

INEEL/CON-02-00146
PREPRINT

Subsurface Pathway and Transport Modeling for the Idaho National Engineering and Environmental Laboratory's Subsurface Disposal Area

S. Magnuson

August 4, 2002 – August 8, 2002

Spectrum 2002

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint should not be cited or reproduced without permission of the author.

This document was prepared as a account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights. The views expressed in this paper are not necessarily those of the U.S. Government or the sponsoring agency.

Subsurface Pathway Flow and Transport Modeling for the Idaho National Engineering and Environmental Laboratory's Subsurface Disposal Area

Swen Magnuson

Idaho National Engineering and Environmental Laboratory

P.O. Box 1625, Idaho Falls, Idaho 83415

smm@inel.gov

Abstract—Migration of contaminants through the complex subsurface at the Idaho National Engineering and Environmental Laboratory's Subsurface Disposal Area was simulated for an ongoing Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) assessment. A previously existing model for simulating flow and transport through the vadose zone for this site was updated to incorporate information obtained from recent characterization activities. Given the complexity of the subsurface at this site, the simulation results were acknowledged to be uncertain. Rather than attempt parametric approaches to quantify uncertainty, it was recognized that conceptual uncertainty involving the controlling processes was likely dominant. So, the effort focused on modeling different scenarios to evaluate the impact of the conceptual uncertainty.

I. INTRODUCTION

As part of an ongoing CERCLA evaluation, the migration of contaminants through the hydrologically complex subsurface at the Idaho National Engineering and Environmental Laboratory's (INEEL's) Subsurface Disposal Area (SDA) was simulated using TETRAD.¹ A previously existing model for simulating flow and transport through the vadose zone beneath the SDA² was updated to incorporate additional information obtained from recent characterization activities. This model used an equivalent porous continuum approach to represent movement of water and contaminants in the subsurface. Full calibration of the model, which depends on both calibration of the source release model and on suitable monitoring data sets, was deferred to 2004. The source release modeling was simulated external to the flow and transport modeling and has its own suite of uncertainty issues, which are not addressed in this paper. Data from an expanded local monitoring network, which includes a newly installed set of monitoring points within and near the buried waste, will be used to calibrate the models. Therefore, the current flow and transport model is based on best judgment and is used to estimate future groundwater concentrations to evaluate risks to hypothetical receptors.

Uncertainty in the three-dimensional flow and transport simulation results derives from both parametric and from conceptual sources. Parametric uncertainty results from the hydrologic and transport properties that are assigned based on measured or interpreted properties. Conceptual uncertainty results from processes or influences in the real system that are not simulated in the model. Because conceptual uncertainty involving the controlling

processes was likely dominant,³ various scenarios were used to assess the possible impacts of the conceptual uncertainties.

II. OVERVIEW OF SITE GEOLOGY AND BASE MODEL DEVELOPMENT

The SDA is 180 meters above the regional Snake River Plain Aquifer. The vadose zone beneath the SDA is composed primarily of fractured basalts. Thick layers of fractured basalt are interspersed with thin, mostly continuous, sedimentary interbeds that were deposited through aeolian and fluvial processes during periods of volcanic quiescence.

The vadose zone model was created with a three-dimensional domain. A conformable gridding approach matched vertical gridding interfaces to kriged lithologic contacts⁴ (see Fig. 1). Multiple concentric refined zones were used to discretize the model to match varying levels of available lithologic detail. The outline of the SDA is shown at the top of each domain. Infiltration at land surface within the SDA was treated as spatially variable and was considered to be controlled by topography and degree of soil disturbance. Three constant rates representing areas with high, medium, and low annual infiltration rates were assigned, as shown in Fig. 2. The equivalent average infiltration calculated from these spatially variable rates is 8.5 cm/year. These spatially varying estimates were based on inverse modeling to site-specific calibrated thermal neutron monitoring in a network of neutron access tubes.⁵ A uniform low infiltration rate of 1 cm/yr annually was assigned outside the SDA. Hydrologic properties for sedimentary interbeds were spatially vari-

able and were kriged based on interbed samples that were hydrologically characterized.⁴ An influence within the vadose zone from

Big Lost River water discharged to the spreading areas approximately 1 km away was included. This model was used to simulate dissolved-phase transport for a suite of contaminants of potential concern.

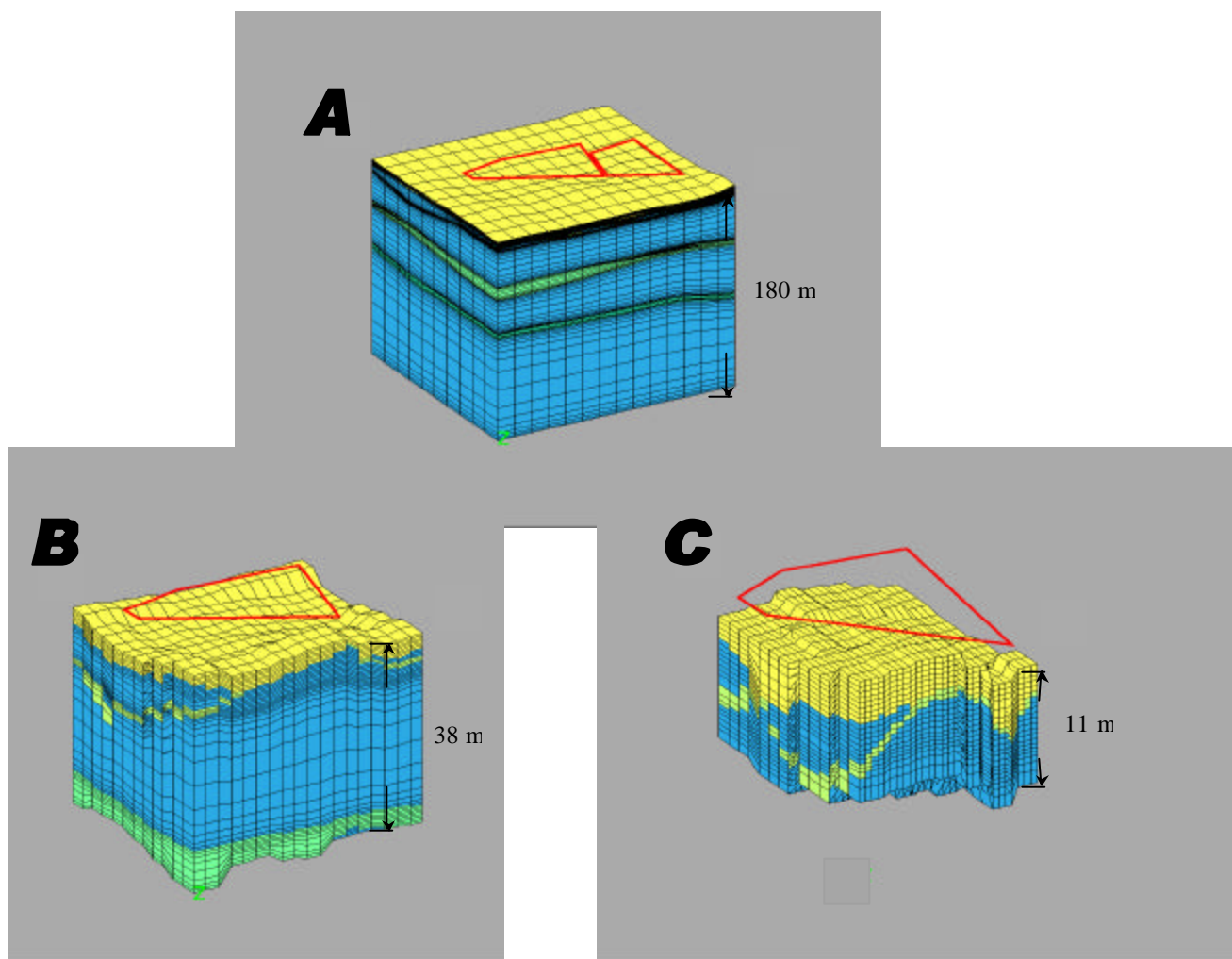


Fig. 1. Conformable grid for base domain (A) and concentrically refined domains (B and C). Surficial sediments are shown in yellow, interbeds in green, and fractured basalt in blue.

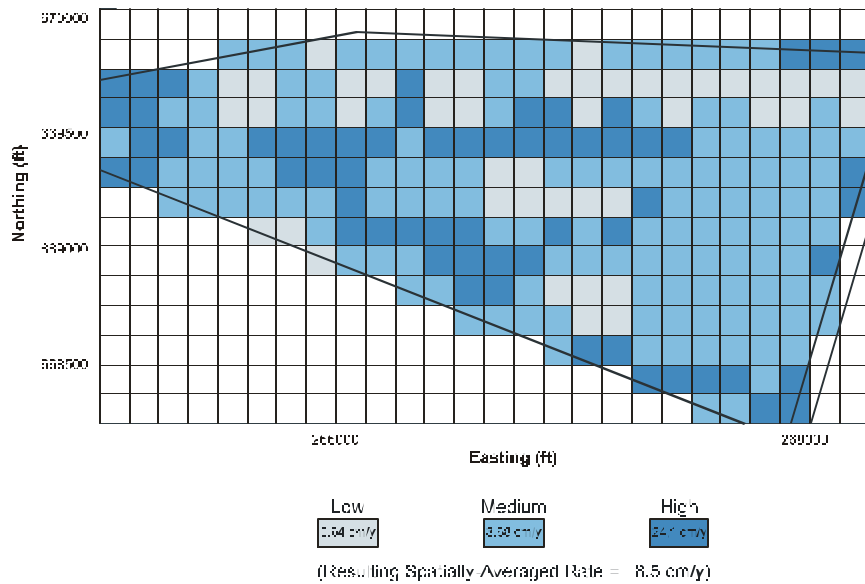


Fig. 2. Spatially varying infiltration rates assigned inside the SDA.

III. CONCEPTUAL UNCERTAINTY SIMULATION RESULTS

Conceptual uncertainties relating to the flow and transport modeling addressed for this paper were spatial variability in infiltration, movement of contaminants via facilitated transport, and variably saturated fracture hydraulic properties. Each is discussed in turn.

III.A. Infiltration rates

To compare the effect of infiltration rates assigned at the surface, an alternate approach was used to assign infiltration rates. Rather than three spatially variable rates, a single equivalent infiltration rate of 8.5 cm/year was assigned. Fig. 3 shows maximum simulated U-238 aquifer concentrations with the base spatially variable infiltration and with the equivalent uniform infiltration. The concentration with the uniform infiltration rate is approximately half an order of magnitude higher than that with the spatially varying infiltration rate, indicating the importance of the amount of water going through the waste zones.

III.B. Facilitated Transport

Infrequent, sporadic, low-level detections of actinides in the aquifer near the SDA have led to the hypothesis that facilitated transport, possibly by actinides associated with colloids, is occurring. Column studies with SDA interbed samples also have shown a very small mobile fraction for plutonium isotopes.⁶ A series of simulations were performed to evaluate the effects of fractional

amounts of the plutonium in the buried waste becoming mobile annually. The assigned fractions were 1×10^{-6} , 1×10^{-4} and 1×10^{-2} . In the subsurface model, a low sediment partition coefficient of 0.1 ml/g was assigned to represent the mobile fraction to allow for comparison to observed interbed sediment concentrations. Fig. 4 shows the simulation results for the base and range of mobile fraction results. In each mobile fraction case, the Pu-239 concentration rapidly rises. Comparisons of the simulated concentrations to concentrations detected in the aquifer and in the interbeds show that none of the simulated mobile fraction results are plausible.

III.C. Variably Saturated Fracture Flow Moisture Characteristic Curve

The simulations include a fractured-basalt, which is conceptualized as a high-permeability low-porosity continuum. The constitutive relations describing moisture content, matric potential, and hydraulic conductivity for the base simulations are described by a Corey-type curve. The parameters for this Corey-type curve were defined through inverse modeling to a wetting front advance from the Large Scale Infiltration Test conducted in 1994 at the INEEL.⁷ Subsequent tensiometer monitoring at one location inside the SDA was used to test the appropriateness of this moisture characteristic curve (MCC) that has been used for the fractured basalt. Two alternative descriptions, one using a differently parameterized Corey curve and one using a van Genuchten curve, were used to describe water movement in the fractured basalt.

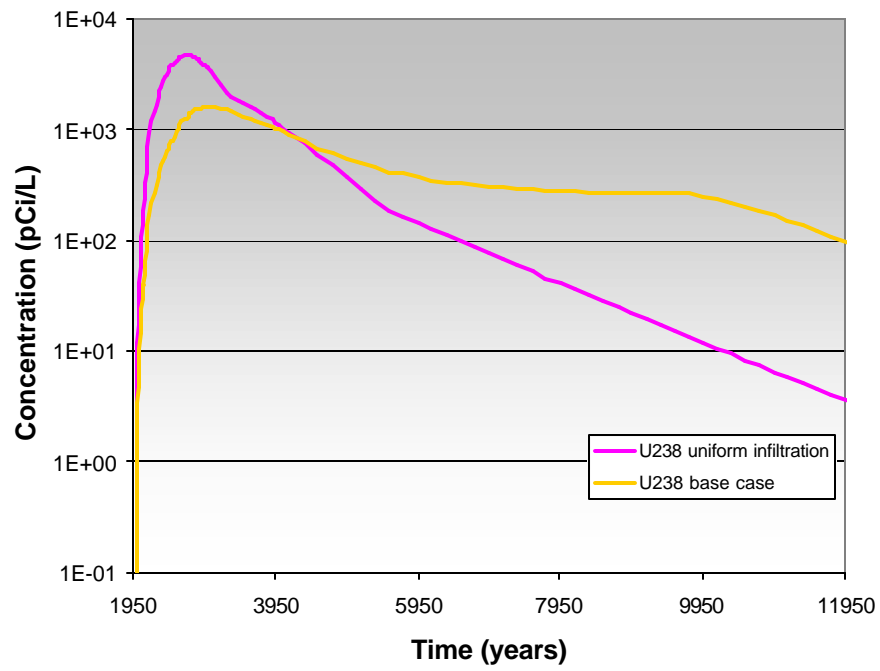


Fig. 3. Spatially variable versus uniform infiltration: effect on simulated aquifer U-238 concentration.

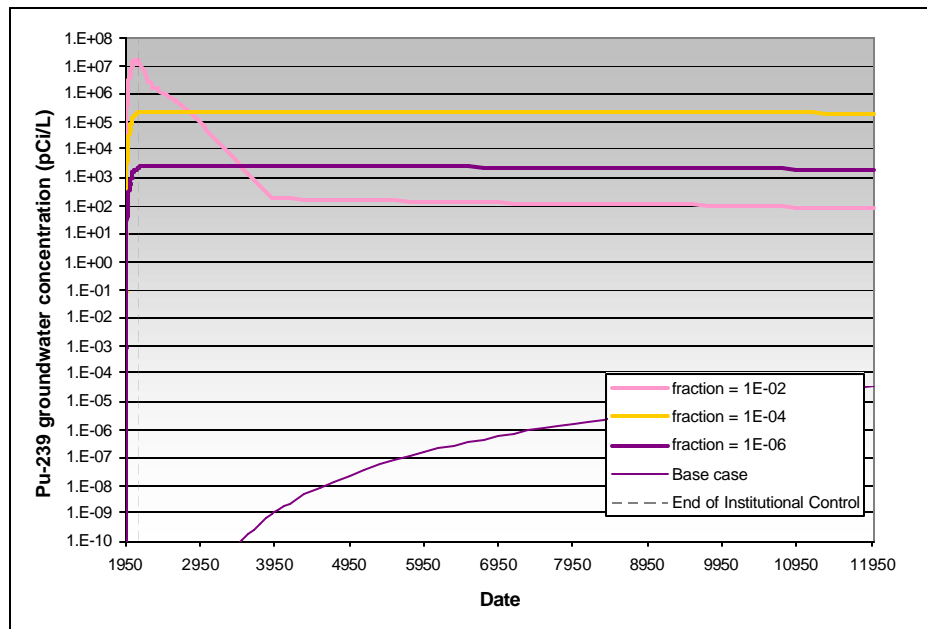


Fig. 4. Simulated aquifer Pu-239 concentrations for base and mobile fraction simulations.

Fig. 5 shows a well construction diagram for a location inside the SDA that has nested tensiometers that recorded the movement of three successive wetting fronts to depth in 1999. Also shown in the figure is a one-dimensional simulation grid that was used to represent this site. Fig. 6 compares observed and simulated matric potentials with three wetting events imposed at land surface. The series of wetting fronts can be seen passing down through the profile during the late winter and early spring of 1999. The intermediate depth (9.4 m) was within a very thin local interbed. The simulated results using a van Genuchten MCC mimic the data reasonably

well, with the combined effect of multiple wetting fronts showing progressively wetter conditions over time. The last plot in Fig. 3 shows simulated water fluxes out the bottom of the domain using the van Genuchten MCC curve, the base case Corey MCC curve, and the alternative Corey MCC curve. The Corey curves show faster and more complete advances of the wetting front through the simulation domain. The base Corey curve shows nearly the fastest simulated wetting front movement through the domain, demonstrating that a conservative approach was used to simulate water movement in the fractured basalt portion of the vadose zone simulations.

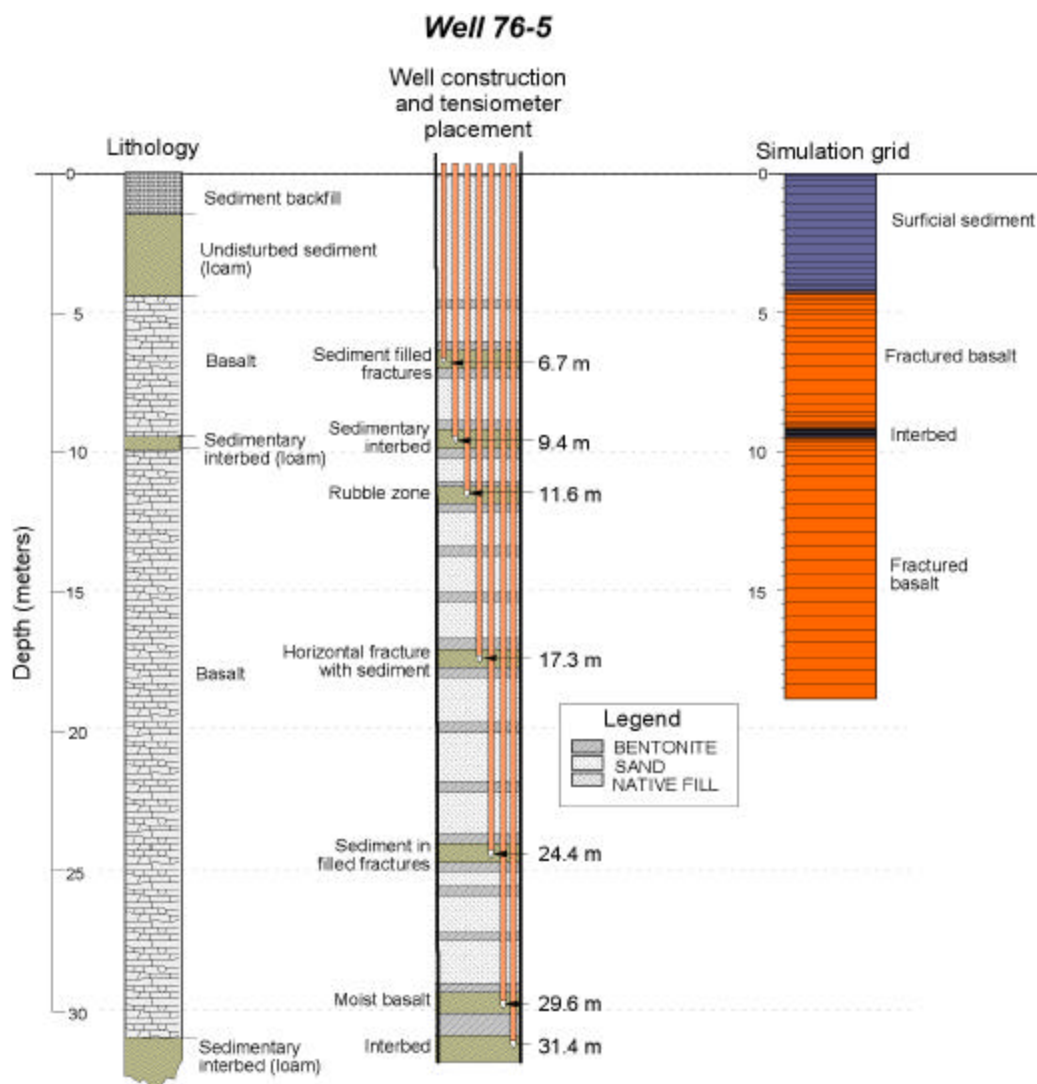


Fig. 5. Construction and simulation grid for Well 76-5.

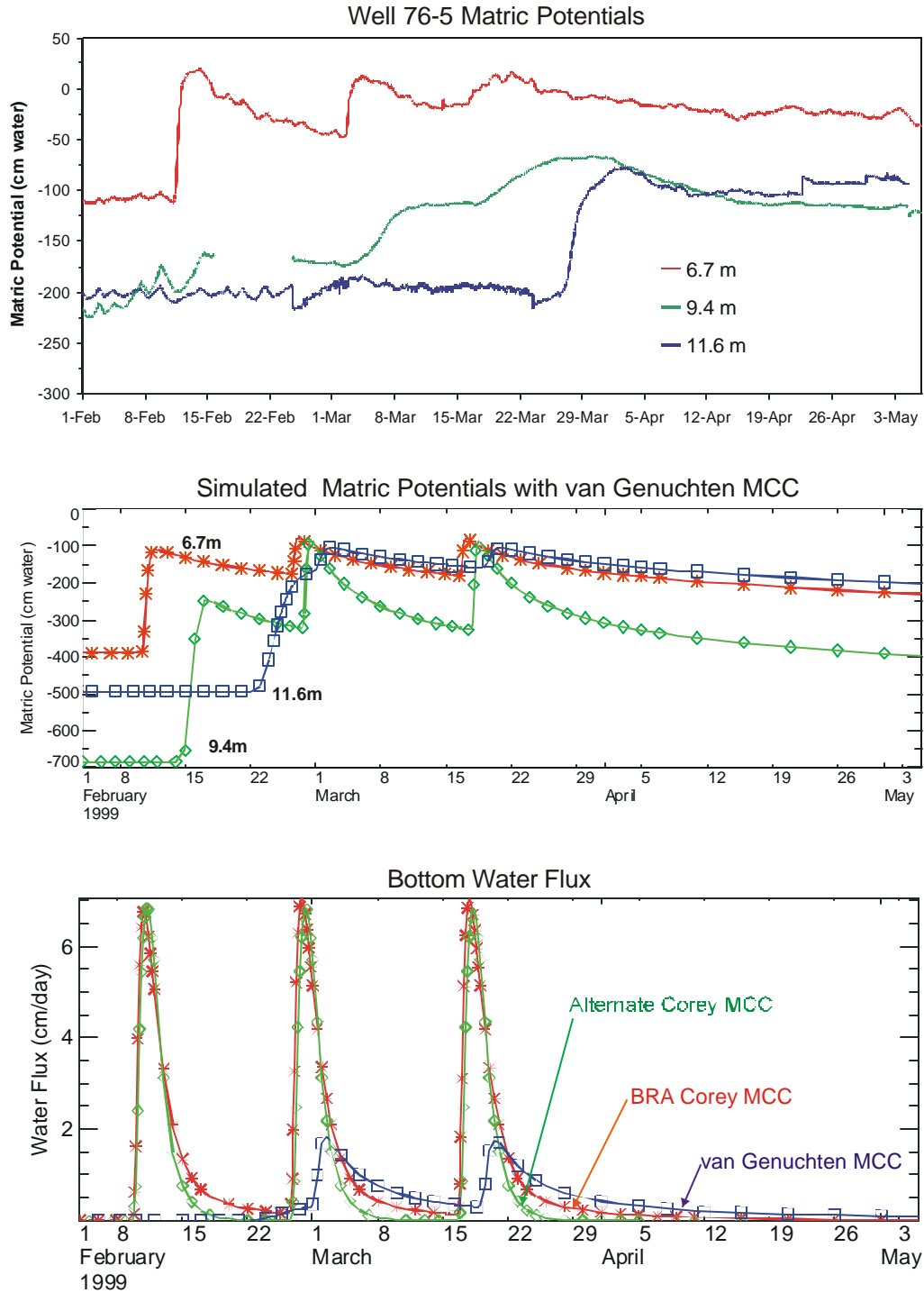


Fig. 6. Observed and simulated matric potentials for a well inside the SDA and simulated fluxes with different moisture characteristic curves.

IV. CONCLUSIONS AND DISCUSSION

A model was refined to simulate flow and transport of contaminants as part of a CERCLA site assessment for the Subsurface Disposal Area (SDA) at the INEEL. Conceptual uncertainties for the model were assessed by im-

plementing conceptual variations such as different infiltration rates at the surface, facilitated transport, and different methods to describe hydraulic properties of variable saturated fractured basalts constituting the majority of the subsurface. The fluxes out the bottom of the vadose zone model were input into an aquifer model to es-

timate aquifer concentrations. The estimated aquifer concentrations were used to evaluate human health risks for a potential future receptor as part of the CERCLA process. The sensitivity of the results to the conceptual variations has been used to guide additional characterization activities at the SDA. Of the sensitivities discussed in this paper, the primary sensitivity has been the amount of water that actually infiltrates through the waste, thereby mobilizing contaminants.

Improvements in modeling for the SDA will derive primarily from calibration to monitoring data within the pits and in the deeper vadose zone. As representativeness is established, uncertainty regarding conceptual errors will be lessened and more emphasis on quantification of the parametric uncertainty can then be accomplished.

ACKNOWLEDGEMENTS

Work supported by the U.S. Department of Energy, Assistant Secretary for Environmental Management, under DOE Idaho Operations Office Contract DE-AC07-99ID13727.

REFERENCES

1. P. K. W. VINSOME and G. M. SHOOK, "Multi-Purpose Simulation," *Journal of Petroleum Science and Engineering*, **9**, pp. 29-38 (1993).
2. S. O. MAGNUSON and A. J. SONDRUP, *Development, Calibration, and Predictive Results of a Simulator for Subsurface Pathway Fate and Transport of Aqueous- and Gaseous-Phase Contaminants in the Subsurface Disposal Area at the Idaho National Engineering and Environmental Laboratory*, INEEL/EXT-97-00609, Lockheed Martin Idaho Technologies Company, Idaho Falls, Idaho (1998).
3. S. P. NEUMAN, "Accounting for Conceptual Model Uncertainty Via Maximum Likelihood Bayesian Model Averaging," *Proc. 4th Int. Conf. on Calibration and Reliability in Groundwater Modeling: A Few Steps Closer to Reality*, Prague, Czech Republic, June 17-20, 2002, *Geologica* (2002).
4. M. K. LEECASTER, *Geostatistic Modeling of Subsurface Characteristics in the Radioactive Waste Management Complex Region, Operable Unit 7-13/14*, INEEL/EXT-02-00029, Revision 0, April, Bechtel BWXT Idaho, LLC, Idaho Falls, Idaho (2002).
5. P. MARTIAN, *UNSAT-H Infiltration Model Calibration at the Subsurface Disposal Area, Idaho National Engineering Laboratory*, INEL-95/0596, Lockheed Idaho Technologies Company, Idaho Falls, Idaho (1995).
6. R. A. FJELD, J. T. COATES, and A. W. ELZERMAN, *Column Tests to Study the Transport of Plutonium and other Radionuclides in Sedimentary Interbed at INEEL*, Department of Environmental Engineering and Science, Clemson University, Clemson, South Carolina (2000).
7. S. O. MAGNUSON, *Inverse Modeling for Field-Scale Hydrologic and Transport Parameters of Fractured Basalt*, INEL-95/0637, Lockheed Martin Idaho Technologies Company, Idaho Falls, Idaho (1995).