# **HLWYM HEmails**

From:	Olufemi Osidele	
Sent:	Thursday, October 05, 2006 12:40 PM	
To:	Osvaldo Pensado; Jude Mcmurry; Scott Painter; David Pickett	
Cc:	James Winterle	
Subject:	Fw: FEIS UZ performance and matrix diffusion study	
Attachments:	note2KeithC10032006.doc	
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All:

The attached report might be of interest since it further reveals how the TSPA takes credit for UZ performance. I made two quick observations: First, it seems Jack Gwo has found a way to turn off matrix diffusion in the UZ in the TSPA-FEIS model, essentially by setting fracture-matrix mass exchanges to zero in the flow field input file. Second, on page 4 and in summary item 3, he makes an argument comparing advective versus diffusive matrix diffusion that I did not observe when I initially extracted the UZ transport module from the TSPA-FEIS. Perhaps our subject matter experts could comment on the merits of Jack's argument. Please let me know if you have any other observations or comments.

Thanks . . . . Femi.

----- Original Message -----From: "Jin-Ping Gwo" <jxg4@nrc.gov> To: "Femi Osidele" <oosidele@cnwra.swri.edu>; "Andy Campbell" <ACC@nrc.gov>; "Allen Fetter" <AHF@nrc.gov>; "Bret Leslie" <BWL@nrc.gov>; "Christopher Grossman" <CJG2@nrc.gov>; "Eugene Peters" <EMP2@nrc.gov>; "Keith Compton" <KLC@nrc.gov>; "Philip Justus" <PSJ@nrc.gov>; "Randall Fedors" <RWF@nrc.gov>; "Timothy McCartin" <TJM3@nrc.gov> Sent: Thursday, October 05, 2006 7:54 AM Subject: FEIS UZ performance and matrix diffusion study

> Folks,

>

> Thanks to Bret for reminding me that I need (though I planned) to send

- > the attached note to Keith to those that may be interested. Basically
- > it's a UZ FEHM model performance study using the GoldSim model pulled
- > out of FEIS by Femi. In one simulation, I put in a square source and
- > another I turned off all the fracture-matrix fluid exchange. The former
- > is to determine the relative performance of fracture and matrix after
- > the termination of source terms and the latter to identify the mechanism
- > of the so-called "matrix diffusion" in the FEIS. Comments are most
- > welcome and feel free to forward to anyone else that may be interested.
- > Regards,
- > Jack
- >

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Recipients: "James Winterle" <jwinterle@cnwra.swri.edu> Tracking Status: None "Osvaldo Pensado" <opensado@cnwra.swri.edu> Tracking Status: None "Jude Mcmurry" <jmcmurry@cnwra.swri.edu> Tracking Status: None "Scott Painter" <spainter@cnwra.swri.edu> Tracking Status: None "David Pickett" <dpickett@cnwra.swri.edu> Tracking Status: None</dpickett@cnwra.swri.edu></spainter@cnwra.swri.edu></jmcmurry@cnwra.swri.edu></opensado@cnwra.swri.edu></jwinterle@cnwra.swri.edu>				
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Expiration Date: Recipients Received: Follow up To: Keith Compton Date: October 4, 2006 Subject: FEIS UZ Performance

## **Background and Assumptions**

A UZ Goldsim model was pulled out of the TSPA-FEIS model earlier on by Femi Osidele at the CNWRA. For convenience of discussion, the pulled-out model is henceforth referred to as the FEIS-FO model. The purpose of the model is to independently test and determine the performance of the UZ model of the FEIS and to identify the major barriers of the UZ in the FEIS model. The principle component of the model is the FEHM UZ model that consists of a three-dimensional model grid of 47,664 nodes for each porosity/permeability. The FEHM model is configured as a collection of double-porosity double-permeability rock formations with 48 hydrogeologic units. The fluid velocities for the pathways connecting the nodes were calculated off-line by TOUGH2. Particle tracking is then performed within GoldSim by the FEHM code to determine radionuclide concentrations and number of particles at the nodes and the discharge rates of radionuclides from the UZ to the SZ of the FEIS model.

A few notable assumptions of the FEIS-FO model that differ from the TSPA-FEIS are:

- 1. Only Tc-99 and Np-237 and its daughter products are released from the EBS. No colloidal Np-237 is assumed to be released from the EBS. In contrast, in the TSPA-FEIS there are 26 soluble and irreversibly bound colloidal species.
- 2. The release rates of both radionuclides are set at 10 g/yr. In contrast, the release rates of radionuclides are calculated by a suite of EBS and other disruptive event models.
- 3. Only the climate condition with mean annual infiltration rates is considered. In this case, the fluid mass velocities in the file ff0200.ini are used to initialize FEHM, which results in a steady-state flow condition in the UZ.

Other GoldSim components of the TSPA-FEIS are either simplified, e.g., EBS, or removed, e.g., the SZ, in the FEIS-FO model. The five source bins (or zones 501 - 505 in the input file fm\_pchm1.zone2) and four discharge bins (or zones 701 – 704 in the input file fm\_pchm1.zone2) are the same as those in the TSPA-FEIS.

In the following discussion, I focus on three studies of the FEIS-FO model, with an aim to build up an analytical capability for full-blown analysis of the TSPA-FEIS model on the Windows 2000/2003 cluster. I also wish to determine the relative performance of the fracture and matrix flow paths and the mechanism that governs the so-called "matrix diffusion" in the TSPA-FEIS. The three studies are:

- 1. The base case scenario of the FEIS-FO as designed by Femi.
- 2. The square step input scenario to identify the signature of "matrix diffusion." In this study, the source term is maintained at the same rate as the FEIS-FO only up to the first 400,000 years.

3. The no "matrix diffusion" scenario, in which the fluid mass exchange rates between the two porosities or fracture-matrix compound are artificially set to zeros. This requires the modification of the fluid flow velocity file ff0200.ini and setting the fluid mass exchange rates to zeros.

The purposes of the three studies are to (1) determine the effect of source term on the relative performance of fracture and matrix as barriers of radionuclide movement in the UZ (scenario 2) and (2) determine the mechanism of "matrix diffusion" of the FEIS-FO model (scenario 3). One has to note that, before a detailed comparison of the FEIS-FO and the TSPA-FEIS input parameters, the conclusions reached here may not be transferred directly to TSPA-FEIS.

### **Result and Discussion**

### Base Case Scenario and Long-Term Performance

The relative contributions of fracture and matrix to UZ discharge for the base case scenario is shown in Figures 1 and 2 for Tc-99 and Np-237, respectively. For both radionuclides, matrix discharges account for about 20% of total long-term radionuclide mass discharge. The discharge rates reach steady-state at about 70,000 years for the fracture and 90,000 years for the matrix for Tc-99. For Np-237, the discharge rates continue to increase over the 1,000,000 years simulation time. The larger retardation factor of Np-237 results in a delay in the initiation of matrix discharge for about 1,250 years and renders its increase of discharge rates more gradual than those of Tc-99. One must note that these discharge rates are measured at the discharge zone, not in individual hydrogeologic units. It is the aggregated performance measure of not only "matrix diffusion" but also the fluid flow field of the matrix. Finer grain analysis of the performance at each hydrogeologic units or flow zones as delineated as flow zones in the input file fm pchm1.zone2 requires three-dimensional, detailed analysis of FEHM output which can only be obtained by reconfiguring FEHM input parameters that are not controllable through the GoldSim interface. As of the writing of this note, the analysis is underway.

The FEIS model divides the UZ discharge into four geographical zones as shown in Figure 3, in which discharge zones 1 - 4 are colored as magenta, green, red and yellow, respectively. Tc-99 and Np-237 display a fine-grain variation across the four discharge zones (e.g., see Figures 4 and 5 for zones 1 and 2 for Tc-99 and zones 3 and 4 for Np-237) as well as inside individual discharge zones. In particular, mean matrix discharge from zone 3 are much higher than others. In comparison, mean fracture discharge rates are relatively more uniform than those of the matrix zones (see Figure 6 for discharge rate statistics). The causes for the relative large matrix discharge rates at zone 3(about 40% of the fracture discharge rates for Tc-99 and 30% for Np-237) cannot be deduced from the aggregated discharge measures. Fine-grain, three-dimensional analysis is being conducted to determine the causes.



Figure 1. Total UZ Tc-99 discharge rates: total, fracture and matrix (upper panel) and relative contributions (lower panel).

#### Matrix Diffusion and Retardation Effect on Tailing

Because of differences in reactivity with solid surface, reactive solutes tend to display discernible effect of retardation in rock matrix. Shown in Figures 7 and 8 are the total, fracture and matrix discharge rates of Tc-99 and Np-237, respectively, with a square source input of 400,000 years. The more gradual increase of Np-237 relative matrix discharge rates (lower panels) after the source is terminated and its longer tailing (upper panel) indicates the larger retardation factor of Np-237. After the source is terminated, discharge rates of the matrix exceed those of the fracture for both Tc-99 (Figure 7) and Np-237 (Figure 8). The gradual increase of Tc-99 contribution (Figure 8) towards the end of the simulation at one million years may be caused by "reverse matrix diffusion" with Tc-99 inside the matrix acting as secondary source. The exact cause of the increase requires more detailed analysis of the fine-grain FEHM output. Nevertheless, the discharge rates after source termination are only a fraction of the maximum discharge rates. One notes the simple source functions in the current study. The conclusions reached here may not be generalized to situations where the source terms fluctuate with time and space. For the FEIS-FO model, the uniform mass (radionuclide and fluid) exchange mechanisms between the fracture and matrix largely simplified the analysis of "matrix diffusion." The size of radionuclides or their relative free water diffusion

coefficients do not impact the mass exchange rates. Rather, it is the inter-porosity, fracture-matrix, fluid mass exchange velocities that affect both the discharge rates and the flow path of the radionuclides in the fracture and matrix.



Figure 2. Total UZ Np-237 discharge rates: total, fracture and matrix (upper panel) and relative contributions (lower panel).

Shown in Figure 9 is the total, fracture and matrix discharge rates of Tc-99 for which the fluid mass exchange rates between the fracture and matrix are artificially set to zeros. All the Tc-99 is discharged through the fracture, indicating the nature of the "matrix diffusion" mechanism. In effect, the movement of Tc-99 between the fracture and matrix is determined only by the inter-porosity fluid exchange rates. The "matrix diffusion" mechanism is essentially an advective mass exchange, akin to mechanical dispersion rather than molecular diffusion, between the fracture and matrix. Without the advective mass exchange, the long-term performance of the UZ does not differ much from that with the advective mass exchange (see upper panel of Figure 10). However, within the first 10,000 years and with the advective mass exchange, "matrix diffusion" does result in lower total discharge rates (see upper panel of Figure 11). Because the fluid flow rates in the UZ are relatively lower than those in the SZ, diffusive "matrix diffusion" as a result of molecular diffusion of radionuclides into or out of the matrix may affect the performance of the UZ. It is likely to include the mechanism in the TSPA-FEIS or the

FEIS-FSO model by changing the parameters of the FEHM model. These together may warrant a detailed analysis using the FEIS-FSO model to determine the relative importance of advective and diffusive "matrix diffusion" over the first 10,000 years and the entire one million years simulation time.

As the regulatory time frame is being extended to one million years, the results above suggest that there may be uncertainty as to what extent advective "matrix diffusion" may contribute to the performance of the potential repository. Nonetheless, one needs to note that the source term here is a simple step function and is steady over the one million years period. Further studies needed to determine the impact of source term spatial and temporal variations by using more realistic source terms or adopt those from the TSPA-FEIS directly into the FEIS-FO model.



TSPA-FEIS Grid and UZ Discharge Zones/Bins

Figure 3. Model Grid and discharge zones of TSPA-FEIS – zones 1 – 4 are color-coded as magenta, green, red and yellow, respectively.

#### Summary

Three studies of the UZ transport model based on the pulled-out model of the TSPA-FEIS by Femi, or the FEIS-FO model, were conducted to determine the relative performance of the fracture and matrix, to identify the signatures of matrix diffusion and the effect of retardation on matrix diffusion, and to determine the mechanisms of the socalled "matrix diffusion" in the FEIS-FO and, possibly, the TSPA-FEIS models. As a result of these studies, detailed three-dimensional distributions of Tc-99 and Np-237 (and its daughter products U-233 and Th-229) concentrations, both temporally and spatially, have been obtained. Detailed analyses on the basis of these concentration distribution histories are being conducted to determine the major barrier formations of the UZ hydrogeologic units in the TSPA-FEIS and to understand the transport pathways (e.g., fracture mostly, fracture  $\rightarrow$  matrix, or fracture  $\rightarrow$  matrix  $\rightarrow$  fracture/secondary source) of the radionculides.

The results of the reported studies here suggest that:

- 1. The matrix flow path contributed about 20% of long-term Tc-99 and Np-237 annual discharge rates. If extrapolated to account for matrix diffusion, one may suggest that matrix diffusion accounts for 20% of the Tc-99 and Np-237 movement through the UZ as the source is released only to the fracture in the EBS. However, for long-term, one million year performance of the UZ, "matrix diffusion" does not render the matrix a major solute transport barrier for the less reactive Tc-99. On the other hand, for the first 10,000 year, "matrix diffusion" does results in reduced discharge rates for Tc-99 and Np-237.
- 2. Spatial variations of radionuclide concentrations as well as discharge rates need to be further investigated in the FEIS-FO and TSPA-FEIS models. This is particular important in terms of identifying individual discharge features and preferential flow paths such as faults. To this end, the aggregated discharge rates obtained for the studies reported here will need to be disaggregated and three-dimensional spatial variations of radionuclide concentrations will need to be examined.
- 3. The governing mechanism of "matrix diffusion" in the FEIS-FO model, and possibly the TSPA-FEIS model, is the movement of fluid mass between the fracture and the matrix. In effect, it is an advective type "matrix diffusion," not a diffusive type. The effect for this advective "matrix diffusion" in the FEHM particle tracking is akin to mechanical dispersion for the aggregated fracture-matrix rock formations. It may be necessary to conduct further FEHM and FEIS-FO model simulations to investigate the efficacy of diffusive matrix diffusion relative to that of advective matrix diffusion.



Figure 4. Discharge rates of Tc-99 in discharge zones 1 (upper panel) and 2 (lower panel).



Figure 5. Discharge rates of Np-237 in discharge zones 3 (upper panel) and 4 (lower panel).



Figure 6. Mean discharge rate statistics of Tc-99 and Np-237 through fracture and matrix.



Figure 7. Total, fracture and matrix Tc-99 discharge rates (upper panel) and relative discharge rates (lower panel) of the square input function simulation of the FEIS-FO model.



Figure 8. Total, fracture and matrix Np-237 discharge rates (upper panel) and relative discharge rates (lower panel) of the square input function simulation of the FEIS-FO model.



Figure 9. Total, fracture and matrix Tc-99 discharge rates (upper panel) and the relative contributions of fracture and matrix to the total discharge rates (lower panel).



Figure 10. Comparison of total discharge rates between the base scenario (with advective "matrix diffusion") and the no-matrix-diffusion scenario (upper panel). Without the advective "matrix diffusion," the fracture carries higher and all the mass flux injected at the repository (lower panel).



Figure 11. Comparison of total discharge rates within the first 10,000 years for the base and no-matrix-diffusion scenarios.