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SANDIA NATIONAL LABORATORIES
WASTE ISOLATION PILOT PLANT

AP-149

Analysis Plan for the Interpretation of Culebra Tracer Tests

Task 1.4.2.3

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1 Introduction and Objectives

1.1 Introduction

In 1996, the Department of Energy (DOE) completed a performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP). The PA was part of the Compliance Certification Application (CCA) submitted to the Environmental Protection Agency (EPA) to demonstrate compliance with the radiation protection regulations of 40 CFR 191 and 40 CFR 194. As required by the WIPP Land Withdrawal Act (Public Law 102-579), DOE is required to submit documentation to EPA for the recertification of the WIPP every five years following the first receipt of waste in order to continue operation of the site. Calculations characterizing probabilities of release are performed to support the recertification process. Releases considered in these calculations and subsequent analyses include those due to cuttings and cavings, spallings, direct brine releases, and groundwater transport releases through the Culebra Dolomite Member of the Rustler Formation. Currently, Culebra transport calculations assume homogeneity of the subsurface geology. Experimental work has been performed that demonstrates that the subsurface geology in the vicinity of WIPP is heterogeneous. It is expected that the inclusion of subsurface heterogeneity in the Culebra transport calculations will provide better agreement between simulated and experimental Culebra transport results.

Revision 1 of AP-149 was made to reflect the changes to how the transport solution will be performed. Rather than modifying STAMMT-L to replace SECOTP2D, SECOTP2D will instead be modified to include the required capabilities of STAMMT-L. Additionally, previously collected Culebra column study data has become available (Lucero et al., 1998), and will be used with STAMMT-L to provide additional data for justification of the new parameters needed in PA.

1.2 Objectives

This analysis plan (AP-149) describes the set of compliance-level calculations (as per NP 9-1) that will be performed using a modified version of SECOTP2D to simulate multi-rate mass transport in the Culebra. A combination of MODFLOW-2000, SECOTP2D, STAMMT-L, and PEST (or equivalent codes, as they become quality assurance (QA)-approved) will be used to numerically re-create tracer tests that have already been conducted, for the estimation of model parameters to be used in future PA simulations. The CCA, Compliance Recertification Application (CRA) 2004, and CRA 2009 PA simulations have used a dual-porosity SECOTP2D for radionuclide transport in the Culebra. Simulating multi-rate mass transport in the Culebra using either STAMMT-L or a modified version of SECOTP2D will require additional parameters not previously needed by SECOTP2D (e.g., multi-rate diffusion coefficients, justified per procedure NP 9-2), which must be estimated from interpretation of tracer tests already performed in the Culebra (e.g., at H-19 (Meigs et al., 2000) and H-11 (Jones et al., 1992)) and from column studies previously performed using Culebra cores (Lucero et al., 1998).

2 Approach

Culebra flow will be simulated using MODFLOW-2000, at a hydropad scale (e.g., several nearby wells at the scale of a few tens of meters), to account for observed heterogeneity and transient behavior witnessed during Culebra tracer tests. This observed hydropad heterogeneity is at a scale smaller than the MODFLOW-2000 Culebra model used for PA (which has 100 meter square finite-difference cells). The MODFLOW model parameters used for the simulation in this analysis will not share any parameters with those from the PA model calibration, since they represent different scales.

STAMMT-R (Haggerty et al., 2000) was previously used to interpret Culebra tracer tests (Meigs et al., 2000). STAMMT-R cannot accommodate heterogeneity or asymmetries in the groundwater flow field and transport parameters, or background regional flow gradients, as this code assumes radial symmetry. By accounting for these deviations from perfect radial symmetry in the simulation, we will estimate parameters (e.g., diffusion rate distribution coefficients) for use in Culebra flow and radionuclide transport on the scale used for PA.

The PA radionuclide transport simulation previously done for PA with SECOTP2D assumes a single rate of diffusion between the matrix and fracture porosities. In contrast, the proposed methodology will use a distribution of diffusion rate coefficients. Either STAMMT-L or a modified version of SECOTP2D will have the capability to use a distribution of mass-transfer coefficients. These distribution parameters will be estimated from analyzing Culebra tracer tests and Culebra column studies; the results of these analyses being added to the PA Parameter Database (PAPDB).

3 Software List

Table 1 lists the main computer codes and their minimum applicable version numbers, which will be used for the Culebra tracer test interpretation. Equivalent codes (different codes and newer versions of those listed) can be substituted for those in Table 1, as new codes become available and comply with the requisite QA standards.

Table 1. Main Computer Codes (and minimum version numbers) to be Used in the Culebra Flow and Transport Analysis

Code	Program Type	Version
MODFLOW-2000	groundwater flow simulation	1.60
SECOTP2D	solute transport in two dimensions	1.41a
STAMMT-L	solute transport in one dimension	3.0[1]
PEST	inverse modeling (parameter estimation using 3 other codes)	9.11
Python	script interpretation / plotting	EPD 6.1

[1] STAMMT-L version 3.0 has not yet finished the QA-qualification process, as of May, 2010.

4 Tasks

This analysis will combine several portions of hydraulic and tracer test analysis into a single consistent result for each hydropad. Hydraulic head data collected at multi-well hydraulic pumping tests will be used as data to constrain parameter estimation; along with tracer concentration data collected during different tracer tests at the same hydropad. PEST will be used to jointly invert the flow and tracer transport solutions to best fit the observed data. The resulting parameter estimates will then be used to simulate Culebra flow and transport conditions believed to be important to PA. The process is fairly generic and can be completed at multiple hydropads, and therefore Table 3 lists estimated time required to complete steps, rather than calendar dates.

4.1 Data Sources

The WIPP Records Center package ERMS 237446: T*racer test sample analyses general [University of Nevada Las Vegas (UNLV) contract aj-8745]* contains both electronic and hard-copy versions of tracer and hydraulic test data from the H-11, H-19, and H-6 hydropads. Beauheim (1989) includes hydraulic test data (in hardcopy form) for the H-11b4 multi-pad pumping test. Jones et al. (1992) includes tabulated tracer test data (in hardcopy form) for the

H-2, H-3, H-6, and H-11 hydropad tracer tests. Background and previous interpretations of the H-19 tracer tests are summarized in SAND97-3109 (Meigs et al., 2000), and the Water Resources Research journal papers Haggerty et al. (2000), Meigs and Beauheim (2001), and Haggerty et al., (2001). Column studies on Culebra cores were performed and reported in SAND97-1763 (Lucero et al., 1998).

Some older tracer and pumping tests were performed before the current QA system was in place. Any data sources (especially older ones) that are not already qualified, will be evaluated for inclusion for this analysis, as the work progresses. The Lucero et al., (1998) Culebra core data, and the H-19 and H-11 tracer test data are already qualified, and will not need to be evaluated.

4.2 Task 1: Qualification of Data

Depending on the status of the data to be used in the analysis, some data sources must be qualified. If any non-qualified data is to be used, it must be qualified. If all data to be used in the analysis is already qualified, this task will already be complete.

4.3 Task 2: Modification of SECOTP2D

The solute transport code SECOTP2D will be modified to add multirate mass transport, similar to that done by STAMMT-L. The modified code will be tested and subjected to QA in accordance with NP 19-1.

4.4 Task 3: Simulation of Groundwater Flow

To allow for non-radial flow fields and heterogeneous flow parameter distribution, MODFLOW-2000 will be used to simulate groundwater flow on the hydropad scale. Model cells will be sized appropriately to capture heterogeneity that is believed to affect the results of both pumping and tracer tests. The required size of the domain, model finite-difference grid spacing, and the boundary conditions assigned at the distal extent of the domain (e.g., no flow or no drawdown) will be investigated as part of the analysis. These modeling assumptions will be made so as to minimally impact the results, while maintaining small computer run times for the codes.

4.5 Task 4: STAMMT-L/SECOTP2D Transport Simulation

The results of Task 3 are groundwater flow velocities, which will be used as inputs to SECOTP2D simulation for pad-scale tracer tests. For one-dimensional column studies, STAMMT-L will be used directly to compute the solution, without need for a separate groundwater flow model. Both the modified version of SECOTP2D and STAMMT-L will use the same transport parameters.

4.6 Task 5: PEST Parameter Estimation

The observed data at a particular hydropad may include observed hydraulic heads during pumping tests, observed hydraulic heads during tracer tests, known tracer inputs during tracer tests, and observed tracer concentrations sampled at extraction wells during tracer tests. The model input parameters that PEST will estimate include both flow and transport inputs. MODFLOW hydraulic parameters include Culebra hydraulic conductivity and storativity (not needed for column simulations). Estimated parameters include both Culebra transport properties (e.g., multi-rate diffusion coefficient distributions, longitudinal dispersivity, and tortuosity), and tracer-specific properties (e.g., free water diffusion coefficient distribution and potential retardation). PEST will be used to adjust the input parameters in a methodical manner, to find a distribution of flow and transport parameters that best reproduce the observed

responses at each hydropad or column study. Tasks 3, and 4 comprise a single forward simulation and will be executed by PEST many times during the optimization process.

4.7 Task 6: Report Preparation

The results of the tracer test reinterpretation will be summarized in one or more Analysis Reports to document the exact steps taken and report the results of the optimization process.

Table 2. Task Completion Dates Summary Table

Task	Estimated Time Required	Responsible Individuals
1	0-3 months	Kris Kuhlman, Bwalya Malama
2	12 months	
3	6 months	
4		
5	4 months	
6	3 months	

5 Special Considerations

There are no special considerations.

6 Applicable Procedures

Analyses will be conducted in accordance with the quality assurance (QA) procedures listed below.

Training: Training will be performed in accordance with the requirements in NP 2-1, Qualification and Training.

Parameter Development and Database Management: Selection and documentation of parameter values will follow NP 9-2. The database will be managed in accordance with relevant technical procedure.

Computer Codes: New or revised computer codes that will be used in the analyses will be qualified in accordance with NP 19-1. Codes will be run on the fully-qualified PA Linux cluster.

Analysis and Documentation: Documentation will meet the applicable requirements in NP 9-1.

Reviews: Reviews will be conducted and documented in accordance with NP 6-1 and NP 9-1, as appropriate.

7 References

Beauheim, R.L. 1989. *Interpretation of H-11b4 Hydraulic Tests and the H-11 Multipad Pumping Test of the Culebra Dolomite at the Waste Isolation Pilot Plant (WIPP) Site*, Sandia National Laboratories, Albuquerque, NM, SAND89-0536.

Haggerty, R., Fleming, S.W., and McKenna, S.A. 2000. *STAMMT-R Solute Transport and Multirate Mass Transfer in Radial Coordinates*, Sandia National Laboratories, Albuquerque, NM, SAND99-0164.

Haggerty, R., Fleming, S.W., Meigs, L.C., and McKenna, S.A. 2001. Tracer tests in a fractured dolomite 2. analysis of mass transfer in single-well injection withdrawal tests, *Water Resources Research*, 37(5), 1129-1142.

Haggerty, R., McKenna, S.A., and Meigs, L.C. 2000. On the late-time behavior of tracer test breakthrough curves, *Water Resources Research*, 36(12), 3467-3479.

Jones, T.L., Kelley, V.A., Pickens, J.F., Upton, D.T., Beauheim, R.L., and Davies, P.B. 1992. *Integration of Interpretation Results of Tracer Tests Performed in the Culebra Dolomite at the Waste Isolation Pilot Plant*, Sandia National Laboratories, Albuquerque, NM, SAND92-1579.

Lucero, D.A., Brown, G.O., and Heath C.H., 1998. Laboratory column experiments for radionuclide adsorption studies of the Cuelbra Dolomite member of the Ruster Formation. Sandia National Laboratories, SAND97-1763.

Meigs, L.C. and Beauheim, R.L. 2001. Tracer tests in a fractured dolomite 1. Experimental design and observed tracer recoveries, *Water Resources Research*, 37(5), 1113-1128.

Meigs, L.C., Beauheim, R.L., and Jones, T.L. (eds). 2000. *Interpretation of Tracer Tests Performed in the Culebra Dolomite at the Waste Isolation Pilot Plant Site*, Sandia National Laboratories, Albuquerque, NM, SAND97-3109.

Walter, G.R. 1986. *1981 Aquifer tests at the H-6 hydropad: Basic data and porous-medium interpretations*, Sandia National Laboratories, Albuquerque, NM, SAND86-7087.

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