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REVIEW OF MODELING EFFORTS ASSOCIATED WITH YUCCA MOUNTAIN, NEVADA

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The Nevada Agency for Nuclear Projects/Nuclear Waste Project Office was created by the Nevada Legislature to oversee federal high-level nuclear waste activities in the state. Since 1985, it has dealt largely with the U.S. Department of Energy's siting of a high-level nuclear waste repository at Yucca Mountain in southern Nevada. As part of its oversight role, NWPO has contracted for studies of various technical questions at Yucca Mountain.

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SUMMARY

Detailed comments are presented on five modeling investigations related to the NNWSI at Yucca Mountain, Nevada. Some comments are common to the five reports reviewed. In general, the quality assurance/quality control (QA/QC) procedures of the modeling efforts are considered to be poor. The reports reviewed indicate model documentation and verification/validation is lacking. Many of the technical assumptions underpinning the theory of the models are not supported by observed field conditions and may be inappropriate for application to the Yucca Mountain flow system. Much of the data is assumed and not field measured. Many of the problems simulated have insufficient information provided to allow reproduction of the computed results. Finally, the accuracy of some of the results is questionable, and lack confidence because good QA/QC procedures, such as mass balance calculations, are not performed or reported with the computational results. The review of these five reports underscores the apparent lack of coordination between field investigations and the overall modeling efforts which will be used to support the licensing proceedings via travel time calculations. For example, some model assumptions used in these reports are not supported by the compiled field observations or cannot be technically justified because the characterization program has yet to collect a particular type of field information.

INTRODUCTION

This report consists of a review of the following five modeling reports associated with the NNWSI at Yucca Mountain, Nevada. The reports reviewed include:

Klavetter, E.A., and R.R. Peters, 1986. Fluid Flow in a Fractured Rock Mass, Sandia Report SAND85-0855.

Wang, J.S.Y., and T.N. Narasimhan, 1984. Hydrologic Mechanisms Governing Fluid Flow in Partially Saturated, Fractured, Porous Tuff at Yucca Mountain, Lawrence Berkeley Laboratory Report LBL-18473.

Lin, Y.T., 1985. SPARTAN - A Simple Performance Assessment Code for the Nevada Nuclear Waste Storage Investigations Project, Sandia Report SAND85-0602.

Peters, R.R., J.H. Gauthier and A.L. Dudley, 1986. The Effect of Percolation Rate on Water-Travel Time in Deep, Partially Saturated Zones, Sandia Report SAND-0854.

Pruess, R., Y.W. Tsang, and J.S.Y. Wang, 1984. Numerical Studies of Fluid and Heat Flow Near High-Level Nuclear Waste Packages Emplaced in Partially Saturated Fractured Tuff, Lawrence Berkeley Laboratory Report LBL-18552.

As part of the review procedure, the following points are addressed for each report:

(1) The particular analytic solution and its assumptions,

(2) The minimum and the optimum data bases for application, and

(3) The technical appropriateness of the actual model application.

Review of Klavetter and Peters (1986)

This report summarizes the mathematical basis for the code used in TOSPAC (see also the review of Peters, Gauthier and Dudley, 1986) for simulating flow in the unsaturated zone at Yucca Mountain, and estimates the relationships of capacitance coefficient (related to storage) versus pressure head, and hydraulic conductivity versus pressure head, for the hydrologic units in the unsaturated zone. A key assumption in the code formulation is that pressures are the same in the matrix and the fractures along any horizontal plane (perpendicular to flow). This assumption may not be valid. Another important basis of the report is the characterization of the fractures; estimated hydraulic conductivity of the fractures is probably incorrect.

The equations used to model the flow are based on separate mass balance equations for water in the rock matrix and in the fractures. A simple linear equation relates the flux between the two media to pressure head differences. Supporting arguments for this formulation are made based upon results of modeling by Travis et al. (1984) and by Martinez (in preparation at this writing). Neither of these reports were available for review. The argument is based on the high pressure gradient that would result upon initial saturation of a fracture located adjacent to a matrix of high moisture tension. There is little doubt that high tensions are present in the tuffs. Both in-situ measurement and measurements from cuttings in USW UZ-1 provide this information (Parviz Martinez, U.S. Geological Survey, personal communication, 1984).

The modeling of both Travis et al. and Martinez apparently assumed a fracture width of 100 micrometers. Mineral coatings on fracture walls are evident in drill cores at Yucca Mountain. The models do not consider effects of these mineral coatings; therefore, they predict the water is quickly sucked into the matrix. If the fracture coatings are of lower permeability than the matrix, the rate of removal of water from the fractures would be decreased, and water would travel further in the fractures. In addition, the amount of water placed in the fracture by Travis is small. A 2.54 cm (1-inch) rainfall on a 1 m^2 surface containing 10 fractures of 1 m length and 100 micrometer width could provide enough water to saturate each fracture to a depth of 25.4 meters (rather than the 2 m depth used by Travis et al.), albeit most of the water would run off. One-inch rainfalls are not that rare, and the water that runs off would be diverted to stream valleys, which typically form in the presence of fracture zones. Thirdly, the vast majority of fractures at Yucca Mountain have apertures less than 100 micrometers. Fractures with larger apertures are also present. These aperture widths are apparent in TV logs of the drill holes, and from results of hydraulic testing of fractured, welded tuffs in the saturated zone. Larger fracture aperture produces a more rapid flow in the fractures, resulting in more water required to be sucked from the fracture to desaturate it, and in general, increasing the importance of fractures in the unsaturated zone.

Tunnels in Rainier Mesa encounter fractures that transmit water. The rock types are similar to those at Yucca Mountain, but welded (fractured) tuffs are less common at Rainier Mesa. Rainier Mesa is also wetter, as indicated by a Pinon-Juniper community at Rainier Mesa, compared with desert scrub species at Yucca Mountain. Isotopic and chemical data indicate a short residence time for water in fractures in the tunnels (refer to the work of Clebsch and Jacobson). While the Rainier Mesa setting is different, it may provide data for validation (or nonvalidation) of some of the proposed models at Yucca Mountain.

Following the assumption that the pressures in the matrix and the fractures are equal, the two mass balance equations are added together. The resulting equation uses bulk properties for the combined matrix-fracture system. At the recharge rates assumed for Yucca Mountain, the properties of the fractures become unimportant for the combined system, and the matrix properties control the results of the calculations. While the combined system will still respond as a fractured system at high recharge rates, the combined equations may overestimate the amount of recharge required to initiate flow in fractures because of the high storage in the matrix and the presence of fracture coatings.

The combined equation is expanded to allow for the determination of hydrologic properties. In general, the effects of changes in saturation of the matrix and fractures were much more important in determining the capacitance coefficient (analogous to an aquifer storage term or heat capacity term) than were compressibility effects of the water, matrix, or fractures.

The hydraulic conductivity (as a function of pressure head) was estimated in two different ways. The first is by addition of estimated hydraulic conductivity versus pressure curves for the matrix and fractures. The curve for the matrix material is estimated using an empirical relationship derived for unconsolidated materials. The use of this equation for consolidated tuffs is unproven. The curve for the fractures is apparently based on the concepts of the degree of connection of water in the fracture as a function of saturation. Because of the potential significance of fracture flow and its effect on travel-time calculations, experimental confirmation of the fracture hydraulic conductivity-pressure relationship is essential.

The second technique used to estimate the hydraulic conductivity-pressure relationships is based on capillary tube theory. Both the fractures and the pores in the matrix were assumed to be representable by capillary tubes. Pore-size distribution for the matrix was determined from mercury intrusion porosimetry. Aperture distribution for the fractures was estimated from permeability values, and may be based on incorrect values (discussed below).

Both techniques yield similar curves. Both assumed the same saturated conductivity, so that the estimated values also should be similar. As both techniques were developed in the field of soil physics, and the parameters used in the first, empirical method are affected by pore-size distribution (the basis of the second method);

it would be surprising if results were greatly different. However, neither may be correct in application to fractured rock.

The saturated conductivities used to develop the conductivity-pressure curves, and reported (calculated) in Table 1, are not consistent with the data. For example, Thordarson (1983) reported saturated hydraulic conductivities for densely welded Topopah Spring in J-13 of about 1 m/day (1.1×10^{-5} m/s). Similarly, Weeks (as reported by Montezer and Wilson, 1984) reported values of densely welded Topopah Spring from 0.4 to 10 m/d (4.9×10^{-6} to 1.1×10^{-4} m/s). Table 1 lists bulk fracture conductivities ranging from 0.69×10^{-9} to 3.1×10^{-9} m/s for the same rocks. The values measured in-situ are approximately four to five orders of magnitude higher than those used in the calculations. This casts doubt on all calculations dependent on the fracture conductivities, and on fracture apertures and porosities.

<ins>Summary</ins>. The development of the simplified equations is an attempt to enable groundwater flow and transport calculations to be made more quickly and easily so that their results may be coupled with other models for performance assessment of the waste package-engineered barrier-host rock system. Such simplification is probably necessary. However, the resulting simplification contains assumptions that have not been adequately field tested, and that are not yet supported by limited in-situ observations. The empirical equations and theories used to develop the conductivity to pressure relationship have not yet been shown to agree with experimental results. In addition, the saturated hydraulic conductivity values used for the Topopah Spring do not agree with measurements; other values should be checked with measurements as well. The code is one-dimensional, and therefore does not agree in concept with the conceptual hydrologic model proposed by Montezer and Wilson (1984), where lateral flow to the structural discontinuities provides an important mechanism for moving water through the unsaturated zone at Yucca Mountain.

Much remains to be learned about moisture movement in the unsaturated zone at Yucca Mountain. More experimentation is needed on the role of fractures (including their mineral coatings), and detailed observations made during construction of the exploratory shaft and related drifts will be needed to substantiate modeling results.

Review of Wang and Narasimhan

Code. Wang and Narasimhan (1984) applied the code TRUST, which is based on the integrated finite-difference method (IFDM), to simulate vertical drainage in a fractured tuff column. The code version used was an updated version of the one cited by Narasimhan et al. (1978). The validation/verification of the code version used for this document is unknown and the code's capability to calculate mass balance is not mentioned in the report.

Major Assumptions. The major assumptions associated with the code and application include:

(1) The flow domain can be represented by contiguous nested elements. Interfaces between nested elements represent fracture planes. The nested elements are basically a one-dimensional approximation of the storage effect in the matrix. It is not clear from the information given in the document whether fluid is allowed to pass through the nested elements.

(2) The relationship between fluid pressure head and fracture saturation is governed by a van Genuchten (1980) curve which is based on the work of Mualem (1976) as well as the phase separation constriction factor and mean noncontracting aperture.

(3) The relationship between fluid pressure head and fracture conductivity is governed by the phase separation constriction parameter, mean noncontracting aperture, and an empirical relationship based on Mualem's theory.

(4) The proportion of the fracture surface that remains wetted is governed by asperities, stress level, and phase separation constriction parameters.

(5) The cubic law is valid.

These assumptions, particularly 2 through 4, are based on theoretical speculation. The authors conceded that, to date, there exists no data from Yucca Mountain to validate their theories. The fifth assumption has been experimentally shown recently by Gale et al. (1985) to be invalid in some situations.

There may be many other assumptions employed in the code TRUST; however, the code, according to the report, has no documentation except for the paper published by Narasimhan et al. in 1978. The updated documentation is not mentioned in the report.

Data. The TRUST code requires a variety of data. In the report, data from the Topopah Spring member were employed. These data were provided in a memorandum from the Sandia National Laboratory (Hayden et al., 1983). Supplementary data were obtained from the literature. Parameter values needed for simulations were not available and were derived using the theoretical deviations given in the report. The SNL memorandum and other literature (USGS reports and minutes of meetings) are not readily available to us. Problem areas with the data include:

(1) Fracture data from well USW-G4 were presented in the report. There is no indication that the representative elementary volume exists.

(2) Fracture characteristics curves were assumed to take the forms similar to those in porous media. Information presented in various petroleum engineering references indicates that this may not be the case.

Application. A test case was set up to simulate fluid flow in partially saturated, fractured, and porous tuff. Simulations of vertical drainage within the Topopah Spring member were performed. Two vertical and one horizontal fracture sets were assumed. The matrix block size and fracture apertures (horizontal and vertical) were assumed to be uniform. It should be noted that the aperture distribution is supposed to be of a gamma type. Not all the details of numerical simulations were given. Examples are time-step sizes and stability criteria.

Some of the simulation results appear to be physically impossible. An example is in Figure 11 (p. 34) in which pressure drop versus time along fractures and inside the solid matrix is reported. It is interesting to see that pressure drop versus time at two points of the same elevation, one inside the solid matrix and one in a fracture, is identical.

This observation implies either that:

(1) there is a conduit between the above two points or, more importantly,

(2) the model cannot simulate the drainage process realistically.

Another example is the calculated zero Darcy velocity in horizontal fractures when the phase separation constriction factor is between 0 and 1 (curves c and d, Figure 15a) and when the phase separation constriction factor is 1 (curve d, Figure 15b). The results do not seem to be physically possible.

Summary. The authors have presented an analysis of variably saturated flow in fractured porous tuff. The conceptual model is based on theoretical speculation with idealized fracture configurations. The model has not been verified experimentally. The code TRUST, which embodies the theoretical development presented in the report, has never been documented, benchmarked or verified. Some of the simulation results do not seem to be physically possible, suggesting the theoretical model itself is not viable.

Review of Lin (1985)

Code. Lin (1985) used the code SPARTAN, which, as the title states, is a simple performance assessment code for the NNWSI. It simulates one-dimensional, dispersionless transport of radionuclides in a multiple-flow-path, homogeneous, geologic medium with sorption in a constant-velocity field. As such, it would be ideal for use in probabilistic modeling; however, it was not used that way in this paper.

On page two, the author states, "It is not the intent of this report . . . to formally document and verify SPARTAN." Unfortunately, no references are provided where this is formally performed. The code does not have a mass balance.

Major Assumptions. The assumptions underlying the model are presented in a Sandia Report SAND 84-1492, which we do not have. Briefly, however, they appear to be:

(1) Total repository area is 6.07×10^6 m^2.

(2) Repository contains 70,000 metric tons of heavy metal spent fuel 10 years out of reactors and emplaced simultaneously.

(3) No waste will dissolve or leach from the emplacement location until the spent fuel is 360 years old.

(4) No thermal effects are considered.

(5) Dispersion is neglected.

(6) The medium is considered homogeneous.

(7) Velocity is constant.

Some of the above assumptions (1-3) concern the source term and are not mathematical in nature. Therefore, no criticism is offered. The final four assumptions (4-7) are not realistic, and any computed results should be viewed with these assumptions in mind.

Data. The author states on page 2, "This simple approach has been taken to estimate radionuclide migration in geologic media because many of the data and parameters needed to simulate a more detailed physical process are not available at this time." Data that are used in the simulations consist of lengths of flow paths (distance to water table 150 - 250 m), sorption values (provided in his Table 2), assumed effective porosities (ranging from 0.001 to 0.2), and water velocities (ranging from 2.5×10^{-3} to 5×10^{-3} m/y). There is no supporting justification for the values used. The uranium solubility used is 4×10^{-4} kg/m^3. Initial inventories are given in his Table 1.

Application. Two cases are considered: problem 1 uses a flux of 0.5 mm/yr whereas problem 2 uses a flux of 5 mm/yr. The flow path from the repository to the accessible environment is vertically downward through the unsaturated zone to the water table, which is considered to be the accessible environment. Three flow paths are considered, defined by different flow lengths and velocities.

The results are compared to an analytical solution. The main conclusion is that the comparison is good and that SPARTAN can be used for these types of applications.

Summary. The code presented is very simplified and should not be used in a deterministic study. Because it is simple, it can be used in a probabilistic analysis in a cost-effective manner. The results, however, should be carefully scrutinized because of the underlying model assumptions.

Review of Peters, Gauthier, and Dudley (1986)

Code. Peters et al. (1986) use a one-dimensional code called TOSPAC. It is a dual porosity, continuum model for simulating variably-saturated flow in a fractured, porous medium. Only the final equations are presented, with no discussion of the solution technique. The code does not account for radionuclide transport.

There was no indication of verification/validation. Also, there was no discussion that the code calculates a mass balance, which is needed to evaluate the technical appropriateness of the model application.

Major Assumptions. The major assumptions associated with the code and application include:

(1) Flow is one-dimensional. The percolation rate is the same in each unit and no lateral water diversion occurs at unit interfaces.

(2) Vapor transport is not considered; therefore, upward movement of water vapor is not included in the mathematical model.

(3) Darcy's equation is valid.

(4) Pressure heads in the fractures and the matrix are identical in a direction perpendicular to the flow lines.

(5) A unit change in the quantity "total saturation times pressure head" at a point causes a unit change in the local stress field.

(6) Bulk rock consolidation results in vertical displacement.

(7) For the problems considered, steady-state flow is assumed.

The assumptions listed above idealize the flow problem at Yucca Mountain. For example, lateral diversion of water at the interfaces between units is thought to occur. Therefore, flow is not one dimensional. Also, the upward movement of water vapor at Yucca Mountain may be a significant mechanism for water movement. Although Darcy's equation is probably appropriate for flow in the matrix, it has not been established that it is appropriate for flow in the fractures. Many of the remaining assumptions are required to support the one-dimensional flow assumption and are not supported by data and observations at the Yucca Mountain site.

Data. Much of the data used in the simulations is referenced to a Sandia Report SAND 84-1471, which we do not have. The data are summarized in Table 1 of their report. Problem areas include:

(1) Residual saturations for the various units range from 0.2 percent to 11 percent. It is not clear how these were determined but they seem low.

(2) The saturation versus pressure head and hydraulic conductivity versus pressure head relationships are based on soil literature. The appropriateness of these relationships for rock has not been demonstrated. Also, it is not clear how the curve fitting parameters in these relationships were determined.

(3) The saturated bulk rock hydraulic conductivity values for the Topopah Spring do not agree with field measurements, and are probably wrong for other units as well. The values used in the report are 4 to 5 orders of magnitude too low.

Application. Six different steady-state cases were simulated where the percolation rate was varied from 0.1 to 4.0 mm/yr and properties of one unit of tuffs were varied from vitric to zeolitized. The objective was to see how fast water traveled through the tuffs and under what conditions flow occurred in the fractures. Conclusions are (p. i) "current estimates of the percolation rate result in water movement confined to the matrix and that the water-travel time from the repository to the water table is on the order of hundreds of thousands of years. This result is sensitive to the percolation rate; an increase in percolation rate of a factor of 10 may initiate water movement in the fractures, reducing the travel time significantly."

These conclusions are valid only for the conditions assumed in the simulations. Recall that transient pulses of recharged water are not considered in the model. Also, lateral water diversion at unit interfaces and subsequent flow down fractures is not considered. Both of these phenomena will affect water travel time. In addition, the use of Darcy's equation with the relative hydraulic conductivity may underestimate flow in the fractures compared to mathematical formulation in terms of two-phase flow, where additional equations for the air phase are included. Finally, sensitivity analysis on rock properties should have been performed. Of special concern is the saturation at which fracture flow begins. The assumed transition point is not supported by field observations or measurements.

One of the more important modeling parameters, the rate of recharge, has not been measured. There is danger that the "current estimates of the percolation rate" are based on a desire that the fractures not carry water, for if they do, travel times will be much shorter than if the matrix transmits all the water. DOE is postulating a percolation rate of less than 1.0 mm/yr, and probably less than 0.2 mm/yr. At present, this argument is based on measurement of high tensions in the matrix, and the assumption that the fractures therefore cannot be transmitting water. This is probably true for the small aperture fractures. However, larger fractures, especially those with mineral coatings, may transmit water quickly without greatly affecting the saturation of the matrix.

<u>Summary</u>. The authors have presented an interesting analysis, within the limits of their assumptions. It represents a first step. Sensitivity analysis is required, as well as further developments to

the code to allow more realistic assumptions. Also, model verification/validation should be presented. The results point out that the steady-state pressure-head solution is a function of percolation rate, characteristic curves, the conductivity, and the pressure head boundary conditions. Accurate estimates of travel times, therefore, require that these data be collected at Yucca Mountain. Detailed review of the site characterization plan should be performed to insure the appropriate field activities are conducted to compile in-situ information under these categories.

Review of Pruess, Tsang and Wang (1984)

Code. Pruess et al. (1984) apply the code TOUGH to two hypothetical cases. The TOUGH code is a numerical model based on the integral finite difference method, where nonlinearities are treated using Newton-Raphson iteration. It considers fluid flow and heat transport in a partially-saturated medium. It does not account for radionuclide transport.

The extent of verification/validation is unknown, but some results are presented in a symposium proceedings. The review team does not have access to these proceedings. Also, there was no mention that the code calculates a mass balance.

Major Assumptions. The major assumptions in the code and application include:

(1) Neglect gravity and infiltration effects,

(2) Darcy's law is valid and generalized relative permeabilities can be used,

(3) Waste packages are infinite in extent,

(4) Fractures are horizontal and infinite in extent,

(5) Two-dimensional r-z symmetry exists, and

(6) Most data can be assumed.

Many details of the problems simulated are not provided so that reproduction of the results would be difficult. For example, it is not clear what heat source was used to generate temperatures. Most of the assumptions listed above are not justified. Obviously, gravity and infiltration effects are important at Yucca Mountain and should be included. The fracture pattern at Yucca Mountain contains more vertical than horizontal fractures, so that the assumption that they are horizontal and infinite is inappropriate and highly idealized. The assumption about cylindrical symmetry also is inappropriate. This assumption affects boundaries and boundary conditions, which they assume are constant at some distance. There will obviously be a pattern of canisters that will disrupt cylindrical symmetry and will cause changes at the boundaries. It is also obvious that the canisters will not extend to infinity. The assumption concerning data is discussed in the next section.

Data. The TOUGH code requires a variety of data, much of which appears to be assumed or attributed to Keith Johnstone (personal communication, 1983). Therefore, the data used are difficult, if not impossible, to substantiate. Most of the data are summarized in Table 2 of the report, and are not repeated here. These values are supposed to represent the densely welded, devitrified, non-lithophysal zone of the Topopah Spring Unit of the Yucca Mountain tuffs. Problem areas with the data include:

(1) A residual (immobile) saturation for water is assumed to be 1 percent. There is no justification for such a low number. In many geothermal and petroleum applications, values of 30 percent are commonly used. This low number is also not supported by the observed (also used as initial) saturation of 80 percent.

(2) In both cases, the problem is linearized by assuming a linear relationship between pressure and saturation. This is probably not true and has a large influence on the computed results.

(3) Relative permeability vs. saturation are simplified and idealized using formulas from the soils literature. There is no evidence that these formulas are valid for rock. These relationships have a strong influence on the computed results.

(4) The matrix porosity is assumed to be 10.3 percent and that for the fractures is 20 percent. These values are not supported and that for the fractures appears to be unrealistic.

Application. The authors state (p. 9) that a single porosity approach may be of limited utility; however, justification for this approach is its computational simplicity. The applications are designed to support this approach by comparing results from the single porosity approach with those from an approach that considers porous blocks with discrete fractures. Unfortunately, only two hypothetical problems are simulated with no sensitivity analysis on equation parameters. For the cases considered, the two approaches give similar results. The authors attempt to generalize their results by stating (p. 20), "The results presented in this report suggest that fracture effects on a regional scale can be adequately handled by means of equivalent continuum models . . . ." This statement is only true for the limited cases considered. There was no sensitivity analysis performed, especially on nonlinear properties such as the characteristic curves. With more realistic data, it is not clear how well the two approaches would compare.

Based on the applications, the authors further conclude that (p. 16), " . . . with liquid immobile in the fractures at all times, it appears that the role of the fractures is solely to provide a high-permeability pathway for gas phase flow, while having no effects on liquid flow." Also, (p. 17), " . . . with liquid mobile in the fractures, the role of the fractures is to provide high-permeability pathways for both the liquid flow and the gas flow while the matrix acts as the fluid source." Again, these conclusions are only true for the cases considered. If a sensitivity analysis had been performed using more realistic data, these conclusions probably would have changed.

Summary. Because of the unrealistic assumptions, and the assumed simplified data and computational approach, the results of this modeling exercise are hypothetical and have little applicability to the Yucca Mountain site. In addition, because no sensitivity analysis was conducted using realistic data, problem geometry, and boundary conditions, even these hypothetical results are suspect.

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