1984, Unit Evaluation at Yucca Mountain, Nevada Test Site: Summary Report and Recommendation. Sandia National Laboratories, Albuquerque, NM, and Livermore, CA, SAND83-0371.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: August 26, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

The report under review presents a unit evaluation of four potential repository horizons at Yucca Mountain. Prior to completion of the report the Topopah Spring Member was selected as the potential repository horizon. Therefore, most of the information presented in the report is outdated and is of little value to the NRC Waste Management Program. The report may be of some interest to mining engineers and geological engineers involved in the construction of the exploratory shaft at Yucca Mountain.

BRIEF SUMMARY OF DOCUMENT:

The report under review presents an evaluation of ranking criteria for four potential repository horizons beneath Yucca Mountain. The potential repository units are the welded, devitrified portions of the Bullfrog and Tram Members of the Crater Flat Tuff, the welded, devitrified Topopah Spring Member of the Paintbrush Tuff, and the non-welded zeolitized tuffaceous beds of Calico Hills. The Topopah Spring Member and the tuffaceous beds of the Calico Hills are above the water table whereas the Bullfrog and Tram Members are below the water table. The four ranking criteria used in the analysis included: (1) radionuclide isolation time, (2) allowable repository gross thermal loading, (3) excavation stability, and (4) relative economics.

According to the report, formal unit evaluation began at the beginning of fiscal year 1982. The report notes that in the middle of the unit evaluation (July 1982) a programmatic decision, prompted by exploratory shaft design needs, was made selecting the Topopah Spring as the reference case target horizon. Because of this fact, much of the information presented in the report is irrelevant with respect to a potential repository within the Topopah Spring Member.

According to the report, studies for the unit evaluation were limited to those which the authors of the report believed would provide discrimination between units and which had a reasonable probability of being completed successfully with the limited amount of data available. The report notes "some studies were performed in spite of the nearly complete absence of real data or by using very preliminary data because they were deemed crucial to the evaluation. The water travel time estimates are an example of such a study".

Most of the report under review is dedicated to a description of the constructability of the repository in the four potential repository horizons as well as a rock mass classification and a far field thermal/mechanical evaluation. The unit evaluation studies described in the report under the heading "Constructability" deal primarily with the minability of the repository and the stability of the repository once it is constructed. While this section is based on very limited data, some of the information presented in the report may be of interest to mining engineers and geological engineers involved in the repository construction. However, it should be noted that much of the information presented in the report is outdated at the present time.

The section on groundwater travel time estimates presented in the report are outdated and are not applicable to the current conceptual model of the USGS. For example, the authors of the report assumed an infiltration flux of 3 mm/yr. This flux is much higher than current USGS estimates of 0.5 mm/yr. In addition, the report states

> The current hydrologic data from Yucca Mountain do not include information about fracture flow nor are the existing transport codes capable of explicit treatment of fracture flow, especially in the unsaturated zone. Therefore, the travel time estimates in both the saturated and unsaturated zones were based on the assumption of porous flow.

While the infiltration flux of 3 mm/yr is considered by the authors of the report to be conservative, the assumption that all flow occurs through the matrix is non conservative. Under the current USGS conceptual model of unsaturated flow beneath Yucca Mountain, a flux greater than the average saturated matrix hydraulic conductivity of the Topopah Spring Member (0.7 mm/yr) would initiate fracture flow. Ignoring fracture flow with an infiltration flux of 3 mm/yr invalidates the estimates of groundwater travel time presented in the report under review.

According to the report, vertical travel times in the saturated zone from a repository in the Bullfrog range from less than one year up to approximately 225,000 years. Estimated travel times from a repository in the Tram range from 2,200 years to more than 2,260,000 years. These estimates are based on very limited data and are outdated at the present time.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The report under review is of little value to the NRC Waste Management Program with respect to a proposed repository in the Topopah Spring Member at Yucca Mountain. The Topopah Spring Member was selected as the proposed repository horizon before the report under review was completed. This fact served to outdate most of the material presented in the report prior to its publication. The report may be of some interest to geological engineers and mining engineers involved in the construction of the exploratory shaft at Yucca Mountain.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The report under review was outdated prior to its publication. The report is of very little value to the NRC Waste Management Program.

SUGGESTED FOLLOW-UP ACTIVITIES

No follow-up activities are suggested.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND83-7475

DOCUMENT: Thompson, F.L., Dove, F.H., and Krupka, K.M., 1984, Preliminary Upper-Bound Consequence Analysis for a Waste Repository at Yucca Mountain, Nevada. Sandia National Laboratories, Albuquerque, NM, and Livermore, CA.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: July 15, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

The report under review presents the results of a preliminary analysis designed to estimate the long-term, cumulative release of radionuclides from a proposed nuclear waste repository at Yucca Mountain. The analysis attempts to delineate upper bounds on the cumulative release of radioactivity to the accessible environment 10 km from the repository boundary. The results of the analysis show that for the highest credible flux of 17 mm/yr, releases of radioactivity to the accessible environment in 10,000 years after closure of the repository are lower than the limits imposed by 40CFR191. However, several limiting assumptions are incorporated into the analysis because of the lack of available field data.

BRIEF SUMMARY OF DOCUMENT:

According to the report under review, the purpose of the study is to estimate upper bounds to the long-term consequences of a release of radionuclides from a potential waste repository considered for location at Yucca Mountain in Nevada. The consequences are presented in terms of cumulative release to the accessible environment and in terms of radiological dose to man. Radionuclides are assumed to be leached by water that infiltrates through the unsaturated zone to the water table. Once the radionuclides reach the water table they are assumed to travel horizontally through the saturated zone to the accessible environment. For the purpose of this study, the accessible environment was considered to be 10 km from the perimeter of the repository. The authors of the report investigated two time periods: 1) 10,000 years after leaching begins, and 2) 250,000 years after leaching begins.

The one-dimensional multi-component mass transport (MMT1D) model prepared by Washburn and others (1980) was used to simulate the movement of radionuclides that might be leached from buried nuclear waste in a repository at Yucca Mountain. According to the authors, the one-dimensional model is designed to represent three-dimensional flow by associating a width and a height with the paths of travel. The MMT1D model is designed to account for convection, dispersion, retardation, and radionuclide decay. The MMT1D model uses a random walk form of the method of characteristics to solve the advection-dispersion equation numerically for solute transport in porous media.

The analysis performed by the authors considers two different locations in the unsaturated zone for the repository horizon. These locations are: 1) the "upper zone," which is composed of welded fractured tuff, and 2) the "lower zone," which is composed of non-welded zeolitized tuff. The upper zone location and the lower zone location are referred to in the report as Case 1 and Case 2, respectively. For the analysis of both cases, the authors assumed that the waste first contacts water 1,000 years after the repository is closed. The spent fuel is considered to be predominantly uranium dioxide (UO_2). The assumed dissolution rate of UO_2 was based on the maximum possible concentration of dissolved uranium. This rate was estimated from the solubility equilibria, pH, and redox potential data for groundwater from well J13. The MINTEQ geochemical model was used to calculate a maximum possible concentration of dissolved uranium. Appendix A presents the details of the geochemical modeling effort.

The analysis of dissolution rates presented in the report is based on pore water velocities ranging from 0.5 mm/yr to 50 mm/yr for Cases 1 and 2. Case 1 consists of a welded fractured tuff similar to the Topopah Spring with a porosity of 5% and a matrix saturation level of 65%. Case 2 consists of a non-welded tuff similar to the Calico Hills with a porosity of 35% and a saturation level of 95%. According to the report, to make the analysis more conservative, the water infiltrating over the entire repository area was assumed to contact the waste. This approach produces the maximum possible dissolution rate (solubility x flow rate).

The report notes that equilibrium solubilities of uranium minerals in water vary with pH, redox potential (Eh), temperature, and the concentration of complexing ligands. According to the authors, the composition and pH of the groundwater from well J13 were used in the analysis. The MINTEQ geochemical model was used to investigate how changes in redox potential and temperature ($T<100^{o}C$) affect predicted equilibrium solubility. The MINTEQ geochemical model was used to estimate the dissolution rate under the following conditions: oxidizing conditions (Eh>200 millivolts), a pH of 7.5, and temperatures between $25^{o}C$ and $100^{o}C$. Under these conditions, the report suggests that concentrations of dissolved uranium would range from $1.48x10^{-6}$ moles/liter to $1.69x10^{-6}$ moles/liter. Based on these calculations, the authors chose a "representative value" of 0.40 mg/L ($0.40x10^{-3}$ kg/m^3) as a solubility value.

According to the report, 28 radionuclides constitute more than 99% of the total injection and inhalation hazard for one million years for spent fuel rods. Table 3 of the report lists the decay constants and initial inventories for these radionuclides. Table 4 of the report lists the radionuclides that were simulated in the consequence analysis and the radionuclide inventories 1,000 years after repository closure.

The authors of the report estimated that the radionuclides would continue to be leached from the repository for a period of $1.14x10^7$ years for Case 1 and $1.1x10^6$ years for Case 2. These estimates are based on the total amount of uranium in the repository 1,000 years after closure divided by the dissolution rate for uranium. Table 5 of the report lists the estimated leachate concentration for each radionuclide released from the repository. According to the report, four radionuclides have release concentrations at the repository that are greater than the maximum permissible concentrations. The report notes that the steady state concentrations which reach the accessible environment will be approximately equal to the repository concentration for radionuclides with long half lives.

Characterization of Flow Tubes

According to the report, a flow tube consists of a collection of streamlines beginning at the repository and ending at the release region. Figure 2 of the report illustrates the assumed travel path for radionuclides from Yucca Mountain to well J12. The analysis for Case 1 consisted of three flow tubes: welded fractured tuff, non-welded zeolitized tuff, and the saturated zone. The analysis for Case 2 consisted of two flow tubes: non-welded zeolitized tuff, and the saturated zone. Table 6 of the report shows the flow tube characteristics.

The Variable Thickness Transient (VTT) code prepared by Reisenauer (1980) was used to model flow in the saturated zone. Appendix B of the report presents details of the VTT modeling. The results of the VTT modeling are presented in Table 7 of the report. The shortest average travel time value from Table 7 was used as input for the MMT1D model. As an additional measure to make the analysis more conservative the authors assumed that the flow volume through the saturated zone flow tube is the same as that through the unsaturated zone. This assumption eliminates the need to consider potential dilution by the greater volume of water in the saturated zone.

According to the report, estimates of flow length and travel time from the VTT modeling were analyzed stochastically to evaluate dispersivity to be used in the MMT1D model. In this analysis, the authors assumed that dispersion within a flow tube is caused by the difference in travel time between streamlines composing the flow tube. The travel time variance for streamlines within a given flow tube was used as the primary measure of macro dispersion. Dispersivity values for the unsaturated zone were considered to be approximately 10% of the flow tube length. According to the report, all streamlines within the unsaturated zone were assumed to have the same length because of the absence of better information.

Radionuclide Retardation Data:

According to the report, estimates for distribution coefficients for radionuclides in porous flow under oxidizing conditions were derived from Serne and Relyea (1982). Table 8 of the report lists the radionuclides, assumed distribution coefficients, and retardation factors considered in the transport analysis for Case 1. Table 8 indicates also that with a Darcian velocity of 2 mm/yr, none of the radionuclides reached the accessible environment in 10,000 years. Table 9 of the report indicates that with the Darcian velocity of 0.2 mm/yr, none of the radionuclides would reach the accessible environment within 250,000 years.

According to the report, if the repository is located in the non-welded horizon (Case 2), the analysis shows that non-retarded radionuclides will reach the accessible environment in about 3,200 years (Table 10 of the report). However, the report notes that radionuclides with a distribution coefficient of one (Kd=1.0) would not reach the accessible environment for about 28,000 years. According to the report, only Case 2 produces results that can be compared with the Environmental Protection Agency (EPA) proposed rule 40CFR191.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The analysis presented in the report under review attempts to quantify a "natural" release scenario for a repository at Yucca Mountain within the limits of the data available. The report is a good example of the type of analyses that the NRC probably will have to evaluate in the future as additional data become available.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The analysis presented in the report under review constitutes a preliminary attempt to quantify a "natural" release scenario within the limits of the data available. A significant number of limiting assumptions had to be made in order to perform the analysis. These assumptions are necessary because of the absence of real field data. The report notes that while the analysis is based on a flux through the unsaturated zone of 5 mm/yr, data and evaluations that have become available since work on this report was completed suggest strongly that the actual flux is less than 1 mm/yr.

Several limitations of the analysis are listed in the report. These limitations are as follows:

1) The source term is based on the assumption of congruent leaching. Departures from congruent leaching increase significantly the maximum radionuclide concentrations at the accessible environment. The report notes, that the assumption of congruent leaching therefore is non-conservative.

2) If fracture flow is the dominant mechanism for transport, then the convective flow rate may be higher than that assumed in the analysis presented in the report. The report notes, however, that evidence obtained to date suggests that flow probably occurs predominantly through the rock matrix rather than through fractures.

3) Use of the maximum possible cross-sectional area increases the conservatism of the results. However, if a smaller cross-sectional area were used the leach rate would be reduced and the duration of leaching increased.

4) The equilibrium solubilities predicted by MINTEQ were based on groundwater of a specified composition, pH, and redox potential. The report notes that the groundwater with a different set of complexing ligands could change the solubility constraint and increase the maximum concentrations of dissolved uranium. In addition, we suggest that the assumption that the groundwater system is in constant chemical equilibrium may be a significant limitation with respect to the analysis for radionuclide retardation.

5) The fact that the retardation factor depends on β (the ratio of bulk density to porosity or moisture content) indicates that increases in saturation level will decrease β. A decrease in β will result in a decrease in the retardation factor. This reduction would reduce the travel time of retarded radionuclides.

6) Lower values of bulk density would increase the conservatism of the results for the retarded radionuclides by decreasing β and, thus, decreasing the retardation factor.

7) Lower values for distribution coefficients increase the conservatism of the results for the retarded radionuclides by decreasing retardation factors.

8) The distribution coefficient is a lumped parameter for evaluating ion transport through a given medium. Like all deterministic model coefficients, predictions of nuclide travel based on laboratory measurements of K_d are valid only to the degree to which field conditions are duplicated. In addition, the distribution coefficients presented in Table 8 of the report are not valid for fracture flow.

The assumptions used in the consequence analyses are presented in Table 1 of the report.

SUGGESTED FOLLOW-UP ACTIVITIES

The report under review is of primary significance to geochemists. The report should be reviewed by a geochemist who is knowledgeable about the use of K_d.

REFERENCES CITED:

Washburn, J.F., and others, 1980, Multicomponent Mass Transport Model: A Model for Simulating Migration of Radionuclides in Ground Water. Pacific Northwest Laboratory, Richland, WA, PNL-3179.

Reisenauer, A.E., 1980, Variable Thickness Transient Groundwater Hydrology Model. Pacific Northwest Laboratory, Richland, WA, PNL-3160, 3 volumes.

Serne, R.J., and Relyea, J.F., 1982, The Status of Radionuclide Sorption Desorption Studies Performed by the WRIT Program. Pacific Northwest Laboratory, Richland, WA, PNL-3997.

SAND83-1778

Cover Letter 1/10/85

REVIEW OF A REPORT TITLED "REPOSITORY SEALING CONCEPTS FOR THE NEVADA NUCLEAR WASTE STORAGE INVESTIGATIONS PROJECT", BY JOSEPH A. FERNANDEZ AND MARK D. FRESHLEY. PREPARED BY SANDIA NATIONAL LABORATORIES, ALBUQUERQUE, NEW MEXICO 87185 FOR THE UNITED STATES DEPARTMENT OF ENERGY

by

Williams and Associates, Inc.
P.O. Box 48
Viola, Idaho 83872

This report includes the following information that was used to develop the concepts for sealing a repository in unsaturated tuff.

1. Descriptions of existing boreholes and associated geology.

2. A summary of the current understanding of the geology and hydrology of Yucca Mountain.

3. A preliminary conceptual layout of the repository.

4. Federal and state criteria, guidelines and standards.

5. Functional requirements and performance criteria for sealing a repository.

6. Hydrologic calculations.

This report also gives preliminary guidance for sealing the proposed repository in Yucca Mountain and provides the concepts that form the basis for the conceptual design of sealing components. Of particular concern in this review are the questions:

1. Are the assumptions valid?

2. Are inflow estimates defensible?

Performance Criteria for a Repository Sealing

Water Flow into a Shaft

The possible rate of water flow into a shaft is calculated in this section. This section is divided into two parts.

1. The water that could infiltrate at the surface of the ground follows the faults at a slope of 73° and ultimately is

intercepted by the shaft. The infiltration rate for this section is considered to be the infiltration rate throughout the entire region which is 2% of the precipitation or 4 mm/yr. The area of influence is a half circle of diameter 220 m. The amount of inflow that this area contributes is 79 cubic meters per year. The other amount of water that is calculated is that which would fall on the shaft itself or in the area surrounding the shaft which has settled. The rate of water flow into this circular region is the same as the amount of rainfall. According to the author's calculations the smaller shaft (3.1 m diameter) could have as much as 22 cubic meters per year of water and the 6.7 m diameter shaft could have as much as 68 cubic meters per year infiltrating from the source. It is not clear from these calculations what diameter was used for the area of influence in this calculation. This diameter should correspond to the area of settlement, but that is not specified. There are several other ways that the inflow could be categorized but it is doubtful that they would be any better than this particular one. The total inflow from these calculations produced a total of 100 cubic meters per year for the 3.1 meter diameter shaft and 150 cubic meters per year for the 6.7 meter diameter shaft. This amount of water then must be accounted for as drainage at the bottom of the shaft. Water producing zones in drifts and ramps and horizontal emplacement holes are considered next. These flow contributions are only about .07 cubic meters per day.

Calculations Used to Establish the Sealing Concepts

The integrated finite difference code TRUST was used for analysis of flow into the emplacement area. A section was modeled that was approximately 15 m in the horizontal plane and 54 m in the vertical direction. The assumptions used in this analysis are as follows:

1. The hydraulic gradient is vertically downward.

2. Porous matrix flow or flow as a continuum was assumed.

3. Steady state results were used to analyze the need for and the extent of sealing.

4. Isothermal conditions prevail.

The first and third of these assumptions are certainly reasonably valid. The second and fourth assumptions however are very questionable, particularly the fourth one which leads to part of the problem with the second one. The assumption of isothermal conditions is completely invalid because of the heat produced by the emplaced wastes. The heat production of the wastes will bring about a completely different flow process than that due to the porous matrix flow. The high temperatures near the waste will tend to vaporize water which will then move away from the waste in the vapor form until it reaches a region where the temperature is sufficiently low that condensation can occur. In this region it will be condensing and the liquid flow gradient will then be back toward the waste area. This results in a circulating system but the flow of liquid water is only half of the system. This has been explained in several of the reports by Dr. Evans at the University of Arizona. The modeling results show that very little, if any, water would move in near the waste package. This is very likely a reasonable estimate and is probably more than would be predicted if a correct model had been used. However, it does not enhance credibility to use a model which has an obviously invalid assumption. One of the conclusions from this section is as follows: "If backfilling is necessary, coarse materials are apparently more satisfactory because of their capacity to drain and act as a capillary barrier." This conclusion was verified by the following results:

1. Generally the fluid flow rate past the waste packages is lower where the drifts are backfilled with sand rather than clay.

2. The clay backfill tends to drain slowly and retains some moisture.

3. The sand backfill drains more rapidly than the clay backfill and under steady state conditions is essentially dry.

This conclusion is correct if the liquid flow of water is all that is considered. However, in the present case where vapor flow would also be occurring this conclusion may not be valid. Coarse material would allow vapor flow more readily than the clay material. It is possible also that gas could move with the vapor and perhaps lead to migration of radioactive material from the emplaced waste. Clay that is slightly wet would completely prevent the movement of gas from the waste.

Approach and Input Used for the Shaft and Drift Drainage Analysis

To provide for drainage from the bottom of the shaft of the water which was estimated to flow into the shaft in the first section in this report, the Glover and Hasberg-Terletskata equations were used. These equations make use of the following assumptions.

1. The length of the shaft in hydraulic contact with the host rock formation is equal to the height of the standing water

column in the shaft.

2. The concept of free surface flow is a valid approximation.

3. The formation below and surrounding the shaft is homogeneous and isotropic. This may be a weak assumption because it was recognized that fracture rock systems usually are anisotropic.

4. Capillary flow is insignificant and gravitational forces dominate flow.

5. Effective hydraulic conductivity of fractured tuff may be determined from the limited information on fractures that is available.

The second of these assumptions, the concept of free surface flow from a borehole, is invalid. Stephens and Neuman (1980) have shown that the free surface flow model from a borehole above the water table is completely invalid. The flow regime which occurs in steady state is a small saturated bulb around the borehole; the remainder of the flow field is unsaturated down toward the water table. This was shown by the use of the mathematical model TRUST in a research project whose objective was to develop a better means for using piezometer tests for measuring hydraulic conductivities above the water table. TRUST is the same model as used in the report under review. Although the analytical solution used in the present report is incorrect the answers probably would differ only slightly from those using TRUST which would consider the unsaturated flow. The final conclusions given for the shaft and drift drainage analysis are:

1. Any reasonably expected inflow can be effectively drained through the bottom of the shaft even when considering conservative values of fracture permeability. This conclusion is reached by comparing the performance criteria value of 100 cubic meters per year for a 3.1 m diameter shaft and 150 cubic meters per year for a 6.7 m diameter shaft.

2. Considering the possible effect of fracture permeability, any reasonably expected inflow into a drift can be drained through a 6 m length of drift floor. This is based on the assumption that water flow in a discrete fault or fracture zone would be similar to flow in the faults encountered in Rainer Mesa.

These conclusions probably are correct even though questions could be raised about the method of analysis. The remainder of this report is concerned with the sealing techniques; they were not reviewed.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND83-2465, PNL-5117

DOCUMENT: Hydrologic Calculations to Evaluate Backfilling Shafts and Drifts for a Prospective Nuclear Waste Repository in Unsaturated Tuff. Mark D. Freshley, F.H. Dove, and J.A. Fernandez, Sandia National Laboratories, Albuquerque, New Mexico, June 1985.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: April 30, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

Computer simulations originally were to be conducted for flow around waste packages oriented either horizontally or vertically to help evaluate whether drift backfill could influence water flow into the waste package. The simulation used the computer code TRUST. Configurations actually simulated consisted of a vertical shaft that extends downward from the surface to the repository and a horizontal repository drift. In the end only vertical orientation of waste packages was considered, as explained below. Coarse- and fine-grained materials were evaluated as backfill in the drift and shaft. Coarse-grained backfill material in general was drier than the fine-grained material during the flow process. The authors planned to simulate flow around a horizontal waste package but they did not understand how to apply a two dimensional analysis to the problem. We suggest that the modeling be repeated using the measured hydraulic properties of the crushed tuff that is to be used for backfill.

BRIEF SUMMARY OF DOCUMENT:

The configurations of waste package orientation that were evaluated, or for which an evaluation was attempted, by the numerical simulation in the report under review are:

1) A repository drift with horizontal emplacement of waste packages.

2) A repository drift with vertical emplacement of waste packages.

3) A shaft intersecting a contact between welded and nonwelded tuff units.

The simulation was performed to determine the effect of various types of materials to be used as backfill in either the drift or the shaft. Coarse-grained material for backfill would be a moderately to slightly crushed tuff while the fine-grained backfill would consist of a highly crushed tuff. Two factors to be considered in the design of seals for shafts and boreholes are:

1) General Design Criteria: Seals for shafts and boreholes shall be designed so that following closure they do not become pathways that compromise the geologic repositories ability to meet the performance objectives for the period following permanent closure.

2) Selection of Materials and Placement Methods: Materials and placement methods for seals shall be selected to reduce to the extent practicable: 1) the potential for creating a preferential pathway for groundwater and 2) radioactive waste migration through existing pathways.

These criteria are more likely to be met if the backfill material is designed such that water does not move into it. The assumptions used in the modeling are as follows:

1) Water flow is assumed to occur in the surrounding rock matrix.

2) Steady state flow was assumed to have been reached when the flux out of the system was less than 5% different than the flux into the system.

3) The steady state influx to the modeled region was assumed to be .4 cm/yr.

4) The predominant hydraulic gradient driving the flow system was assumed to be vertically downward.

5) Fluid flow was assumed to occur only in the liquid phase; vapor transport was not considered.

6) Isothermal conditions were assumed to exist; the material properties did not change in either space or time.

7) Hysteresis of moisture retention characteristics for the materials simulated was not considered.

8) The rock matrix was assumed to be incompressible.

Most of these assumptions are common for such problems. The hydraulic characteristic curves for volcanic tuffs were obtained from Gee (1982). No attempt was made to correlate a particular tuff core with the stratigraphy of the borehole from which they were removed. The hydraulic characteristics of the backfill were for sand and clay as obtained from Mualem (1976). It should be noted that crushed tuff is proposed to be used for backfill. Since tuff is a volcanic material pores may be present in the actual grains. In such a case the hydraulic characteristics of an ordinary (quartz) sand may not be the same as the crushed tuff because quartz sand grains may not have pores within the grains. Crabcreek sand, which is a volcanic sand, was used for the simulation but it is unknown whether the pores in the grains of Crabcreek sand are similar to that of the crushed volcanic tuff. Hydraulic properties should be measured for the crushed tuff so that the proper characteristic curves can be used in simulation.

Although the project was designed initially to investigate flow around horizontal emplacement of waste packages it became apparent to the authors that two dimensional analysis was invalid in such a case. Consequently they did not conduct this portion of the investigation. We note, however, that if the investigators had turned the plane of reference perpendicular to the drift that contains the waste, then horizontal emplacement could have been investigated using a two dimensional analysis. Ultimately a three dimensional model should be used to simulate horizontal emplacement because whether or not water moves into the waste package is dependent on the spacing between the disturbed emplacement areas. The emplacement drifts must be far enough apart to allow water to flow downward between the tunnels without increasing the degree of saturation to the point where water would flow into the drift. In the present report the investigators state that the sand backfill formed a capillary barrier to water flow. It should be noted that the backfill was able to accomplish this effect only because the distance between the packages was large enough to allow flow between the drifts.

The authors conclusions are as follows.

1) From a hydrologic perspective numerical simulations performed by approximating an open drift with the hydraulic properties of coarse sand show that backfilling the drifts and shafts does not appear to be essential because backfill material does not significantly influence flow past the waste packages.

2) If backfilling is required, results from the numerical simulation indicate that coarse materials perform more satisfactorily as barriers to water flow through drifts and shafts than do fine materials.

3) Regardless of the backfill material modeled, more water flows into the repository drift when the surrounding host rock formation is at a high level of saturation (high moisture content).

Nothing is unusual about any of these conclusions. The authors present a good discussion of hydraulic properties of the materials with a sample of permeability vs. pressure head curves, and moisture content vs. pressure head curves for a number of different samples of tuff as well as for the sand and clay that were used for backfill in the simulations. It should be noted that the curves for sand are considerably different than the curves for any of the tuff samples. This difference reemphasizes our previous statement that hydraulic characteristics should be obtained for the crushed tuff that would be used for backfill.

The fluid properties were referenced to 32 degrees Celsius and conditions near the repository were assumed to be isothermal. This condition will not be the case in the vicinity of the repository. The temperature near the repository is estimated to reach well over 100 degrees Celsius. This higher temperature would have considerable effect on the viscosity of the water and on the applicability of the outcome of the simulation.

One of the interesting aspects of this study is that some work was done to determine the proper grid spacing for the node points in the grid of the model. Experiments with various spacings were conducted and the computational time as well as the changes in average pressure and total number of iterations were investigated. This procedure made possible the use of the coarsest possible mesh while still maintaining accuracy. Use of the coarsest possible mesh optimized the use of computer time.

An analysis of a repository drift is presented in the report. The attempt to model the horizontal emplacement by extending the two dimensional plane through the emplacement tunnel is discussed. In this configuration all water would be forced to go through the backfill whereas in the actual repository water could flow around it also. As we noted above, if the plane of simulation had been taken perpendicular to the tunnel the horizontal emplacement could have been investigated.

Two vertical planes of symmetry were used to define the flow region. One is at the centerline of the drift and the waste package hole; the other is at the centerline between drifts. The simulation perhaps would have been more realistic if an axisymmetric mode had been used with the centerline of the drifts at the centerline of simulation. Since steady state flow was being investigated, the program was run until the outflow was essentially equal to the inflow. In the several configurations investigated with various backfill materials, little disturbance of the flow field occurred at distances greater than 10 m from the emplacement location. Several experiments were conducted by increasing the permeability of the host rock. This increase produced little effect on flow through the drift. Decreasing the host rock permeability an order of magnitude below the permeability of the clay backfill caused the drift to remain at much higher moisture content. This effect would be expected because when the host rock permeability is decreased, a much higher moisture content is required to conduct the specified (fixed) flux of .4 cm/yr. A vertical repository shaft backfilled with sand or clay that intersects a contact between two tuff units was investigated to determine whether a perched water table would develop at the contact. A relatively wet area did develop but this was only a transient condition after which the high moisture content layer dissipated.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The flow of water in the rock surrounding the waste repository must be understood fully in order to predict the rate of movement of water through the waste. This information is necessary for prediction of travel times to the accessible environment.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

Flow around the horizontally emplaced waste should have been investigated by a two dimensional simulation oriented perpendicular to the axis of the tunnel. The hydraulic properties of crushed tuff also should have been obtained and used in the simulation. More realistic temperature and water viscosity values also should have been used in the simulation.

SUGGESTED FOLLOW-UP ACTIVITIES:

The simulation of the flow around the waste packages should be conducted in three dimensions using measured hydraulic properties for crushed tuff.

REFERENCES:

Gee, G.W., 1982, Laboratory Report on the Unsaturated Flow Characteristics of Core Samples from Nevada Test Site Well USW GU-3, Interim Status Report to SNL for PNL, October, 65 p.

Mualem, Y., 1976. A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media. Water Resources Research, vol. 12, no. 3, p. 522-523.

Review of:

Rice, W.A. 1984. Preliminary Two-Dimensional Regional Hydrologic Model of the Nevada Test Site and Vicinity. Sandia National Laboratory Contract Report SAND83-7466, Albuquerque, New Mexico

Introduction

The stated objective in the Introduction section of this document, to the extent that I am able to determine it is as follows: "In particular the regional hydrologic model can be used to establish the boundary conditions for a more detailed local model of the site and can be used to predict the following: ground water flow paths, ground water discharge points, subsurface flux, pluvial climate effects and man-influenced effects." It is not obvious that this document accomplishes any of these objectives satisfactorily. The document contains no figure that presents a single flow line, although figure 12 does present the hydraulic heads for the study area as predicted by the model. These heads are for steady-state confined conditions. They are presented in the form of a contour map. The report does contain one figure (figure 10) that designates the discharge areas of the regional model. Unfortunately, the text explains (page 28) that these discharge areas "were digitized from maps and plates and then overlayed on a node map so that an appropriate net discharge value could be assigned to a node or distributed over several nodes." In other words, the discharge areas shown in figure 10 were not predicted by the model, they were input to the model. The document does present certain characteristics of subsurface flux as predicted by the model. These results are presented in table 5. Only two aspects of flux through the model are presented. These are the estimate of net discharge from pumping, springs and evapotranspiration along with the underflow leaving the model in Death Valley and along a southern boundary of the model. No flux is presented for the discharge areas individually as identified in figure 10. Without such fluxes and without flow paths it is difficult to see how boundary conditions can be established for a more detailed local model of the Yucca Mountain site. Pluvial climate effects are not predicted in the model at all. The document states that the regional model could be used for this purpose. The last of the items that page 1 of the document states that the model can predict (man-influenced effects) is restricted to pumping, presumably for purposes of irrigation. Table 5 of the document lumps this discharge mechanism with that of springs and evapotranspiration (misspelled). I can find no other discussion of this man-made impact anywhere in the text. No discussion is presented about the distribution of pumping or how it was input into the model or whether it was output from the model or whether it was simply extracted from another source and lumped with the model discharge in table 5.

It is in this context that the reader is introduced to the document. Since at best only one of the five items that page 1 of the report states that the model can predict is in fact addressed in the document, it is appropriate to proceed with a point by point critique of the document. Although not stated in the report, apparently the real objective of the modeling effort is to input existing composite head data for the study area and existing data pertinent to recharge and discharge into a single layer, isotropic, steady state model that is restricted to horizontal flow lines and then to "adjust the transmissivities of blocks of rock within reasonable limits in order to minimize the difference between the hydraulic heads simulated by the model and hydraulic heads measured at well locations." The model used requires confined conditions even though some of the water level measurements reflect confined conditions and some do not. As discussed below, these assumptions place considerable constraint on the utility of the model.

Review of Technical Aspects of the Subject Document

1. The study area encompassed by the model covers approximately 30,000 square miles of the Basin and Range Physiographic Province in southern Nevada and central California. The Yucca Mountain site is included within the study area. However, the size of the area covered by the model and other constraints, as discussed below, limit the significance of the treatment of the Yucca Mountain site considerably. In other words, the size of the Yucca Mountain site is so small relative to the size of the area modeled that the significance of the results relative to the flow system within Yucca Mountain is limited.

2. The hydrogeology of the study area is known to be complex. The area contains Precambrian and Paleozoic sediments that were folded and faulted during the Mesozoic. During the Cenozoic, volcanism and additional block faulting occurred. Other studies have lumped the older sedimentary rocks into a unit called the lower clastic aquitard. This unit is comprised of low permeability sandstones and shales that range in age from Precambrian to Cambrian. Limestones and dolomites overlie this aquitard. These units crop out in the southern and eastern part of the study area. Their ages range from Cambrian to Devonian. These units have been

called traditionally the lower carbonate aquifer. This unit appears to be a major aquifer beneath Yucca Mountain. A unit of less permeable rocks, collectively called the Eleana Formation overlies the lower carbonate aquifer. The Tertiary Tuffs that have been analyzed in other studies at Yucca Mountain overlie the Eleana Formation. The most recent sequence is the valley fill alluvium overlying the tuffs. All of these units have been affected by tectonic forces. Geologic structures have created large-scale folding and fault blocks, intense folds that have fractured the limestones and dolomites (thereby creating secondary permeability features) and lastly, folding and faulting that has created barriers to water movement that ultimately have produced the springs in the study area. This complex hydrogeologic framework is important because of its implications relative to the simplifying assumptions that have been used to characterize the hydrogeology in the model discussed in the subject document. These simplifying assumptions are as follows:

A. Ground water flow is horizontal. The hydrogeology discussed above suggests that ground water flow cannot be horizontal throughout the study area. The existence of the confining layers mentioned above preclude the validity of this assumption. In addition, the climate of the area is such that precipitation is much greater in regions of higher elevation than in regions of lower elevation. Because of the location of the outcrops of the carbonate aquifer in particular, one can conclude with confidence that vertical flow occurs beneath the areas of higher elevation at least. Similarly the discharge areas noted on figure 10 could not exist without the occurrence of vertical flow. Finally, the hydraulic head versus depth data for well UE-25P#1 presented in USGS Water Resources Investigations Report No. 84-4197 indicate a difference of 20 m in the hydraulic head between the depth interval 383 to 500 m and the depth interval 1,297 to 1,805 m. A 20 m variation in hydraulic head over this depth interval suggests that some vertical component of flow exists. Consequently, it is safe to conclude that the assumption of no vertical flow, as used in the construction of the model, is not valid.

B. The model assumes a steady state condition throughout the study area. This assumption ignores fluctuations in the potentiometric surface caused by recharge in the spring and it ignores fluctuations caused by pumping for irrigation. In spite of these realities, the assumption of steady state flow probably is the most defensible assumption in the model.

C. The report states that the aquifers are assumed to be isotropic with respect to transmissivity. In reality, the model does not contain aquifers. It contains only one aquifer. The entire geologic column discussed above is treated as one aquifer. The model consists of one layer. The carbonate rocks, the Eleana Formation, the lower clastic aquitard, the tuffs, and the alluvial aquifer are not differentiated in the model. The existence of these hydrogeologic realities makes the assumption of isotropy and a single layer as used in the model completely indefensible.

D. The model is based on the assumption of confined conditions. In other words, the single aquifer that is supposed to characterize the study area does not contain a phreatic surface. This assumption is contrary to the assumptions presented in USGS Water Resources Investigations Report 84-4197. Page 3 of that document contains the following statement, "The water levels generally represent water table or unconfined conditions; potentiometric levels show little variation with depth in the upper part of the saturated zone." Consequently the assumption that the aquifer is confined is not consistent with the assumption inherent in the potentiometric surface map presented by the USGS in Water Resources Investigations Report No. 84-4197. This distinction is significant because, as stated above, the introduction section of the document under review claims that the boundary conditions for a Yucca Mountain model can be derived from this model.

3. The model selected for this effort is a Battelle Pacific Northwest Laboratory model described by the two-dimensional, variable thickness, transient code developed by Reisenauer in 1980. The model is described in Battelle's document PNL-3160. After a grid is assigned to the study area, the model solves the appropriate differential equations for the hydraulic head at each node. The parameters that define the aquifer system (in this case only one aquifer was used) that must be assigned each node are as follows:

Elevation of land surface,
Elevation of the top of the aquifer,
Elevation of the bottom of the aquifer,
Elevation of the initial potentiometric surface input,
Transmissivity or hydraulic conductivity of the aquifer,
Recharge to the aquifer,

Discharge from the aquifer,
Boundary conditions for the region that is modeled.

In the case of the document under review, the elevation of the land surface should be relatively reliable. The elevation of the top of the regional aquifer probably is not reliable because the model considers only a single confined aquifer. The hydraulic head data used as initial input to the model do not differentiate confined from unconfined water levels or water levels among different confined aquifers. Consequently these data probably are not reliable. The elevation of the bottom of the aquifer is not known. Transmissivity is obtained by trial and error methods that rely on matching model output head data to measured data. The transmissivity is treated as that of a single layer and it is treated as isotropic. Neither of these approaches reflect the hydrogeologic complexity discussed above. The recharge to the aquifer, as used in the study, probably is as defensible as it can be based on the existing knowledge of the climate of the area. The discharge from the aquifer assigned to the discharge areas shown in figure 10 (discharge from different discharge areas are not distinguished) probably also is as valid as it can be based on current knowledge.

As stated above, the regional system was modeled in the subject document as a one-layer flow system that combines valley fill, volcanic and carbonate aquifers into a single unit. Boundaries for this unit were established along the following topographic highs. The north boundary consists of the topographic highs in the Palmetto Mountains and in the Catus, the Kawich, the Reveille and the Grant Ranges. The east boundary consists of the the topographic highs for the Pahranagat Range, the Sheep Range, and Spring Mountain. The south boundary consists of the topographic highs in the Kingston Range and the Saddle Hills. The western boundary is the topographic low corresponding to Death Valley. This boundary was fixed as a discharge boundary. The boundaries on the north and east were held at water table elevations of a hand-contoured hydraulic head map provided to PNL by the Denver office of the USGS. These head measurements undoubtedly are a combination of water table conditions and confined water levels. They appear to be composite water levels in all cases.

This information sets the stage for the performance of the model. Clearly, the hydrogeologic framework is oversimplified drastically in the model and clearly the hydraulic head data that constitute the match data and the boundary conditions reflect a combination of water table conditions and multiple layer confined conditions that have been converted to data that are supposed to represent a single aquifer that is supposed to simulate the minimum of four (perhaps more and/or perhaps some that are not layers) hydrostratigraphic units listed above.

This model was used to produce a head distribution subsequent to variations in transmissivity that produced matches to measured heads from 240 wells shown in figure 6 of the document. Interestingly enough, page 22 of the document lists the hydraulic head measurements in the 240 wells as water table measurements even though the aquifer model requires confinement.

As stated above, PNL used a hand-contoured ground water elevation map interpreted by the Denver office of the USGS for purposes of matching heads produced by the PNL model discussed in the document under review. In addition, PNL used Kriging to calculate a "statistically unbiased hydraulic head distribution that optimally fits the 240 <u>water table</u> measurements shown in figure 6". The document under review states that the "uncertainty in the USGS interpreted hydraulic head distribution was determined by comparing the USGS hand-contoured distribution with water table measurements at well locations." This reviewer does not understand this statement. Presumably the water level measurements <u>were the basis</u> for the contour map. If this is not the case, then the document should have described the basis for the USGS contour map; the only data mentioned are the 240 water table measurements shown in figure 6. Since I do not understand the difference between the 240 water level measurements and the basis for the USGS contour maps, I cannot understand the PNL method of estimating the error between these two data sources (assuming that they are two different data sources which does not make sense).

The authors of the document under review also calculated the Kriging or estimation error in an effort to measure the uncertainty in the hydraulic head distribution. This method is a statistical procedure that is primarily a function of well spacing and changes in head among measured points versus the distance between the points. The technique does not address error caused by the aforementioned problems of water table measurements versus measurements in different confined aquifers that subsequently are compared to the output of the single layer isotropic model. It is important in this context to reemphasize the meaning of the word error. This error estimation measure does not take into account the most important sources of error in the data base relative to the requirements of the model. It is a statistical manipulation that has very little meaning in the context of the extent to which the model results match the hydraulic head data base. It is for this reason that errors of the following type are cited in the document under review as being most important (page 25). "Areas of greatest error occur in mountainous regions where well data are <u>most deficient</u>; here the hydraulic head may be in error by more than 100 m." "Where farming activity has <u>increased the number of wells</u> as in the Pahrump Valley, Sand Spring Valley, and the Armogosa Desert, the hydraulic head error is reduced to 30 m. The regional hydraulic head uncertainty near Yucca Mountain exhibits an intermediate error between 25 and 75 m." It is my considered opinion that this type of error is not the major source of error that should be considered when evaluating the results of the model output.

The major source of error that should be considered most important consists of the transfer of a combination of water table measurements, undifferentiated confined aquifer measurements, and composite water level measurements to a single aquifer in the model wherein the aquifer is confined and isotropic and consists of only a single layer. It is essential that the reader understand the distinction between these two types of errors in order to put the model output into proper perspective.

As stated above, two of the required inputs to the model consist of the elevation of the top and bottom of the aquifer. Neither of these elevations is known. In order to circumvent this requirement, the document under review uses transmissivity rather than permeability as the hydraulic property for adjustment to match head values; but transmissivity is the product of hydraulic conductivity and saturated thickness. In this case, the saturated thickness is the entire thickness because the model requires the assumption of confinement. Page 25 of the document under review justifies this manipulation by the following statement, "Since the purpose of this hydrologic model is to determine flux, the use of transmissivity does not present a problem." Strictly speaking, this statement is correct, but it is clear that the ultimate purpose of this modeling effort is not restricted to the determination of flux. The evidence for this conclusion, as discussed previously, is presented in the introduction to the document. To repeat, the introduction states (page 1) "In particular the regional hydrologic model can be used to establish the boundary conditions for a more detailed local model of the site and can be used to predict the following: ground water flow paths, ground water discharge points, subsurface flux, pluvial climate effects, and man-influenced effects." With the possible exception of subsurface flux, virtually all of these determinations would require the use of permeability rather than transmissivity as the critical hydraulic property. Thickness of the aquifer system certainly would affect the use of the model output "to establish the boundary conditions for a more detailed local model of the site."

Recharge and discharge to the model are discussed on pages 27, 28, and in appendices A and B. The nature of these calculations is somewhat beyond the area of this reviewer's expertise; consequently, I do not choose to comment beyond the statement made previously to the effect that it appears that the recharge and discharge calculations are about as defensible as they can be under the constraints of the existing data base. This type of calculation must always be considered approximate, especially over such a large area wherein elevation varies over a large range.

Page 31 of the document under review states that "model calibration involves adjusting of transmissivities within reasonable limits in order to minimize the difference between the hydraulic heads simulated by the model and hydraulic heads measured at well locations. The transmissivity distribution that introduces heterogeneity into the isotropic, single-layer, confined model is presented in figure 11 of the document. The document does not provide information about the process whereby transmissivity values were assigned to different blocks other than to say that "initial estimates of transmissivity for the regional model were taken from the USGS regional hydrologic model prepared by Wadell in 1982." The decision making process via which adjustments were made from these initial inputs in order to approximate model output head data is not described in the paper. Consequently I am not able to comment on the assignment of transmissivity values for head matching purposes.

It is interesting to note that the entire Yucca Mountain block is assigned a homogeneous, isotropic transmissivity value of less than 10 m^2/day. It is of interest to compare this assigned transmissivity value with that obtained by Moench (1984) by the application of a dual porosity model to drawdown data from wells UE-25B#1 (pumping well) and UE-25A#1 (observation well). Moench calculated the permeability of the fracture system in the welded tuffs to be 1.157 m/day. He concluded on the basis of a borehole flow survey that 400 m of aquifer were contributing water during the pumping test. These numbers translate to a transmissivity value of 4.63×10^2 m^2/day. Moench also calculated hydraulic properties of nonfractured portions of the borehole; these values are lower but presumably the fracture system would constitute the aquifer that controls flow on a regional scale as portrayed by the steady state model in the document under review. If one accepts the 400 m figure for aquifer thickness and if one accepts the fact that the fractured aquifer controls the regional flow system, then one would argue that the transmissivity of the Yucca Mountain block in figure 11 in the document under review should have been about two orders of magnitude higher than that shown. If the value of permeability calculated by Moench is multiplied by the entire saturated thickness beneath Yucca Mountain to obtain the transmissivity of the Yucca Mountain block (as required by the assumptions in the model), the number would be two or more orders of magnitude higher yet, depending on how one defined the saturated thickness. The point of this discussion is that if the results of this model were in fact used to define boundary conditions for a smaller hydrologic model around Yucca Mountain, those boundaries would be in error because the transmissivity assigned to Yucca Mountain itself is too low, if the results of the aforementioned pumping test are in fact valid. U.S. Geological Survey Water Resources Investigations Report 83-4032 also provides supporting data to the effect that the fractured aquifer portion of the Yucca Mountain block has transmissivity greater than that shown in figure 11 of the document under review. These data are the results of pumping tests performed on test well USWH-1. The analytical methods used to derive the transmissivity values were the Theis equation and the Jacob straight line solution. A dual porosity model was not considered in these derivations. The transmissivity of the most permeable zones in the Prow Pass Member range between 154 and 183 m^2/day. This reasoning again assumes that the flow through the regional model would be controlled by the most permeable portions of the fractured aquifer system rather than the low permeability portions.

The absence of a discussion of the procedure whereby transmissivity values were assigned to the blocks shown in figure 11 of the document under review precludes comment on how these differences might be explained. The most obvious explanation is that the Yucca Mountain block and probably the other blocks shown in figure 11 of the subject document do not behave hydraulically as a single layer as required by the model. All the data available in the USGS reports of investigation suggest that the Yucca Mountain block behaves as a heterogeneous block wherein transmissivity varies by several orders of magnitude in the vertical dimension. The borehole flow surveys alone that have been conducted on wells in the Yucca Mountain block justify this conclusion. In this particular type of hydrogeologic environment, transmissivity may not be a very useful term because the thickness of the fracture portions of the aquifers that control flow varies by orders of magnitude. Consequently the application of models such as those utilized in the document under review may lead to very erroneous results even if the determination of flux alone is the primary objective of the modeling effort.

Statements in the text of the document under review indicate that the writer of the document is aware of some of the shortcomings and the limitations of the modeling effort. These limitations are caused in large part by the fact that the model simply does not simulate the hydrogeologic environment that is known to exist near the Yucca Mountain site on the basis of borehole flow surveys, borehole geophysical logs, and pumping tests. The output of the model is controlled to a large extent by this deficiency and by the assignment of hypothetical boundary conditions as initial input to the model. In order to alleviate some of the uncertainties that are inherent in this approach, the author of the subject document recommends the following as procedures that might improve the reliability of the model.

A. Calibrating the model under unconfined conditions.

B. Incorporating the latest USGS measurements of hydraulic head into the hydrologic model.

C. Analyzing well logs of the 240 wells considered in the study and incorporating only the reliable hydraulic head measurements and aquifer tests into the model.

D. Calibrate the model with a statistical parameter estimation technique that minimizes the difference between predicted and observed hydraulic heads and estimates the uncertainty in the predicted hydraulic heads and calibrated transmissivities.

E. Construct a three-dimensional hydrologic model consisting of two layers. The top layer would represent the alluvial and volcanic aquifers and the bottom layer would represent the carbonate aquifer. Such a three-dimensional model would more accurately simulate the physical system, particularly where vertical flow occurs. Analysis of well logs and keying the hydraulic heads and aquifer tests to specific hydrostratigraphic units would allow construction of a three-dimensional model.

These suggestions are all reasonable but they are not sufficient to authenticate the reliability of results of a reconstructed model. The major limitation lies in the fact that a two-layer model also would not simulate the real hydrogeologic environment that is evidenced by borehole geophysical logs and borehole surveys near the Yucca Mountain site. These data suggest that the aquifers at the site are fracture controlled and that they are not horizontal. They also are not restricted to two layers. None of the data available to date suggests that hydraulic continuity exists among high permeability fractured units in the horizontal plane near the Yucca Mountain site. If such layers do exist, it is essential that field data be obtained that authenticates their existence in order for the assumptions required by a two-layered or even a three-layered model be satisfied. The list of recommendations on pages 39-40 of the subject document needs to be lengthened by the addition of an item which prescribes a field investigation that will provide evidence for the existence of whatever hydrogeologic framework is selected for modeling. It is not reasonable to launch into a two-layer modeling effort without ascertaining that two layers exist in the study area. Without such an investigation that documents field conditions, this follow-up modeling procedure, if implemented, would constitute the classical case of the model dominating the prototype.

Recommendations

The principal recommendation of this reviewer is that the results of this model not be used for purposes of performance assessment of the vicinity of the Yucca Mountain site. The model clearly is too simplistic and based on too limited a data base for its results to be considered valid. The assumptions required by the model are not compatible with most of the hydraulic property data base in the vicinity of Yucca Mountain. This statement applies particularly to the model requirement that homogeneity exists throughout the hydrogeologic section in the Yucca Mountain block. Pumping tests and borehole flow surveys from wells in the vicinity of Yucca Mountain make quite clear the fact that permeability varies in the vertical dimension in the tuffs by at least four orders of magnitude and that producing zones are distributed unevenly throughout the length of boreholes. Under these conditions it is not defensible to identify boundaries for a smaller model from the output of this model or from the output of a double layer model that is suggested as a follow-up study by the author of the document under review. It also is not defensible to accept the flux values produced by the model as valid. These flux values in essence are a consequence of the assignment of boundary values at the recharge boundaries and the discharge boundaries of the model. The assignment of such values, as I understand the model, determines to a large extent the underflow entering the model on the north and east boundaries. According to the text of the document under review, the assignment of these boundary values is based on topography of the various mountain ranges rather than on potentiometric measurements in the aquifers themselves (as opposed to aquifer itself).

The primary concern of this reviewer is that this model or a succeeding two-layer model will be used for performance assessment purposes at the Nevada Test Site. This fear is based primarily on the following statement presented on pages 39-40 of the document under review. That statement is: "The model-predicted hydraulic head distribution presented in figure 12 indicates that PNL has a working regional model of the Nevada Test Site. Water balances within the model region indicate that calculated estimates of recharge and discharge are in good agreement with published values." In reality, it is not possible to conclude that the model under review herein constitutes a <u>working regional model</u> of the Nevada Test Site. As explained above, field data collected from the Yucca Mountain block alone suggest that transmissivity varies over at least four orders of magnitude and that permeability is by no means uniform in the vertical dimension as assumed in this model. It cannot be overemphasized that it is not justifiable to conclude that this is a defensible working model of the Nevada Test Site.

This concludes my review of the documents addressed in your letter of October 17, 1984. If you have any questions, please call.

Sincerely,

Roy E. Williams
Ph.D. Hydrogeologist
Registered in Idaho

REW:sl

cc: GeoTrans

SAND 84-0192

WMGT DOCUMENT REVIEW SHEET

FILE NO:

DOCUMENT: Effect of Host-Rock Dissolution and Precipitation on Permeability in a Nuclear Waste Repository in Tuff.

REVIEWER: Williams and Associates, Inc.

DATE REVIEW COMPLETED: December, 1984

BRIEF SUMMARY OF DOCUMENT: DATE APPROVED:

This report constitutes the results of an investigation (mathematical model) that was conducted to determine whether thermally induced, host-rock mineral dissolution and precipitation processes could decrease the isolation capability of the potential high-level nuclear waste repository in tuff by significantly altering the permeability of the formation. The report under review describes the modeling rationale and conservative assumptions used to predict the effects of rock dissolution and/or mineral precipitation. The effects of porosity changes due to rock dissolution and/or mineral precipitation were calculated as a function of time, depth, emplaced waste power density, and water flux for both matrix and fracture flow.

The purpose of the investigation was to evaluate the effect of thermally induced dissolution and precipitation of the host rock on alterations of the hydrologic properties of the tuffs at Yucca Mountain to determine whether the proposed site satisfies the isolation-related DOE siting guidelines (960.4-2-3) (U.S. Department of Energy, 1984).

For the purpose of this investigation, the repository horizon was assumed to be at a constant depth of 390 m below the land surface. This hypothetical repository would be contained in a thick ash flow section of the Topopah Spring unit that is densely welded, relatively nonporous, highly fractured, and highly transmissive. Below this layer is a relatively thin, densely welded, vitric layer, underlain by a thick interval of nonwelded, highly porous, but relatively unfractured and nontransmissive argillic and zeolitic bedded and ash flow tuffs. The hypothetical repository located at 390 m would be within the unsaturated zone with a thickness of approximately 500 to 600 m. The primary purpose of the investigation was to evaluate whether heating and subsequent cooling of recharge water could induce host rock dissolution and precipitation, which, in turn, could change the local permeability of the tuff layers. According to the report under review, the effective vertical unsaturated hydraulic conductivity of the tuff layers appears to be sufficient to allow all of the recharge water to flow through without saturating the formation; any net rock dissolution would only further increase the effective vertical unsaturated hydrualic conductivity and thus would have a negligible impact on water flow characteristics. Decreases in permeability due to mineral precipitation could potentially affect the isolation characteristics of the host rock by causing the rock to saturate. These two changes could potentially increase radionuclide release rates from the waste package and decrease radionuclide travel time. According to the report under review, after consideration of these factors, the most important aspect of the investigation was to determine whether any significant decreases in permeability could occur. Because of this fact, the approach used in the investigation was to place bounds on the effect on permeability by using assumptions that lead to conservatively high estimates of matrix in fracture porosity changes. Information and justification for the approach used in the investigation are presented in the following three subsections of the report: 1) Identification of the Controlling Mineralogy, 2) Environmental Effects on Amorphous Silica Solubility, and 3) Temperature Distribution.

Identification of the Controlling Mineralogy

The potential repository horizon within the Topopah Spring Member of the Paintbrush Tuff is composed primarily of alkali and plagioclase feldspars and several forms of silica (SiO_2) which include quartz, cristobalite, and tridymite. Minor mineralogic constituents include mica, clay and Fe-Ti oxides. The analysis of the dissolution and precipitation of minerals contained within Yucca Mountain was simplified by assuming that the ground water always maintains saturation with respect to amorphous silica. According to the report under review, this approach is justified for the following reasons: 1) The mineralogy can be described as consisting of two major phases: feldspars and silica polymorphs. The quantity of these phases that will dissolve depends on the ground water chemistry, the temperature and pressure, leach kinetics, and the amount of reaction time. The kinetics of some silica reactions are so slow that equilibrium with a solution is thought to be unattainable on a laboratory time scale. However, from a dissolution standpoint assuming that equilibrium can be achieved allows one to estimate the maximum quantity of material that can be dissolved for a given temperature, pressure, and solution composition. 2) Some published descriptions of sandstones that have undergone diagenesis and/or pressure solution suggests that quartz is more susceptible to dissolution in precipitation than are feldspars. Other investigators have observed strong dissolution of both feldspars and quartz. Thus, the amorphous-silica assumption is more conservative than the assumption that the ground water maintains saturation with respect to the feldspars, since feldspars must precipitate whenever the silica concentration exceeds 0.0006 mole/L. 3) A comparison was made between the quantity of rock dissolved experimentally under isothermal conditions and a prediction using the amorphous silica assumption under similar conditions. Wafers of Topopah Spring core were submerged in representative ground water and heated to 150 °C for various periods of time up to a month at the Lawrence Livermore National Laboratory. Most of the weight loss occurred during the first two weeks. The weight loss observed after one month was 1.4%. The weight loss calculated for similar conditions using the amorphous silica solubility equation was 1.8%. This result demonstrates the conservative nature of the model. 4) Numerous experimental studies have shown that the solubility of amorphous silica is approximately two to four times that of cristobalite and four to 19 times that of quartz for temperatures up to 200 °C. According to the report under review, the following three boundary assumptions produced conservative results such that the potential for reducing permeability beneath the repository horizon is maximized: 1) silica concentrations in ground water are determined by equilibrium saturation with amorphous silica, 2) cristobalite is the solid phase contributing most of the silica to the ground water, 3) amorphous silica is the solid phase precipitating from cooling ground water.

Environmental Effects on Amorphous Silica Solubility

Several studies have found that the presence of moderate quantities of cations such as sodium, potassium, calcium and magnesium either has no effect or decreases amorphous silica solubility. Silica solubility is not affected significantly by changes in pH at moderate values for pH (4 to 9). The effects of pressure and temperature have been studied extensively. All the studies have shown that silica concentrations in water increase with increasing temperature, where the dissolving solid is quartz, silica glass, amorphous silica, or granite. Previous studies have found that pressure has a slight to negligible effect on solubility.

Temperature Distribution

Dissolution and precipitation of the host rock would be driven by temperature changes produced by the emplacement and decay of several radionuclides contained in the high level wastes. A thermal mechanical study was completed recently in which the temperature distribution as a function of time along the vertical center line intersecting the repository area was predicted for two different areal power densities. This far field analysis assumed that the spent fuel was uniformly distributed throughout the repository at a depth of 390 m below the surface. According to the report under review, use of the temperature distribution along the center line is again a conservative approach since it includes both the maximum absolute temperatures and the maximum temperature gradient.

According to the report under review, some portions of the rock will heat up for some time to temperatures that exceed 100 °C. Since the proposed repository would be in a highly fractured, unsaturated zone, atmospheric pressure will not, in general, be exceeded. Therefore, the water in these high temperature regions could vaporize, and the rock could dry out. In some of the evaluations conducted in this investigation, water vaporization was included to determine whether the precipitation of the solids initially dissolved in water, because of the geothermal gradient, could cause a significant decrease in permeability. A number of evaluations were made in which this dry out possibility was ignored and temperatures in the aqueous phase were allowed to exceed 100 °C. According to the report under review, this latter approach was initially viewed as probably being conservative because temperature has an important influence on silica solubility and thus on the quantity of rock that dissolves and subsequently precipitates.

Model

A Fortran computer program was written to predict the temperature distribution, as a function of time and position, the corresponding amorphous silica solubility, the incremental quantity of silica dissolved or precipitated, and the cumulative change in porosity. The effects of water flow rate, initial rock porosity, power density, and time on the porosity change were evaluated. The hydraulic system of Yucca Mountain was simulated by dividing the 600 m of rock along the vertical center line of the repository into six stratigraphic units. It was assumed that the initial matrix porosity of each of the units was constant and uniformly distributed.

Results for Constant Porosity

The effect of a number of parameters on the cumulative change in porosity was first calculated assuming that only matrix flow occurs and that a single initial matrix porosity exists throughout the entire unsaturated zone being studied. A case with a 57-kW/acre (14 W/m²) spent fuel gross thermal loading, 0.5 mm/yr water percolation rate, 100-% pore saturation, no water vaporization, and 12% matrix porosity was considered to be the base case with which most comparisons were made.

The effect of time on the cumulative porosity change for the base case conditions is shown in figure 5 of the report under review. All of the evaluations in which water percolation rate, matrix porosity, and thermal conditions were varied produced similar profiles. The maximum dissolution occurs at the point of highest temperature (the repository horizon) and decreases with increasing time. According to the report under review, the following results are particularly worth noting: 1) the cumulative porosity changes are extremely small, 2) net porosity decreases did not occur.

The effect of assuming a different initial matrix porosity is shown in figure 7 of the report under review. The base case initial porosity of 12% was changed to 33%. Figure 7 of the report under review shows that the magnitude of the porosity change is directly proportional to the difference in the initial matrix porosity. The effect of percolation rate in pore saturation on cumulative porosity change is shown in figure 8 of the report under review. As shown in figure 8, the effect of percolation rate under the assumed conditions is limited. Acccording to the report under review, the lack of effect probably results because the quantity of solids transported between areas is dominated by temperature differences and not by the actual flow of water. A decrease in saturation has the same effect as reducing the initial matrix porosity.

Figure 9 of the report shows the effect of higher temperature (due to increased power density) on the cumulative porosity increase. Higher rock temperatures increased the magnitude of the porosity changes. The effect of allowing water to vaporize and therefore the rock to dry out is shown in figures 10, 11, and 12 of the report. According to the report under review, regions in which cumulative porosity changes were negative occurred only when the water was allowed to vaporize.

Results for Variable Matix Porosity

The effect of time on the change in porosity for the two areal power densities being considered is shown in figures 13 and 14 of the report. According to the report under review, the deviation in the general shapes of the responses shown in figures 13 and 14 compared to the results for constant porosity is due to the fact that higher initial matrix porosity values decrease the quantity of rock with which a given volume of water can interact.

The effect of percolation rate on the cumulative porosity change for matrix flow conditions is shown in figure 15 of the report. According to the report under review, the impact of percolation rate under the currently expected conditions of matrix flow is not significant.

Results for Permeability Changes

Peters and Gauthier (1984) showed that matrix flow should dominate the hydraulic system for all of the unsaturated units beneath Yucca Mountain. Assuming this is correct, most dissolution and precipitation reactions should occur within the pores. According to the report under review, using the largest observed relative increase, the initial 15% matrix porosity would increase to 15.0016%. The largest observed cumulative decrease would change the initial 12% matrix porosity to 11.9988%. These small calculated effects would be undetectable among naturally occurring variations.

According to the report under review, fracture flow was only studied in the Topopah Spring unit because these are the only units in which a net precipitation of silica occurred; the change in permeability is affected by initial fracture aperture, the fracture density, and the volume of material dissolved or precipitated. Scott et al. (1983) indicate that fracture densities range from approximately 16 to 32 fractures per meter in densely welded tuffs and about 7 fractures per meter in the vitrophyre of the Topopah Spring. According to the report under review, apertures of these fractures have not been measured; it was assumed, based on the work by Klavetter (1984), that hydraulic apertures will range from 5 to 50 um. According to the report under review, since equivalent hydraulic apertures are smaller than actual geometric apertures, the porosity change described will have a larger relative effect using this assumption.

According to the report under review, since fluctuations in the flow rate great enough to exceed the conductivity of the fractures are unlikely, the fractures should be able to transmit all water from above that penetrates the matrix. Figure 16 of the report shows the porosity changes for the matrix flow as well as for fracture flow with two different fracture porosities. The report under review points out correctly that material precipitated in the fractures will decrease conductivity to a more significant extent than the same quantity of precipitate would decrease matrix conductivity.

According to the report under review, the maximum precipitation of material occurs when the water vaporizes, and this vaporization would have the largest effect at the repository horizon. Precipitation would cause a reduction in the fracture aperature which according to the report under review would reduce the hydraulic conductivity of the fractures by about 70%. The results of the model show that under the assumed maximum fracture flux of 4 mm/yr, and an initial fracture hydraulic conductivity of 66 mm/yr, a 70% decrease in the fracture hydraulic conductivity to approximately 21 mm/yr will not prevent the fractures from transmitting all of the available water. Dissolution within the fractures will increase the hydraulic conductivity of the fracture system. However, according to the report, since even the initial fracture conductivity is greater than that necessary to transmit the anticipated water flux, this increase will not have a significant impact on the flow patterns.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

Significance in EAs

Reference to the report under review occurs on page 6-186 in Section 6.3.1.3 Rock Characteristics--under subheading Evaluation of Host Rock Permeability Changes. The results of the report under review are used in the EA to support the contention that flow rates through the porous matrix in fractures due to potential porosity/permeability changes are not significant.

The report under review constitutes the primary source of information pertaining to potential mineral dissolution and precipitation due to heating and subsequent cooling of ground water as it flows through the host rock. The report evaluates the potential changes in permeability due to mineral dissolution and precipitation. The magnitude of changes in permeability that would adversely affect isolation have not been identified. The report under review is the primary source of experimental data pertaining to potential porosity/permeability changes due to heating in the vicinity of the repository.

PROBLEMS, DEFICIENCIES, OR LIMITATIONS OF REPORT:

The report under review presents fairly strong evidence that increases or decreases in matrix and fracture porosity due to mineral dissolution and/or precipitation is insignificant for the experimental conditions. The analysis of the dissolution and precipitation of minerals is simplified by making the following assumptions: 1) Silica concentrations in ground water are determined by equilibrium saturation with amorphous silica (mass of rock dissolving and subsequently precipitating), 2) cristobalite is the solid phase contributing most of the silica to the ground water (volume of silica dissolving), 3) amorphous silica is the solid phase precipitating from cooling ground water (volume of silica precipitating). According to the report under review, these three bounding assumptions produced conservative results in that the potential for reducing permeability beneath the repository horizon was maximized.

SUGGESTED FOLLOW-UP ACTIVITY:

REFERENCES CITED:

Scott, R.B., et al., 1983. Geologic Character of Tuffs in the Unsaturated Zone at Yucca Mountain, Southern Nevada. in Mercer, J. (ed.) Role of the Unsaturated Zone in Radioactive and Hazardous Waste Disposal. Anarbor Science, Anarbor, Michigan, p. 289-335.

Klavetter, E.A., 1984. Fracture Hydrologic Property Data. memo to distribution, April 17, 1984.

Peters, R.R., and Gauthier, J.H., 1984. "Results of TOSPAC Hydrologic Calculations for Yucca Mountain". SNL memo to F.W. Bingham, 6312, April 30, 1984.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND84-0369

DOCUMENT: Vadose Water Flow Around A Backfilled Drift Located in Tuff. L.A. Monde, B.L. Baker, R.L. Eaton, Sandia National Laboratory, Albuquerque, New Mexico, July 1985.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: April 30, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

The computer program SAGUARO is used to model flow around vertically emplaced waste containers in tuff. The authors had severe numerical instability problems due to the low values of hydraulic conductivity used for the sand backfill. In our review, however, we suggest that incorrect hydraulic conductivity values were used in the model which may have been part of the problem. The principle recommendation of our review is that the hydraulic properties of the material to be used for backfill be measured and the modeling be repeated with correct properties used as input.

BRIEF SUMMARY OF DOCUMENT:

The computer code SAGUARO for unsaturated flow is used to model flow around vertically emplaced waste containers beneath a drift in tuff. The modeling simulated either sand or clay backfill in the drift. The authors conclude that backfilling a drift does not provide a significant reduction of flow in the vicinity of a vertically emplaced waste package. The proposed tunnels or drifts in the repository will be approximately 5 m wide and 6 m high. The vertical emplacement would consist of a shaft approximately 7-1/2 m long and 1 m in diameter, excavated in the bottom of the drift. The waste canister would fill approximately the bottom 4 m of the hole. The remainder of the shaft would be filled with an impermeable isolating plug. The work under review here was done to determine the effect of backfilling of the drift on the flow past the waste canister. This flow was modeled in a two-dimensional mode using the computer code SAGUARO, recently developed at Sandia Laboratory. A finite element mesh consisting of 234 node points was used for the simulation. The size of the mesh was 15 m across by 135 m in height. The left boundary was at the plane of symmetry through the waste package while the right boundary was through the plane of symmetry between two adjacent waste packages.

Material properties used in the simulation were taken from Mualem (1976) for the clay and sand, and from Gee (1985) for the tuff. The values of saturated conductivity used for the clay and sand are incorrect. The value used for clay was 3.92×10^{-14} m^2 while that for sand was 1.93×10^{-13} m^2. Checking of these values in Mualem shows that the correct values are 2.3×10^{-14} m^2 for clay and 1.31×10^{-11} m^2 for sand. The error in saturated hydraulic conductivity was nearly two orders of magnitude for each material.

There also are errors in the determination of unsaturated flow characteristics. The actual procedure used for calculation of such values is not described but the values of relative conductivity presented differ by as much as six orders of magnitude from comparable values determined by the Brooks-Corey relationships. The Brooks-Corey values of unsaturated flow characteristics for these materials have been verified with laboratory data (King, 1964). These errors may be the reason for problems that were encountered in maintaining a stable numerical solution when sand was used in the drift. Usually sand does not cause numerical instabilities that are as severe as those produced when a material such as clay is used. In the report under review, the numerical difficulty was encountered with the sand because of its low permeability. In a portion of the simulation a fictitious value was used for the conductivity of the sand at high capillary pressures in order to bring about a stable solution. With such gross errors in the input values of conductivity of these materials it is questionable whether the results of the experiment are valid.

The authors state on page 23, "We feel that refining the mesh is the least effective way to overcome the numerical instabilities because the sand permeability can change over seven orders of magnitude with a change of .1 m in pressure head and because the number of elements allowed in SAGUARO is limited to 1,000." This statement is incorrect. The probable intended meaning is that a change in pressure head of one order of magnitude produces a seven order of magnitude change in permeability. Use of the proper values for the hydraulic conductivity of sand probably would have reduced the numerical difficulties.

On page 25, the velocity in the sand is calculated as approximately 1.7×10^{-15} m/sec downward. This calculation is incorrect because the flux rate was not divided by either the moisture content or the degree of saturation multiplied by porosity. Assuming the moisture content is about .1, the velocity should be about 1.7×10^{-14} m/sec.

Several plots of the pressures in the flow field around the drift and waste emplacement area are presented. Plots of velocity in the flow region are presented also. Although the actual values are suspect due to the problems discussed above it is doubtful that correct values of conductivity for sand and clay would change the flow patterns significantly. We recommend, however, that the actual material to be used for backfill, such as finely crushed tuff or coarsely crushed tuff, be compacted and tested in the laboratory to determine the correct hydraulic characteristics for these materials. The current experiment (modeling) could then be repeated with correct hydraulic characteristic values; this procedure would increase the credibility of the experiment (modeling).

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The water flux through the actual waste canister should be determined to facilitate the prediction of post emplacement travel times to the accessible environment. Modeling of unsaturated flow around the canister is the first step in the determination of flux. This determination is required for evaluation of compliance with the EPA standard (40CFR191).

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The most serious problem with the work under review is the erroneous values of hydraulic conductivity used for simulating pressure distribution in and flow through the backfill material. These errors probably produce the severe numerical instabilities encountered during the simulation.

SUGGESTED FOLLOW-UP ACTIVITIES:

This experiment should be repeated using correct hydrogeologic parameter values, after experiments have been conducted to obtain defensible properties of backfill materials.

REFERENCES CITED

Gee, G.W., 1985, Laboratory Report on the Unsaturated Flow Characteristics of Core Samples from the Nevada Test Site Well USW-GU3 (NTS). Draft Letter Report Prepared for Sandia National Laboratories by Pacific Northwest Laboratory, Richland, Washington.

King, L.G., 1964, Imbition of Fluids By Porous Solids. Colorado State University, Ph.D. Thesis.

Mualem, Y., 1976, A Catalog of the Hydraulic Properties of Unsaturated Soils. Hydrodynamics and Hydraulic Laboratory, Technion Israel Institute of Technology, Haifa, Israel, Research Project 442.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND84-0747

DOCUMENT: FEMTRAN-A Finite Element Computer Program for Simulating Radionuclide Transport Through Porous Media. M.J. Martinez, Sandia National Laboratories, Albuquerque, NM, January 1985.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: May 28, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E Williams

FEMTRAN is a finite element computer code for numerical simulation of two-dimensional transport of radionuclide decay chains through saturated/unsaturated absorbing porous media. The program requires input of a velocity field from either of the programs FEMWATER, MARIAH, or SAGUARO. Several optional solution schemes are used in operation of the program. The program is designed for the Cray 1S computer. Comparison of simulation results with analytical results show excellent agreement.

BRIEF SUMMARY OF DOCUMENT:

FEMTRAN is a finite element computer program for numerical simulation of two-dimensional transport of decaying radionuclides through saturated/unsaturated adsorbing porous media. The transport mechanisms considered include advection, hydrodynamic dispersion, diffusion, equilibrium and adsorption and radioactive decay and evolution. The resulting equations are solved by the method of weighted residuals and the finite element method. The ordinary differential equations are integrated in time by standard finite difference methods such as Crank Nicholson, backward difference or central difference. In formulating the governing equations for radionuclide transport the Darcian velocity field is assumed to be a known input. FEMTRAN requires the computation of Darcian velocities from the programs FEMWATER, MARIAH or SAGUARO which are then used in the transport equations.

A large number of alternate numerical schemes are in use for the operation of the program. These schemes are Crank Nicholson backward difference, mid difference, two different systems of weighting functions, the Galerkin, and upstream and mass matrix lumping may or may not be used. The authors present limited user instructions. The program is designed to be used on the Cray 1S computer at Sandia National Laboratory. The authors present several sample problems for comparison with analytical results. The comparison shows excellent agreement. User instructions are brief but probably are sufficient for a person familiar with the Cray computer and with similar numerical programs.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

This program appears to be useful for determining the travel time to the accessible environment if the solution for water flow velocity is available, and if the actual water travel times are large enough that the time for adsorption and decay is not significant.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The most significant limitation appears to be the necessity for having a solution to the hydrodynamic equations before using the program.

SUGGESTED FOLLOW-UP ACTIVITIES

No follow-up is necessary.

WMGT DOCUMENT REVIEW SHEET

FILE #:

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A large number of alternate numerical schemes are in use for the operation of the program. These schemes are Crank Nicholson backward difference, mid difference, two different systems of weighting functions, the Galerkin, and upstream and mass matrix lumping may or may not be used. The authors present limited user instructions. The program is designed to be used on the Crav 1S computer at Sandia National Laboratory. The authors present several sample problems for comparison with analytical results. The comparison shows excellent agreement. User instructions are brief but probably are sufficient for a person familiar with the Crav computer and with similar numerical programs.

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PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The most significant limitation appears to be the necessity for having a solution to the hydrodynamic equations before using the program.

SUGGESTED FOLLOW-UP ACTIVITIES

No follow-up is necessary.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND84-0878

DOCUMENT: PETROS--A Program for Calculating Transport of Heat Water, Water Vapor and Air Through a Porous Material. G.R. Hadley, Sandia National Laboratories, Albuquerque, NM, May 1985.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: April 30, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E Williams

This program calculates transport of water, water vapor, inert gas, such as air, and heat through a partially saturated porous medium. Gas transport includes effects due to Knudson diffusion and binary gaseous diffusion of each gas component, plus Darcian flow of the gas mixture. The expression used for gas permeability is incorrect which casts some doubt on the validity of the program, particularly at medium values of degree of saturation. A description of the model assumptions is presented; the resulting equations together with numerical techniques used to obtain problem solutions are presented also. Instructions are included for running the program along with a sample problem output.

BRIEF SUMMARY OF DOCUMENT:

This code originally was written to study transport of water and water vapor in the inner region of a nuclear waste repository. In repositories located above the water table movement in all three phases (air, water and water vapor) may be important. In addition, the treatment of the binary gas system includes effects due to Darcian flow as well as Knudson diffusion of each gas species into the other. This more complete treatment of the gas phase was motivated by the need to handle transport in a tight geologic material which displays a small average pore size. Heat transport includes conduction, convection by all three phases and latent heat effects. The transport equations, except for the heat equation, have been written in integral form and then differenced on a stationary Eulerian grid. This procedure allows the solution of problems with extremely steep saturation gradients.

Differencing in time is fully implicit and uses a predictor-corrector scheme to handle the nonlinear terms. Provisions are made for the inclusion of several user defined properties such as capillary pressure, relative permeability, and thermal conductivity. Surface tension effects are presented so that pressure effects as well as saturation and temperature effects are included. Hysteresis is not included. The program is listed as one-dimensional; however, it is either one dimension in a plane, in a cylinder or a sphere. The mesh which is used for the discretization is simply a line with points I, I-1, I+1, etc. All primary variables such as vapor pressure, air pressure, saturation, and temperature are defined at node points while all fluxes are defined at the mid node points. These lines represent the boundary of a control volume with the node point at the center.

Transport equations are integrated over the control volume. In most of the equations all variables are continuous. However, at interfaces between materials, degree of saturation will be discontinuous because different materials have different capillary pressure-saturation curves. This discontinuity is handled numerically by defining degree of saturation at the interface node as an arithmetic mean of the discontinuous values. This procedure makes possible the determination of capillary pressure at the interface in terms of the two saturations across the interface. Capillary pressure itself is a continuous function. The time step procedure for this program is quite complex because the strong nonlinear coupling between equations together with possible nonlinear boundary conditions makes any simple procedure inadequate to prevent numerical oscillation.

The reason behind this procedure is to obtain estimates of the advanced variables to use for nonlinear terms so as to dampen numerical instabilities.

The program has a mesh generation scheme which involves a ratio of the spacing between nodes. Between adjacent nodes it is controlled between .8 and 1.25. Internally supplied routines determine the viscosity of water, the saturation vapor pressure of water, the Knudson diffusion coefficient, binary diffusion coefficient, liquid and gas relative permeabilities, capillary pressure, and thermal conductivity. All these appear to be standard except the relationship for gas relative permeability. The gas phase relative permeability is equated to one minus the liquid relative permeability. This procedure is not correct because gas permeability plus liquid permeability is not equal to one. Such an error appears to be a very serious problem with the program except when the medium is completely filled with gas or with liquid.

The program solves a set of coupled nonlinear equations. No comparison with analytical solutions is presented as a complete problem. The various parts of the program can be checked with analytical solutions for heat transfer and liquid mass transfer separately. When such a comparison was made the errors in all cases were less than 2 percent.

The user instructions and documentation for the program are brief but they probably are adequate for a person who is already familiar with the CDC 7600 computer system. In cases where the material properties are not available in functional form, a data table may be used in the program and a quadratic interpolator program is used to evaluate the material properties. An option also is available for using a spline fitting routine available from math libraries. A spline fit equation has the advantage of having a continuous first derivative. The program appears to be satisfactory except for the incorrect method of determining the relative permeability for the gas phase.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The program is a contribution toward the simulation of water vapor and heat movement in Yucca Mountain. Correct analysis of these phenomena is necessary to predict the flux of water through the repository and the resulting travel time to the accessible environment.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The program is limited to one dimensional flow and the calculation of gas permeability is related incorrectly to liquid permeability.

SUGGESTED FOLLOW-UP ACTIVITIES

The program should be revised with a correct method of determining the gas permeability.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND84-1076

DOCUMENT: Ortiz, T.S., and others, 1985, A Three-Dimensional Model of Reference Thermal/Mechanical and Hydrological Stratigraphy at Yucca Mountain, Southern Nevada. Sandia National Laboratories, Albuquerque, NM, and Livermore, CA, SAND84-1076, 72 p.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: July 16, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

The report under review presents a discussion of a three-dimensional model of the thermal/mechanical and hydrogeological reference stratigraphy at Yucca Mountain. The reference stratigraphy is based on porosity and grain density. The model consists of a set of surface representations. Sixteen reference units and one mineralogical surface have been defined. The primary purpose of the model is to assist in the interpolation of the stratigraphy among data points (drill holes). The model is shown to be a powerful tool; however, the limited data base constrains the usefulness of the model at the present time.

BRIEF SUMMARY OF DOCUMENT:

The purpose of the report under review is to present a geometric representation of the rocks at Yucca Mountain. The intent of the report is to use the geometric representation along with associated material properties in the performance assessment and repository design calculations. The stratigraphy used in the model presented in the report is based on porosity and grain density. According to the report, the stratigraphy can be correlated to thermal, mechanical, and hydrogeological properties.

The geometric model presented in the report consists of a collection of three-dimensional surface representations. A separate surface is used to define the base of each thermal/mechanical and hydrological reference unit. The model incorporates a method of analytically interpolating among sparse and irregularly spaced data. According to the report, the method generates a single, continuous analytical surface equation from a collection of three-dimensional coordinates.

An example of the development of a three-dimensional model is shown schematically in figure 3 of the report. The example shown in figure 3 illustrates the results of combining the method of generating an analytical surface equation with information on the location of faults. In this example pre-faulted coordinates of units were used as input data to obtain pre-faulted surfaces. The set of equations used to represent the pre-faulted surfaces is then combined interactively with the fault information.

The report notes that the actual surfaces were assumed to be smooth and continuous when originally formed; deviations from the smoothed surfaces, such as erosion features, or igneous structures cannot be assessed in the model. The report notes also that contrary to the earlier three-dimensional model by Nimick and Williams (1984), locations of pinch-outs are predicted by the model.

For the purpose of the model sixteen reference stratigraphic units have been defined. A description of these units is presented in table 1 of the report. According to the report, in addition to the reference stratigraphic units, the upper level of prevalent zeolites has been modeled as a surface.

Data sources for the model consisted of drill hole locations, lithologic logs, geophysical logs, physical properties, X-ray analyses, gyroscopic surveys. The x, y, and z coordinates input into the model are based on surface positions of drill holes. According to the report, at Yucca Mountain the x and y coordinates are defined in Nevada state plane coordinates; the z coordinates are the absolute elevations above mean sea level for the prefaulted units. All coordinates are presented in feet.

According to the report, a structural block containing drill holes USW G-1, USW G-3, USW GU-3, USW H-3, and USW H-4 was selected as a reference region. This region was assumed to be unfaulted and all fault offsets were determined relative to this block. According to the report,

> three assumptions were made about the faulting at Yucca Mountain: 1) the assumed offset along known faults does not change with depth along the fault; 2) the dip of the fault does not change at least to the maximum depth of interest; and 3) no faults exist at Yucca Mountain other than those mapped.

Tables B-1 through B-12 in Appendix B of the report summarize the input data obtained from drill holes. Table B-13 lists the dates on which surveys for each drill hole were made. Table B-14 lists the faults used to adjust the input data, along with the vertical offset and apparent dip estimated for each fault. Figure 4 of the report shows the location of faults, drill holes, and cross sections discussed in the report.

Evaluation of the reliability of the reference stratigraphy model consisted of the comparison of four cross sections from the model to a geologic map, cross sections, and interpretations presented by Scott and Bonk (1984). According to the report, locations of surface outcrops agree within 40 feet (vertical) and thicknesses were consistent.

Figure 9 of the report is an isopach map of the Topopah Spring welded unit. The model predicts a zone of thickening in the west central portion of the area. This prediction is due to the rapid change in observed thickness between test well UE-25a#1 and test well USW G-4. Figure 10 is an isopach map of the vitrophyre near the base of the Topopah Spring Member. Figure 10 shows that the vitrophyre thins gradually from west to east. The model predicts regions in the eastern portion of the study area where the vitrophyre is absent; the thickness is predicted to be 80 feet at the western edge of the study area. According to the report, the thickness of the vitrophyre probably is less variable than indicated.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The report under review presents a geometric representation of the rocks at Yucca Mountain. The model is an attempt to simulate the stratigraphy in the vicinity of Yucca Mountain based on limited data. The primary use for the model appears to be the interpolation of geological characteristics among data points (drill holes). Thus, the model may prove useful by assisting investigators in interpolating among data points.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The model presented in the report under review may prove to be valuable in the interpretation of the geology in the vicinity of Yucca Mountain. The model is a powerful tool; however, the absence of geological data in three dimensions limits the usefulness of the model significantly. The report notes that the current fault descriptions lack the detail sufficient to automate the removal of fault movement from input data or its reinsertion into calculated surfaces. For this reason the effects of faulting are handled interactively in the model.

SUGGESTED FOLLOW-UP ACTIVITIES

Future additions of the model presented in the report under review may prove to be valuable in the simulation of the geology and hydrogeology in the vicinity of Yucca Mountain. We recommend that all new models be evaluated to determine their significance to the NRC Waste Management Program.

REFERENCES CITED:

Nimick, F.B., and Williams, R.L., 1984, A Three-Dimensional Geologic Model of Yucca Mountain, Southern Nevada. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, SAND83-2593.

Scott, R.B., and Bonk, J., 1984, Preliminary Geologic Map of Yucca Mountain, Nye County, Nevada with Geologic Sections. USGS Open-File Report 84-494.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT: Peters, R.R., Klavetter, E.A., Hall, I.J., Blair, S.C., Heller, P.R., and Gee, G.W., 1984, Fracture and Matrix Hydrologic Characteristics of Tuffaceous Materials from Yucca Mountain, Nye County, Nevada: SAND84-1471 Sandia National Laboratories, Albuquerque, New Mexico 87185 and Livermore, California 94550, for the U.S. Department of Energy.

REVIEWER: Williams and Associates, Inc.

DATE REVIEW COMPLETED: November 1985

BRIEF SUMMARY OF DOCUMENT: DATE APPROVED:

This report concerns the measurement of unsaturated flow properties of the tuffaceous materials from Yucca Mountain, Nevada. Yucca Mountain is composed of tuffaceous formations that must be characterized to estimate the rate at which radionuclides would migrate to the water table. In order to determine the flux of water in the unsaturated zone, the unsaturated flow properties of these materials must be known. Tests were run on 19 samples of tuff taken from drill hole USW GU-3 and 29 samples taken from drill hole USW G-4 on the NTS to determine the hydraulic properties in the pressure range of -10 to -1,000 meters. Direct measurement of unsaturated conductivity was not done since this is extremely time consuming. Capillary pressure water retention data were obtained which allows calculation of the unsaturated conductivity. Four samples of unfractured tuff from drill hole USW GU-3 and five fractured samples taken from drill hole USW G-4 were tested at elevated confining pressures to determine saturated conductivity. This report concerns methods used to obtain these data and methods to analyze the results.

MATERIALS AND METHODS:

Pacific Northwest Laboratories (PNL) performed three types of tests. These included 1) water retention tests, 2) unconfined saturated hydraulic conductivity tests, and 3) confined saturated hydraulic conductivity tests. Micromeritics Instrument Corp.

performed mercury intrusion tests to provide a check on the water retention curves determined by psychrometric measurements. Water retention characteristics were obtained on 48 cylinderical samples. These samples were 1.4 x 1.2 cm (diameter by length) that were subcored from the original core samples. Unconfined saturated conductivity tests were also run in the cylinders as well as saturated conductivities at elevated confining pressures. Unfractured samples which were tested at elevated confining pressure consisted of 5.4 x 1.9 cm (diameter by length) wafers. The criteria for selecting the fractured core samples were that the fracture was natural and met the orientation of the fracture testing.

TESTING METHODS:

All samples were vacuum saturated by standard methods before testing with the thermocouple psychrometer. The psychrometer was used to measure potential of the matrix water in the range of 10 to 10,000 meters of water. Samples were weighed to determine the moisture content. The determination of suction head from psychrometer measurements was by use of a relationship from Campbell (1977) The total water potential was equated to the sum of the osmotic, matric, gravitational, pressure, and overburden potential components. In the unsaturated rock sample, the major component of total potential is the matric potential. It should be noted that the neglect of gravitational potential was only for the laboratory testing of the core and not in general for the tuff.

Mercury intrusion tests were performed on 1.2 cm by 2 cm cylinderical samples by standard testing procedures. The sample was first evacuated and mercury then was forced into the pores under a pressure of up to 60,000 psi. The saturation of the mercury was calculated from the volume that had been intruded. The equivalent head or pressure of water was evaluated from the mercury data. In this calculation surface tension of water was used as 72 dynes/cm. This value, however, is the value for pure water; it may be preferable to use the measured surface tension of the water used in the experiments.

Unconfined saturated hydraulic conductivity was measured by a constant head method. The samples were positioned in a specially built plastic permeameter sealed in place with a silicon rubber compound, then vacuum saturated and allowed to soak for 24 hours before testing. Elevated pressures up to 3 bars were used for this experiment. Fractured samples were tested with a confining pressure and pore pressure of 35 and 30 bars, respectively. A pressure difference was introduced across the sample and flow through the sample was measured by either a flow meter or a piston displacement of the pore fluid supply pump.

EXPERIMENTAL RESULTS:

Complete data from all the experiments are presented in the appendix of the report. These data include porosities, densities, hydraulic conductivities, and the water retention characteristics at various suction heads. In several samples, the porosity was not the same as the total water content at saturation. This discrepancy may be due to inaccuracy of the single grain density measured for that particular sample because of tuff material variability within the sample. The samples also may contain small disconnected pores that could not be saturated. For these reasons the maximum volumetric water content rather than porosity was used as a basis on which to calculate the relative saturation.

The mercury intrusion data and psychrometer data generally agree over the pressure range where both tests are valid. In the few cases, there was disagreement; assumptions made to convert the mercury intrusion data may miss important effects due to sample structure and mineralogy that may be present in some samples and not in others. An equation from Van Genuchten (1978) was used to fit the saturation-suction data because it yields an analytical expression which may be used to calculate the unsaturated conductivity. The calculation process was used for unsaturated conductivities because there is no direct way to measure such low values in a reasonable time period. Saturation data versus suction head data, and experimentally fitted curves are presented for all the various units. The data appear to be more consistent than the fitted curves in some cases. The most striking factor about these data are the extremely high displacement or entry pressure heads. These are all greater than 10 m and many are as high as 80 m. There is good discussion of the various individual sample data. The saturated hydraulic conductivity data are presented in plots of porosity versus the conductivity for each sample in the non-welded vitric tuffs. There appears to be a fairly consistent relationship between porosity and hydraulic conductivity. In most of the other materials there is considerable scatter in the data. In one sample there is rapid loss of conductivity noted in pressures between 50 and 150 bars. This effect was caused by a well developed crack and is consistent with crack closure and deformation with increased pressure. Data from fractured tuff samples are presented as a table of conductivity and calculated aperture widths. These aperture widths were calculated from the cubic law and an empirical equation developed for the relation between effective pressure and the change of conductivity due to pressure.

SUMMARY:

The authors give conclusions which are paraphrased below.

1) The relationship between water content and suction head for each individual sample is unique for the specific core matrix material.

2) A comparison of psychrometric and mercury intrusion data for 22 individual samples indicates the two testing methods give results that are for the most part in good qualitative agreement.

3) The data on water content versus suction head data for the limited number of samples taken from a particular rock group form a reasonably coherent group for comparison of Havercamp and Van Genuchten curve fits of data.

Conclusions for the saturated matrix hydraulic conductivity data are as follows:

1) The nonwelded vitric tuff samples had conductivity orders of magnitude higher than those of either the welded tuff samples or the nonwelded zeolitic tuff samples.

2) As individual groups the nonwelded vitric tuff samples and the welded devitrified samples appear to have a general correlation between the porosity and the hydraulic conductivity.

3) The reduction in conductivity as confining pressures increased to approximately lithostatic load is fairly small compared to the reduction due to other factors such as the degree of saturation.

Conclusions for the fracture saturated hydraulic conductivities are as follows:

1) Saturated conductivity of the fractures is several orders of magnitude higher than that of the matrix.

2) Flow through all fractured samples were substantially reduced at elevated pressures.

3) Fractured samples that were composed of strong rock regained 75 to 100 percent of initial conductivity when pressure was lowered to initial levels.

The remainder of the report consists of about 100 pages of tabular data and graphical presentations of these data.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

This report presents a tremendous amount of laboratory data which will be useful in order to understand the flow regime in Yucca Mountain. It should be recognized that these are small samples and therefore represent point values of the various formations. However, the data appear to be consistent, well presented and obtained by well accepted procedures.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

There are not major problems or deficiencies in the report.

SUGGESTED FOLLOW-UP ACTIVITY:

No follow-up activity is suggested at the present time.

REFERENCES CITED:

Campbell, G.S., 1977, An Introduction to Environmental Biophysics: Springer Verlag, New York, New York.

Van Genuchten, R., 1978, Calculating the Unsaturated Hydraulic Conductivity with a New Closed Form Analytical Model: Water Resources Bulletin, Princeton University Press, Princeton University, Princeton, New Jersey.

WMGT DOCUMENT REVIEW SHEET

FILE #:

SANDIA NATIONAL LAB #: SAND84-1492

DOCUMENT: Preliminary Bounds on the Expected Postclosure Performance of the Yucca Mountain Repository Site, Southern Nevada, by Sinnock, Lin and Brannen (1984)

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: July 1985

BRIEF SUMMARY OF DOCUMENT: DATE APPROVED:

General Assumptions, page 6. Assumption 7 states that the amount of water that is moving through the repository is a small percentage of the amount of surface water that infiltrates. It appears that they have not considered all of the ramifications of the cross-sectional area through the repository. This issue is discussed on page 7 of this review.

Chapter 3, Site Conditions. The hydrogeologic properties of the matrix and fractures of the units at Yucca Mountain are well documented with confidence limits given. The data are taken primarily from core samples as measured in the laboratory. This chapter also presents a good discussion of the various approaches used to estimate the downward flux. The first two methods discussed are climatic methods based on water budget considerations. Two types of flux measurements are considered. The first is based on the geothermal gradient; the second is based on moisture content and hydraulic pressures in rocks from the unsaturated zone. On the basis of the water budget methods, the authors conclude that an upper bound on the flux rate is a few millimeters per year through the unsaturated zone. From the geothermal approach it is estimated that water is moving downward at a rate of 1 to 10 mm/yr in the lower unsaturated zone. But in the upper portion of the unsaturated zone geothermal data suggest an upward flux. The authors conclude that the geothermal approach provides an independent estimate of recharge that strengthens the evidence that the flux is very low, certainly less than 10 mm/yr and probably less than 1 mm/yr. The last method used to estimate flux through the unsaturated zone was based on measurements of moisture content, pressures and effective hydraulic conductivities of rocks along unsaturated flow paths. They state correctly that this approach provides the most direct evidence about unsaturated flux. The in-situ pressure measurements of -20 to -40 bars correspond to saturations of less than 50 to 80% based on moisture content pressure head relations determined from core samples by Blair and others (1984). The corresponding hydraulic conductivities of the order of .01 to .1 mm/yr indicate that a .5 mm/yr flux constitutes a conservative upper limit on the flux through the rock matrix (Peters, 1984). The analysis used is correct.

Other analyses from the literature are presented to show that the transition from fracture flow to matrix flow would occur at higher pressures in the rock than those indicated. Wang and Narashimhan (1984) determined that the hydraulic conductivity corresponding to the calculated pressure threshold of fracture flow is about .5 to 1 mm/yr. Peters and Gauthier (1984) calculated that flux in excess of .5 mm/yr would nearly saturate most rocks in the unsaturated zone. They argue therefore that since the rocks are not completely saturated, the flux must be under .5 mm/yr.

The next paragraph considers the effect of having high recharge events in limited areas such as beneath the washes. They point out that the tendency would be for flow to occur in the horizontal plane away from the nearly saturated zones. Quoting the authors (page 15), "Given this reasoning, we tentatively conclude that pulses of flux through fractures at restricted places are not very likely, at least not as episodic events occurring at regular and frequent intervals at the same place. This conclusion needs to be confirmed by detailed modeling that calculates the lateral gradients of moisture content and pressure, if any, that can be sustained by local pulses of fracture flow of various intensities and frequencies."

In the next paragraph (page 16) they summarize the evidence that indicates that the average flux through Yucca Mountain is probably less than about .5 mm/yr. Again quoting (page 16), "Before this conceptual model of flux through the unsaturated zone can be firmly established, however, more widely distributed data are needed for in-situ moisture content, pressure heads, and hydraulic conductivities."

Section 3.1.3.1 Flow in the Unsaturated Zone. In this section the authors discuss the velocities of flow downward through Yucca Mountain. They point out that even if the downward flux did exceed the capacity of the matrix to transmit flow, only the very finest fractures would be required to transmit water and thus the actual velocity of flow in the fracture may not increase as abruptly as is considered ordinarily.

In the next paragraph (page 17) the effect of a pluvial climate is considered. The discussion leads to the preliminary conclusion that not more than 10 or 20 mm/yr flux would be available to pass through the unsaturated zone at Yucca Mountain under wetter climatic conditions. They point out that if that much infiltration had occurred during the pluvial climate, the entire profile would have been saturated. They then question whether in the 10,000 to 20,000 years since the pluvial climates ended the profile would have drained to the present value of saturation. They state that detailed modeling of this drainage process must be considered when attempting to establish the probable change in flux through the unsaturated zone due to the potential onset of another pluvial climate. In summation they state that the flux probably is less than .5 mm/yr in which case the flow would be entirely through pores in the rock matrix and travel times would be very long.

Some portions of the waste emplacement area are underlain by the zeolitic Calico Hills Unit. Flow to the water table in these portions probably would be almost entirely by rapid fracture flow for flux greater than 1 mm/yr. They conclude that this is the most likely situation but additional measurements should be made during the characterization stage to get better confidence in the above conclusion.

Chapter 4, Performance in Relation to Regulatory Requirements. In this section the authors calculate the travel times with three different definitions of the accessible environment. The first considers that the saturated aquifer immediately beneath the repository is the accessible environment. The second considers that a 2 kilometer distance from the repository is the accessible environment and the third considers that a 10 kilometer distance is the accessible environment. In all these cases the majority of the travel time occurs through the unsaturated Calico Hills Unit. Using a flux of 1 mm/yr, the travel time would always be greater than 10,000 years. With lower flux rates the time would be much longer. They next analyze the situation where the flux through the unsaturated zone is greater than 1 mm/yr in which case fracture flow occurs in the unsaturated zone. If the accessible environment is at a distance of 10 kilometers, the travel time for flux greater than 1 mm/yr is slightly greater than 1,000 years. In the case of the accessible environment at either 2 kilometers or at the water table, the travel time is less than 1,000 years. Quoting from their summary paragraph (page 30), "The one millimeter year value for flux above which significant fracture flow would occur, generally corresponds to the saturated flow of the Topopah Spring and zeolitic Calico

Hills units. Because the actual transition value varies within each unit and among different units, intervals of local fracture flow may be interspersed with intervals of local matrix flow. More widely distributed data are needed on both the vertical and the horizontal components of both saturated and unsaturated effective hydraulic conductivity of the rock matrix to allow more accurate characterization of this transition value throughout the unsaturated zone at Yucca Mountain."

Section 4.2 Waste-Dissolution Rate (page 31). Case 3 under this section considers the assumption that all water flowing vertically to the area of mined openings will interact with the waste. They go on to say, "According to current information, quite the opposite would probably happen. Openings created by the repository, even if backfilled, would tend to act as capillary barriers, thus diverting flux away from, rather than into, excavated areas (Fernandex and Freshly, 1984). This case conservatively assumes that mining of repository drifts will remove about 25% of the rock at the level of the underground facilities." It is correct that the flow probably would be diverted away from the excavated areas. However, if a sufficient amount of rock is excavated for the repository, the amount of flow that is diverted through the formation may be sufficient to cause fracture flow or even saturated zones in which case the water probably would flow into the repository.

Section 4.3.2 Unlikely Scenarios Involving Fracture Flow (page 41). In this section the performance of the repository under flux of up to 20 mm is considered. At such rates the flow in the vitric Calico Hills unit is in the matrix because the unsaturated hydraulic conductivity is nearly 1,000 mm/yr (in text page 41) or 410 mm/yr (Table 3). The flow in the zeolitized Calico Hills unit would be in the fractures at the flux of 20 mm/yr. The proportion of areas of these two units is considered in analyzing the movement of radionuclides to the accessible environment. Several plots are presented of the amount of radioactivity which would be released as a function of time after closure. For flux rates of up to 5 mm/yr the amount released is below EPA limits. This analysis does consider the decay rates of the various isotopes.

Chapter 5 Conclusions. One of their concluding statements is as follows (page 53): "Therefore site characterization and theoretical research should focus on establishing the flux through the unsaturated zone at Yucca Mountain, including the manner in which it is temporally and spatially distributed. Such efforts require information about the spatial distribution of hydraulic conductivity as a function of moisture content, development of better understanding of the conditions that dictate the transition between fracture and matrix flow, and empirical and theoretical studies of the magnitude of the diffusion process in unsaturated fractured media. Until the level of understanding for these items is improved, the pattern of results presented in this report must be considered provisional."

In summary we feel that this report constitutes a more defensible product than the analogous information presented in the Environmental Assessment. The authors consider ranges of values of pertinent parameters and determine the consequences of using those ranges; however, they tend to emphasize the low end of the ranges in most cases. The analysis of the unsaturated flow process is logical. The most probable value for flux is considered to be less than 1 mm/yr. This estimate probably is defensible; however, the authors recognize that additional field work must be done to determine whether that number is valid over the entire extent of the proposed repository.

1.0 INTRODUCTION

WWLNUM:	2
DOCUMENT NO.:	SAND84-1492
TITLE:	"Preliminary Bounds on the Expected Postclosure Performance of the Yucca Mountain Repository Site, Southern Nevada"
AUTHORS:	Scott Sinnock, Y. T. Lin, Joseph P. Brannen
PUBLICATION DATE:	December, 1984
REVIEWER:	Water, Waste & Land, Inc.
DATE REVIEW COMPLETED:	June 27, 1986
SCOPE:	General review of concepts and methods emphasizing theoretical considerations and assumptions. Specific review with respect to input data. Reviewed in the context of support of licensing activities.
KEY WORDS:	Pre-emplacement Groundwater Travel Times; Radionuclide Annual Release Rate; Deep Infiltration; Unsaturated Flux; Retardation Factors; Solubilities.
DATE APPROVED:	mjL 7/7/86

2.0 SUMMARY OF DOCUMENT AND REVIEW CONCLUSIONS

2.1 SUMMARY OF DOCUMENT

The general purpose of the report was to provide information which demonstrates the capabilities of the geohydrologic regime at Yucca to isolate nuclear waste materials in compliance with regulatory requirements. The applicable regulatory requirements considered are:

1. The 1,000 year pre-waste emplacement groundwater flow time from the disturbed zone to the accessible environment [10 CFR 60.113; 10 CFR 960.4].

2. The annual release rate of any radionuclide from the engineered barrier system after closure of the repository shall not exceed 1 part in 100,000 of the total amount of that radionuclide calculated to be present 1,000 years after permanent closure [10 CFR 60.115].

3. Reasonably foreseeable releases of radionuclides to the accessible environment shall be less than quantities calculated using procedures prescribed by the U.S. Environmental Protection Agency (EPA) [40 CFR 191.1; 10 CFR 60.112; 10 CFR 960.41].

The following general assumptions were used to analyze for compliance with the above regulatory requirements:

1. The repository will be located in the lower Topopah Spring welded unit.

2. The repository will contain 70,000 metric tons of heavy metal (MTHM) in 35,000 canisters.

3. The total area encompassing the waste will be approximately 607 ha.

4. No waste will dissolve until either 300 or 1,000 years after closure of the repository.

5. All waste released from the repository will be caused by ground water moving through the repository.

6. Dissolution of the uranium oxide matrix of spent fuel will saturate the flowing water with uranium. Additional radionuclides contained in the spent fuel will dissolve at a rate equal to the uranium dissolution rate multiplied by the ratio of the radionuclide to uranium.

7. The solubility of uranium will remain constant for the entire post-closure period.

8. The amount of water available to dissolve and transport waste will be a fraction of the total water moving through the repository level.

9. The flow path from the repository to the accessible environment is vertically down to the water table and then horizontally along the water table to a distance of 2 or 10 km.

10. Transport velocity of radionuclides is water velocity divided by a total retardation factor for each radionuclide and each material through which water flows. Retardation factors are the combined effects of sorption, precipitation, and diffusion.

11. Radioactive decay is considered.

12. Uniformity is assumed within each hydrogeologic unit.

2.1.1 Data Review

The report summarizes site conditions including brief descriptions of the geologic and hydrologic units. Data collected for each of the units is also presented. In the following subsections, the important data with regard to evaluating regulatory compliance are briefly discussed.

2.1.1.1 Unsaturated Flux

The authors review various estimates of deep percolation (unsaturated flux) provided by other investigators. These different estimates result from regional water budget, geothermal, and empirical analyses. Using regional water budget, methods an upper bound of 4 mm/yr was estimated based on current climatic conditions. The geothermal approach provides evidence that the flux is "certainly less than 10 mm/yr and probably less than 1 mm/yr." Using measured pressure head measurements of -20 to -40 bars and an assumed hydraulic conductivity vs. pressure head relationship, a flux range of 0.01 to 0.10 mm/yr is calculated.

Generic descriptions of fracture contributions to unsaturated flow are briefly discussed. The authors point out that fracture flow does not occur until the matrix is very nearly saturated and capillary pressure heads approach zero. These discussions are based on the assumption that the fractures behave as 'large pores'.

The paper also presents discussion concerning the effects of changes in climatic conditions on unsaturated flux. As other investigators have reported, wetter climatic conditions could result in increased deep percolation. This in turn is likely to cause a larger portion of the flow to occur in the fractures.

Based on the above observations, the authors conclude the following with regard to unsaturated flux:

1. Under current climatic conditions, the flux is probably less than 4 mm/yr and the most likely value is 0.5 mm/yr.

2. Sustained fracture flow is unlikely under current site conditions.

3. Flux in excess of 1 mm/yr (the approximate saturated conductivity of the matrix) would tend to cause significant fracture flow in and beneath the repository horizon.

4. A change in pluvial conditions could cause initiation of fracture flow.

2.1.1.2 Saturated Zone Conductivity

The authors also review data and interpretations regarding the hydraulic conductivity of the saturated zone. Analyses of Carbon-14 ages of ground water in the vicinity of the proposed repository results in conductivities on the order of 25 m/yr. Results of aquifer tests indicate conductivities of about 365 m/yr for the Topopah Springs unit and 0.07 m/yr to 700 m/yr for the Calico Hills unit and older tuffs. The higher values occurred in the upper portions of the water table. Results of packer tests indicate saturated conductivities of between 2 m/yr and 50 m/yr.

Results of numerical modeling activities for the saturated region were also discussed briefly with regard to saturated zone flux and hydraulic conductivity. The authors demonstrate that the modeled flux in the saturated zone would require extreme aquifer thicknesses (1,000 - 200,000 m) or very large conductivities (several thousand m/yr) to maintain the gradient which has been measured in the vicinity. It was concluded these extreme values were unreasonable.

Finally, the authors state that evidence indicates that most of the flow occurs in intervals less than about 100 m in thickness. In addition, most of these highly permeable zones are presumed to occur in close proximity to the water table. They conclude that the average effective conductivity of the saturated zone is 25 m/yr with a bounding range from 1 m/yr to 50 m/yr.

2.1.1.3 Geochemistry

Based on predictions of temperature gradients for the repository in various other reports, the authors conclude that temperatures less than 100°C will occur at the wall of the emplacement holes before the end of the containment period (300 years). Therefore, the authors conclude that "decay heat from the waste will not significantly affect waste solubility."

The chemical composition of water percolating through the repository was estimated since samples from the unsaturated zone are unavailable. Extrapolations were made from water obtained from the saturated zone in wells around Yucca Mountain. These waters can be characterized as a low total dissolved solids, sodium-bicarbonate type water with neutral to slightly alkaline pH (7-8). Because the repository is to be located in the unsaturated zone, free oxygen is assumed to be present resulting in an oxidizing Eh of about 700 mV. Based on these considerations, the authors conclude that the water flowing through the repository will not be highly corrosive.

Solubility of uranium was calculated using two geochemical models of equilibrium chemical reactions. The two models, EQ3 and MINTEQ, predicted uranium solubilities of from 3×10^{-4} mol/l to 5×10^{-11} mol/l, depending on assumed values of Eh and pH. Based on the results of those computations, the authors conclude that the solubility of uranium in spent fuel is less than about 10^{-4} mol/l and may be as low as 10^{-7} to 10^{-6} mol/l. It was also assumed that the release of other radionuclides occurred proportionately with their mass ratio to the mass of uranium in the spent fuel.

Once the radionuclides are released, a retardation factor, R_d, is used to determine the velocity of radionuclide movement relative to ground water movement. This retardation factor combines all of the processes which tend to cause the contaminant velocities to be less than water velocities. Some of the processes contributing to this slowing are mineral precipitation, ion exchange, adsorption, and absorption. Retardation factors can range from zero to greater than 100, depending on the particular radionuclide and the geochemical properties of the hydrologic unit in which flow is occurring. If the flow is in fractures, the retardation by sorption is less effective than for flow through the matrix. However, the authors indicate that under conditions of significant fracture flow, the difference in radionuclide concentration between water in fractures and water in the matrix will create a concentration gradient which will cause transfer of contaminants from the fracture water to the matrix water. It is concluded, therefore, that significant retardation of radionuclides will occur regardless of whether or not flow occurs in the fractures.

2.1.2 Results

As with the report being reviewed, the results have been divided into three sections - one dealing with groundwater travel times, the second dealing with waste release rates and the third dealing with releases to the environment. In each, the authors strive to demonstrate that the results presented are based on conservative assumptions.

2.1.2.1 Groundwater Travel Time

Groundwater travel times are calculated for three interpretations of the 'accessible environment':

A. The water table is assumed to represent the accessible environment. The flow path for this scenario is vertically downward from the base of the Topopah Springs unit to the water table. Therefore, the flow will occur through unsaturated Calico Hills tuff.

B. The accessible environment is located 2 km in a horizontal direction from the waste emplacement area. The flow path is vertically downward as described for Case A above and then laterally along the top of the aquifer for 2 km.

C. This case is identical to Case B above except the accessible environment is assumed to be a horizontal distance of 10 km from the waste emplacement area.

Although the above implies that calculations were performed for various values of conductivity for the saturated zone, this is not the case. A saturated zone travel time of 200 years was assigned to Case B. This corresponds to a velocity of 10 m/yr which when coupled with the observed gradient of 0.00034 and effective fracture porosity of 0.002 leads to a hydraulic conductivity of about 59 m/yr. Case C was assigned a travel time of 2,000 years which results in a velocity of 5 m/yr and a hydraulic conductivity of about 29 m/yr assuming a gradient and effective porosity of 0.00034 and 0.002, respectively. Presumably, the lower average conductivity for Case C is due to the increased length of the flow path. Travel times for Case B were calculated by adding 200 years to the Case A travel times. Case C travel times were calculated in a similar manner using 2,000 years.

The travel times for Case A were calculated by assuming the existence of a unit gradient. Under these conditions the hydraulic conductivity is equal to the flux. Using an effective porosity of 0.2, the travel times were calculated for flux values of about 0.05 mm/yr up to 1 mm/yr. The calculated travel times range from about 10,000 years for a flux of 1 mm/yr to over 100,000 years for a flux of 0.1 mm/yr. Travel times for Cases B were about 10,200 years and 100,200 years for fluxes of 1 mm/yr and 0.1 mm/yr. Corresponding Case C travel times were 12,000 years and 102,000 years.

Calculations were also conducted for fluxes in the range of 1 mm/yr to 20 mm/yr. Case A travel times ranged from about 5 years for a flux of 20 mm/yr to about 100 years for a flux slightly great are than 1 mm/yr. Case B travel times ranged from about 200 to 300 years and Case C travel times ranged from about 2,000 to 2,100 years.

The authors reached the following conclusions with regard to travel times as a result of the previously described calculations:

1. Under expected site conditions, travel times are well in excess of 1,000 years.

2. For the predicted flux range (less than 1 mm/yr), total travel time is not very sensitive to travel time through the saturated zone.

3. For fluxes greater than about 1 mm/yr, the location of the 'accessible environment' must probably be at least 10 km from the repository to comply with the regulatory requirements.

2.1.2.2 Waste-Dissolution Rate

The radioactive waste will be protected from contacting water by stainless steel canisters. Other barriers to the contacting water will be the zircalloy cladding and the uranium oxide itself. The authors considered three scenarios to determine the release rates:

1. Vertical canister emplacement which allows 0.25% of the total flux passing through the repository level to interact with the waste.

2. Horizontal canister emplacement which allows 2.5% of the total flow passing through the repository level to interact with the waste.

3. All water flowing vertically to the area of mined openings will interact with the waste which allows 25% of the total flux passing through the repository level to interact with the waste.

As might be expected, the results of the calculations showed that at the largest flux considered, 20 mm/yr, the largest amount of radionuclides will be released for the third case (the ratio of the amount of radionuclides released annually to the amount of waste contained in the repository was estimated to be 2×10^{-7}). For the first case, the annual fractional release rate was about 2×10^{-9} for a flux of 20 mm/yr. They also show that for flux less than 1 mm/yr and complete containment for 300 years, total curies remaining in solution will never exceed the EPA cumulative release limits, even if 25% of the total flux interacts with the wastes. They conclude that a repository at Yucca Mountain could comply with NRC requirements for slow release rates even without engineered barriers.

2.1.2.3 Releases to the Accessible Environment

The results of the calculations show that for a flux of 1 mm/yr, no releases to the accessible environment should occur during the 10,000 year period of compliance required by the EPA standard. This result holds even if the accessible environment occurs at the water table directly below the repository. This is a direct result of the long travel times (greater than 10,000 years) calculated for flux rates of 1 mm/yr or less.

The short-lived fission products, predominantly cesium and strontium, are responsible for most of the hazards during the first few hundred years after emplacement. These elements were determined to be completely contained within the immediate vicinity of the repository. The main source of radioactivity for longer time periods, the long-lived actinides and their short-lived daughter products are sufficiently retarded that they will be contained near the repository for millions of years. The author's calculations also show that the difference between 300 year or 1000 year periods of containment (as far as cumulative releases to the water table is concerned) is negligible.

The above conclusions are based on the authors determination of the most likely conditions at Yucca Mountain. The authors also consider performance "under less likely, but possible, site conditions." Five separate conditions were examined, four of which have to do with fracture flow. A flux of up to 20 mm/yr was used to provide a conservative basis for evaluation of fracture flow. The calculations showed that only if 25% of the flux were to become saturated with respect to uranium immediately upon contacting the waste, would the cumulative releases exceed the EPA limits. The basic conclusions reached indicate that the authors believe that even if these 'unlikely' events occur, a repository at Yucca Mountain would suitably isolate nuclear wastes from the environment. The authors did indicate that the performance of the waste packages and the buffering isolation of the saturated zone would become "more significant elements in the overall performance of a repository at Yucca Mountain" if the retardation due to diffusion was not assumed to occur under conditions in which fracture flow is significant.

2.1.3 Summary of Document Conclusions

A probable scenario resulting from the above results is that groundwater travel times to the water table from the repository probably exceed 10,000 years and may exceed 100,000 years. Combining the low flux with the long travel times keeps the radiation releases well within the allowable set by the NRC. If the current estimates of the flux are low or if future climatic conditions increase the flux, short flow times to the water table could occur because of fracture flow. However, the geochemistry of the site is such that even under these circumstances, it is unlikely that regulations regarding cumulative releases to the environment would be violated.

2.2 SUMMARY OF REVIEW CONCLUSIONS

The primary problems identified with the report have to do with the lack of actual physical data that is available from within the potential repository block. The authors have used the available information to derive the flow characteristics within the unsaturated and saturated zones. Until more physical data becomes available and the statistical interpretation of each unit's flow characteristics is determined, the validity of the travel times and radionuclide loading at the accessible environment as determined in this report is difficult to assess. The detailed review in Section 4.0 addresses six topics pertaining to uniformity of properties, unsaturated flux, flow in the unsaturated zone, flow in the saturated zone, solubility, and radionuclide retardation. In summary, the document demonstrates that the Yucca Mountain site should not be eliminated from consideration as a potential high level nuclear waste disposal area and indeed, if the assumptions are correct, that the site should provide excellent isolation of the radionuclides.

3.0 SIGNIFICANCE TO THE NRC WASTE MANAGEMENT PROGRAM

Using a number of simplifying assumptions, the performance of the Yucca Mountain site for a mined repository is assessed. Some of the critical parameters affecting the performance are identified, both for the travel time calculations and the radioactivity calculations. Areas needing further investigation are identified. The report shows that if the given assumptions are correct, the regulations can be met. As such, the report is highly significant to the NRC Waste Management Program, not only in concerns related to licensing but also as an aid in evaluating site characterization plans.

4.0 DETAILED REVIEW (Problems, Deficiencies and Limitations)

The document under review provides data, information, and calculations which indicate that the Yucca Mountain site can probably meet regulatory standards regarding disposal of high level nuclear waste. As such it is thought to be a reasonable 'first-cut' approach to estimating performance characteristics of the proposed repository. However, due to the paucity of actual data on which to base such performance analyses, the calculations are based on many assumptions. Therefore, most of the comments contained in the following sections have to do with those assumptions and their possible effects on the interpretation of the results. In general, we agree with the authors with regard to the following points:

1. Preliminary performance assessment indicates that the Yucca Mountain site is capable of providing a reliable location for development of a repository for disposal of high level nuclear wastes.

2. Additional data should be collected to verify as many of the assumptions invoked to perform the calculations. These data will allow the performance assessment to be refined and will hopefully provide statistical confidence in the results obtained.

4.1 LOCAL VARIATION OF HYDROLOGIC PROPERTIES

As noted earlier, it was assumed that hydrologic properties were uniform in each individual unit considered. While the report admits that there is undoubtedly variations within each unit, it is concluded that these variations are minor when compared with the variations between units. The actual physical properties (permeability, porosity, saturation, etc.) were available from two wells in the potential repository block, USW G-4 and USW GU-3. Because of the sparse amount of data available from the repository block, the actual variation of physical properties within each unit is unknown. Review of published literature regarding properties at Yucca Mountain indicates that while data for both the matrix and the fractures is sparse, there is substantially more data for the matrix materials. Much of the fracture data is inferred or based on theoretical considerations rather than on measured values. Fracture properties within each unit may vary substantially and thus be very influential on the fluid flow phenomena occurring within that unit. In addition, the areal extent of the hydrologic units, particularly the zeolitic and vitric zones of the Calico Hills nonwelded unit, are poorly defined. Cumulative release rates from the repository are extremely difficult to determine without additional resolution of the extent and hydrologic properties of the individual units at Yucca Mountain.

4.2 UNSATURATED FLUX

The report does not make clear why the value of 0.5 mm/yr constitutes a conservative upper limit on the flux. The report cites data from in-situ pressure head measurements of 20 to 40 bars (about 20,000 to 40,000 cm of water) for the Topopah Spring Member in hole USW UZ-1 at Drill Hole Wash just north of the target emplacement area. Using assumed relations between hydraulic conductivity and suction head, the report states that the corresponding hydraulic conductivities for these pressure head measurements are of the order of 0.01 to 0.1 mm/yr. The report further states that significant fracture flow does not occur until the flux is greater than about 0.5 to 1 mm/yr. It is not clear from the report as to how this range of values was determined. The authors do qualify these statements by indicating that additional data is needed to firmly establish the conceptual model of flux through the unsaturated zone. It is interesting to note that the most probable value of flux as used in this report is also the value of flux in which fracture flow may be initiated.

4.3 FLOW IN THE UNSATURATED ZONE

Both matrix and fracture flow are possible in the unsaturated zone at Yucca Mountain. The report states that if the flux is less than the saturated permeability of the matrix, flow occurs within the matrix materials. It is further stated that if the flux is greater than the matrix conductivity, the portion of the flux greater than the matrix conductivity will flow through the fractures. This implies that fracture flow occurs only when the imposed flux passing through a unit is greater than the saturated matrix conductivity. Fracture flow can also occur when the imposed flux is less than the saturated matrix conductivity (Peters et al, 1985).

Flux in excess of the saturated matrix conductivity was assumed to travel in the fracture system. To determine the travel time for the water in the fracture system of any unit, the velocity was first determined and the thickness of the unit was divided by that velocity to determine the travel time. Constant effective porosities were used to determine the fracture velocity. The effective porosity of the fracture is also a function of the imposed flux and as the flux is increased, the effective porosity increases. The velocity calculations for the fracture system apparently do not take into account the changing values of the fracture effective porosity.

4.4 FLOW IN THE SATURATED ZONE

The report asserts that the saturated zone has a "significant capacity to transmit water." However, the report also discusses the possibility that high conductivities which were estimated with drill-stem tests and large regional flux estimates based on groundwater modeling conducted by Waddell (1982), may be discontinuous and isolated. It is postulated that under such conditions the average flow velocity would be dominated by flow through the less permeable regions. The evidence available from well J-13, which has been pumped for a number of years, tend to refute this statement. Well J-13 has been pumped intermittently for 18 years yielding as much as 1.26×10^6 m^3/year in pumping tests, while the water level has stayed about the same. The hydraulic gradient has been estimated between well J-13 and well USW H-4 as 0.00033. The distance between the wells is approximately 6.1 kilometers (DOE, 1986).

It should also be noted that results of drill-stem tests indicate that the more permeable zones within the saturated region occur near the water table. The two cases, B and C, which included the saturated zone as part of the flow path to the 'accessible environment' were formulated as flow laterally along the top of the water table. Based on the currently available data and the transport model conceptualization used in this report, it may be that the travel times used for flow through the saturated zone are nonconservative. It is apparent that additional investigation will be required to further define the hydrologic properties of the saturated zone should the DOE wish to take credit for travel time through the saturated zone as may be the case if it is shown that significant fracture flow is occurring.

4.5 SOLUBILITY

The solubility of uranium was calculated by two geochemical models of equilibrium reactions using the chemical characteristics of water from the saturated zone near the site as a basis for the computation. The results of the calculations indicated that the solubility of uranium in spent fuel would be less than 10^{-4} mol/l and possibly as low as 10^{-6} or 10^{-7} mol/l. A value of 4×10^{-4} kg/m^3 of water was used for uranium solubility in the calculations.

This equates to an uranium solubility of about 1.7×10^{-6} mol/l (4×10^{-4} kg/m^3 x 1 mole/.238 kg x 1 m^3/1000 liters). Since this is substantially lower than the upper limit of 10^{-4} as calculated with the computer models, the results obtained may not be conservative especially in light of the fact that the chemical composition of the water in the unsaturated zone was extrapolated from water samples collected beneath the water table. Oxygen should be readily available and may have unanticipated effects on redox potential as well as pH values. It would seem prudent to evaluate annual release rates as well as cumulative releases to the environment under the more conservative conditions which may occur.

The report states that radioactive species with higher solubilities than uranium are known to be present in the spent fuel and that some of those elements may be segregated, e.g. carbon in the zircalloy cladding, iodine in gaps between the cladding and fuel, and cesium in the fuel. There is no reference given as to where this information was obtained, nor is there any statement or analyses as to the effect which this segregation may have on radioactive release rates. Again it may be more conservative to relax the assumption that dissolution of such elements is proportional to the dissolution rate of uranium.

4.6 RADIONUCLIDE RETARDATION

The report provides ample discussion about the retardation capacities of tuff matrix. This serves to further increase the length of time necessary for waste particles to reach the water table when the flow occurs through the matrix. The water travel times through the matrix are on the order of 10,000 years or greater even under saturated conditions because of the low permeabilities and large thicknesses. Therefore, the ability of a repository at Yucca Mountain to meet EPA cumulative release standards is not extremely sensitive to retardation coefficients of the matrix materials, if fracture flow is not significant.

The authors acknowledge the fact that during fracture flow sorption is less effective than during matrix flow, because less rock is in contact with the contaminated water. Relationships between fracture aperture width and retardation factor were presented. While the theory and concepts presented appear to be reasonable, it should be noted that the retardation factors are based on laboratory estimates of distribution coefficients. Mass transport literature provides abundant evidence that laboratory values of parameters are often substantially larger than those observed under field conditions. It is probably more conservative, therefore, to neglect retardation effects especially when evaluating contaminant transport through fractures until more data is available and the theory is better understood.

5.0 RECOMMENDATIONS

The effect that the high temperatures will have on radionuclide transport by the vapor phase is still unknown. Transport calculations for vapor phase need to be performed, as the vapor phase may provide the quickest route for radionuclide release to the accessible environment.

The interaction between the fracture system and the matrix in the unsaturated zone needs further investigation. Since the fractures may provide the quickest method for water transport to the accessible environment, the type of flow occurring within the fractures needs to be determined. Some fracture flow in the unsaturated zone has been observed at Yucca Mountain in test wells. There is not enough data available at this time to determine if fracture flow is occurring across much of the unsaturated zone.

The mechanisms by which the spent fuel will be dissolved and the rates at which the individual elements will be dissolved need further clarification. If some of the elements with high solubilities can become segregated in the spent fuel, the dissolution of these species and subsequent release may be higher than this report estimates. In addition, it is recommended that additional tests be scheduled to enhance confidence in the retardation factors used in the computations.

6.0 REFERENCES

DOE (U.S. Department of Energy) Office of Civilian Radioactive Waste Management, May, 1986. "Environmental Assessment, Yucca Mountain Site, Nevada Research and Development Area, Nevada.

Peters, R. R., Gauthier, H. H., and Dudley, A. L., 1985. "The Effect of Percolation Rate on Water-Travel Time in Deep, Partially Saturated Zones" SAND85-0854C, Sandia National Laboratories, Albuquerque, New Mexico.

Waddell, R.K., 1982. "Two-dimensional, steady-state model of ground-water flow, Nevada Test Site and vicinity, Nevada-California", Water Resources Investigations 82-4085, 72 pp., U.S. Geological Survey, Denver, CO.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT: Bixler, N.E., 1985, NORIA-A Finite Element Computer Program for Analyzing Water, Vapor, Air and Energy Transport in Porous Media: SAND84-2057, Sandia National Laboratories, Albuquerque, New Mexico 87185 and Livermore, California 94550 for the U.S. Department of Energy

REVIEWER: Williams and Associates, Inc.

DATE REVIEW COMPLETED: November 1985

BRIEF SUMMARY OF DOCUMENT: DATE APPROVED:

This report describes a finite element computer program that solves four non-linear, parabolic, partial differential equations simultaneously. The four equations describe the transport of water, water vapor, air and energy through partially saturated porous media. The Galerkin finite element method is used for the spatial discretization of two-dimensional domains with planar symmetry or axisymmetry. The time integration is done by a third order predictor correcter scheme that uses error estimates to automatically adjust time step size so as to maintain uniform local time truncation errors throughout the calculation. The user is not required therefore to select time step size except at the first step. Most material properties can either be set to constant values or defined as functions of dependent or independent variables by user supplied subroutines. The report includes discussions of the theory of two phase transport in porous media and the numerical procedure used in NORIA.

GENERAL TECHNICAL DISCUSSION:

Introduction. This section is a general discussion of the various types of finite element and finite difference programs which are available to solve various types of flow problems. The author notes that NORIA is intended for non-isothermal problems in which large gradients are expected in the gas pressure. Other programs which have been developed at Sandia Labs are SAGUARO which considers gas flow but with little or no pressure gradient and MARIAH which is for saturated flow. There are only three other programs that can solve the same types of problems that are solved by NORIA. These are PETROS which is a one-dimensional finite difference program, TUFF which is an integrated finite difference program, and WAVE which is a finite difference program. The author feels that the finite element program NORIA is more suitable than the finite difference programs.

Section 2 Theory and Mathematical Model. The assumptions which the author uses are 1) the two phases consist of a single component in liquid and vapor phases and a second component that is an inert gas. The liquid phase is assumed to be water and the inert gas is assumed to be air, but other constituents can be modeled equally well by NORIA. 2) Both air and vapor are assumed to be ideal; thus the partial pressure of each component is described by the ideal gas law and the partial pressures are additive. 3) The three phases are taken to be in local thermal equilibrium; thus the temperatures of the rock matrix, liquid water and gas are all equal locally. 4) All viscous flow is laminar and obeys Richards equation which is a form of Darcy's law for unsaturated media. 5) The liquid phase behaves as a Boussinesq fluid. In other words, the density is independent of pressure and varies only slightly in proportion to the difference between local temperature and the referenced temperature. 6) The porosity and density of the porous matrix are constant over each material. Up to ten materials are allowed. The remainder of Section 2 is a formulation of the four non-linear partial differential equations which define the flow of the four phases. This formulation appears to be reasonable.

Section 3 Galerkin Finite Element Formulation. This is a fairly standard Galerkin formulation with development of the basis functions, and the use of parametric and subparametric elements. There is also a discussion of the various types of boundary conditions.

Section 4 is the time integration scheme in NORIA. This is quite different than other models currently available. The user only selects an initial time step and all succeeding time steps are adjusted automatically to give the same truncation error in each time step. The time step may be increased or decreased at a particular interation. The basic process is to use a predictor corrector method coupled with a Newton iteration procedure to move ahead in time. The Adams-Bashforth predictor cannot be used in the first two time steps because rates of change of the dependent variables are not known prior to the initial condition. The start-up procedure used is to take two backward difference steps before starting the two step time integration procedure. This process helps to damp out discontinuities that may be present in the initial data.

Section 5 Program Description. The first stage of operation of NORIA involves assigning nodal point locations. The mesh is then generated. Boundary and initial conditions are next specified. The solution procedure then is pursued. Next, derived quantities such as heat or water vapor or air velocities are computed. The output data thus may be plotted as desired. Several different types of meshes such as eight point isoparametric or subparametric elements as well as six node subparametric or isoparametric elements may be used. The options give a great deal of flexibility in fitting a mesh to irregular boundaries. Boundary conditions involve either flux boundaries or constant potential boundaries. There are several options in calculation of derived quantities such as heat fluxes or determination of water vapor and velocities. The plotting package will generate plots of nodal point locations, finite element mesh outlines of materials, contours and profiles of the dependent variables.

The remainder of the report presents the actual specifications of the cards to run the program. On reviewing the use of this program, the obvious question raised is whether the huge amount of data on materials would ever be available to model a field type problem. The program is very large containing 10,000 source statements and must be run on a relatively large computer such as the Cray 1S. Development of the program is a large step that is necessary to define the flow of vapor, liquid water and heat in the neighborhood of the repository. The amount of data required to run the program, however, would be mind boggling.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The report under review is one of many computer models that are being developed to simulate multiphase flow in porous media.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

There are no major problems or deficiencies in the report. However, the program is very large and will require an immense amount of data to be useful.

SUGGESTED FOLLOW-UP ACTIVITY:

No follow-up activity is suggested at the present time.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND83-2593

DOCUMENT: Nimick, F.B., and Williams, R.L., 1984, A Three-Dimensional Geologic Model of Yucca Mountain, Southern Nevada. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, SAND83-2593.

REVIEWER: Williams & Associates, Inc., James F. Osiensky

DATE REVIEW COMPLETED: November 2, 1987

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

The report under review describes an initial version of a three-dimensional trend surface generation model for the geology of Yucca Mountain. The trend surface model was designed for use with sparse and irregularly distributed input data. The purpose of the trend surface analysis is to provide a quantitative method for the interpolation and extrapolation of data between data points (drill holes). The main limitation of the model for use in the vicinity of Yucca Mountain is the lack of a comprehensive three-dimensional field data based description of faults that occur in this area. It is anticipated that trend surface analysis of this type will become more significant as additional data become available during site characterization.

BRIEF SUMMARY OF DOCUMENT:

The report under review describes the development of a three-dimensional geometric framework of the geology of Yucca Mountain using trend surface analysis. The framework was developed to aid in the interpolation and extrapolation of known geologic features that occur in the vicinity of Yucca Mountain. The report describes the initial version of a 3-D geologic framework model of Yucca Mountain. In addition, the report describes the modeling method and configuration, the input data used, and an analysis of the interpolative and extrapolative ability of the model.

The geometric framework model consists of a collection of three-dimensional trend surface representations; the base of each stratigraphic zone is defined as one trend surface. Information concerning the nature and distribution of rock units and geologic structures at Yucca Mountain is limited to maps of surface outcrops, and drill hole logs. Because these data are very sparse and irregularly distributed, Sandia National Laboratories (SNL) developed an estimation technique to handle sparse and irregularly spaced data. This technique is called trend modulation by multi-kernel summation (Williams and Nimick, 1984). The method generates a single, continuous analytical surface equation (trend surface equation) from a collection of three-dimensional coordinates. The interpolation technique used to generate trend surfaces is discussed in Appendix A of the report. According to the report, the interpolation method is the core of the implementation of the trend surface analysis. Data such as fault location, orientation, and offset are used to transform coordinates for the base of a unit to the coordinates of the unit prior to faulting. The data are manipulated by the mathematical estimation technique to generate a set of analytical equations; each equation represents the surface at the base of a single defined unit. According to the report, the assumption has been made that the actual geologic surfaces were smooth and continuous when the layers of pyroclastic materials originally were deposited.

Data for the model are input on three-dimensional coordinates, x, y, z. For Yucca Mountain, x and y coordinates are the east and north locations in state plane coordinates; the z coordinate is the absolute elevation above mean sea level.

Data used in the model include drill hole locations, lithologic logs, and gyroscopic surveys. The x, y, z coordinates for a given lithologic unit are based on drill hole data. The effect of faults which occur between data points (drill holes) must be removed prior to calculation of the geologic surfaces. According to the report, only vertical (z) offsets on faults were accommodated. All fault offsets were accounted for relative to a structural block containing drill holes USW G-3, USW GU-3, USW H-3, and USW G-1. This structural block was presumed not to have moved due to faulting.

Lithologic units that were found to be missing in certain drill holes were assumed (for the purpose of the model) to reach zero thickness at the location of the drill holes where they are missing. According to the report, the model can be adjusted as more information becomes available. Tables 3 through 11 of the report summarize the input data for the individual drill holes used for the model.

The model was evaluated using two types of analyses. In the first analysis, the accuracy of the generated surface was evaluated by comparing the model surfaces with data measured for drill holes not included in the model. The second type of analysis consisted of generating a number of cross sections from the model. Predicted data were compared to real field data from drill holes USW G-4, UE-25B#1, USW H-1, USW H-3, and USW H-5. The results of the comparisons for drill hole USW G-4 are presented in tables 15 and 16 of the report. The results for the comparison of predicted and actual elevations and thicknesses at drill hole USW H-1 is presented in table 17 of the report. The authors of the report suggest the comparisons for drill hole

USW G-4 are reasonable on average but can be imprecise in detail. This statement basically is true for the other drill holes.

Figures 5, 6, 7, and 8 of the report present cross sections which illustrate the predictive capability of the model. According to the report, the cross sections should be viewed as representative of the information available as a result of calculating the surfaces described in the report and as a result of inserting fault offsets manually via the graphics system. The authors of the report suggest that the cross sections are consistent with various publications of the USGS.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The report under review presents a method for the interpolation and extrapolation of geologic data in the vicinity of Yucca Mountain. The trend surface generation model is capable of yielding a three-dimensional trend surface of the geologic stratigraphy at Yucca Mountain. The model is capable of generating cross sections along any chosen path; in addition, the model can be used to produce maps of the elevation or thickness of selected generated trend surfaces (stratigraphic units). The primary significance of the model is its ability to extrapolate data in the form of trend surfaces to areas in which no geologic data are available.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The primary limitation of the model under review is the lack of available input data, especially for faults that occur within the area. As would be expected, the ability to ascertain the accuracy of the generated trend surfaces is severely limited by the data available for input.

SUGGESTED FOLLOW-UP ACTIVITIES

No follow-up activities are suggested at the present time. However, it is anticipated that this type of model will become more significant as additional data become available during site characterization. It is very likely that model representations of the type presented in the report will be standard application materials to be evaluated by the NRC during licensing of a repository.

REFERENCES CITED:

Williams, R.L., and Nimick, F.B., 1984, A Technique for the Geometric Modeling of Underground Surfaces. Sandia National Laboratories, Albuquerque, NM, SAND84-0307.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND84-2642

DOCUMENT: Klavetter, E.A., and Peters, R.R., July 1986, Estimation of Hydrologic Properties of An Unsaturated, Fractured Rock Mass. Nevada Nuclear Waste Storage Investigations Project, Sandia National Laboratories, Albuquerque, NM 87185.

REVIEWER: Williams & Associates, Inc., George L. Blomberg

DATE REVIEW COMPLETED: December 15, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

Theoretical relationships are developed for combined matrix and fracture flow in the unsaturated zone of Yucca Mountain. Two methods are used: a microscopic method in which the actual geometry and size of pores are considered, and a macroscopic procedure in which the conceptual model of Wang and Narasimhan (1985) is used. Agreement between the two methods is good. Composite curves for hydraulic conductivity as a function of capillary pressure are presented for flow in both the matrix and the fractures. It is assumed and justified that the pressure in the matrix and fractures at a particular elevation is the same during steady downward flow. This report appears to be a good first step in developing the theory for combined matrix and fracture flow.

BRIEF SUMMARY OF DOCUMENT:

The report presents two theoretical developments for the analysis of flow in fractured rock masses in which matrix flow also occurs. The authors first present a general discussion of the Yucca Mountain hydrogeologic system reviewing the various stratigraphic units in the formation. The authors accept the basic conceptual model of the USGS in which there may be diversion of flow along the contact between units. However, this conceptual model is not used in their theoretical development.

The authors also use the conceptual model of Wang and Narasimhan (1985) for the analysis of unsaturated flow within the fractures. They assume an average fracture aperture of 25 micrometers and an average matrix pore diameter of 0.03 micrometers (Peters et al., 1984). These numbers are justified in an appendix of the report from the analysis of mercury injection data. The Wang and Narasimhan (1985) analysis shows that under relatively low values of saturation in the fractures, flow will occur across the fractures from one porous block to another. At high fracture saturation values, the flow will be parallel to the fractures. The implications of this conceptual model are that

1) The fracture conductivity for water movement across the fracture is probably much larger than the adjacent matrix conductivity, thus flow across the fracture is controlled by the adjacent matrix conductivity. The fracture conductivity across the fracture can be replaced by the matrix conductivity in flow calculations.

2) The average fracture conductivity for water movement in the plane of the fracture is a highly non-linear function of fracture saturation or pressure head. If the flux is less than the saturated conductivity of the matrix then the water will tend to flow only in the matrix. If the flux is greater than the saturated conductivity of the matrix then the matrix will saturate and the fractures will also carry water.

The discussion in this report assumes that the distribution of flux in the horizontal direction is uniform and that a definite value of hydraulic conductivity exists for each unit. The variability of hydraulic properties within each unit is not considered. The theory in this report is being used for development of the computer code TOSPAC. The code is not presented in the present report. The development is based upon the equation for conservation of mass (continuity equation) in the absence of either sources or sinks. The equation includes terms for the rate of change of moisture content with time within an element, the flux in and out of an element and a term allowing deformation of the porous medium. When the Darcy equation is substituted into the conservation of mass equation, Richard's equation is obtained. The authors discuss the following two alternatives to modeling a situation where water movement may occur in both fractures and the matrix:

1) Model the fractures explicitly by simulating them in the computational mesh as a second region that has different properties than those of the matrix.

2) Use an equivalent porous medium taking into account that there are two porosity systems: the matrix porosity and the fracture porosity.

In the present situation it is necessary to use the second method since the fractures are small scale and numerous. It would not be possible to map all fractures. Equation development is done on both macroscopic and microscopic scales. The macroscopic model assumes that the fracture and matrix properties are representative statistically of a large volume of rock. Samples of the rock must be used to determine the conductivity and saturation values as a function of pressure head for a representative sample, but there is no actual knowledge of the physical structure of the system. Basically the volume of rock is treated as a black box with the constitutive equation as a transform function and hydrologic properties as coefficients to be determined to relate the input and output parameters.

The microscopic approach considers the microscopic structure of the system, a theoretical analysis of fluid flow in the pores and storage of fluid in the pores, and determines relative conductivity and saturation values as a function of pressure head. The description of size and distribution of pores is based on mercury injection data. Both derivations use capillary bundle theory in their evaluation of hydrologic coefficients.

The authors state that the "calculation of the rise in height of water in a capillary tube as a function of tube radius indicates that for tubes with a radius on the order of a few millimeters, the fluid rise, due to capillary forces, is the same as the tube radius." This statement gives an erroneous impression that this relationship is valid if the radius of the tube is sufficiently small. Such an impression is not valid because the rise is equal to the radius of the tube only at a diameter of 3.86 mm. The quoted statement is then used to justify the limit of applicability for capillary bundle theory to tubes having radii on the order of millimeters. This limit actually has nothing to do with the statement that is quoted above.

The macroscopic derivation consists of writing the continuity equations separately for flow in the matrix and in the fractures. A term is included to allow for flow between the matrix and fractures which is dependent on the pressure difference between the fluids in the fractures and matrix. The authors present considerable discussion to justify the assumption that the pressure in the fractures and that in the matrix is the same. The assumption is justified and completely consistent with information from Yucca Mountain. The justification is based on the fact that pulses of water from the surface are damped out within a matter of a few meters below the surface of Yucca Mountain. Travis et al. (1984) and Martinez (in press) have shown by independent calculations that the penetration distance into fractures in densely welded tuff of low conductivity (similar to those in Yucca Mountain) are on the order of 10 m or less if the fracture apertures are 100 micrometers or less. Wang and Narasimhan (in press) have simulated episodic flooding events which concentrate the estimated annual flux at Yucca Mountain over many years into a time period of 0.2 years. This concentration of annual flux caused little change in hydrologic condition. Wang and Narasimhan (1985) also have simulated drainage of fractures in a welded tuff cube of approximately 1.5 cubic meters. They have shown that the pressure in the fractures and matrix will be the same at the same elevation. The form of the continuity equation which the authors use can be considered to have two general parts:

1) Consideration of all storage aspects of the water within a unit volume, and

2) Flow in and out of the volume due to flow both in the fractures and in the matrix.

The storage terms are written in terms of saturation and are grouped such that one coefficient (capacitance coefficient) is given as a function of pressure head. The capacitance coefficient includes the sum of the storage due to the change of saturation, and compressibility of the matrix, fractures, and water. Curves for the capacitance coefficient as a function of pressure are presented for each of the materials in Yucca Mountain. Information about hydraulic conductivity as a function of pressure head also is presented in the form of a curve for the matrix, a curve for the fracture, and a composite curve for each unit. These curves were calculated from capillary pressure-saturation data by the methods of Brooks and Corey, and Mualem. The two methods are similar.

The microscopic derivation begins with a discussion of the actual geometry of the tuff and uses mercury intrusion data to obtain values for pore sizes and pore size distributions. Data are presented for each of the hydrogeologic units of interest. Analyses of these data show that the fracture aperture was about 25 micrometers while the pore sizes were considerably smaller, although no actual number is given. The Burdine equation was used to calculate the relative permeability from the capillary pressure-saturation data. Both of the above approaches (microscopic and macroscopic) enable the calculation of hydrologic parameters for an unsaturated fractured rock mass. Both methods incorporate the assumptions that the pressure is the same in the matrix and in the fractures and that capillary theory is valid. The latter assumption implies that laminar flow exists and that fracture apertures are small enough for capillary pressure to have meaning. A lognormal aperture width distribution also is assumed. A comparison is made of the hydraulic conductivity vs pressure head for each of the materials for the two methods of analysis. In general, good agreement exists between the microscopic model and the macroscopic model. In the case of the Tiva Canyon unit some discrepancy exists between the two models for pressure heads between 100 and 1,000 meters.

In summary, this is an excellent start in developing the theory of flow in a combined matrix/fracture situation for Yucca Mountain. The development is relatively easy to understand and the results appear to be excellent. Future work should concentrate on the development of a computer code for the use of the author's equations and evaluation of the best method for modeling the variation in hydraulic properties of the various units. The present work assumes that one characteristic sample exists for each of the units in the formation; the variation of hydraulic properties is ignored. The appendices of the report under review contain a detailed derivation of the flow equation and a comparison of several models of relative hydraulic conductivity. The four models used include the Brooks-Corey, the Mualem, the Fatt and Dykstra and the Burdine equations. The Mualem, and Brooks-Corey relationships are the most consistent.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

This is one of the better papers to date which focuses on development of a theoretical equation to describe the flow in the matrix/fracture systems. The authors' assumptions are well justified and their theoretical development is easily followed. The development includes the compressibility of water, the matrix, and fractures, due to pressure changes. No field data are presented in the report. This report is a first step in developing capability for correctly modeling the unsaturated zone in Yucca Mountain.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

The main deficiency of the report under review is that variability of hydraulic properties within each unit is not considered. After a code is developed to handle variable hydraulic properties within each unit, it will be necessary to obtain some field verification of the code.

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Wang, J.S.Y., and Narasimhan, T.N., 1985, Hydrologic Mechanisms Governing Fluid Flow in Partially Saturated, Fractured, Porous Tuff at Yucca Mountain. Sandia National Laboratories, Albuquerque, NM, SAND84-7202.

Peters, R.R., Klavetter, E.A., Hall, I.J., Blair, S.C., Heller, P.R., and Gee, G.W., 1984, Fracture and Matrix Hydrologic Characteristics of Tuffaceous Material from Yucca Mountain, Nye County, Nevada. Sandia National Laboratories, Albuquerque, NM, SAND84-1471.

Travis, B.J., Hodson, S.W., Nuttal, H.E., Cook, T.L., and Rundberg, R.S., 1984, Preliminary Estimates of Water Flow and Radionuclide Transport in Yucca Mountain. Mat. Res. Soc. Symp. Proc., vol. 26, 1039-1047.

Martinez, M.J., in press, Capillary Driven Flow in a Fracture Located in a Porous Media. Sandia National Laboratory, Albuquerque, NM, SAND84-1697.

1.0 INTRODUCTION

WWLNUM: 73

DOCUMENT NUMBER: Sand 84-7202

TITLE: "Hydrologic Mechanisms Governing Fluid Flow In Partially Saturated, Fractured, Porous Tuff at Yucca Mountain"

AUTHORS: J.S.Y Wang and T.N. Narasimhan

PUBLICATION DATE: April, 1985

REVIEWER: Water, Waste & Land, Inc.

DATE REVIEW COMPLETED: March 7, 1986

DATE APPROVED: L.A. Davis 3/21/86

Mark J. Logsdon, WWL Project Manager 3/31/86

2.0 SUMMARY OF DOCUMENT AND REVIEW CONCLUSIONS

2.1 Summary of Document

The paper presents a conceptual model for the hydrology of a partially saturated, fractured medium. A general statistical theory is developed to describe the flow phenomena in fractures and the flow phenomena which occurs between the matrix and fractures. The theory yields expressions for fracture saturation, fracture permeability and effective areas of matrix fracture flow as functions of pressure. Using these expressions in a numerical model, the drainage of a fractured tuff column was simulated. Specific physical parameters from Yucca Mountain were used for model input. The model indicated that fracture flow properties are important only during highly transient changes in flow from fully saturated to partially saturated conditions. For a partially saturated, fractured, porous system the fluid flow could be simulated approximately without taking fractures into account once the fractures have desaturated.

2.2 Summary of Review Comments

We believe that the model proposed in this report is an important advance in the understanding of the mechanisms governing fluid flow in partially saturated, fractured, porous tuff. Further advances will probably require:

a. Inclusion of film flow on fracture surfaces.

b. Realistic simulation of fracture orientation.

c. More vigorous development of the relation between the hydraulic properties of individual fractures and the overall bulk permeability.

d. A more realistic calculation of the phase-separation constriction factor.

The model should be used to simulate problems of infiltration as well as drainage. It is expected that the relation between fracture and matrix flows will be substantially different for the two cases. Further, it is expected that inclusion of the effects of the air in the matrix blocks will eventually be required. Finally, vapor transport in the fractures is expected to play a significant role in the overall water balance at Yucca Mountain. If so, a liquid flow model uncoupled from vapor transport may give misleading results.

3.0 SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM

Because the licensing of the Yucca Mountain Site will be based to some extent on the results of numerical modeling, the initial work performed in this paper will be important to determining the flow characteristics in the unsaturated zone at the site. The results from the paper make possible a more detailed numerical simulation capability, as more hydrogeologic data becomes available, for the unsaturated zone.

4.0 DETAILED REVIEW (Problems, Deficiencies and Limitations)

4.1 Conceptual Model

The conceptual model developed uses basic principles of soil physics to quantify the flow phenomena which can take place in unsaturated, fractured porous media. The concept that the largest pores will desaturate first as the water phase pressure in the porous medium is decreased below atmospheric pressure is translated to the desaturation of fractures. As desaturation occurs, water will tend to flow across fractures from one matrix block to another through pendular rings located at asperities. Once fracture desaturation initiates, a relatively continuous air phase produces a large resistance to flow parallel to the fracture, significantly reducing the effective fracture permeability. The effect of the unsaturated fractures is to introduce a macroscopic tortuosity to the porous media.

To quantify the hydrology of a fractured porous medium, three relations are developed from theoretical grounds. The relationships required are fluid pressure head/fracture saturation, fluid pressure head/fracture conductivity, and proportion of fracture surface that remains wetted. In the development of these relationships, the following factors are ignored:

1. Film flow on partially saturated rock surfaces.

2. Vapor transport from evaporation-condensation across the liquid phase.

3. Drying processes of isolated liquid pockets surrounded by gaseous phase.

4. Solubility of air in water.

The authors state that it is possible to include these phenomena into the developed quantitative statistical theory.

As stated in the DOE Draft Environmental Assessment and Montazer and Wilson's Conceptual Model of Flow in the unsaturated zone, Yucca Mountain, Nevada (1984), a geohydrologic unit above the host rock exists which would divert the downward infiltration of water beyond the limits of the emplaced waste. Part of this barrier consists of a capillary barrier which is probably formed between the matrix of Paintbrush non-welded unit and the fractures of the Topopah Spring welded unit. The barrier is formed where the water filled pore sizes in the non-welded unit are smaller than the aperture of fractures in the underlying welded unit. From a theoretical standpoint, no flow into fractures can occur until atmospheric pressure exists at the base of the pores. As stated by Montazer (1984), the pore and fracture opening sizes and saturation conditions are such that some sheet flow can occur along the walls of the fracture in quantities that are greater than the flow into the matrix of the welded unit.

Since the model developed by Wang and Narasimhan and described in the paper reviewed ignored film flow on partially saturated rock surfaces, the utility of the model in evaluating some of the flow phenomena at Yucca Mountain is decreased. It is recommended that film flow on partially saturated rock surfaces be incorporated into the model.

4.2 Fracture Orientation

Fracture orientation data used in the numerical model were based on information obtained at test hole USW G-4. Fractures and fracture orientation were analyzed from the core samples and downhole television camera and compass. The fractures can be divided into two major categories:

1. Joints, which are defined as fractures where fracture faces show no apparent evidence of differential movement.

2. Shear fractures, which show evidence of differential movement in the form of minor offsets of pumice fragments, slickensides, and associated brecciation.

The frequency of fractures is strongly influenced by the degree of welding. In the densely welded zone of the Topopah Spring Member, measurement of fracture inclinations indicated that approximately 36 percent are inclined between 0^{o} and 30^{o} (Spengler and Chornack, 1984). Fractures inclined between 61^{o} and 90^{o} account for about 46% of the fractures (Spengler and Chornack, 1984).

The authors have grouped the fractures into two categories:

1. Nearly vertical - 56% of the fractures have steeply dipping inclinations ($>45^{o}$).

2. Nearly horizontal - 44% of the fracture have small inclinations ($<45^{o}$).

The averages of the cosine of the dip angles for the two groups are $(COS)_V$ = 0.27 and $(COS)_H$ = 0.92. Using these values, the average vertical fracture would have an inclination of 74^{o} and the average horizontal fracture would have an inclination of 23^{o}.

For the fractured tuff column simulations of the Topopah Spring Member using the TRUST numerical model, two vertical fracture sets and one horizontal fracture set were used to partition the tuff formation into discrete fracture blocks. Only one vertical column of blocks bounded by four vertical fractures were modeled since the midplanes of the bounding vertical fractures are no-flow boundaries due to symmetry. Horizontal fractures were explicitly simulated.

Because the actual orientation of fractures in the welded Topopah Spring Member are not vertical and horizontal, the results from the numerical model presented are difficult to translate into actual conditions. While the advantages of specifying a set of vertical and horizontal fractures relative to setting up a numerical model are obvious, the differences between model results and actual flow phenomena are hard to relate quantitatively. It is recommended that the TRUST model should be used with the stated average fracture orientations to determine if significant differences in matrix/fracture flow behavior occur.

4.3 Simulation of Drainage

The simulation of drainage of a column of fractured porous medium demonstrated several salient features of the interaction between the fractures and the matrix. However, other important phenomena are not demonstrated by the drainage problem. The relative fracture/matrix components of the flux during an infiltration event are equally important as during drainage and are likely to be very different.

4.4 Equivalent Bulk Permeability

The development of the hydraulic properties of a single fracture were rather carefully and fully developed in terms of the distribution of apertures for the single fracture. Relatively little was presented on the relation between the properties of a single fracture and the behavior of the bulk medium containing many fractures with presumably different properties. Apparently, calculation of the hydraulic properties of a single fracture from a field measured permeability as was done in this report is tantamount to assuming that all fractures in the bulk medium have the same hydraulic properties.

4.5 The Phase-Separation Constriction Factor

Incorporation of a parameter or function to account for increased tortuosity of flow along the fracture as the saturation decreases is an important feature of the model. It was necessary for the authors to assume a very simplified geometry to enable calculation of their phase-separation constriction factor. It seems likely that it will be necessary to calculate this factor for random location of asperities and more complex geometries of the pendular water associated with the asperities.

5.0 RECOMMENDATIONS

It is recommended that the model be updated to include film flow, vapor transport, and air solubility. Some of these phenomena are considered important in the conceptual model presented by Montazer and Wilson (1984). Improving the model to include them may provide insight into their relative importance to the overall flow field at Yucca Mountain.

It is also recommended that the model be reformulated using more realistic fracture orientations. The results of such modeling efforts would demonstrate the importance (or lack of) of fracture orientation on the solution obtained.

It is further recommended that infiltration events be modeled. As the authors point out, fractures are important during the transient-flow period. An infiltration event followed by drainage period represents a highly transient flow phenomena. Modeling of such an event may provide additional insight into the details of combined fracture and matrix flow.

6.0 REFERENCES

Montazer, P. and W. E. Wilson, 1984. "Conceptual Hydrologic Model of Flow in the Unsaturated Zone, Yucca Mountain, Nevada," USGS Water Resources Investigations Report 84-4345, 55 pages.

Spengler, R. W. and Chornack, M. P., 1984. "Stratigraphic and Structural Characteristics of Volcanic Rocks in Core Hole USW G-4, Yucca Mountain, Nye County, Nevada," USGS Open File Report 84-789, 77 pages.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND84-7202

DOCUMENT: Wang, J.S.Y., and Narasimhan, T.N., 1984, Hydrologic Mechanisms Governing Fluid Flow in Partially Saturated, Fractured, Porous Tuff at Yucca Mountain, Lawrence Berkeley Laboratory, Berkeley, CA, 47 p.

REVIEWER: Williams & Associates, Inc., George J. Bloomsburg

DATE REVIEW COMPLETED: January 20, 1987

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

This report discusses the development of a conceptual model for saturated and unsaturated flow in a fractured porous medium such as that which occurs beneath Yucca Mountain, Nevada. The concept used in the development of the model is that flow will occur along the fractures only when they are saturated; otherwise flow will occur across the fractures. Flow across the fractures will occur at the points of contact across the fractures.

A gamma distribution is assumed for the distribution of aperture widths. A statistical analysis combined with limited data on the flow properties of the porous matrix then is used to develop relationships between pressure, saturation and relative conductivity for the combination of fracture and matrix flow. These relationships then are used in the computer code TRUST to simulate flow in a single column of porous matrix which is surrounded by four vertical fractures. The results show that in some cases a very long response time is needed for water to move from the interior of a porous block to a fracture; however, this characteristic is very sensitive to the fracture properties. The authors believe that detailed data on the fracture density and geometry are not necessary for a steady flow analysis of the flow field but they believe that such data may be necessary for analysis of transient conditions caused by episodic recharge events.

BRIEF SUMMARY OF DOCUMENT:

The purposes of this report were 1) to develop a theory, 2) to contribute to the understanding of partially saturated flow in a fractured porous tuff, and 3) to determine the effects of fractures and the porous matrix on the transient and steady state fluid flow behavior.

The Topopah Spring Member of the Paintbrush Tuff at Yucca Mountain is a densely welded devitrified, nonlithophysal zone. Although these welded tuffs usually have low matrix hydraulic conductivities, the numerous fractures may be highly transmissive. Under saturated conditions water tends to move relatively rapidly along the fractures; for unsaturated conditions the movement tends to be across fractures from one porous block to another. Under unsaturated conditions the small effective area for flow across the fractures restricts the flow from one block to another. The conceptual model used includes fractures of varying widths to account for the small effective area for flow at these points of contact across the fractures between the blocks. Between the fractures the pore sizes of the porous matrix are considerably smaller than the width of the fractures.

Under unsaturated conditions the degree of saturation is dependent upon the size of pores in which the air/water interfaces occur. The pressure difference between the air and water phases also depends on the size of pores in which the interfaces occur. Therefore, a relationship exists between the liquid pressure in a porous media and the degree of saturation. Because the fractures are considerably larger than the pores, a near discontinuity will occur in the capillary pressure-saturation relationships.

The authors state that three basic relationships are required to evaluate the hydrology of a fractured porous medium: 1) the relationship between pressure head (which is less than atmospheric pressure under partial saturation) and fracture saturation; 2) the relationship between pressure head and fracture conductivity; and 3) the proportion of the fracture surface that remains wetted at a particular capillary pressure.

At the time this report was written no data were available on these relationships for the fractured materials in Yucca Mountain.

The authors present a statistical description of a rough walled, variable aperture fracture using an aperture distribution function. The mechanical stress in the rock is brought into this analysis, recognizing that at zero stress the fracture surfaces are in point contact (zero contact area) between the walls. As stress is increased the area of fracture surfaces in contact will increase. A relationship is developed for the saturated conductivity of a variable aperture fracture using the cubic law for flow in a fracture. The tortuosity of flow paths introduced by the flow around contact areas is not taken into account. An equation is developed for a so-called phase separation constriction factor which indicates the degree of connectedness of the water films around the various contact points, assuming a particular geometric arrangement. A gamma distribution is fitted to the aperture measurements and analytical expressions for the fracture relative permeability K_r, saturation S, and effective fracture matrix flow area are developed.

The matrix data used for simulation consisted of laboratory measurements of core samples from various boreholes at Yucca Mountain. These data were supplemented with matrix characteristic curves and matrix relative permeability curves developed by the method of van Genuchten (1980) following a theory of Mualem (1976).

Fracture pattern orientation spacing was measured in borehole cores and from surface mapping. The fracture permeability value used for simulation was obtained from well tests in well J-13; this value is assumed to represent the equivalent fracture continuum. However, the high in-situ conductivity measured in well J-13 may be due to faults and associated fractures in the formation. The saturated hydraulic conductivity value chosen for the Topopah Spring Member is 10^{-2} cm/sec. The authors recognize that hydraulic conductivity is one of the most important coefficients in determining the flow field at Yucca Mountain.

The available data and formulae derived from the aperture distribution were used to calculate the partially saturated hydraulic properties of the fractures as functions of negative pressure head; the data also were used in the computer simulation with the TRUST program. Relationships between the fracture saturation levels, discrete fracture permeability and effective fracture-matrix flow area were calculated as functions of negative pressure head; they are presented graphically. At 100 percent saturation, the permeability of each discrete fracture is approximately eight orders of magnitude greater than the matrix permeability. However, at small suctions in the range of 10^{-1} to 10^{1} m the discrete fracture permeabilities decrease considerably. At a suction of 112 m, fracture flow is negligible and matrix flow dominates. Matrix flow is impeded as it crosses fractures; it is limited by the available area on the fracture surfaces where fluid can be transmitted. The computer program TRUST was modified to consider the flow across the fractures as well as the flow through the porous blocks between the fractures.

The first effort simulated vertical drainage within the Topopah Spring Member. Two vertical fracture sets and one horizontal fracture set partitioned the tuff formation into blocks. The simulation included only one vertical column bounded by four vertical fractures; lateral flow was being allowed between the vertical fractures and the matrix blocks. The available area for flow across the fracture/matrix interface was determined by the fracture saturation level. Initially the system was 100 percent saturated and the pressure distribution was hydrostatic. The constant negative suction head at the lower boundary then induced transient changes in the flow field throughout the tuff column. Five cases of flow were considered with various combinations of fractures, phase separation, and constriction factors with and without the porous matrix.

The results are presented as graphs of pressure head and saturated permeability, effective fracture-matrix flow area and Darcy velocity for various times at different locations in the matrix. Curves of changes in saturation level versus time show that it may take up to one year for saturation to change in the interior of the matrix as a result of a pressure change in the fractures. Such information is useful in planning laboratory experiments. Darcy velocity studies show that when a fracture is saturated, the fluid flow is parallel to the fracture. After the fractures desaturate the fluid velocity in the fractures is essentially zero.

The following statements are made in the summary of the report.

1. The highly transient changes in flow from fully saturated conditions to partially saturated conditions are extremely sensitive to the fracture properties.

2. The ambient steady state flow field of a partially saturated fractured porous tuff system probably can be understood without detailed knowledge of the discrete fracture network properties.

3. Detailed information on fracture network geometry and discrete fracture characteristics is needed to understand fully the responses of a fractured porous system to perturbations such as extreme flood events which may cause transitions between partially saturated and fully saturated conditions.

The authors believe that the basic conceptual model based on the extension of physics of heterogeneous systems to a fractured porous media is sound. Better data and experimental verification will be necessary in some instances to show the validity of certain assumptions.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The report probably is the best conceptual model to date for describing the flow in a fractured porous medium, although it is based on rather limited experimental data. The authors appear to have done an excellent job of developing capillary pressure/conductivity/saturation level relationships for a fractured porous medium. The model should be verified and the assumptions should be validated before the model is used in an actual field situation.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

Few experimental data are available with which to verify the conceptual model. At this point it is not clear how a model such as this would be applied to Yucca Mountain.

REFERENCES CITED:

Mualem, Y., 1976, A New Model for Predicting the Hydrologic Conductivity of Unsaturated Porous Media. Water Resources Research, vol. 12, p. 513-522.

van Genuchten, 1980, A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. Soil Sci. Soc. Am. J., vol. 44, p. 892-898.

WMGT DOCUMENT REVIEW SHEET

FILE #:

DOCUMENT #: SAND84-7212

DOCUMENT: Jacobson, E.A., Freshley, M.D., and Dove, F.H., 1985, Investigations of Sensitivity and Uncertainty in Some Hydrologic Models of Yucca Mountain and Vicinity: SAND84-7212, Sandia National Laboratories, Albuquerque, New Mexico, and Livermore, California, 93 p.

REVIEWER: Williams & Associates, Inc.

DATE REVIEW COMPLETED: April 21, 1986

ABSTRACT OF REVIEW: APPROVED BY: Roy E. Williams

The emphasis of the report under review is directed toward estimating groundwater travel times through the unsaturated zone and the saturated zone in the Yucca Mountain area. The travel time is treated as a random variable and two analytical procedures are used to study it: a first-order approach provides estimates of the mean and variance of travel time based on the assumed mean and variance of one specified input parameter. Secondly a Monte Carlo simulation provides estimates of the mean, variance, and pdf (probability density function) of travel time. The first-order analysis provides a method of studying the sensitivity of travel time to various input parameters. The report uses the word uncertainty throughout. But the word is used incorrectly in a statistical sense. In most cases the word uncertainty in the report should be replaced by the word variation.

BRIEF SUMMARY OF DOCUMENT:

Uncertainty Analysis of Groundwater Travel Time in the Unsaturated Zone

The purpose of the report under review is to investigate the use of statistical methods that relate variations in hydrologic parameters to variations in groundwater travel time. Three statistical methods are used in the report to evaluate sensitivity and uncertainty of input hydrogeologic parameters. These statistical methods are: 1) the perturbation approach to determining sensitivity coefficients, 2) first-order analysis of uncertainty, 3) Monte Carlo approach to uncertainty analysis. Uncertainty is used in the context of a variable that can have a distribution of input values.

The perturbation approach to estimating sensitivity coefficients consists of repeated simulations with a model while varying the input hydrogeologic parameters among simulations. The first-order analysis of parameter variations involves combining the sensitivity coefficients determined by the perturbation approach with parameter variations to relate variations in the input parameters to variations in the estimated water travel times. The Monte Carlo approach is a direct method for relating uncertainty of input parameters to variations in water travel time. The Monte Carlo approach involves generating a large number of "realizations" of input parameters (hydrogeologic parameters) and their spatial distributions, then calculating the corresponding values of groundwater travel time, then determining the mean, variance, and probability density function of travel time as generated by the variations in input hydrogeologic variables.

The report under review presents statistical analyses of water travel time through the unsaturated zone and through the saturated zone in the vicinity of Yucca Mountain. According to the report, a one-dimensional, steady state analytic solution for vertically downward unsaturated flow was used to investigate the effect of water travel time of variations on estimates of percolation through Yucca Mountain. The percolation rate estimate was considered the primary parameter controlling variations in predicted travel time through the unsaturated zone. According to the report, the analysis was used to quantify the possible variations in travel time resulting from variations in the estimates of percolation.

The analytic solution for one-dimensional, vertically downward, unsaturated flow through Yucca Mountain was applied to a simplified geologic profile based on the geologic log of well USW G-4. The hydrogeologic characteristics of the stratigraphic units in the profile were based on data from core samples reported by Peters and others (1984).

According to the report, moisture-retention characteristics, or characteristic curves, were developed by use of Haverkamp's formula (McKeon and others, 1983) for moisture retention. Haverkamp's formula is as follows:

$$\theta \quad \frac{\alpha(\theta_s-\theta_r)}{\alpha+|\psi|\beta} + \theta_r$$

where θ is the volumetric moisture content at pressure head ψ, θ_s is the moisture content at saturation, θ_r is the residual moisture content, and α and β are empirical constants derived from fitting the data. Characteristics curves relating hydraulic conductivity to pressure head for core samples G4-8, G4-12, and G4-13 are presented in figure 7 of the report. These curves were obtained by Haverkamp's formula for unsaturated hydraulic conductivity:

$$K(\psi) = K_s \frac{A}{A+|\psi|^B}$$

where K_s is the saturated hydraulic conductivity, and A and B are empirical coefficients used to fit the unsaturated hydraulic conductivity values.

According to the report, saturation levels based on pressure heads estimated by the analytic solution were matched with saturation levels reported in Fernandez and Freshley (1984) to obtain a partial calibration of the analytic solution. Calibration was attempted by adjusting the estimated percolation rate rather than the measured hydraulic properties of the tuff. According to the report, a percolation rate of 0.02 cm/yr gave the best calibration. According to the report, a percolation rate of 0.02 cm/yr and the resulting distributions of pressure head and saturation levels were assumed to represent the baseline case for the uncertainty analysis. The total travel time from the proposed repository depth to the water table for the baseline case was estimated to be 2.17×10^8 years.

A sensitivity analysis and a first-order analysis of the effect of variations in percolation rate were performed by the authors of the report. According to the report, variations from the baseline percolation rate of 0.02 cm/yr ranging from +0.015 cm/yr to -0.015 cm/yr were used to investigate the effect of the magnitude of perturbations in the input parameter on the resulting sensitivity coefficient. The report indicates that calculation of the sensitivity coefficient converges to -1.03×10^7 near 10^{-3} cm/yr perturbation of the percolation rate.

The first-order analysis of percolation variations and their effects was performed with an assumed (no field data were used) range of percolation through Yucca Mountain. The upper bound on the range of percolation was assumed to be 0.1 cm/yr. The lower bound for the range of percolation was determined to be 3.0×10^{-3} cm/yr. According to the report, these values were obtained from the graph of travel time versus perturbation of recharge. The procedure is not clear.

The authors of the report used natural logarithms of the values because the assumed distribution of percolation values was not symmetric about the mean. The authors of the report assumed that the estimates of percolation are log normally distributed; this assumption forces the distribution of log percolation values to be symmetrical, i.e., a transformed normal distribution.

Table 6 of the report presents a range of percolation estimates for the first-order analysis. The authors of the report assumed that 1.61 (the smaller of the two differences in table 6) represents a multiple of the standard deviation. According to the report, if 1.61 is assumed to be three standard deviations of the log percolation flux, the resulting variance in standard deviation of travel time are 1.42×10^{10} yr^2 and 1.19×10^5 years, respectively.

A first-order analysis of travel time based on hydraulic conductivity variations was performed by the authors to compare variations in travel time resulting from variations in hydraulic conductivity with that caused by variations in percolation through Yucca Mountain.

According to the report, a wide range of variations to a baseline hydraulic conductivity of 0.06 cm/yr was used to determine the sensitivity coefficient for travel time with respect to hydraulic conductivity. Table 8 of the report lists the travel times and sensitivity coefficients associated with variations of the hydraulic conductivity. According to the report, the sensitivity coefficient appears to converge near -1.76×10^5 yr^2/cm at small variations of hydraulic conductivity. The lower limit of hydraulic conductivity was assumed to be equal to the assumed baseline percolation flux of 0.02 cm/yr. The upper limit of hydraulic conductivity was assumed to be one order of magnitude higher than the assumed baseline hydraulic conductivity.

Table 9 of the report lists the range of saturated hydraulic conductivities used the first-order uncertainty analysis. According to table 9, differences between the natural log of saturated hydraulic conductivity are 1.082 and 2.302. According to the report, if 1.08 is assumed to be three standard deviations of the log saturated hydraulic conductivity, the resulting variance and standard deviation of travel time are 1.5×10^7 yr^2 and 3.88×10^3 years, respectively. It is not clear why 1.08 was used in this calculation. The conservative choice (for travel time) would be the difference between baseline and the larger hydraulic conductivity (i.e., 2.302) rather than 1.08.

According to the report, the variances of travel time indicate that variations in the estimates of percolation through Yucca Mountain contribute more to variations in travel time than variations in saturated hydraulic conductivity for the range of values considered. The report indicates also that travel time is influenced more by the percolation rate than by saturated hydraulic conductivity of the lowermost layer of the profile.

Uncertainty Analysis of Groundwater Travel Time in the Saturated Zone

The authors of the report used the Monte Carlo and first-order analysis techniques to calculate the variations in groundwater travel time caused by variations in transmissivity and effective thickness (effective porosity times the thickness of the zone producing the water).

To estimate groundwater travel time from the proposed repository in Yucca Mountain to the accessible environment (defined at a distance of 10 km from the repository), the authors considered seven pathlines extending from the vicinity of wells USW G-1 and USW H-3 to an area just south of well J12. The variation in groundwater travel time was calculated for seven different cases in which the hydrogeologic information was varied. According to the report (p. 44),

> The various combinations of hydrologic parameters were chosen in order to investigate the effect on travel time uncertainty of 1) the use of simulated hydraulic heads from the aquifer parameters versus a fixed distribution of hydraulic head that may not reflect a mass balance solution for the flow system, 2) the representation of effective porosity by either one value over the entire flow domain or differing values in selected zones to allow for spatial variability, and 3) the treatment of the effective porosity as a deterministic parameter (known values with no uncertainty) or a random parameter. In all seven cases, transmissivity was treated as a spatially varying, random parameter.

Two models of the spatial variability of effective porosity were considered to investigate the effect of variations in effective porosity on travel time uncertainty. In the first model, the effective porosity was assumed to be a spatial variable having one probability distribution over the entire study area. In the second model, the effective porosity was assumed to have a distinct probability distribution in each zone of different transmissivity. Effective porosity was assumed to be distributed normally.

The authors of the report calculated the variations in groundwater travel time for the first three cases using the first model of effective porosity. For each of the groundwater flow simulations a new, uniform effective porosity was used to calculate travel time. Based on the Monte Carlo analysis for Cases 1 and 2 and this model of effective porosity, the authors of the report conclude that use of the USGS-interpreted hydraulic heads leads to an "over estimation" of groundwater travel time. However we do not believe that this is a safe conclusion. The Monte Carlo technique may be an underestimate of groundwater travel time. According to the report, the comparison of the magnitudes of the sample means of groundwater travel time for Cases 1, 2, and 3 shows that when the USGS hydraulic head interpretation was used (Case 1), the travel times were four times larger than when consistent hydraulic head data were used (Cases 2 and 3). A sensitivity analysis and first-order analysis were conducted for Cases 2 and 3 using the first model of effective porosity. According to the report, a sensitivity analysis and first-order analysis were not conducted for Case 1 with the USGS hydraulic heads because the authors do not consider Case 1 to be representative of the flow system.

Table 16 of the report presents values of mean, standard deviation, and coefficient of variation of travel time obtained from Monte Carlo and first-order analysis for Cases 2 and 3 using the first model of effective porosity. Table 16 shows that the first-order analysis provided lower estimates of the mean and standard deviation compared to those determined by the Monte Carlo approach for Cases 2 and 3. The mean travel times calculated by the Monte Carlo and first-order analysis approaches vary from 760 to 920 years.

An analysis was performed for four cases assuming locally stationary effective porosity (termed spatially varying effective porosity in the report). The authors of the report calculated variations in groundwater travel time for Cases 4, 5, 6, and 7, in which the probability density function (pdf) of effective porosity varied in the different zones near Yucca Mountain. The Monte Carlo analysis with spatially varying (Model 2) effective porosity was performed for Cases 4 through 7. The authors of the report performed a sensitivity analysis for Cases 6 and 7. According to the report, Cases 4 and 5 were not analyzed because they used hydraulic heads that were not completely representative of the groundwater system. A first-order analysis also was performed for Cases 6 and 7. Table 19 of the report presents estimates of mean, standard deviation, and coefficient of variation for travel times calculated from the Monte Carlo and first-order analyses. According to the report, the fact that the coefficients of variation obtained from the first-order analysis are smaller than the values calculated from the Monte Carlo approach indicates that the first-order analysis underestimates the travel time uncertainty. However, this conclusion assumes that the Monte Carlo approach was correct, valid, and rigorous, which is somewhat ridiculous. The mean travel times calculated by the Monte Carlo and first order analyses range from 990 to 1,090 years.

SIGNIFICANCE TO NRC WASTE MANAGEMENT PROGRAM:

The report under review presents hypothetical analyses of travel time in the unsaturated zone and in the saturated zone in the vicinity of Yucca Mountain. The purpose of the report was to "demonstrate methods that relate uncertainty in hydrologic parameters to variations in groundwater travel time." The report is significant with respect to the NRC Waste Management Program because it presents the types of analyses that may be used to define groundwater travel times at all potential repository sites.

PROBLEMS, DEFICIENCIES OR LIMITATIONS OF REPORT:

Unsaturated Zone:

A reliable and realistic baseline value for percolation rate or for saturated hydraulic conductivity is critical to the first-order sensitivity and other analyses because sensitivity coefficients and travel time variances depend directly on these baseline values (see table 5 and table 8). The results of a study that would alter the baseline values and recalculate sensitivity coefficients and travel time variances would be interesting. We suspect that little difference would be observed in the sensitivity coefficients (probably less than an order of magnitude) and that a moderate difference would be observed in the travel time variances primarily due to the assumption that percolation rate and hydraulic conductivity are lognormally distributed.

In using a realistic range of values to select a standard deviation of the percolation rate, the difference between the upper limit and the baseline value was chosen apparently to coincide with a conservative (short) estimate of travel time (p. 32). If this is the case, then why is the difference between the lower limit and the baseline value chosen for the hydraulic conductivity (p. 36)? If conservatism is not the issue and the smaller difference was selected arbitrarily for both percolation and conductivity, then it should be noted that by selecting the larger difference to control standard deviation, the resulting standard deviation in travel time is increased by approximately one-half order of magnitude.

If percolation rate (q) is assumed to be lognormally distributed, then the distribution of ln(q) is a normal distribution (symmetrical, bell-shaped). In order for ln(q*) to be the mean of this normal distribution, the value of q* must equal the median (not the mean) of the raw percolation (q) distribution. Thus, the baseline value of percolation rate, 0.02 cm/yr, must be considered the median percolation and not the mean percolation, as implied by the authors. The same comments apply to hydraulic conductivity.

A Monte Carlo simulation was not conducted for the unsaturated zone. Derivations for the first-order analysis given in Appendix B appear to be valid.

Saturated Zone

The groundwater flow system in the Yucca Mountain area is modeled as an unlayered aquifer with regional flow in a southerly direction. Input parameters that are treated as random variables in estimating groundwater travel time are the transmissivity and effective porosity. Transmissivity is assumed to be lognormally (base 10) distributed and locally stationary in four areal zones and to be constant in three other zones (see table 11, p. 48). Effective porosity is assumed to be normally distributed and locally stationary in the same four areal zones mentioned above (see table 12,, p. 51). The mean value of log T (transmissivity) is calculated incorrectly, as was the case for lognormal variables studied in the unsaturated zone. The logarithm (base 10) of the median, not the mean, transmissivity is equal to the mean of the normal distribution of log T (see p. 47).

The information presented in fig. 16 (p. 49) and fig. 18 (p. 53) actually corresponds to a test of the psuedo normal random number generator used by the computer in the Monte Carlo simulation. Very rarely will 100 simulated values stabilize about mean zero with the desired standard deviation. However, as stated on p. 48, the goal of the study is not to provide definitive results but only to demonstrate the use of the procedures. Along these same lines of thought, it is not correct to state that "... 100 realizations were not sufficient for the statistics to converge to their final value" (p. 67). There is no such thing as a final value in a Monte Carlo simulation; the result is a reasonably small range of values about which the results of the simulation will stabilize.

Uses of the terms "uniform" and "spatially varying" throughout the latter parts of the report are confusing. A much better approach would rely on terms such as globally stationary or globally constant versus locally stationary or locally constant. A random variable such as effective porosity is considered to be globally stationary if its pdf is the same throughout the entire area of study. One that is locally stationary would have a constant pdf only over a zone within the study area, such as Zones 1, 2, 3, and 4 for the Yucca Mountain study.

We question the physical validity of assuming perfect correlation between effective porosity and log transmissivity (p. 53), induced by using the same random number to sample from the effective porosity distribution and the log T distribution in a given Monte Carlo pass. We realize this assumption is made to elicit an effect in the estimated travel time variation, and thus must be considered as the limiting case. In reality, effective porosity sometimes may be correlatable to transmissivity but only for specific, homogeneous materials at one scale of testing. The relationship between effective porosity and transmissivity for one material certainly cannot be applied to any other material. A new relationship must be developed for each material and the material must be homogeneous.

The statement is made in several places that the first-order uncertainty analysis underestimated the mean and standard deviation of travel time. It is not valid to say that a given method underestimates a parameter when its true value is not known. The first-order analysis provides lower parameter estimates than Monte Carlo, but even a rigorous Monte Carlo analysis (p. 70-71) can provide only an estimate of the travel time distributions that might be possible. Monte Carlo methods incorporate more variety in possible conditions and allow for multiple interaction of different random variables. For this reason, the technique is considered to provide a more realistic representation of the physical system. However, results from most Monte Carlo models are quite sensitive to spatial correlations in separate random variables and to interdependencies between random variables. Thus, simulation procedures and interpretations of results must be tempered with common sense and professional judgment about the conceptual model and the prototype.

Monte Carlo methods can be used to indicate which parameters are contributing most to output variations. All parameters are held constant except the one of interest, and the simulation is conducted. The procedure is then repeated for each input parameter to be considered. The outcome from all of the simulations are compared to see how the resulting pdf's reflect the sensitivity of the dependent parameter (in this case travel time) to each of the input parameters. This issue is discussed on p. 71.

SUGGESTED FOLLOW-UP ACTIVITIES:

Probabilistic approaches to estimate groundwater travel times at proposed repository sites are in their infancy. We recommend that all similar documents be reviewed in detail so that the NRC can maintain records of the most useful and valid methods for estimating groundwater travel time. We recommend also that the NRC research the importance of scale of testing on the distributions of input parameters. Papers of the type reviewed herein illustrate the fact that scale of testing is becoming more and more important to stochastic models that predict distributions of groundwater travel time. In addition, the meaning of the word uncertainty should be clarified. It is not used correctly in this report.

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