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ACTIVITY/PROJECT SPECIFIC PROCEDURE

SP 9-9
PREPARATION OF CULEBRA POTENTIOMETRIC
SURFACE CONTOUR MAPS
Revision 0

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1.0   Purpose and Scope

This procedure prescribes the Sandia National Laboratories (SNL) Waste Isolation Pilot Plant (WIPP) process for creating contour maps of groundwater flow model generated freshwater head and a conservative particle track beginning at the WIPP waste handling shaft consistent with freshwater head values observed in Culebra monitoring wells over a specified time period. The particle track, contour maps, and associated summary statistics will be used to satisfy New Mexico Environment Department (NMED) regulations associated with WIPP.

Beginning with the ensemble of calibrated groundwater flow model transmissivity (T) fields used in WIPP performance assessment (PA), a single average T field is used as input to a groundwater flow model to simulate freshwater heads in and around the WIPP land withdrawal boundary (LWB). A parameter estimation (i.e., inverse modeling) code is used to adjust the boundary conditions of the model to obtain the best-fit match between the observed freshwater heads from approximately one month in a calendar year and the model-predicted heads. The output of the averaged,calibrated groundwater flow model is contoured and used to compute an advective particle track forward from the WIPP waste handling shaft. The contour map, particle track, associated summary fit statistics, and Quality Assurance (QA) run control information are submitted to records in an analysis report.

This Activity/Project Specific Procedure (SP) is intended to direct SNL technical personnel in the procedures needed to produce high-quality results that meet SNL QA standards. All future calculated contour maps, particle tracks, and associated statistics will be documented in analysis reports to file in the WIPP records center referencing this SP. This SP is governed by Nuclear Waste Management Procedure (NP) 9-1 Analyses, which directs analyses associated with routine calculations and programmatic decisions.

Acronyms and definitions for terms used in this procedure may be found in the Glossary located at the Sandia National Laboratories (SNL) WIPP Online Documents web site.

1.1   Executive Summary of Process

The potentiometric surface map for a given time period shall be generated using the following steps:
- ➢ Examine hydrographs to identify the time period having the largest number of Culebra water levels available with the fewest wells affected by pumping or other anthropogenic events.
- ➢ Convert water levels from target time period to equivalent freshwater heads using fluid densities appropriate to the date.
- ➢ Fit trend surface through freshwater heads.
- ➢ Extrapolate the trend surface to the boundaries of the model domain used in Performance Assessment (PA) and define initial fixed-head boundary conditions based on the trend surface.
- ➢ Using the ensemble-average Culebra transmissivity field from the PA, optimize the model boundary heads to improve the fit of the model to the freshwater heads at the wells using optimization software interactively with the groundwater flow model.
- ➢ Run the groundwater flow model with optimal boundary conditions fit.
- ➢ Contour groundwater flow model head results on WIPP site.
- ➢ Compute particle path and travel time from the waste handling shaft to the Land Withdrawal Boundary.

2.0   Implementation Actions

2.1   Safety

The activities described in this SP shall conform to SNL Environmental Safety and Health programs (ES&H). All activities described in this SP will be conducted in the SNL office facility.

2.2   Responsibilities

The Technical Staff are responsible for performing the calculations as outlined in this procedure, documenting all required information described in this SP, and assuring the latest revision of this document is followed.

If the procedure cannot be worked as written, the user has the responsibility to stop work and resolve all concerns with the principal investigator (PI) and/or QA as appropriate, prior to proceeding with the work.

2.3   Equipment (Software List)

The equipment required to perform the work outlined in this SP is limited to a computer with the requisite software, and a working knowledge of how to use the computer and software. The software utilized in this SP includes both commercial off-the-shelf (COTS) software and software previously qualified for use in WIPP Performance Assessment (PA).

The groundwater flow simulations, particle track, and boundary condition parameter estimation are performed using the most recent qualified versions of MODFLOW (Harbaugh et al., 2000), DTRKMF (Rudeen, 2003) and PEST (Doherty, 2002), respectively (see Table 1). These programs have already been qualified for use on WIPP PA. The contouring of the head results, plotting of the particle track, and plotting of the summary statistics will be done using one or more available COTS plotting

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programs (e.g., Golden Software Surfer, GnuPlot, or Microsoft Excel, etc.), as appropriate for each required result.

Table 1. Software Used

Software	Description	Status
MODFLOW-2000	Flow model	Acquired; qualified under NP 19-1 (Harbaugh et al., 2000)
PEST	Inverse model	Developed; qualified under NP 19-1 (Doherty, 2002)
DTRKMF	Particle tracker	Developed; qualified under NP 19-1 (Rudeen, 2003)

2.4 Procedure for Computing Modeling Results

The steady-state groundwater flow simulations are carried out using the same simulation code used to create the calibrated fields used as inputs when possible. The groundwater flow model T field used here to compute the freshwater heads and flow vectors is an ensemble average of the Culebra T fields used for WIPP PA. To clearly distinguish between the two, the original groundwater flow model, which consists of multiple realizations of calibrated parameter fields (obviously a pre-requisite for this analysis) will be referred to as the "*PA groundwater flow model*". The model derived here from the PA groundwater flow model, to be used to construct the resulting contour map and particle track, will be referred to as the "*averaged groundwater flow model*". The calibrated model parameters, boundary conditions, and other model input files are appropriately averaged across all realizations to produce a single averaged steady-state groundwater flow model that can be used to predict regional Culebra groundwater flow across the WIPP site.

The calibration process that resulted in the calibrated model realizations of the PA groundwater flow model adjusted spatially variable model parameters using the inverse modeling software, while holding the groundwater model boundary conditions constant to best fit both snapshots of undisturbed conditions across the site and transient responses to large-scale pumping tests.

The resulting heads from the inverse model calibrated ensemble-average flow model will be contoured over the region surrounding the WIPP site (a subset of the complete groundwater flow model domain) using COTS contouring software. The track made by a conservative (i.e., non-dispersive and non-reactive) particle released from the waste handling shaft to the WIPP land withdrawal boundary will be computed from the flow field computed by the groundwater flow model using qualified particle-tracking code. Plots of statistics summarizing the fit of the calibrated model to the observed freshwater head at Culebra monitoring wells will be created and included in an Analysis Report including Run Control documentation as per the reporting standards in NP 9-1 (specifically Appendix B). The Analysis Report will be submitted to technical, QA, and management review according to NP 6-1, Document Review Process.

2.4.1 Creating Ensemble-Average Groundwater Flow Simulation

An ensemble-average groundwater flow model is used to compute both the freshwater head and flow vectors across the model domain; the heads are then contoured and the cell-by-cell flow vectors are used to compute particle tracks. The ensemble-averaged inputs are used to create a single average simulation that produces a single output, rather than averaging the multiple realizations of the Culebra flow model used for WIPP PA.

The model inputs from the PA groundwater flow model will be checked out of the proper version control system repository. The input files and parameters associated with the most recent calibrated Culebra PA groundwater flow model should be used. The model inputs can be divided into two

groups. The first group is the model inputs that are the same across all calibrated realizations; these include the model grid definition, the boundary conditions, and the model solver parameters. The second group is the model inputs that are different for each realization; these include *x*-direction hydraulic conductivity, vertical recharge, and the horizontal anisotropy ratio. The model inputs in the first group are used directly in the averaged groundwater flow model, while the inputs in the second group must be averaged across all realizations. Hydraulic conductivity (and any other parameter that varies over multiple orders of magnitude) will be log-transformed before averaging.
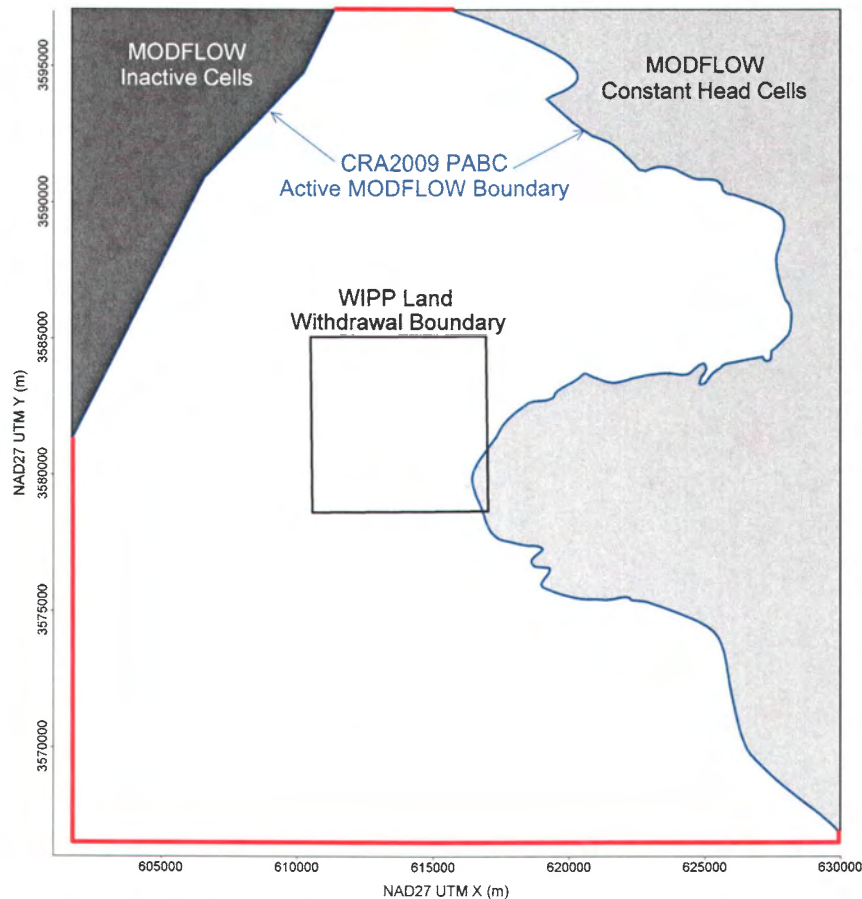
Figure 1. CRA-2009 PABC model domain and different types of boundary conditions

The boundary conditions belong to the first group of inputs (they are constant across all PA groundwater flow model realizations), but are discussed separately here because of their importance to the current work. The boundary conditions taken from the PA groundwater flow model in the version control system repository are used as the baseline condition, from which the inverse model calibration can be compared. There are two types of boundary conditions in both groundwater flow models. The first type of condition includes geologic or hydrologic boundaries, which correspond to known physical features in the flow domain. For example, from the CRA-2009 PABC, the no-flow boundary along the axis of Nash Draw is a hydrologic boundary (i.e., the boundary along the dark gray region in Figure 1). Also from the CRA-2009 PABC, the constant head boundary along the halite margin corresponds to a geologic boundary (i.e., the eastern irregular boundary adjoining the light gray region in Figure 1).

Physical boundaries are assumed to be known, and are not adjusted in the inverse model calibration. The second type of boundary condition includes the constant head cells along the rest of the model domain; the linear southern, southwestern, and northern boundaries that coincide with the rectangular

frame surrounding the model domain are all of this type (shown as a heavy red line in Figure 1 for CRA-2009 PABC). The value of specified head used along this second boundary type will be adjusted in the inverse model calibration process (Table 2 summarizes the parameter connections between the PA and averaged groundwater flow models).

Table 2. Summary of connections between PA groundwater flow model inputs and those in averaged groundwater flow model

PA groundwater flow Model Input Parameters (averaged groundwater flow model inputs in red)
1. **variable** across all realizations (e.g., hydraulic conductivity, anisotropy) ← averaged
2. **constant** across all realizations
a. boundary conditions (BC)
i. **geological / hydrological** boundary conditions   ← used directly
ii. other **model-required** boundary conditions   ← inverse modeled
b. **non-BC** constant model parameters (e.g., grid geometry)   ← used directly

2.4.2 Inputs to Inverse Model Calibration of Averaged Groundwater Flow Model to Observations

There are three major inputs to the inverse model. The first type of input includes the set of observed freshwater head values used as targets for the inverse model calibration. The second class of inputs includes the entire groundwater flow model setup described in the previous section, along with any pre- or post-processing scripts or programs needed; this comprises the forward model that the inverse model runs repeatedly to estimate sensitivities of model outputs to model inputs. The third type of input includes the inverse model input files, which include parameter and observation groups, indicating which parameters in the groundwater flow model will be adjusted in the inverse simulation.

The freshwater head values that are used as target values should be representative of "quiescent" conditions at WIPP, when there are minimal observable transient responses occurring due to anthropogenic (e.g., pumping tests, well rehabilitation, or nearby oil field activities) or natural (e.g., rainfall) causes. For each calendar year for which a potentiometric surface map is needed, hydrographs of all wells monitored during that year will be prepared. Through evaluation and comparison of all the hydrographs, the month in which the largest number of wells showed the least transient response to the types of factors listed above will be identified. If no data are available for specific wells during the chosen month, data may be interpolated for those wells from prior and later water-level measurements, if the analyst concludes that a defensible basis for that interpolation exists. All interpolations will be fully explained in the analysis report prepared for this task. The water-level data from the chosen month will then be converted to equivalent freshwater heads using fluid densities calculated following the procedure outlined in SP 9-11, when possible. When near-simultaneous pressure and water-level data are not available to calculate the density of the fluid in a well, historical records of activities and other measurements in the subject well will be examined to develop a basis for estimating fluid density. The methods used to establish fluid densities for all wells will be fully documented in the analysis report prepared for this task.

The forward simulation includes a trend surface extrapolation script or program which takes the adjustable parameters for the surface as inputs and creates a groundwater flow model starting-head array as output. The choice of type and degree of trend surface is left to the analyst, but it should be sufficiently flexible and general to allow the inverse model to improve the fit of the model to observed heads, without over-parameterizing the problem. Inputs to this pre-processing program are controlled by the inverse model during calibration. A post-processing script or program is used to extract and interpolate the model-predicted heads at observation locations from the groundwater flow model

output files. The inverse model reads the output from post-processing to compute the fit of the model to the observed target heads. The entire forward simulation includes the pre-processing surface extrapolation, the forward groundwater flow simulation, and the extraction of the model-predicted head at desired locations.

The inverse model specific input files make up the third type of input; these are largely dependent on the specific types of parameters and observations described in the previous paragraphs. It is left to the analyst to determine the appropriate optimization options or features to use. Inverse model calibration should try to find the set of boundary conditions that best re-creates the observed freshwater heads in the Culebra monitoring network while still producing physically plausible results across the model domain. Some extreme combinations of boundary head values may improve model fits at observations at the expense of producing physically improbable model-predicted heads between observations.

2.4.3   Producing Deliverables from Calibrated Groundwater Flow Model

The groundwater flow model is run predictively using the ensemble-averaged model parameters, along with the inverse model calibrated boundary conditions. The resulting cell-by-cell flow budget is then used to compute a particle track from the map location of the waste handling shaft (in the Culebra) to at least the edge of the WIPP land withdrawal boundary. The particle tracking code will be used to compute the conservative particle track.

The resulting particle track and contours of the model-predicted head will be plotted using a COTS contouring or plotting program for an area including the WIPP land withdrawal boundary, similar to the region shown in previous Annual Site Environmental Reports (ASERs); e.g., Figure 6.11 in DOE (2008). Surfer (Golden Software, 2002) or equivalent COTS can be used to plot the results in an acceptable format for inclusion in the resulting analysis report.

A scatter-plot showing the relationship between measured and modeled freshwater heads, along with a summary statistic indicating the goodness-of-fit for the linear correlation (e.g., R^2) at wells is the minimum required information to be included in the memo with the contour map and particle track.

2.5   Special Considerations

The work outlined in this SP depends on the results of the PA groundwater flow model calibration (AP-114 Task 7 - Beauheim, 2008 - for CRA-2009 PABC) and any prerequisites that are identified therein.

2.6   References

Beauheim, R.L. 2008. "Analysis Plan for Evaluation and Recalibration of Culebra Transmissivity Fields, AP-114, Revision 1", ERMS# 548162, Sandia National Laboratories WIPP Records Center, Carlsbad, NM.

DOE (Department of Energy). 2008. *Waste Isolation Pilot Plant Annual Site Environmental Report for 2007*. DOE/WIPP-08-2225. Carlsbad, NM: U.S. DOE.

Doherty, J. 2002. *PEST: Model Independent Parameter Estimation*. Brisbane, Australia: Watermark Numerical Computing.

Golden Software, Inc. 2002. "Surfer for Windows User's Guide". Golden, CO: Golden Software, Inc.

Harbaugh, A.W., E.R. Banta, M.C. Hill, and M.G. McDonald. 2000. *MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model -- User Guide to Modularization Concepts and the Ground-Water Flow Process.* Open-File Report 00-92. Reston, VA: U.S. Geological Survey.

Rudeen, D.K. 2003. User's Manual for DTRKMF Version 1.00. ERMS 523246. Carlsbad, NM: Sandia National Laboratories.

3.0   Records

The following QA records, generated through implementation of this procedure, shall be prepared and submitted to the WIPP Records Center in accordance with NP 17-1 (Records). Two analysis reports are to be prepared, with the contour map generation report depending on the results of the freshwater head calculation report. This will allow the data to be subjected to full review and QA before the analysis is performed, since the quality of the data is critical to the rest of the method.

<div align="center">QA Record</div>

- Analysis Report documenting freshwater head calculation including a table of values to be used in contour map generation and justification of density values.
- Analysis Report documenting contour map generation with Run Control documentation
- Contour map with particle track from waste handling shaft
- Scatter plot showing modeled and measured observations summary fit statistics

4.0   Appendices

There are no appendices associated with this document.

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