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SANDIA NATIONAL LABORATORIES
WASTE ISOLATION PILOT PLANT

AP-144

Analysis Plan for the Calculation of Culebra Flow and Transport for CRA2009PABC

Task 1.4.2.3

Effective Date: 07/20/09

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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.

A new set of PA calculations will be included in the CRA-2009 PABC submittal to EPA (Cotsworth, 2009; Moody, 2009). Analysis Plan AP-145 (Clayton, 2009) presents the full set of PA calculations required for the CRA-2009 PABC and lists the series of analysis plans that describe the specific details for each component model that will be run. This analysis plan (AP-144) describes the set of calculations that will be run to simulate Culebra flow and transport in the vicinity of the repository for 10,000 years, given the 100 calibrated Culebra parameter fields (Hart, 2009). The horizontal hydraulic conductivity (proportional to transmissivity), horizontal anisotropy, and vertical recharge are parameter fields included in the calibration.

1.2 Objectives

This Analysis Plan directs the modification of the 100 calibrated realizations of Culebra transmissivity (T) inside areas that would be affected by the removal of potential potash deposits (Cranston, 2009). The mining-modified T fields are substituted back into the original MODFLOW-2000 model and re-executed to get the predicted Culebra flowfield under the influences of potash mining. Then the MODFLOW-2000 flow modeling grid (100 m square) is refined to smaller 50 m square elements and both boundary conditions and parameter fields are interpolated onto the finer mesh. The flow budgets from the MODFLOW-2000 simulation using the 50 m mesh are used as inputs to the SECOTP2D solute transport modeling. The SECOTP2D model computes radionuclide transport over a period of 10,000 years; its results are inputs to CCDFGF, for computing the CCDF for releases through the Culebra.

2 Approach

Culebra flow is simulated using MODFLOW-2000, given the 100 parameter fields realizations resulting from the PEST calibration efforts of Hart (2009). Culebra transport will be simulated using the SECOTP2D, which uses the Culebra flow field computed by MODFLOW-2000 as input.

Different boundary conditions and different sets of adjustable parameters are used in the CRA-2009 PABC MODFLOW-2000 model, compared to the CRA-2004 PABC MODFLOW-2000 simulations. The MODFLOW-2000 domain has also been enlarged, with the eastern boundary moved 6 km east, compared to CRA-2004 PABC.

2.1 Modification of Transmissivity Fields for Mining

After the CRA-2009 PABC T fields are calibrated to steady-state water levels and transient hydraulic-response data (Task 7 of AP-114, Beauheim, 2008), they are modified to account for the potential effects of future potash mining, using definitions of the mining areas from the Bureau of Land Management (Cranston, 2009). The mining modification is performed in two stages. The "partial-mining" modification is performed by increasing the transmissivity of the Culebra over areas that might be mined in the future (yellow mining zones in Figure 1) outside the WIPP land-withdrawal boundary. For each of the calibrated T fields, the Culebra T in the affected regions is increased by a random factor between 1 and 1000 produced by Latin Hypercube Sampling (LHS). For the "full-mining" modification, the T multiplier is applied to all areas that might be mined, both outside and within the WIPP land-withdrawal boundary. For a given T field, the same T multiplier is used for both the partial-mining and full-mining modifications.

The mining modification analysis will largely follow the procedure taken in the analysis report associated with Task 5 of AP-088 (Lowry, 2004). The most significant procedural change will be a modification of the boundary conditions in mining-affected areas. In areas where the mining zones intersect the constant head boundary conditions, shown in Figure 1 as overlapping yellow (mining zones) and the light gray areas (constant head regions east of the halite margins), the constant head cells are changed to active cells, while still maintaining a single column or row of constant head cells along the perimeter of the model domain. This represents the conversion of the very low permeability zones east of the halite margin to active flow regions, based on the increase in permeability associated with the mining modification.

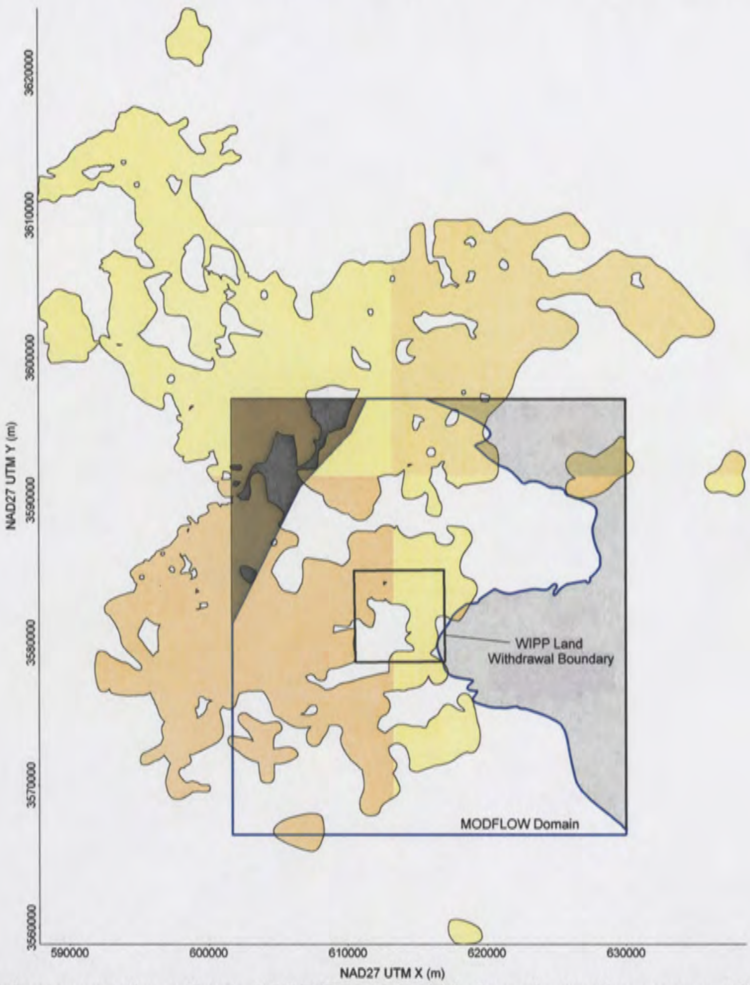

Figure 1. Potash mining zones (in yellow), MODFLOW-2000 domain (active area outlined in blue, inactive cells shaded dark gray, constant head cells shaded light gray) and WIPP Site Boundary (black square)

2.2 Culebra Transport Calculations

Radionuclide transport in the Culebra will be simulated using a two-dimensional dual-porosity or dual-continuum solute transport model to account for the fractured nature of the porous medium. The model assumes parallel-plate-type fracturing where fluid flow is restricted to the fractures (the advective continuum). Advection and hydrodynamic dispersion are considered to be the dominant physical transport processes within the fractures, while molecular diffusion is the dominant physical transport mechanism within the rock matrix (the diffusional continuum). The dual-porosity model includes diffusional mass transfer between the rock matrix and the fractures. Retardation is permitted in both the advective and diffusive continuum assuming a linear equilibrium sorption process. Radioactive decay is accounted for in the model through the use of multiple straight decay chains.

The Culebra radionuclide transport calculations will be performed using the SECOTP2D code. SECOTP2D is an implicit finite volume code that is second-order accurate in space and time. Advective terms are discretized using a Total Variation Diminishing (TVD) scheme. Diffusion terms are treated using central differences. The time discretization is a generalized three-level scheme. SECOTP2D uses a staggered finite volume mesh in which the velocity components are defined at cell faces while concentrations are defined at cell centers.

The physical domain used in the transport calculations will be a subregion of that used for the groundwater flow calculations (Figure 2). This subregion will be approximately 7.5 km by 5.4 km, aligned with the principal directions of the groundwater flow domain. The transport domain will extend beyond the boundaries of the WIPP in the east-west direction (approximately 200 m in the west and approximately 700 m in the east). Since the groundwater flow direction is generally north to south, the transport domain will extend from a point midway between the waste panels and the northern WIPP boundary to approximately 1000 m beyond the southern WIPP boundary. The transport calculations will use a uniform computational grid composed of 50 m square cells.

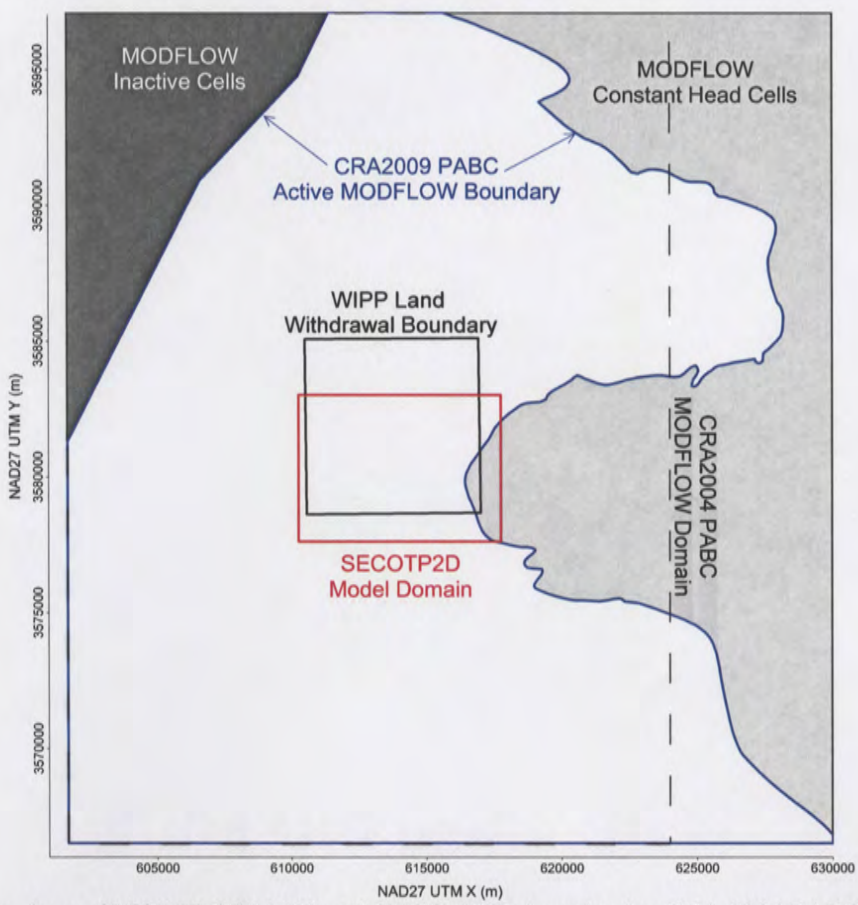

Figure 2. Comparison of MODFLOW-2000 and SECOTP2D domains for CRA-2004 PABC and CRA-2009 PABC. Inactive and constant head cells refer to CRA-2009 PABC MODFLOW-2000 model.

3 Software List

The main computer codes and their applicable version numbers, which will be used for the Culebra mining modification and SECOTP2D radionuclide transport calculations, are listed in Table 1.

Table 1. Main Computer Codes to be Used in the Culebra Flow and Transport Analysis

Code	Version
ALGEBRACDB	2.35
DTRKMF	1.00
GENMESH	6.08
GROPECDB	2.12
MATSET	9.10
MODFLOW-2000	1.60
POSTLHS	4.07A
POSTSECOTP2D	1.04
PRESECOTP2D	1.22
RELATE	1.43
SECOTP2D	1.41A
SUMMARIZE	3.01

4 Tasks

The work that is covered under this AP is follow-on work to that conducted under AP-114. AP-114 outlines the tasks necessary to generate new T fields for the CRA-2009 PABC. Once the T-fields are generated and have been modified for both full- and partial-mining conditions, several additional steps are involved in adapting them for use in the Culebra transport calculations. This analysis plan outlines the tasks necessary to use the new T fields in the Culebra transport calculations. The input from the work performed under AP-114 for the tasks outlined here are 100 unaltered T, anisotropy, and recharge fields, boundary conditions, and the other ancillary input files and parameters related to the steady-state MODFLOW-2000 simulation.

4.1 Task 1: Evaluation of Mining Scenarios

For CRA-2004 PABC, the potential effects of future potash mining on flow and transport in the Culebra were evaluated by increasing the transmissivity of the Culebra in the areas that might be affected by mining. For each realization of the calibrated Culebra T fields, the T within the area potentially affected by mining was increased by a randomly chosen factor between 1 and 1000. Model boundary conditions were left unchanged during this exercise. Two different scenarios were considered, denoted the partial-mining and full-mining cases. The partial-mining case assumed that all potash was mined from leased areas outside the WIPP land-withdrawal boundary. The full-mining case assumed that all economic-grade ore was also mined from within the WIPP land-withdrawal boundary. For each T-field realization and each case, the flow path and groundwater travel time from a point above the center of the WIPP disposal panels to the WIPP land-withdrawal boundary were calculated.

Full-mining and partial-mining cases will be evaluated in exactly the same manner using the transient-calibrated T fields generated under Task 7 of this AP-114. The flow path and groundwater travel time from a point above the center of the WIPP disposal panels to the WIPP land-withdrawal boundary will be calculated using DTRKMF for each modified T field, and CDFs of travel time for the partial-mining and full-mining cases will be generated. The CDFs generated from the mining-altered T fields used in the CCA will be compared to the new CDFs to determine if the new T fields produce results that are significantly different from those presented in the CCA. Deliverables for this task will consist of the T fields modified for partial- and full-mining conditions and the CDFs of travel time to the WIPP land-withdrawal boundary.

4.2 Task 2: Conversion to 50 m Grid

The T fields being generated under AP-114 use a uniform grid of 100 m square cells. The radionuclide transport calculations require a finer mesh with 50 m square cells. Hence, the MODFLOW-2000 domain used for T field generation will be refined by creating a new grid with 50 m cells, and mapping the distributed flow properties and model parameters from each of the old 100 m cells directly into the corresponding four 50 m cells. T, horizontal anisotropy, recharge, and cell activity (i.e., no-flow, constant head, or active MODFLOW-2000 IBOUND flag) are copied uniformly from the 100 m grid to the 50 m grid. The specified head boundary condition values for the refined grid will be linearly interpolated onto the 50 m grid from the heads assigned for the 100 m grid.

The product of this task will be 600 T fields on a 50 m grid: Three replicates of both the 100 T fields altered for partial mining (outside the controlled area), and the 100 T fields altered for full mining (both inside and outside the controlled area).

4.3 Task 3: MODFLOW Runs to Generate SECOTP2D Input

After the mining-modified T fields are migrated to the 50 m grid, a forward steady-state MODFLOW run will be performed for each field to generate a cell-by-cell flow budget file that can be used as input to SECOTP2D. The product of this task will be 600 flow budget files.

4.4 Task 4: Extraction of Flow Field Values for SECOTP2D

Because the physical domain used in the transport calculations will be a subregion of that used for the groundwater flow calculations, the flow budget information for the transport subregion will be extracted from the full budget files calculated by MODFLOW-2000, for the full CRA-2009 MODFLOW-2000 model domain using VTRAN (see Figure 2). The product of Task 4 will be 600 extracted water budget files: three replicates of each of the 100 partial-mining T fields; and the 100 for full-mining T fields.

4.5 Task 5: Radionuclide Transport Calculations

This task first involves application of a scaling factor to the groundwater velocity fields from Task 4 to account for climate change, as input to the calculation of radionuclide transport through the Culebra.

Section 6.4.9 of the CCA (DOE, 1996) discusses how potential changes in the future climate might affect groundwater flow in the Culebra, and how the effects of those changes are incorporated in transport modeling. The regional, three-dimensional effects of climate change can be reasonably approximated in performance assessment through direct scaling of specific discharge in the two-dimensional, steady-state groundwater velocity field for the Culebra. Radionuclide transport in the Culebra is then calculated by SECOTP2D using the scaled velocity fields.

Scaling of the two-dimensional velocity field is done using the Climate Index, which is a dimensionless factor by which the specific discharge in each grid block of the MODFLOW domain is multiplied. As summarized in CCA Appendix PAR (Parameter 48), the Climate Index is a sampled parameter in the performance assessment, with a bimodal distribution ranging from 1.00 to 1.25 and from 1.50 to 2.25. A single value of the Climate Index is chosen in LHS for each sample element and held constant throughout the 10,000-year SECOTP2D simulation. Each realization of disposal system performance thus represents a different approximation of future climate. Those realizations (25%) in which the sampled value is close to its maximum of 2.25 represent the most extreme changes in groundwater flow that may result from climatic change. Sampled values close to the minimum of 1.00 (75%) represent climatic changes that have little effect on groundwater-flow velocities. Because all sampled values of the Climate Index are greater than 1.00, climate change as implemented in the performance assessment can only increase the rate of groundwater flow. The Climate Index is applied to each velocity field by the code PRESECOTP2D.

Radionuclide transport in the Culebra will then be calculated using SECOTP2D. SECOTP2D will be run for 600 cases: three replicates of 100 vectors each for both full- and partial-mining conditions. Each replicate applies a different random sampling of the Climate Index to the velocity fields. The output from the SECOTP2D calculations will be used in CCDFGF to calculate the CCDF for releases through the Culebra over 10,000 years. The results of Task 6 will be documented in an analysis package.

4.6 Task 6: Reporting

An analysis report will be written, which summarizes the results of the analysis outlined here. The analysis report will contain material analogous to that contained in the 2003 and 2004 reports related to AP-088 Task 5 (Lowry, 2004) and AP-100 (Lowry, 2003; Kanney, 2003). A run control summary will also be included as an appendix to the analysis report.

Table 2. Task Completion Dates Summary Table

Task	Estimated Completion Date	Responsible Individual
1	August 31, 2009	Kris Kuhlman
2	September 7, 2009	
3	September 14, 2009	
4	September 21, 2009	
5	October 19, 2009	
6	January, 31, 2010	

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. All other codes unchanged since the PAVT are qualified under multi-use provisions of NP 19-1. Codes other than MODFLOW-2000 will be run on the fully-qualified WIPP PA Alpha cluster. MODFLOW-2000 will be run on the fully-qualified i686 Intel PC cluster running Red Hat Linux.

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.. 2008. "*Analysis Plan AP-114, Revision 1, Analysis Plan for Evaluation and Recalibration of Culebra Transmissivity Fields*". ERMS#548162. Carlsbad, NM, Sandia National Laboratory.

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Moody, Dave. 2009. "*Response to EPA May 21, 2009 Letter on CRA-2009 – changes included in the Performance Assessment Baseline Calculation*". ERMS#551565. Carlsbad, NM, Department of Energy Carlsbad Field Office.