Analysis Plan for Evaluation and Recalibration of Culebra Transmissivity Fields

Task 4.4.1.1.1

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# Table of Contents

1. Introduction........................................................................................................................................ 3
2. Motivation for Study.......................................................................................................................... 5  
   2.1 Inclusion of New Data .................................................................................................................. 5  
   2.2 Evaluation of Steady-State Optimization Targets ....................................................................... 5  
   2.3 Incorporation of Mills Ranch Pumping Data .............................................................................. 5  
   2.4 Optimized Boundary Conditions ............................................................................................... 5  
   2.5 Code Updates ............................................................................................................................. 6  
3. Information Sources......................................................................................................................... 6  
   3.1 Water Levels and Pressures ........................................................................................................ 6  
   3.2 Transmissivity ............................................................................................................................ 6  
4. Analysis Tasks................................................................................................................................... 6  
   4.1 Task 1—Evaluation of Steady-State Head Optimization Targets ........................................... 6  
   4.2 Task 2—Development of a New Steady-State Head Approach for T-field Optimization .......... 7  
   4.3 Task 3—Updated T Values and Multi-Pad Pumping Test Optimization Targets ................. 7  
   4.4 Task 4—Investigation of the Impact of Boundary Conditions on the Model Domain .......... 7  
   4.5 Task 5—Update Flow and Optimization Codes ........................................................................ 8  
   4.6 Task 6—Evaluation of Mills ranch Pumping Data as Optimization Targets ...................... 8  
   4.7 Task 7—Calibration of Revised T Fields ................................................................................... 9  
5. Software List ..................................................................................................................................... 9  
6. Special Considerations..................................................................................................................... 10  
7. Applicable Procedures ..................................................................................................................... 10  
8. References ......................................................................................................................................... 10
1. Introduction

This Analysis Plan directs the evaluation and recalibration of transmissivity (T) fields for the Culebra Dolomite Member of the Rustler Formation near the Waste Isolation Pilot Plant (WIPP) site. Culebra T fields are used to model groundwater flow for performance assessment (PA) calculations for the WIPP. For the 2004 WIPP Compliance Recertification Application (CRA-2004; DOE, 2004), T fields were developed by McKenna and Hart (2003) using MODFLOW-2000 v. 1.6 (MF2K; Harbaugh et al., 2000) and PEST v. 5.51 (Doherty, 2000; McKenna, 2003) that were calibrated to heads assumed to represent equilibrium-state conditions as well as to transient heads arising from hydraulic testing activities. These fields were recalibrated by Hart et al., (2009) after generating revised base T fields (Hart et al., 2008). The same T fields calculated for the CRA2009 PABC were used for CRA 2014 (DOE 2014).

Under this Analysis Plan (AP), the sensitivity of the base T fields to different boundary conditions and hydrogeologic parameterizations will be evaluated. The conceptual model of T fields has remained unchanged since the 2008 Peer Review (Burgess et al., 2008). New T fields will be calibrated incorporating data from wells added since or excluded from the 2014 conceptualization (Figure 1).

The factors/features to be evaluated include:
1) New/updated T values for wells not included in CRA-2014 or wells that have been replaced and retested since CRA-2014 (DOE 2014)
2) A multi-pad pumping test as an optimization target
3) An evaluation of non-anthropogenic heads for optimization targets
4) Incorporation of the Mills Ranch pumping event information
5) Optimized boundary conditions
6) Updated flow and optimization codes

The first three of these factors will be evaluated as part of the development and calibration of new T fields. The fourth factor will require evaluation of the pumping event as a viable optimization target given that the typically necessary data is incomplete, specifically a lack of pumping rate data. The fifth item involves an update of the code versions for both forward model calculations and optimization.

As the resulting T fields are intended as input to the 2024 Compliance Recertification Application, the analyses of this Analysis Plan are categorized as a Compliance Decision.
Figure 1. Locations of Culebra wells providing new information for modeling from the two Reports described in Task 2.
2. Motivation for Study

The T fields in this AP will be developed using a reasonable numerical implementation of the conceptual model of the Culebra. However, alternative ways of implementing features of the conceptual model, as well as slight variations on the conceptual model, are possible and should be examined to ascertain their potential effects on calibration metrics. The principal alternatives to be considered are discussed below.

2.1 Inclusion of New Data

The T fields generated in the AP used all Culebra T data available as of September 2021. T data are now available from tests completed at two additional new wells (SNL-6, IMC-461) and six replacement/retested locations (AEC-7R, H-9bR, H-10cR, H-11b4R, H-12R, and H-15R. A long-term (~30 days) pumping test involving numerous observations wells was performed at well H-9bR in 2012 to provide transient-response data near the southern model boundary that can be used in T-field calibration. Head data used for the steady-state component of new T-field calibrations is discussed in the following sub-section.

2.2 Evaluation of Steady-State Optimization Targets

Head values used for steady-state optimization targets for CRA-2014 T-fields were measured from wells exclusively in May 2007. This approach is limited in that singular head measurements, per well, may not be representative of long-term steady-state head and in that it excludes all measurements made outside of a snapshot in time. Alternatively, a more representative dataset may be found using the statistics associated with non-anthropogenic head measurements from monitoring network wells. This approach allows for the potential inclusion of more monitoring data in evaluating steady-state heads. The statistical approach may be influenced by temporal data density or bias.

2.3 Incorporation of Mills Ranch Pumping Data

The Mills Ranch pumping response (MRPR) began in 2013 with recovery in some wells concluding in 2020. Pumping rate information is not available. The MRPR was the most impactful pumping event measured by the WIPP monitoring well network. The MRPR data cannot be used in an identical fashion as a traditional multi-pad pumping tests for transient optimization targets. Methods to incorporate this data will be investigated.

2.4 Optimized Boundary Conditions

Uncertainty in the model peripheral constant head boundary conditions will be investigated by allowing each geostatistical realization of the Culebra forward model to have a unique set of constant head boundaries in the north, south, and southwestern borders of the model domain. In past iterations of T fields, these boundary conditions are based upon recent Annual Site Environmental Report (ASER) values. For this iteration of T fields, unique sets of head conditions will be applied to each T field and optimized. The optimized head boundary values will be evaluated.
2.5 Code Updates

The previous iteration of T field calibration used MODFLOW 2000 (flow code) and PEST v. 9.11 (optimizer). The run time to produce calibrated T fields was on the order of months. Modern and supported versions of these codes, MODFLOW 6 (v.6.2.2) (Langevin et. al., 2017) and PEST++ (v.5.1.6) (White et. al., 2020), will be reviewed and evaluated for computational improvement. While the methodology of T-field generation will mostly remain unchanged by the updated codes, the computational methodology is significantly different (simultaneous realization calibrations) and is likely to decrease code run times.

3. Information Sources

The modeling described in the previous section will require different types of data from various sources. The types of data required and the sources for each are discussed below.

3.1 Water Levels and Pressures

Observed water levels and pressures in Culebra wells provide the basic data against which Culebra T fields are calibrated. Water levels are measured monthly in all wells by Washington Regulatory and Environmental Services (WRES). Sandia receives a monthly data transmittal letter from WRES, and the same data are published annually in the WIPP Site Environmental Reports (e.g., WRES, 2022). Sandia also measures water levels and fluid pressures in monitoring wells under Test Plan (TP) 03-01 (Schuhen, 2010a) and TP 06-01 (Schuhen, 2010b) and the data are recorded in Scientific Notebooks.

3.2 Transmissivity

Hydraulic tests have been and are being conducted in new and recompleted wells under TP 03-01 (Schuhen 2010a). The data from these tests were analyzed under AP-070 (Bowman, 2020) to provide estimates of T, storativity (in the case of tests with observation wells), and flow dimension. All new T and S data will be added to the modeling process.

4. Analysis Tasks

4.1 Task 1— Evaluation of Steady-State Head Optimization Targets

This task entails a review of depth-to-water data captured at each historical WIPP monitoring network well. The depth-to-water measurements recorded by both WRES and Sandia will be filtered for anthropogenic affects, such as changes due to oil field exploration, to build a set of water level data that is representative of the natural, or as natural as possible, state of the Culebra dolomite aquifer. Data recorded between the inception of each well and January 2018 will be evaluated. The analysts for Task 1 are Dale Bowman and Mike Fort. An analysis report of the evaluated data was produced in 2019.
4.2 Task 2—Development of a New Steady-State Head Approach for T-field Optimization

This task will use the output of Task 1 to evaluate a new approach to calculating heads representative of steady state in the Culebra Dolomite aquifer. The analysis will investigate a centrality approach to replace the previous approach that designated May 2007 monitoring network freshwater heads as singularly representative of a steady-state aquifer. Non-anthropogenic water levels will be evaluated using histograms and various centrality criteria to generate a new potentiometric surface for T field optimization. The resulting potentiometric surface, and the data used to generate it, will be evaluated against the May 2007 data for acceptance. If the approach is found valid, wells that were excluded in the calculation of previous iterations of the potentiometric surfaces will be incorporated and evaluated. The analysts for Task 2 are Dale Bowman and Mike Farinacci. Two analysis reports were planned for this task under AP-150 (Bowman 2021) and were completed in FY21 and FY22.

4.3 Task 3—Updated T Values and Multi-Pad Pumping Test Optimization Targets

This task will involve the incorporation of new optimization targets and updated aquifer parameters, specifically T and S, as products of well test analyses of new and replacement wells. In contrast to past application, the updated values will only be used as part of the calibration process and were not incorporated in the generation of new base T-fields. New wells to be included are wells IMC-461 and SNL-6; replacement wells to be included are wells AEC-7R, H-9bR, H-10cR, H-11b4R, H-12R, and H-15R. Additionally, a multi-pad pumping test was conducted in well H-9bR with observation response from four monitoring network wells (H-4bR, SNL-12, SNL-14, SNL-17) and one cattle production well (Engle). The multi-pad pumping test is intended to be used as a transient optimization target. The analyst for Task 3 is Dale Bowman. The new/updated aquifer parameters will be derived from several analysis reports under AP-070 that were completed between 2005 and 2017. The multi-pad pumping test data, captured under TP 03-01, was recorded in 2012.

4.4 Task 4—Investigation of the Impact of Boundary Conditions on the Model Domain

The north-south hydrologic gradient observed in the site model is controlled by boundary conditions in the form of constant head cells along the boundaries of the model domain. These constant head cells are extracted from an interpolated surface of potentiometric head values using the following equation:

$$ h_{x,y} = A + B \times (y + D \times \text{sign}(y) \times \text{abs}(y)^{\text{exponent}}) + C(E \times x^3 + F \times x^2 - x) $$

Where x and y represent the row and column of the model and the variables A, B, C, D, E, F and exponent are adjustable.

Due to the nature of using this stochastic approach, uncertainty in the potentiometric surface may propagate into the flow solution for the final 100 calibrated T fields. The effect of this uncertainty will be investigated by generating 1,000 geostatistical realizations that have unique sets of constant head boundaries in the north, south, and southwestern borders of the model domain. The investigation will be performed by adding the seven variables in the equation as adjustable...
parameters to the calibration workflow. After this is complete, an ensemble of constant heads may be included as a fifth parameter set to the final T fields based on their effect on model calibration.

This task will be performed in tandem with Task 7 by including parameters that can adjust the boundary conditions in the form of a constant head file for MODFLOW 6. The analysts for Task 4 are Ross Kushnereit and Jeremy White. This task is scheduled to be completed by January 2023 and will be documented in an analysis report.

4.5 Task 5—Update Flow and Optimization Codes

The previous iteration of T field calculations utilized the flow software MODFLOW 2000 and calibration software PEST 9.11. There have been two core versions of the MODFLOW suite since MF2K; the current supported version is MODFLOW 6. MODFLOW 6 has more robust pre- and post-processing python libraries which are advantageous in passing flow results to the PEST optimizer code. Active development of PEST has migrated to the refactored software PEST++. Using PEST++ software package allows us to take advantage of the ensemble calibration capability of the iterative ensemble smoother algorithm for drastically faster optimization times. Specifically, the code versions being qualified for this iteration of T fields are MODFLOW 6 version 6.2.2 and PEST++ version 5.1.6. The utility of these codes require review prior to implementation into the generation of T fields. The general path for each will be:

1) Test if the new codes are functional in the context of the established T fields calculation/optimization process
2) Evaluate the changes internal to each code (e.g., solver differences, input/output format)
3) Qualification of each software per NP 19-1
4) Update the calculation/optimization process to account for changes found in 2) and verified in 3).

The code qualifiers for Task 5 are Sarah Brunell and James Bethune. This task was scheduled and successfully completed in June 2022.

4.6 Task 6—Evaluation of Mills ranch Pumping Data as Optimization Targets

A private production well at the Mills Ranch was pumped intermittently between 2013 and 2018. While the observation response of the pumping was captured by the monitoring well network, the pumping rates were not made available. As a result, the Mills Ranch pumping events cannot be included as optimization targets with defined withdrawal rates and target drawdowns.

In this Task, a methodology will be developed and evaluated to include the observation well data from the WIPP monitoring well network affected by Mills Ranch pumping in the optimization process of T fields. As the observation well data is sound, the process will focus on treating the Mills Ranch pumping rate as a fitting parameter. The analysts for Task 6 are Ross Kushnereit and Jeremy White. The initial incorporation of Mills Ranch Data was scheduled for March of 2022; final decisions on its application are scheduled for November 2022. The final incorporation of this data as part of the testing structure for calibrating T fields will be performed in tandem with Task 7, if accepted, which is scheduled to be completed by January 2023.
4.7 Task 7—Calibration of Revised T Fields

This task is conceptually similar to the first revision of Task 7 (Hart, Beauheim & McKenna, 2009) and will use the inputs below:

- 1,000 stochastically generated geospatial transmissivity realizations produced in Task 5, AP-114 Revision 1 (Hart, Holt & McKenna, 2008)
- Freshwater head calculations to represent steady state head conditions (Task 2)
- Transient heads from several multi-well pumping tests (Task 3)
- Transient heads for the WIPP monitoring well network, developed for an anthropogenic pumping event in the Culebra near the WIPP boundary between late 2013 to 2018 (Task 6)
- Single well diffusivity information obtained from hydraulic-test interpretations (Task 3)

These inputs will be used to generate 100 final calibrated T fields from 1,000 realizations, which will include: hydraulic conductivity, horizontal anisotropy, recharge, specific storage, and potentially, constant head values, in a format compatible with the groundwater flow modeling software MODFLOW6 v. 6.2.2.

The most notable change from the previous calibration of the T fields will come from upgrading the parameter optimization software from PEST v. 9.11. to PEST++ v. 5.1.6 (White et. al., 2020). The PEST++ Iterative Ensemble Smoother (IES) algorithm allows for faster run times and incorporation of significantly more parameters, due to the use of the ensemble Kalman filter (EnKF) and the Gaussian Levenberg Marquart (GLM) optimizer. This method will allow for more exploration of parameter space, for providing an ensemble of calibrated T fields in significantly less time. Additional measured data, such as the anthropogenic pumping event and new hydraulic-test interpretations, will also be included to help constrain the calibrations.

The analysts for Task 7 will be Ross Kushnereit and Jeremy White. An analysis report will be prepared describing the analysis procedure and results. This task is scheduled to be completed by January 2023.

5. Software List

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

- ESRI ArcInfo 8.1 (off-the-shelf software);
- nSIGHTS v.2.41a (qualified under NP 19-1);
- MF2K (MODFLOW-2000) v. 1.08 (qualified under NP 19-1);
- MODFLOW 6 v.6.2.2 (qualified under NP 19-1);
- PEST v. 9.13 (qualified under NP 19-1);
- PEST++ v.5.1.6 (qualified under NP 19-1);
- Python v. 3.6.8 (off-the-shelf software);
- Advanced Python packages FloPy and PyEmu (off-the-shelf software); and
- DTRKMF v. 1.02 (qualified under NP 19-1).
Calculations will be performed on the Sandia WIPP computing cluster FWM running the CentOS operating system. Whenever computer platforms (hardware and/or operating systems) change, kt3d, sgsim, MODFLOW 6, PEST++, and DTRKMF will be requalified per NP 19-1.

Off-the-shelf spreadsheet programs, such as Excel, and graphing programs, such as Grapher or SigmaPlot, may also be used for data manipulation and plotting on individual workstations.

6. Special Considerations

No special considerations have been identified.

7. Applicable Procedures

All applicable WIPP 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 or NP 9-1 as applicable. 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.

8. References


Harbaugh, A.W., E.R. Banta, M.C. Hill, and M.G. McDonald. 2000. MODFLOW-2000, the U.S.


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