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Capturing Uncertainty in Unsaturated-Zone Flow Using Different Conceptual Models of Fracture-Matrix Interaction

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I. INTRODUCTION

A key part of Performance Assessment (PA) calculations is the examination of the effects of data uncertainty on performance measures. In the evaluation of Yucca Mountain as a potential nuclear waste repository, the unsaturated zone (UZ) is a critical portion of the natural barrier for mitigating radionuclide migration. There are many parameters needed to model unsaturated zone flow for which there is much uncertainty. Many past PA calculations have accounted for the uncertainty in parameters by randomly sampling from parameter distributions and using sampled parameters in flow models [1,2]. One of the problems with this approach is the possibility of getting a combination of parameter values that does not reproduce what is known about the system (e.g., measured matrix saturations) when used in a flow model.

Another aspect of the Total System Performance Assessment (TSPA) calculation is the "abstraction" process. This process takes the necessary information from detailed process-level models and simplifies it for use in the TSPA calculations. In the past this simplification has been performed by using several one-dimensional columns with different stratigraphics based on the locations of the columns [1,2].

For the Total Systems Performance Assessment - Viability Assessment (TSPA-VA) of Yucca Mountain, a novel approach is being used to model UZ flow. With the continuation of data collection since the last TSPA calculations[2], a three-dimensional (3D) model has been developed that is calibrated to the matrix saturations, water potentials, perched water body locations and the geochemistry of the system[3]. This model will be used to generate flow fields that can be used to simulate transport of radionuclides directly in the TSPA calculations. Use of this model not only ensures that the flow fields used in the TSPA calculations will be calibrated to the available data, but also allows for use of multidimensional UZ flow for the TSPA-VA. Since lateral flow above the zeolitized units below the repository is considered important[4], moving to multidimensional simulations from use of one-dimensional flow columns is a significant improvement.

Even with the calibrated 3D flow model, there is a considerable amount of uncertainty in the system. There is enough uncertainty in the system that the calibration is non-unique and several different conceptual models can be developed that equally well capture what is known about the system. One of the major uncertainties in the groundwater flow system is the degree of interaction between fractures and matrix.

It is proposed here that by using different conceptual models of fracture-matrix interaction and by varying a few key parameters, uncertainty in the UZ flow fields can be adequately captured.

II. APPROACH

In order to capture the uncertainty in fracture-matrix interactions, two conceptual models were developed. The first was developed by the flow modelers at Lawrence Berkeley National Laboratory[3]. Parameters used in this model were generated using inverse modeling to match the *in-situ* saturation and water potential data. Both inverse and forward flow modeling are done using the dual permeability model (DKM). This conceptual model allows for flow within and between the matrix and fracture domains. One of the key parameters that was calculated in the inversions is referred to as X_{fm}. This parameter is a reduction factor that is multiplied by the fracture-matrix interaction area. This reduction in fracture-matrix interaction is conceptualized as being due to fingering of flow along fracture faces and the fact that not all fractures have water flowing through them[5]. Once the parameters are determined from the inversions, they are used in the 3D flow model. Local changes are made to the parameters to make sure that the 3D model includes perched water and other important components of the system. It should be noted that for the subset of parameters for which there are measurements, the inversion technique forced the parameters to stay within these ranges. This model is referred to as the DKM/Base-Case model.

The second conceptual model is similar to the Weeps model described in Chapter 15 of TSPA-93[1]. This conceptual model of groundwater flow treats Yucca Mountain like a "sieve" where water moves quickly only through the fractures. In this instance a dual permeability formulation is used to imitate the Weeps model. This model is referred to as the DKM/Weeps model. Parameters used in this model are derived from the available data[3,6]. Fracture-matrix interactions are reduced to a greater extent than in the DKM/Base-Case model by using the upstream relative permeability $(k_r)*X_{fm}$ as the reduction term[7]. One value of X_{fm} is calculated for the entire system using inverse modeling.

With these two parameter sets using different fracture-matrix conceptual models, several parallel steps are taken: 1) reasonable bounds are determined for the different parameter sets; 2) sensitivity analyses are performed on the different parameters to determine which parameters are most sensitive; 3) simulations are run using the ranges in parameters and the two conceptual models; and 4) performance measures (e.g., pore water velocities and mass flow rates) are examined. The bounds determined on the different parameters can be based on several factors depending on information available for each parameter. These factors include standard deviations determined from the inversions and ranges or standard deviations calculated based on available data.

This exercise was run on a one-dimensional column located at borehole SD-9 (N234,086m, E171,267m). Simulations were run using the EOS3 module (two-phase flow) of TOUGH2[8] (Sandia configuration management version 3.4.1). The DKM was used for both conceptual models. The upper boundary condition was set to a constant infiltration rate of 3.6 mm/yr. The lower boundary was set to a constant saturation of 1. Simulations were run to steady state (inflow = outflow).

III. RESULTS

Mass flow rates are sensitive to van Genuchten[9] fracture alpha values (α_f). This sensitivity is especially apparent in the DKM/Base-Case model (Figure 1a) in which there is greater fracture-matrix interaction. As the α_f increases, the suction pressure of the fractures decreases. This leads to decreased flow in the fracture domain and increased flow in the matrix domain. With the DKM/Weeps model, the interaction between the fractures and the matrix is so small that α_f does not have as strong an effect on partitioning the flow between the fracture and matrix domains. Pore water velocities are shown not to be sensitive to α_f.

This set of simulations also shows that use of the two conceptual models allows for a greater range in the generated performance measures. It can be seen that the differences in the fluxes between the two models are greater than the differences in the fluxes within a single model. The flow rates are greater in the DKM/Base-Case model than in the DKM/Weeps model in the Topopah Springs welded unit (TSw), but less than in the DKM/Weeps model in the Calico Hills non-welded unit (CHn). In the non-welded units (Paintbrush Tuff non-welded unit (PTn) and CHn), the fracture-matrix interaction is greater and there is a general transfer of flow from the fractures to the matrix. This transfer is larger for the DKM/Base-Case model (mass flow in the PTn is almost entirely in the matrix for this model, not shown in Figure 1). However, there is still some transfer of mass from the fractures to the matrix in the DKM/Weeps model. At the PTn/TSw contact the flow is transferred back into the fractures in the DKM/Base-Case model, but not in the DKM/Weeps model. Again, this is due to the greater fracture-matrix interaction of the DKM/Base-Case model.

There are two other points that should be made related to the pore-water velocities. The difference in pore-water velocities between the two models are primarily due to different van Genuchten fracture betas used in the two models (not shown). Also, fracture porosities would have a great effect on the transport of radionuclides. Since these simulations are run to steady-state and the porosity appears in the storage term, changes in the porosities do not affect the results shown.

IV. CONCLUSIONS

Preliminary calculations show that the two different conceptual models of fracture-matrix interaction presented here yield different results pertinent to the performance of the potential repository at Yucca Mountain. Namely, each model produces different ranges of flow in the fractures, where radionuclide transport is thought to be most important. This method of using different flow models to capture both conceptual model and parameter uncertainty ensures that flow fields used in TSPA calculations will be reasonably calibrated to the available data while still capturing this uncertainty. This method also allows for the use of three-dimensional flow fields for the TSPA-VA calculations.

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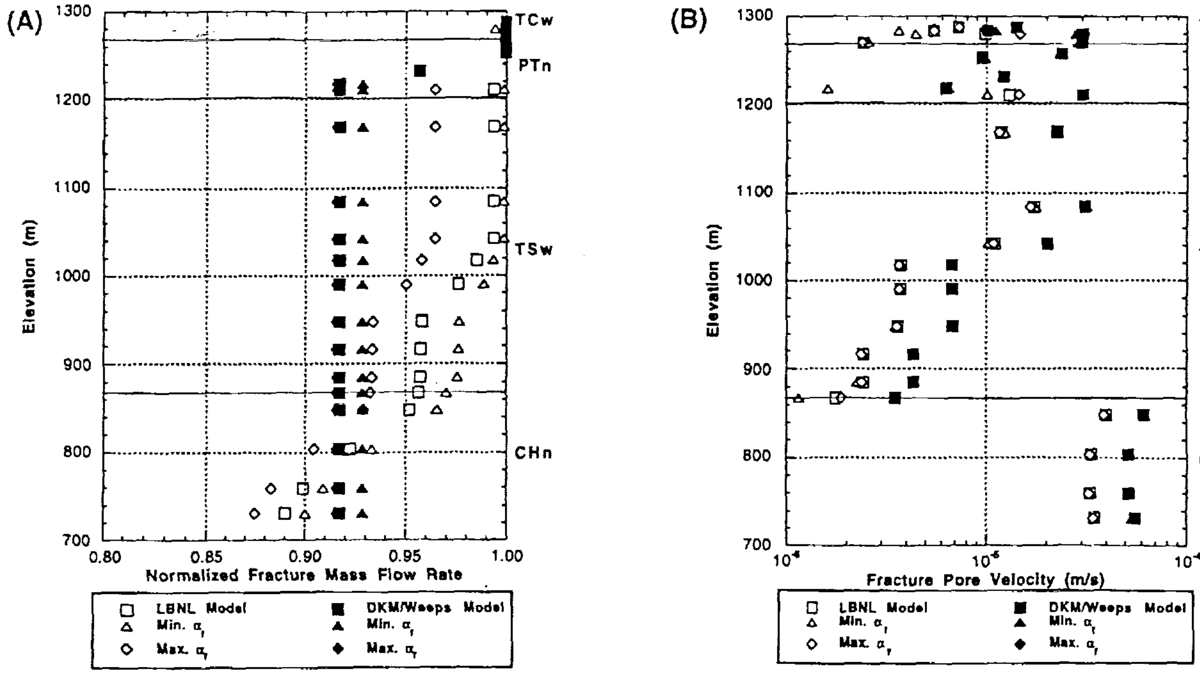

Figure 1: Simulated normalized mass flow rates (A) and porewater velocities (B) on one-dimensional columns used to compare the results of two different conceptual models of fracture-matrix interaction. Mass flow rates are normalized to the mass flow (infiltration) into the upper boundary. Van Genuchten α_f was varied within reasonable ranges to test whether use of the two different models can capture the uncertainty in UZ flow performance measures. The DKM/Base-Case model allows for more fracture-matrix interaction than the DKM/Weeps model. Note that since the scale of the normalized mass flow rates has been cut off at 0.80, it cannot be seen that the mass flow is almost entirely in the matrix in the PTn for the DKM/Base-Case model.

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