ANALYSES OF DATA BIAS:
A Follow On Report Based On Presentations
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By

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Introduction

The following information is with regard to questions and discussions brought forth at the Nuclear Waste Technical Review Board meetings in Reno, Nevada on April 21 and 22, 1993. This report relates mainly to the presentation by Linda Lehman of L. Lehman & Associates (LLA), and Edward Kwicklis of the U.S. Geological Survey. These presentations showed research involving the unsaturated flow mechanisms and hydrologic conditions at Yucca Mountain which was sponsored by the State of Nevada and the U.S. Department of Energy. This report describes additional analyses done as a result of the meeting as well as some additional conclusions and recommendations.

Background

A short review of the important relationships in unsaturated flow follows. The basic equation governing unsaturated flow is the well known Richard's equation[1]:

$$div(K(\theta)\,grad\ h) = -\rho g\left(\frac{d\theta}{d\psi}\right)_{\theta}\frac{\partial h}{\partial t} \qquad (1)$$

where: $K(\theta)$ is the hydraulic conductivity as a function of water content θ
- h is the hydraulic head
- ρ is the fluid density
- g is the gravitational acceleration
- ψ is the capillary suction
- t is the time.

Equation 1 can also be written taking $\psi/\rho g$ as the unknown, or even θ. This non-linear equation is solved numerically and requires knowledge of the water retention properties relating conductivity to water content or capillary suction, and water content to capillary suction.

Water retention properties are generally modeled using two functions which may be fitted to measurements by adjusting some of the parameters. The first function (Equation 2) is usually a mathematical description of the relationship between water content (or degree of saturation) and water potential (or pressure). The second function describes the relationship between degree of saturation and hydraulic conductivity (Equation 3). Several pairs of mathematical functions are often used such as the van Genuchten equations or others based on work by Mualem, or Brooks and Corey. Both LLA and the USGS have used variations of the van Genuchten equations[2]:

$$S = (1 - S_r)\left[\frac{1}{1 + |Ah|^M}\right]^{\left(1-\frac{1}{M}\right)} + S_r \tag{2}$$

$$\frac{k(S)}{k_{sat}} = [1 + |Ah|^M]^{-\frac{N}{2}} \left\{1 - \left[\frac{|Ah|^M}{1 + |Ah|^B}\right]^N\right\}^2 \tag{3}$$

where: S is the saturation

S_r is the irreducible or residual saturation

h equals the pressure head

k(S) is the conductivity as a function of saturation

k_{sat} is the saturated conductivity

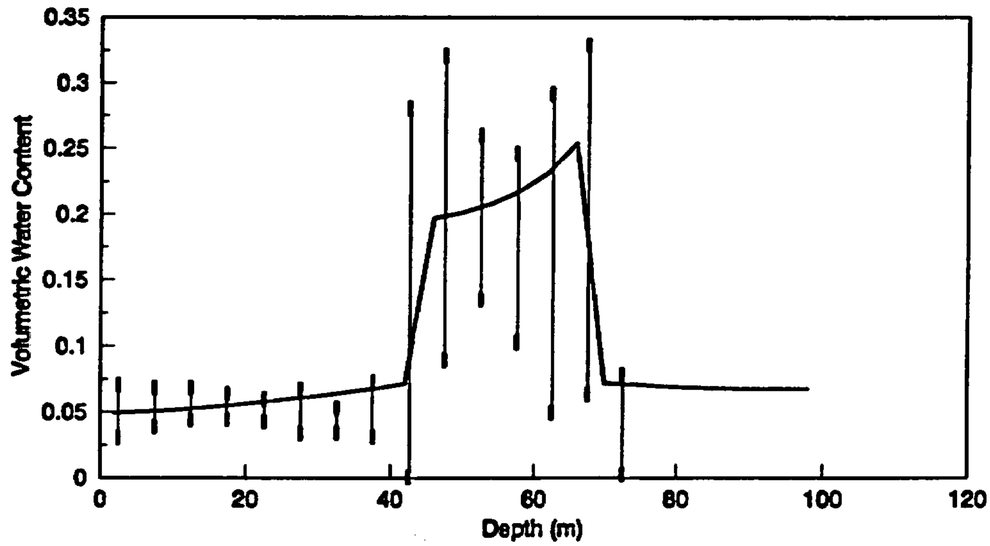
A and M with N = 1-1/M are the van Genuchten parameters.

Parameters generally adjusted to fit data or estimated properties include A and M. M is often taken as the same value for Equations 2 and 3, though not necessarily.

L. Lehman & Associates (LLA) presented to the NWTRB the work done for the State of Nevada on the INTRAVAL Unsaturated Zone Test Case for Yucca Mountain. The LLA work used matrix porosity, saturated conductivity, and laboratory pressure/saturation relationships measured by the USGS on samples from a transect and three shallow boreholes. The LLA work also utilized estimated fracture properties to show that the water content profiles measured at these same boreholes were best modeled by including fracture flow mechanisms along with the matrix properties. Figure 1a shows our fracture model result compared to the INTRAVAL data. LLA also showed that several different combinations of the most uncertain parameters, such as infiltration rates and fracture properties, can lead to very similar water content profiles. Thus the conclusion that the INTRAVAL validation problem as posed has several non-unique solutions.

Edward Kwicklis presented research which involved a fracture network model as well as a 1-D model of unsaturated flow at borehole UZ-5. For his 1-D matrix flow model he

a. Fracture model result compared with hole data



b. 1-D calibrated model result compared with hole data

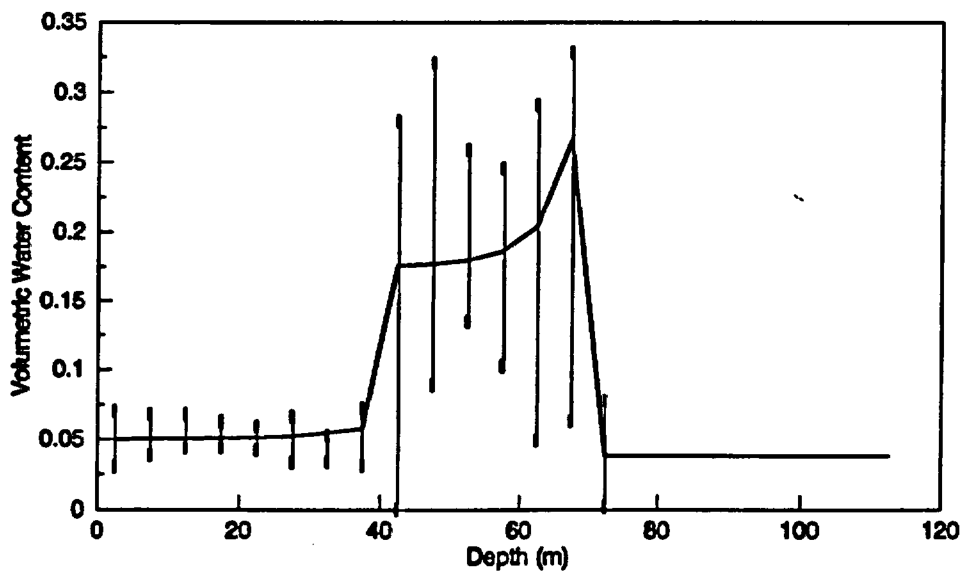


Figure 1. Results from both the dual porosity fracture model and the 1-D model calibrated using water retention curves compared with 2 standard deviations either side of the mean of measured water contents.

calibrated the modeled water potentials to those measured by adjusting the parameter A in Equation 2. He concluded that the water potential (h) can be locally variable in the presence of fractures and that 1-D matrix flow is probably not sufficient to capture the important unsaturated zone flow mechanisms at Yucca Mountain. Kwicklis also speculated that the need to adjust A in Equation 2 to obtain reasonable results may reflect some systematic bias in the data measurements.

The primary differences between the two modeling approaches are the measures used for calibration and the type of data used. The Kwicklis model was calibrated against water potential measurements by adjusting A in Equation 2. The LLA model was calibrated against water content measurements by adjusting infiltration rates and fracture properties because no insitu data were available on water potential (h), for the boreholes used. Lab measurements of water potential vs. saturation were available to use for fitting Equation 2. Since no data were available for fitting Equation 3, M was assumed the same value for both equations.

Another difficulty in comparing the results of the two models is that two separate locations were modeled which had significant differences in stratigraphy.

Discussion Of New Analyses

After the NWTRB meeting LLA decided to test the idea that a measurement bias exists. The 1-D model was forced to match the measured water content profiles. This was done by adjusting the parameter M in Equations 2 and 3. Previously LLA had only adjusted the input parameters for which no measurements existed in an attempt to fit the measured water contents, rather than to force a fit by ignoring the measured data. Figure 1b shows our 1-D model results compared to the INTRAVAL data. Note that the modeled profile of 1a is nearly identical to 1b yet the two models have major differences in conceptualization and matrix unsaturated properties.

For this forced calibration, the degree of adjustment relative to the original functions used varied from unit to unit. The original functions were derived from actual measurements, whereas this forced calibration simply chose the needed parameter value to match water contents. Figure 2 shows the adjusted pressure/saturation curves (Equation 2), compared to our measurement based curves. The average values of the measured data are also shown. The welded units in the model required forced adjustments of similar magnitude (a factor of 2-3) while the non-welded unit required little or no adjustment. This observation does not support a uniform measurement bias across all units. However, it does not rule out systematic biases by unit type. For example, the LLA model needed a similar magnitude change in M for the welded units. Kwicklis essentially only modeled the non-welded units and a 2-fold increase in A (a different parameter than M) was needed. Therefore, the possibility cannot be ruled out that a systematic bias may exist for the non-welded units which is different from the welded units.

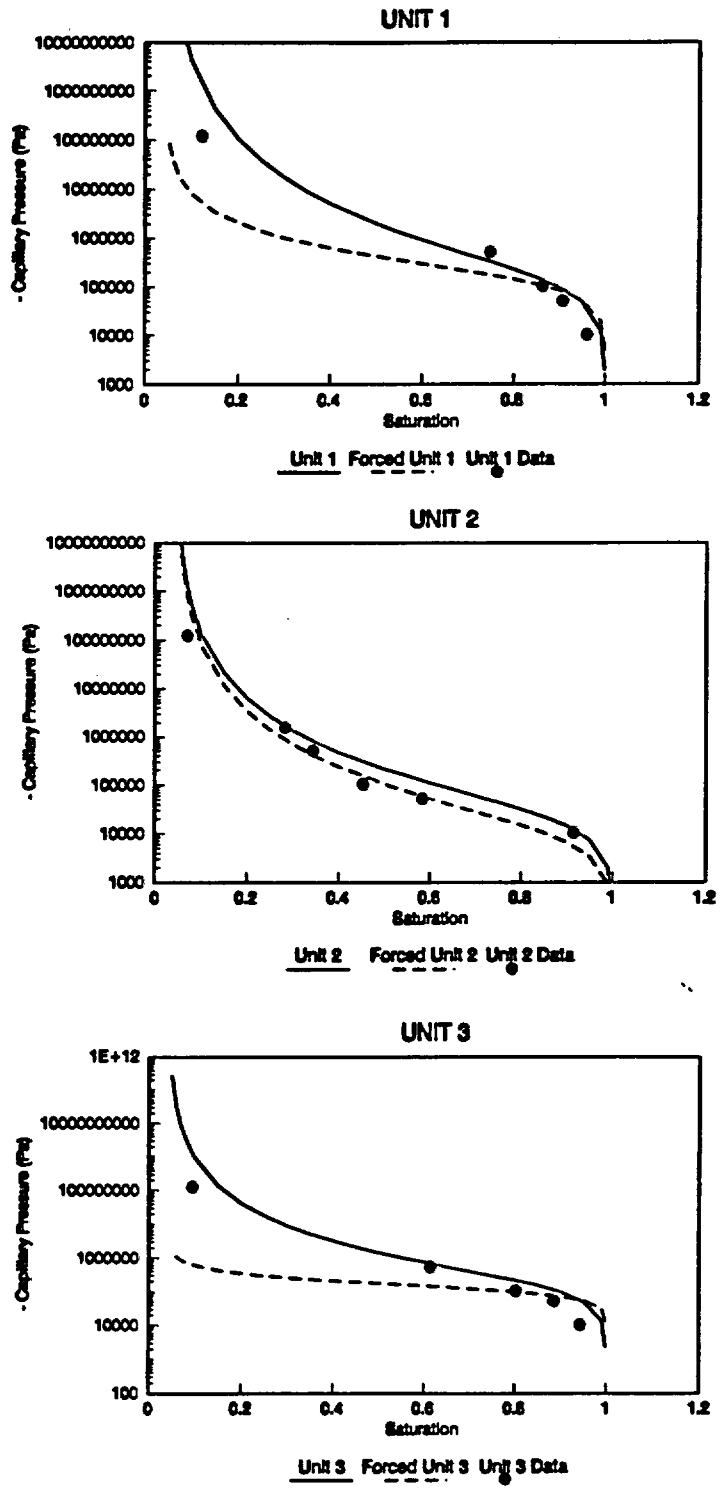


Figure 2. Water Retention Curves based on data (solid lines) and forced to fit measured water content (dashed).

One should not be too quick to interpret a bias in the data measurements, because the choice of conceptual model may be the most important issue. The INTRAVAL group has been assured that these data are reproducible. These INTRAVAL data are different from those used by Kwicklis in that they were analyzed by different people in addition to being different parameters measured at different locations. Some biases may be inherent though and not easily overcome, such as heat generated in drilling through the welded units driving off water. Independent verification of these data would be a good way to put this issue to rest quickly.

If these data are good and reproducible, then one must ask about their usefulness and how they are to be utilized in a performance assessment calculation. Also how many of these measurements are needed? If one concludes, as has LLA, that fracture flow probably dominates the flow field then the focus of data collection must change to acquiring fracture properties on a large scale and probably pneumatically. This is not to say that DOE should stop collecting matrix properties, but perhaps only a limited number of samples to determine matrix properties may be necessary. This number must be statistically derived to be representative and will in part depend upon the conceptual flow models and layering schemes (stratigraphy) utilized.

The choice of conceptual model for the unsaturated flow can also have a large effect on the model output. It was found during the course of the INTRAVAL modeling activity that measured water content profiles could be reasonably duplicated by incorporating fracture flow and recharge rates on the order of mm/yr, without adjusting the measured data available.

In addition to the water retention properties, other important model parameters could be adjusted to give reasonable results. Both the stratigraphic unit conductivities, and the infiltration rate will have a large effect on the modeled water content and water potential profiles.

Other problems, such as whether or not the van Genuchten curves are representative for a media which has fracture distributions exhibiting fractal characteristics, have not been addressed; especially if the distribution of fractures is controlling water potentials and/or saturations.

The possibility that some parameters may scale could also contribute to the differences between what was measured and what was needed to fit the models. Many studies and much modeling experience have shown that often lab scale measurements do not translate well to the field scale. This is especially true of hydraulic conductivity. Since the unsaturated conductivities are derived from Equation 3, and based on the van Genuchten parameters and the saturated conductivity measurements, this unsaturated conductivity may be only representative locally. Much of the uncertainty outlined above could be due to such scaling and so any field scale model will need to consider this source of uncertainty.

Conclusions

The preceding discussion outlined how the 1-D model developed for INTRAVAL (which did a poor job of predicting water content) could be forced to fit by adjusting the water retention curves outside the measured range of data. In principle any conceptualization of the flow field must be consistent with measured data. LLA believes a fracture model to be more reasonable, as no concrete evidence exists to justify ignoring the measured data in order to force matrix flow, at this point in time.

The above discussion begins to illuminate the large uncertainty associated with any model of the unsaturated zone which uses current information. Not only is there a potential for measurement bias, but many important variables are as yet unmeasured, for example, infiltration rates and fracture properties.

Probably most significant to uncertainty is the conceptual model selection. The modeling analyses undertaken to date by LLA indicate that all adjustments in laboratory measured data led to a model which is more like a fractured media than strictly a porous media. Referring again to Figure 2, the lower slope seen in the middle section (near 50% saturation) of the adjusted curves is generally a characteristic of the retention properties of fractures[3]. Increasing the parameter A in Equation 2, as was done by the USGS, also moves this curve closer to what is expected of fracture relationships. It seems most logical that these matrix flow models are not be accounting for fracture flow when laboratory measured matrix properties are used. The forced adjustments from the measured properties may simply indicate the degree to which the system deviates from a 1-D, matrix dominated conceptual model.

There are several improvements in the collection and analysis of data that may improve the quality of models developed, and therefore the understanding of the unsaturated zone at Yucca Mountain. These recommendations are as follows:

1. Water retention data should be more fully characterized and independently verified. Measurements of conductivity vs. saturation, as well as pressure vs. saturation, need to be undertaken for statistically representative samples from each individual unit deemed significant. For example, if a unit occupying 1 meter of the vertical stratigraphy is found to have a hydraulic properties statistically separate from surrounding units, then enough samples from this horizon should be measured to insure confidence in the result.

2. A full set of hydrologic properties for fractures needs to be developed. This should include information such as saturated conductivity, effective porosity or water retention properties, aperture or effective aperture distributions, fracture coating information as well as information on distribution and orientation of fractures and faults. Some of this may need to be accomplished through pneumatic tests.

3. More emphasis should be given to determining ambient downhole conditions and fracture properties as opposed to lab scale matrix properties.

4. The effects of scaling up the above measurements should also be investigated as well as the possibility of obtaining some of these properties insitu.

5. Recommendations 2, 3 and 4 may have implications for the ongoing exploratory shaft studies which could alter insitu properties. Completion of the exploratory shaft will likely alter the field scale conductivities and flow paths in the areas adjacent to it and may make insitu measurement of these properties impossible. It may be prudent to investigate the possibility of obtaining as much insitu information as possible before massive disruption of the natural system occurs.

6. Modeling activity should involve more diverse groups of qualified modelers, not with the aim of producing a definitive model, but to explore and discuss areas of model uncertainty and improvements in data availability and utility. The INTRAVAL program provides a good example of how this type of cooperation may be implemented with significant benefit to the quality of technical information. The Yucca Mountain project should also provide this type of interaction, especially among affected parties.

References

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