# Summary of the Matrix Diffusion Workshop

## 1.0 Introduction

Matrix diffusion may affect aqueous transport of radionuclides in the unsaturated zone; however, DOE and NRC differ in regard to the importance of matrix diffusion. NRC and CNWRA staff held a workshop on matrix diffusion on July 16–17, 2007, to discuss the issues related to the representation of matrix diffusion, its effect on flow processes, and to assess consequences with regard to radionuclide transport. This workshop was a joint effort for staff working on the Flow Paths in the Unsaturated Zone and Radionuclide Transport in the Unsaturated Zone Integrated Subissues. The workshop examined test data, process-level models, and performance assessment abstractions for matrix diffusion and related fracture–matrix interactions. The two-day workshop involved presentations and discussions aimed at promoting a common understanding of the conceptualization and importance of the matrix diffusion process. These discussions identified specific tasks to be performed in FY2008 including (i) using independent models to evaluate specific processes such as scale dependency, multirate diffusion processes, and heterogeneity in matrix and fracture properties, and (ii) performing sensitivity analyses using TPA to understand the risk significance.

## 2.0 Objectives

Objectives of the workshop included

1. Increase understanding of DOE process-level models and abstractions related to matrix diffusion
2. Identifying and evaluating sources available in literature related to matrix diffusion (including journal articles published by DOE)
3. Evaluating the role of active fracture concept in flow and transport models
4. Planning the use or development of alternate transport models to assess the effect of matrix diffusion in the unsaturated zone
5. Developing staff consensus about risk significance of matrix diffusion relative to other unsaturated and saturated zone barriers based on performance assessment models (TSPA and TPA)

A detailed agenda of the workshop is given in the Appendix.

## 3.0 Summary of the Discussion

- A summary of recent journal articles about matrix diffusion indicated that DOE process-level studies have examined (i) scaling dependency of the matrix-diffusion process in regard to multiple, local flow loops formed by small-scale fractures around major percolation paths (Liu et al., 2007, Zhou et al., in press); (ii) potential effects of dry fractures as a capillary barrier in the matrix-diffusion process (Seol et al., 2003); (iii) multisite (multirate) matrix diffusion processes (Zhang et al., 2006; Zhou et al., 2006); (iv) potential sensitivity of the active fracture exponent to injection/infiltration rates (Seol et al., 2006); and (v) potential uses of the active fracture model for fractal flow patterns in fractures (Liu et al., 2003; 2005). However, conclusions from these studies have not been directly incorporated into TSPA abstractions. The matrix diffusion process in TSPA is simulated via a molecular diffusion process after correction by the matrix tortuosity using an empirical relation by Reimus et al., 2003.

- Staff presented a summary of data and the underlying modeling assumptions used to estimate the reduced fracture-matrix interfacial area in DOE process-level models and the TSPA abstraction. These data included (i) matrix and fracture properties and (ii) an active fracture model exponent ($\gamma$) based on field and numerical analyses conducted by DOE. In TSPA, $\gamma$ is treated as a fracture property; its value remains unchanged with different climate scenarios. The workshop discussion noted that the representation of uncertainty associated with $\gamma$ needs to be evaluated in detail given its importance to matrix diffusion.

- Workshop participants discussed the application or development of independent process-level models to test the importance of the matrix-diffusion process independently under different scenarios. Several alternative models were proposed including a 1D analytical model, a stochastic pathway model, and a streamtube model. Workshop participants will develop and apply these models in FY2008.

- Risk significance of matrix diffusion in the unsaturated zone relative to other unsaturated and saturated zone barriers was also discussed. Other unsaturated zone barriers considered by DOE include direct release of radionuclides to the welded Topopah Spring (TSw) matrix, flow through the matrix in the vitric Calico Hills unit (CHv), and colloid-associated transport barriers. Saturated zone barriers, other than matrix diffusion in the saturated fractured tuff, include matrix flow through alluvium and long travel distances through alluvium, both of which increase the opportunity for retardation of radionuclides by sorption.

- Staff reviewed the caveats related to matrix diffusion and the active fracture model in the relevant KTI agreements and listed specific questions in preparation for the Appendix 7 meeting with DOE about unsaturated zone field tests.

A detailed report describing the main workshop topics will be transmitted to NRC as a joint intermediate milestone in FY2008. This report will be a consolidation of current understanding of matrix diffusion topics and issues and will include a description of results from the proposed independent models.

## 4.0 References

Liu, H.H., G. Zhang, and G.S. Bodvarsson. "The Active Fracture Model: Its Relation to Fractal Flow Patterns and Evaluation Using Field Observations." *Vadose Zone Journal.* Vol. 2. pp. 259–69. 2003.

Liu, H.H., R. Zhang, and G.S. Bodvarsson. "An Active Region Model for Capturing Fractal Flow Patterns in Unsaturated Soils: Model Development." *Journal of Contaminant Hydrology.* Vol. 80. pp. 18–30. 2005.

Liu, H.H., Y.Q. Zhang, Q. Zhou, and F.J. Molz. "An Interpretation of Potential Scale Dependence of the Effective Matrix Diffusion Coefficient." *Journal of Contaminant Hydrology.* Vol. 90. pp. 41–57. 2007.

Reimus, P.W., M.J. Haga, A.L. Adams, T.J. Callahan, H.J. Turin, and D.A. Counce. "Testing and Parameterizing a Conceptual Solute and Transport Model in Saturated Fractured Tuff Using Sorbing and Nonsorbing Tracers in Cross-Hole Tracer Tests." *Journal of Contaminant Hydrology*, Vol. 62. pp. 613–636. 2003.

Seol, Y., H.H. Liu, and G.S. Bodvarsson. "Effects of Dry Fractures on Matrix Diffusion in Unsaturated Fractured Rocks." *Geophysical Research Letters.* Vol. 30. No. 2. Article No. 1075. 2003.

Seol, Y., T.J. Kneafsey, and K. Ito. "An Evaluation of the Active Fracture Concept in Modeling Unsaturated Flow and Transport in a Fractured Meter-sized Block of Rock." *Vadose Zone Journal.* Vol. 5. pp .1–13. 2006.

Zhang, Y., H.H. Liu, Q. Zhou, and S. Finsterle. "Effects of Diffusive Property Heterogeneity on Effective Matrix Diffusion Coefficient for Fractured Rock." *Water Resources Research.* Vol. 42. W04405. 2006.

Zhou, Q., H.H. Liu, F. Molz, Y. Zhang, and G.S. Bodvarsson. "Field-Scale Effective Matrix Diffusion Coefficient for Fractured Rock: Results From Literature Survey." *Journal of Contaminant Hydrology.* To be published.

Zhou, Q., H-H. Liu, G.S. Bodvarsson, and F.J. Molz. "Evidence of Multi-Process Matrix Diffusion in a Single Fracture from a Field Tracer Test." *Transport in Porous Media*, Vol. 63. pp. 473–487. 2006

**Appendix**
**Matrix Diffusion Workshop Agenda**
**CNWRA – San Antonio**
**Bldg. 189, Room A137**

**Monday July 16**

2:00 Introduction and objectives of workshop (Jude McMurry and Randy Fedors)
2:20 Status of KTI agreements and caveats (John Bradbury)
2:50 Matrix diffusion in TSPA (Jack Gwo)
*3:45* *BREAK*
4:00 Matrix diffusion research: Recent papers (Hakan Basagaoglu)
*5:00* *END FOR THE DAY*

**Tuesday July 17**

Field Data
8:15 (1) Key UZ transport-related field tests (Jude McMurry)
8:45 (2) How field tests are used in DOE models (Randy Fedors)
Active Fracture Model
9:15 (1) Representation of the active fracture model (AFM) in flow models (Gary Walter)
9:45 (2) DOE's use of the active fracture model (Hakan Basagaoglu)
*10:15* *BREAK*
Alternative numerical approaches for matrix diffusion
10:30 (1) LB pore scale model, including episodic flow (Hakan Basagaoglu)
11:00 (2) Inferences from fracture characteristics (Randy Fedors)
11:15 (3) Streamtube network (Hakan Basagaoglu)
*11:45* *LUNCH BREAK*
1:00 (4) 1D analytical model (Jim Winterle)
1:30 (5) Stochastic pathway (SKB) model (Scott Painter)

Sensitivity analyses
2:00 (1) DOE matrix diffusion sensitivity analyses (Jude McMurry)
2:15 (2) NEFTRAN and -D analytical model, potential sensitivity analyses (Jim Winterle)
2:45 (3) Other methods to evaluate risk significance? (Chandrika Manepally)
*3:00* *BREAK*
Other considerations
3:15 (1) Potential factors affecting matrix diffusion (John Bradbury)
3:45 (2) Effect of heterogeneous flow paths on matrix diffusion (Jude McMurry)
4:00 Summary Discussion (Chandrika Manepally)
– Key messages from presentations
– Open questions about DOE implementation of matrix diffusion
– Planning the workshop documentation
*5:00* *END OF WORKSHOP*