Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Plan for Justifying Software Changes for Culebra Flow and Transport Calculations

AP-081

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1. Introduction

As part of the Technical Baseline Migration (TBM) for the Waste Isolation Pilot Plant (WIPP), a performance assessment (PA) will be conducted to compute the complementary cumulative distribution function (CCDF) for possible normalized radionuclide releases to the accessible environment. Specifically for the Culebra Dolomite Member of the Rustler Formation, single-phase groundwater flow and radionuclide transport will be numerically/computationally simulated. Similar performance assessments were conducted in 1996 as part of the Compliance Certification Application (CCA, 1996) and in 1997 as part of the Performance Assessment Verification Test (PAVT, 1997); however, calculations for the TBM will differ in several important aspects. Most notably, newly qualified flow and transport codes will replace outdated programs.

This document describes the analysis plan (AP) for the migration of the Culebra flow and transport codes from the old software suite to the updated set of programs. A list of both old and new codes is provided and major assumptions are discussed. Comparison testing of the new software will support their accuracy when agreement with the old codes is found. Where comparison tests demonstrate significant deviation between old and new code output, discrepancies will be justified and a rationale for the outcome established.

2. Analysis Overview

The cumulative release of radionuclides through the Culebra and to the accessible environment will be estimated using a flow code developed by the United States Geological Survey (USGS) and transport codes developed by Sandia National Laboratories (SNL). Overall, the calculations for the Culebra flow and transport for the TBM will require significant computational resources. One hundred partial mining and one hundred full mining transmissivity fields generated for the PAVT by GRASP–INV (Lavenue, 1996) to approximate the geology of the Culebra will be used again for the TBM. Latin hypercube sampling will be used to select necessary hydrogeologic properties for the flow and transport codes from Sandia's PA qualified parameter database. These fields/parameters will be used by MODFLOW–2000 (McDonald and Harbaugh, 1988; Harbaugh *et al*., 2000) to generate steady state flow fields. Each flow field will be simplified to a single, representative travel time and corresponding path length by the particle tracking code, DTRKCDB, for each release point/intrusion location. (The number and location of release points for the TBM is yet to be determined.) The representative velocities and path lengths will be used by STAMMT–L to establish a collection of breakthrough curves (one for each release point in each transmissivity field). Finally, these breakthrough curves will be used as input to the code CCDFGF that generates complementary cumulative distribution functions (Helton and Johnson, 1996; Smith *et al*., 1996). These complementary cumulative distribution functions may be interpreted as overall probabilities of contaminant release.

The scientific goal described in this AP is not to perform complete Culebra flow and transport calculations. Rather, it is intended to provide a rationale for the new suite of flow and transport codes to be used for the TBM. Three primary codes (MODFLOW, DTRCKCDB, and STAMMT–L) will be evaluated for suitability and accuracy of solution for flow and transport in the Culebra. Six transmissivity fields will be selected from the 200 fields generated by GRASP–INV for the PAVT for comparison testing. Steady-state flow fields resulting from the six transmissivity fields will be calculated using the well-known modular software package, MODFLOW, and output will be compared to results from SECOFL2D (the flow code used for the CCA and PAVT). Note that MODFLOW calculations will be performed as closely as possible to corresponding PAVT calculations, although runs for the TBM will likely deviate to some degree based upon a better current understanding of the hydrogeologic system. The particle tracking software, DTRKCDB, will be used to supply a velocity and path length (derived from MODFLOW flow field results) for each transmissivity field. Only a single release of 1 kg of a radionuclide over 50 years from the center of the waste panel area will be examined for each transmissivity field in this analysis. Using the results from DTRKCDB, the one-dimensional, semi-analytical, transport code, STAMMT–L will produce breakthrough and normalized concentration curves for each transmissivity field as well as cumulative mass released. Comparisons will be drawn between the curves resulting from STAMMT–L and those of SECOTP2D (the transport code used for the CCA and PAVT) from the PAVT. Necessary pre- and post-processors for all codes are listed and will be verified according to the QA requirements for software.

3. Software List

The software to be used in the TBM analysis is shown in Table 1. Table 1 also lists software and version number used in the PAVT. Relevant comments for each code are given.

4. Comparison Testing

In general, comparison testing will be conducted in accordance with the AP for the TBM (Wall, 2001). The codes listed in Table 1 will be run on the COMPAQ Alpha platform using OpenVMS AXP, version 7.2. Six transmissivity fields generated for the PAVT by the program GRASP–INV will be retrieved from Sandia’s CAMDAT database and used as input for MODFLOW. In both the CCA and PAVT, SECOFL2D was run iteratively, first on a coarse regional grid, and then on a more refined local grid. Between runs, bilinear interpolation was used to relate regional and local grid hydrogeologic parameters and boundary conditions. MODFLOW will also be run for both coarse and fine grids with a data processor used between runs to coordinate regional and local grids. Because it was recognized as a shortcoming, higher order interpolation may be used to relate regional and local grid information. The data processor performing this task will be verified according to all software QA requirements. Any further pre- and post-processing of MODFLOW data will be completed and the resulting flow fields will be presented as vector plots using an appropriate software tool (e.g., Tecplot). Appropriate measures for

Table 1: Relevant codes used/to be used in the PAVT and TBM PA calculations.

Code name*	PAVT Version	TBM Version	Comments
SECOFL2D	3.03	N/A	PAVT flow code with results to be compared to MODFLOW.
MODFLOW	N/A	1.5	MODFLOW is a well-known, user friendly, modular flow code. To be qualified (TBQ).
SECOTP2D	1.41	N/A	PAVT transport code with results to be compared to DTRKCDB/STAMMT–L.
DTRKCDB	N/A	1.00	Particle tracking code to calculate velocity and travel distance for STAMMT–L from MODFLOW flow fields. TBQ.
STAMMT–L	N/A	2.00	Semi-analytical, one-dimensional solute transport code. TBQ.
Pre-MODFLOW	N/A	TBA	Organizes transmissivity fields and other parameters for MODFLOW. TBQ.
Post-MODFLOW	N/A	TBA	Prepares MODFLOW output for use by DTRKCDB. TBQ.
Post-DTRKCDB	N/A	TBA	Prepares DTRKCDB output for use by STAMMT–L. TBQ.

* More pre-and post-processors may be added as needed

data traceability will be taken. Vector plots of SECOFL2D flow fields corresponding to the same transmissivity fields will be put side-by-side with the MODFLOW results if such data is available. Furthermore, a statistical analysis of the flow field data will measure the means, variances, and correlation of the two data sets. These visual and statistical comparisons will reveal how closely the flow fields from these codes agree with one another.

Similar to the PAVT, allowances for climate change will be incorporated. The post-processor for MODFLOW will multiply the magnitudes of the components of the velocity field by the appropriate climate index factor from the PAVT input vector. DTRKCDB will use the resulting flow fields.

DTRKCDB is a particle tracking code with results that embody each spatially variable flow field from MODFLOW as a single, representative velocity and path length for each particle release point. Analytical solutions to ordinary differential equations are used to determine the total travel distance and necessary travel time for the particle to exit the system (Treadway and Rudeen, 2000). In this analysis, a particle will be released at the center of the waste panel area and followed until it reaches the land withdrawal boundary (LWB) for each flow field considered. The particle path and travel time yield a description of the velocity field experienced by radionuclides discharged from the corresponding release point. STAMMT–L uses these parameters to estimate radionuclide transport characteristics. As no equivalent particle tracking code was used in the PAVT, there is no comparison test to be performed for DTRKCB.

STAMMT–L is a one-dimensional, steady state, dual porosity, multi-rate transport code that numerically inverts the Laplace transform of the governing advection–diffusion equation (Haggerty and Reeves, 2000). For each run of STAMMT–L the path length and velocity (path length divided by transport time) yielded from DTRKCDB will be used to generate contaminant breakthrough and normalized concentration curves at the LWB. Because of the different physical models used in DTRKCDB/STAMMT–L and SECOTP2D, variations in the breakthrough and normalized concentration curves are expected. STAMMT–L is a one-dimensional model (although the multi-rate parameters add a quasi-second dimension) and therefore without transverse diffusion. One hypothesis is that the contaminant plume from STAMMT–L may demonstrate a sharper peak than the corresponding plume from SECOTP2D where contaminants are allowed to disperse perpendicularly to the primary flow direction. Further, because SECOTP2D is a finite difference code, it suffers from numerical dispersion that grows in proportion to the grid size. Because the dimensions for the finite volume grid used for the PAVT are quite large (upward of 50 m), the numerical dispersion inherent to the technique becomes a significant detractor from solution accuracy. It was this large numerical dispersion as well as mass conservation concerns in SECOTP2D that prompted the development of the alternate transport code. STAMMT–L does not suffer from numerical dispersion and it has proven to yield accurate solutions (Haggerty, 1995; Haggerty and Gorelick, 1995). Note that SECOTP2D correctly models the decay of the radionuclides, while STAMMT–L does not account for this process to err on the side of conservatism. By not accounting for decay, more radionuclides will be present in the system for possible release to the environment, reaffirming the conservative nature of the model. Furthermore, in STAMMT–L, daughter products expected to form by decay are assumed initially present as 1 kg releases over 50 years. Again, this equates to a conservative estimate for radionuclide release because more radionuclides than would otherwise be present will be used for the initial condition. The five radionuclides of interest are ^{241}Am, ^{238}Pu, ^{239}Pu, ^{230}Th, and ^{234}U (Helton *et al*., 1998, p 4–44). In the PAVT the only radionuclide with significant releases was ^{234}U, therefore only this isotope will be used for these comparison tests.

5. Tasks

Scott James will handle coordination and management of the comparison testing of the TBM codes with the PAVT results. Bruce Baker will be responsible for MODFLOW runs, David Rudeen will perform all DTRKCDB runs, while Mike Wallace executes STAMMT–L. Amy Gilkey will be responsible for all pre- and post-processing. Stephen Tisinger will provide database support. Rodger Coman will provide CMS support. Scott James will coordinate analysis and documentation. The technical, QA, and management reviewers will be Sean McKenna, Mario Chavez, and M. Kathryn Knowles, respectively. Report to be submitted to DOE/CBFO November 30, 2001.

6. Special Considerations

No special considerations have been identified for this analysis.

7. 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 SP 9–1. The database is to 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. All other codes unchanged since the PAVT are qualified under multi-use provisions of QAP 19–1. Codes will be run on the Compaq Alpha platform using OpenVMS AXP, version 7.2.

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.

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