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SANDIA NATIONAL LABORATORIES
WASTE ISOLATION PILOT PLANT

Analysis Plan for Evaluation of the Effects of Head Changes on Calibration of Culebra Transmissivity Fields

AP-088

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1. INTRODUCTION AND OBJECTIVES

This Analysis Plan directs the development of transmissivity (T) fields for the Culebra Dolomite Member of the Rustler Formation at the Waste Isolation Pilot Plant (WIPP) site to evaluate the effects of head changes on T-field calibration. Culebra T fields are used in WIPP Performance Assessment (PA) modeling of groundwater flow and radionuclide transport. The Culebra T fields used for PA modeling for the WIPP Compliance Certification Application (CCA; US DOE, 1996) were calibrated to heads assumed to represent steady-state conditions as well as to transient heads arising from hydraulic testing and shaft activities. Monitoring subsequent to the CCA has shown heads at many wells to be outside the uncertainty ranges for steady-state conditions, raising questions about the validity of the calibration. We hypothesize that while the assumption of Culebra heads being in steady state may have been unwarranted, this would have no effect on the calibration of the T fields. As long as the heads used for calibration were in equilibrium with the boundary conditions on the system and both were reasonably defined in the model, an appropriate representation of the Culebra T fields should have been obtained. Thus, the major objective of this activity is to develop T fields using heads from three different time periods to show whether or not the calibration is significantly affected if the equilibrium state of the overall system changes. The groundwater travel time from above the center of the WIPP disposal panels to the WIPP site boundary (accessible environment) will be used as the metric by which a "significant" change to the T-field calibration is judged. A secondary objective of this activity is to produce Culebra T fields that can be used to evaluate scenarios thought to have the potential to affect observed Culebra water levels, such as leaking boreholes and potash tailings ponds. The T fields developed under this Analysis Plan may be used for Compliance and/or Programmatic Decisions.

An approach will be taken under this Analysis Plan to produce Culebra T fields that are consistent with Sandia's hydrogeological conceptual model of the Culebra. Preliminary regression studies suggest a strong statistical relationship between hypothesized geological controls and values of Culebra transmissivity at WIPP wells. We will extend these results and develop a regression-based approach for predicting Culebra transmissivity based on geologic information and observed Culebra transmissivity data. The T fields generated using the regression-based approach will then be conditioned to observed heads that were presumably equilibrated with the boundary conditions at the time and also to transient heads.

2. APPROACH

The approach to be taken in development of the Culebra T fields involves, first, defining a statistical correlation between Culebra transmissivities measured at individual wells and geologic factors such as thickness of overburden and amount of dissolution of the upper Salado Formation. This correlation will then be used in combination with contour maps of the geologic factors to create 100 equally likely realizations of the Culebra transmissivity distribution ("base" T fields) over the domain of interest. The modeling domain will be similar in extent to that used in the CCA, but will be oriented with its long axis extending from north to south, parallel to the principal flow direction in the Culebra, like the model domain of LaVenue et al. (1990). These base T fields will then be conditioned to Culebra hydraulic heads representing equilibrium conditions at 10-year intervals (e.g., 1980, 1990, and 2000) and the "steady-state" conditions presented in the CCA using a pilot-point method. To determine how much effect the differences in head have on the resulting T fields, cumulative distribution functions (CDFs) of the groundwater travel times from a point above the center of the waste-disposal panels to the WIPP site boundary will be generated for each set of 100 realizations, and the CDFs will be compared to each other. One or more of the sets of T fields conditioned to equilibrated heads will also be conditioned to transient heads arising from activities in the WIPP shafts and hydraulic tests conducted in the Culebra. The CDF of travel times for these transient-calibrated T fields will be compared to a CDF generated of travel times used in the CCA. Finally, the transient-calibrated T fields will be altered to represent the potential effects of future potash mining as was done for the CCA. Again, CDFs of travel times for the mining cases will be compared to the CDFs generated of travel times used in the CCA.

The data that will be needed to accomplish these tasks includes some or all of the following:

- transmissivity values at wells;
- well locations;
- ground surface elevation at wells;
- stratigraphic information;

- equilibrated heads at defined times;
- Culebra fluid density at wells;
- transient pressure data;
- transient flow-rate data; and
- boundaries of potential mining areas.

Each task report that is prepared (see Section 4) will include a description of the verification methods employed for gathering and interpreting the data used.

3. SOFTWARE LIST

The following computer codes may be used for different tasks associated with development of Culebra T fields:

- ESRI ArcInfo 8.1 (off-the-shelf software);
- WinGSLib/GSLIB90 (acquired; routines to be qualified under NP 19-1);
- Mathcad 2001i (off-the-shelf software);
- MODFLOW 2000 v. 1.6 (to be qualified under NP 19-1);
- PEST v. 5.5 (to be qualified under NP 19-1); and
- DTRKCDB (to be qualified under NP 19-1).

Off-the-shelf spreadsheet programs, such as Excel 2000, and graphing programs, such as Grapher 3 or SigmaPlot.0, may also be used for data manipulation and plotting. Any pre- or post-processors needed for data manipulation and transfer between codes will also be qualified as part of the analysis package.

4. TASKS

Development of Culebra T fields and assessment of their differences with respect to the CCA T fields has been divided into five principal tasks, described below. All tasks will be documented according to NP 9-1 *Analyses* by the task analyst as the analysis progresses. Analysis packages will be prepared, reviewed, and submitted by the responsible analyst according to Appendices B and C

(*Analysis Records* and *Routine Calculation Requirements*, respectively) of NP 9-1 at the completion of each set of related analyses.

Task 1 Construction of Geologic Contour Maps

The first task is to construct maps of the geologic factors affecting transmissivity. These geologic "controls" include the thickness of overburden above the Culebra, the thickness reduction in the upper Salado Formation due to dissolution, and the spatial distribution of halite underlying and overlying the Culebra. These maps will be hand-contoured using the best geologic judgment of the analyst to preserve consistency with known geologic information and Sandia's conceptual hydrogeological model.

The principal analyst for Task 1 will be Dennis Powers. Data sources for this task will include well location and elevation survey information, geophysical well logs, and core logs. Deliverables will be contour maps of the three geologic controls discussed above. The contour maps are expected to be completed by April 1, 2002.

Task 2 Estimating Base Transmissivity Fields

An estimate of the spatial distribution of mean transmissivity is required for generating conditional realizations of Culebra transmissivity. In the past, the transmissivity distribution in the Culebra was determined using a geostatistical approach that incorporated transmissivity data (e.g., variography and kriging) but neglected geologic information. Sandia's current conceptual model for the Culebra relies on geological explanations for the variability of Culebra transmissivity and defines possible geologic controls on Culebra transmissivity (e.g., Beauheim and Holt, 1990; Corbet, 2000). Preliminary studies suggest that Culebra transmissivity values can be accurately estimated ($R^2 > 0.9$) using a linear regression of transmissivity against the thickness of Culebra overburden, the thickness reduction in the upper Salado Formation due to dissolution, and a mode indicator (e.g., high versus low transmissivity). Data on geological controls are much more abundant than hydraulic property data and can be used to provide an improved estimate of the distribution of Culebra transmissivity.

We will develop a geologically based predictor of mean Culebra transmissivity using a standard linear regression approach. We will first formalize a conceptual model for geological controls on Culebra transmissivity. Transmissivity data will then be regressed against our hypothesized controls, and regression results will be verified and validated. The regression will allow the estimation of Culebra transmissivity across the WIPP region. A qualitative mathematical model will also be developed for extending transmissivity predictions to the east of the WIPP site where no Culebra transmissivity data exist.

Maps cannot be created for the transmissivity mode indicator from geologic data alone. The spatial location of Culebra modes will be determined using non-parametric geostatistical methods (e.g., indicator variography, indicator kriging, and conditional indicator simulation). The result will be a series of equiprobable location maps of the mode indicator. Base Culebra transmissivity fields will be developed using the maps of transmissivity controls and the regression parameters.

The principal analyst for Task 2 will be Robert Holt, University of Mississippi. Data inputs for this task will include well location information, inferred transmissivities at wells, values of the geologic controls at the wells, and the maps of geologic controls produced in Task 1. Deliverables will be 100 equally probable realizations of the Culebra mean T field with stochastic variability in the location of the high-T zones. These realizations will not yet be conditioned to heads. The base T fields are expected to be completed by May 15, 2002.

Task 3 Conditioning of Base T Fields to Equilibrium Heads

Four subtasks have been identified under this task:

Subtask 3.1 Analysis of Pilot Point Geometry

A major development in the field of stochastic inverse modeling that has occurred since T fields were constructed for the CCA is that inverse techniques are now capable of simultaneously determining the optimal T values at a large number of pilot points. In the T fields constructed for the CCA, pilot points were added one at a time and calibrated prior to the addition of the next pilot point. In order to determine the optimal number and placing of pilot points, a known hypothetical test problem, similar to the Culebra, will be constructed and inverse modeling will be done with varying numbers of pilot points located on a grid. Results of this test problem will provide a defensible basis for the number and location of the pilot points used for the Culebra T fields. A memo documenting the results of this subtask will be completed by July 31, 2002.

Subtask 3.2 Estimation of Boundary Conditions and Construction of Seed Realizations

Model boundary conditions for each time period for which T fields will be calibrated will be determined by fitting a surface to the freshwater head data available for that time period. Residuals between the fitted surface and the measurements will be used to create a geostatistical estimation of the residuals across the model domain. These residuals will be added to the surface to get the estimates of head at all locations in the model domain. The estimated values of head at the model boundary will provide the specified-head boundary conditions to be used in model calibration. Estimated heads values in the interior of the model domain will be used as the initial head estimates for the groundwater flow model solution. Estimation of boundary conditions will be completed by July 31, 2002.

The base T fields created by Bob Holt in Task 2 do not honor the measured T data at the measurement locations. Prior to the forward or inverse flow modeling, these base transmissivity fields must be conditioned to the measured T data. This conditioning is done by geostatistically simulating a zero mean residual field that is conditional to the residuals at the measurement locations. When this residual field is added to the base T field, it reproduces the true measured T values at the measurement locations and since the mean of the field is zero, it changes the base T-field as little as possible. The combined base T-field and residual filed is the seed T field that will be used as input to the stochastic inverse modeling. The seed T fields will be completed by June 30, 2002.

Subtask 3.3 Forward Modeling

As an initial test of the available data, boundary conditions, and the flow model setup, the seed realizations will be used in a set of forward models. Heads, fluxes, and particle travel times will be retained from these forward models for comparison with the results obtained after the inverse modeling step. This subtask will be completed by July 31, 2002.

Subtask 3.4 Steady State Inverse Models

The base realizations created in Task 2 will be used as input to the inverse model using the pilot point method. The number of pilot points and their locations will be based on the results of Subtask 3.1. For this task, the calibration of 100 T fields will be done to three sets of equilibrium-state head measurements approximately recorded in 1980, 1990, and 2000, while a fourth set of T fields will be calibrated to the “steady-state” heads presented in the CCA. Results of this task will include the T fields and heads and fluxes calculated on those T fields as well as data comparing the modeled and observed heads at the observation wells. 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 also be calculated for each T field. Ensemble average T fields will be prepared for each set of realizations, and difference maps will be prepared showing how the transmissivities differ among the three ensemble average fields. The CDFs of travel times for each set of realizations will be compared statistically to determine the degree to which they differ. The CDFs generated from the calibrated T fields used in the CCA (not modified for the effects of potash mining) will also be compared to the new CDFs. Deliverables for this task will consist of four sets of 100 T fields conditioned to equilibrium-state heads and a memo summarizing the comparison among the sets and the CCA T fields. This task will be completed by October 31, 2002.

The principal analyst for Task 3 will be Sean McKenna, 6115.

Task 4 Conditioning of Base T Fields to Transient Heads

Assuming that the four sets of T fields developed under Task 3.4 show no significant differences, at least one of the sets (probably the one representing the most recent conditions (year 2000)) will be conditioned to both equilibrated and transient head data. If the four sets of T fields do show significant differences, then at least some of the realizations from each set will be conditioned to both equilibrated and transient head data. Results of this task will include the T fields and heads and fluxes calculated on those T fields as well as data comparing the modeled and observed heads at the observation wells. 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 also be calculated for each T field. The CDFs generated from the transient-calibrated T fields used in the CCA will also be compared to the new CDFs. Deliverables for this task will consist of the T fields conditioned to transient heads and a memo summarizing the comparison to the CCA T fields. This task will be completed by January 31, 2003.

The principal analyst for Task 4 will be Sean McKenna, 6115.

Task 5 Evaluation of Mining Scenarios

For the CCA, 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's within the areas potentially affected by mining were 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 4 of this Analysis Plan. 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 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 a memo summarizing the comparison of travel-time CDFs. This task will be completed by February 28, 2003.

The principal analyst for Task 5 will be Sean McKenna, 6115.

5. SPECIAL CONSIDERATIONS

No special considerations have been identified.

6. APPLICABLE PROCEDURES

All applicable NWMP quality-assurance procedures will be followed for these analyses. Training of personnel will be done in accordance with the requirements of NP 2-1 *Qualification and Training*. Analyses will be performed and documented in accordance with the requirements of NP 9-1 *Analyses* and NP 20-2 *Scientific Notebooks*. All software used will meet the requirements of NP 19-1 *Software Requirements*. The analyses will be reviewed following NP 6-1 *Document Review Process*. All required records will be submitted to the WIPP Records Center in accordance with NP 17-1 *Records*.

7. REFERENCES

Beauheim, R.L., and R.M. Holt. 1990. "Hydrogeology of the WIPP Site," *Geological and Hydrological Studies of Evaporites in the Northern Delaware Basin for the Waste Isolation Pilot Plant (WIPP), New Mexico, GSA Field Trip #14 Guidebook*. Dallas, TX: Dallas Geological Society. 131-179.

Corbet, T.F. 2000. "A groundwater-basin approach to conceptualize and simulate post-Pleistocene subsurface flow in a semi-arid region, southeastern New Mexico and western Texas, USA," *Hydrogeology Journal*. Vol. 8, 310-327.

LaVenue, A.M., T.L. Cauffman, and J.F. Pickens. 1990. *Ground-Water Flow Modeling of the Culebra Dolomite, Volume I: Model Calibration*. SAND89-7068/1. Albuquerque, NM: Sandia National Laboratories.

US Department of Energy. 1996. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant*. DOE/CAO-1996-2184. Carlsbad, NM: US DOE Waste Isolation Pilot Plant, Carlsbad Area Office.