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Analysis Report for Preparation of the 2022 Culebra Potentiometric Surface Contour Map

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1. Introduction

This report presents the workflow used to generate the 2022 Culebra potentiometric surface map and corresponding particle pathway at the Waste Isolation Pilot Plant (WIPP). The Culebra potentiometric surface map is prepared every year, as required by the Stipulated Final Order sent to the New Mexico Environment Department on May 28, 2009 (Moody, 2009). The analysis documented in this report follows the Activity/Project Specific Procedure SP 9-9 (Kuhlman, 2009), which is consistent with the methodology outlined in Paragraph 10.a of the 2009 Stipulated Final Order.

For this report, an ensemble of 100 calibrated parameter (transmissivity (T), horizontal anisotropy (A), and recharge (R)) fields were used. The calibrated parameter fields were taken from the data used in the CRA-2009 Performance Assessment Baseline Calculation (PABC), and subsequently used in CRA-2014 & 2019 PAs. For each parameter, the average of the 100 realizations was computed. These averaged parameter fields were then used with MODFLOW-2000 to simulate hydraulic head distribution within and near the WIPP Land Withdrawal Boundary (LWB). To obtain a good fit between observed and simulated hydraulic heads, the parameter estimation software PEST was used to adjust the model boundary conditions. Hydraulic heads measured in November 2022 were used as optimization targets during PEST calibration. The simulated hydraulic heads, based on the optimal boundary conditions, were then contoured to produce the Culebra potentiometric surface map. In addition, the velocity field derived from the final set of simulated hydraulic heads was used to compute the advective particle pathway from the WIPP waste handling shaft to the WIPP LWB.

2. Scientific Approach

The steps involved in generating the Culebra Potentiometric Surface map and advective particle pathway are as follows (Kuhlman, 2009):

- 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 using the 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 (e.g., PEST) 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 map.
- Compute particle path and travel time from the waste handling shaft to the LWB.

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2.1. Water level Data

Groundwater level data used for calibration targets were obtained from the Regulatory Environmental Services (RES) monthly monitoring events (Regulatory Environmental Services, 2022). For each well, the data provided by RES includes the depth to water, the groundwater head, and the Culebra midpoint elevation. To convert the groundwater heads to freshwater heads, the 2021 specific gravity calculations from Farinacci (2022) were used. The specific gravity values for wells H-5bR, WQSP-4, WQSP-5, and WQSP-6 were not included in Farinacci (2022). For each of these four wells, the specific gravity value provided by RES was used to convert groundwater heads to freshwater heads. Note that the specific gravity values provided by RES are hydrometer measurements from sampling events. After reviewing the 2022 hydrographs of Culebra wells, the groundwater levels from November 2022 were selected and used in this analysis. The month of November was chosen because it is the period when a majority of the wells was not impacted by well maintenance or anthropogenic activities within the WIPP well network. Wells SNL-6 and SNL-15 were not used in this analysis because they are still recovering from the original drilling and development. Wells H-9bR, H-12R, and H-16 were also not included because representative water levels were not available. Table 1 presents the water level measurement date, calculated freshwater head, and the specific gravity for each of the observation wells. The specific gravity value corresponds to the calculated density value normalized by the density of freshwater at 70°F. The "Code" column in Table 1 indicates the status and cardinal position of each well.

Table 1: Observation wells and corresponding hydraulic head. Data provided by RES. Code: N=North, S=South, C=Central, and X=not used.

Well	Code	Observation Weight	Measurement Date	Freshwater Head (ft. AMSL)	Specific Gravity (Freshwater at70° F
AEC-7R	N	0.4	11/8/2022	3060.57	1.069
C-2737	S	2.5	11/8/2022	3003.64	1.028
H-4bR	S	1.0	11/7/2022	2991.74	1.023
H-5bR	N	2.5	11/8/2022	3070.50	1.105
H-6bR	N	2.5	11/9/2022	3061.55	1.040
H-9bR**	X	0.4	11/7/2022	2959.42	1.004
H-10cR	S	0.4	11/7/2022	3030.28	1.091
H-11b4R	S	2.5	11/7/2022	2988.94	1.081
H-12R**	X	0.4	11/7/2022	3005.75	1.105
H-15R	C	2.5	11/7/2022	3002.98	1.126
H-16**	X	2.5	11/9/2022	3029.87	1.032
H-19b0	S	2.5	11/7/2022	2995.65	1.067
IMC-461	C	0.4	11/9/2022	3033.15	0.999
SNL-1	N	0.4	11/8/2022	3073.21	1.031
SNL-2	N	1.0	11/8/2022	3060.18	1.011
SNL-3	N	0.4	11/8/2022	3070.76	1.029

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Well	Code	Observation Weight	Measurement Date	Freshwater Head (ft. AMSL)	Specific Gravity (Freshwater at70° F
SNL-5	N	1.0	11/8/2022	3061.97	1.007
SNL-6*	X	0.4	11/8/2022	3475.01	1.262
SNL-8	N	1.0	11/8/2022	3051.03	1.092
SNL-9	C	1.0	11/9/2022	3045.13	1.017
SNL-10	C	2.5	11/9/2022	3044.90	1.013
SNL-12	S	0.4	11/7/2022	2983.47	1.012
SNL-13	S	1.0	11/7/2022	2999.61	1.026
SNL-14	S	1.0	11/7/2022	2984.38	1.045
SNL-15*	X	1.0	11/7/2022	3117.20	1.232
SNL-16	S	0.4	11/7/2022	3007.71	1.017
SNL-17	S	1.0	11/7/2022	3002.51	1.015
SNL-18	N	0.4	11/8/2022	3064.84	1.013
SNL-19	N	0.4	11/8/2022	3060.26	1.006
WIPP-11R	N	1.0	11/8/2022	3069.90	1.032
WQSP-1	N	2.5	11/8/2022	3064.41	1.044
WQSP-2	N	2.5	11/8/2022	3066.27	1.033
WQSP-3	N	2.5	11/8/2022	3060.41	1.141
WQSP-4	S	2.5	11/7/2022	2997.03	1.077
WQSP-5	S	2.5	11/7/2022	2995.42	1.028
WQSP-6	S	2.5	11/7/2022	3010.05	1.016

* Water levels have not fully recovered from original drilling

** Water levels impacted by oil field activities and shaft excavation

2.2. Modeling Overview

The generation of the Culebra potentiometric map follows three main steps. First, the average of the 100 calibrated parameter fields is computed. The ensemble of 100 calibrated parameter fields includes those developed for the CRA-2009 Performance Assessment Baseline Calculation (PABC), and subsequently used in CRA-2014 & 2019 PAs. These averaged parameter fields (T, A, R) were used as inputs for the MODFLOW-2000 groundwater model. The version of MODFLOW-2000 and boundary conditions of the groundwater model are identical to those used in CRA-2019 PA. Groundwater flow simulations are performed under steady state conditions. The second step of the analysis consists of adjusting the model boundary conditions such that the mismatch between simulated and observed hydraulic heads is reduced. The parameter estimation software PEST is used during this calibration phase. This calibration process differs from that used in the CRA-2019 PA. Here, only a subset of boundary conditions (Figure 1) is adjusted; the other parameters (T, A, R) are not changed during the calibration process. The optimal boundary conditions derived from the PEST calibration are used to simulate hydraulic head distribution within and near the WIPP LWB. The simulated hydraulic heads are then contoured to produce the potentiometric surface map. The hydraulic head contours span the entire active MODFLOW-

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2000 domain shown in Figure 1. The direction of groundwater flow in the WIPP LWB is also presented. The last step of this analysis uses the flow field/budget file from MODFLOW-2000 to simulate the pathway of a single conservative particle from the WIPP waste handling shaft to the LWB. The DTRKMF software is used for particle tracking. Table 2 gives the list of software used in the analyses described in this report and their quality assurance (QA) status. The following sections present a detailed description of the modeling steps. Section 2.3 describes how the averaged MODFLOW-2000 model is generated. In Section 2.4, the boundary conditions adjusted during the calibration process are presented. Sections 2.5 and 2.6 describe the calibration process and the particle tracking simulations, respectively.

Table 2: List of software used in analysis

Software	Version	Description	QA Status
MODFLOW-2000	1.08	Hydrologic modeling software	Acquired; qualified under NP 19-1 (Harbaugh et al., 2000)
PEST	9.13	Parameter estimation software	Developed; qualified under NP 19-1 (Doherty, 2002)
DTRKMF	1.02	Particle tracking program	Developed; qualified under NP 19-1 (Treadway, 2014)
Python	2.7.5	Programming language	Commercial off the shelf
Bash	4.2.46	Scripting language (file manipulation)	Commercial off the shelf

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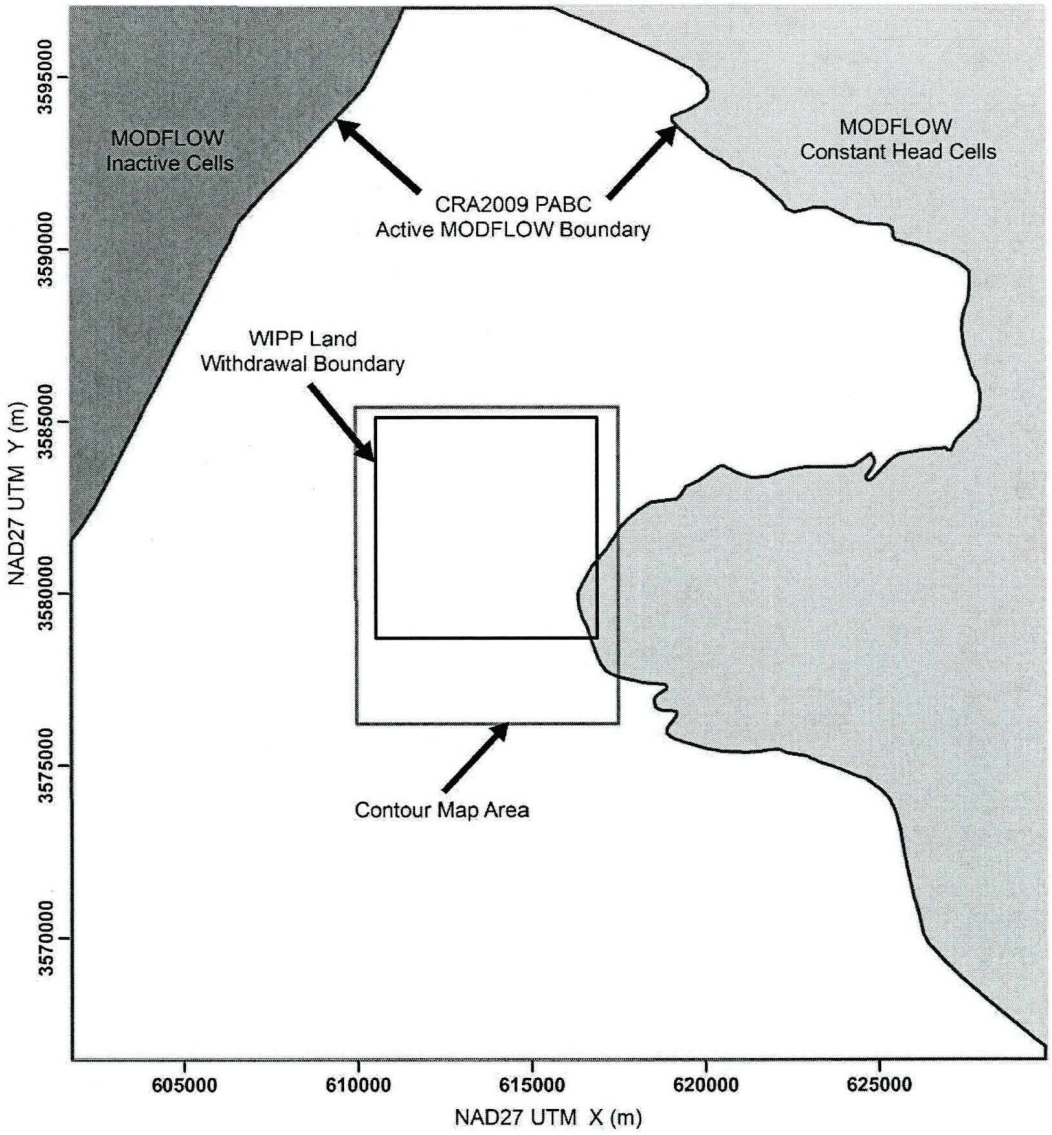


Figure 1: MODFLOW-2000 model domain. Boundary conditions adjusted during PEST calibration are shown in red. The green rectangle represents the contour map area (modified from Kuhlman, 2017).

2.3. Creation of the Averaged MODFLOW-2000 model

The MODFLOW-2000 model grid is discretized into a single layer (thickness=7.5m), 307 rows, and 284 columns. Each grid cell is 100m×100m in size. The model domain spans from 601700 to 630000 meters in the x-direction, and 3566500 to 3597100 meters in the y-direction; these coordinates refer to the NAD27 UTM projection system (Figure 1).

To compute the averaged parameter fields, the ensemble of 100 calibrated fields is obtained from the PA version control repository, using the checkout_average_run_modflow.sh script (scripts are listed in Section 6; input and output files are available from the WIPP version control system in the repository /nfs/data/CVSLIB/Analyses/SP9_9). The model grid settings, the boundary conditions, and the model solver parameters are identical for all 100 calibrated model

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realizations; only the parameter fields (T, A, and R) are different. The average_realizations.py script computes the geometric mean of T, A, and R over the 100 realizations.

2.4. Boundary conditions

The model boundary conditions used in CRA-2019 and in this analysis can be subdivided in two types. The first type corresponds to geologic and hydrologic boundaries derived from WIPP site characterization. The no-flow boundary (the boundary along the dark gray region) in the northwestern section and the constant head boundary (the eastern irregular boundary adjoining the light gray) of the model domain belong to the first type of boundary conditions (Figure 1). Boundary conditions in the first type are not adjusted during the calibration process, because they correspond to well-defined geologic/hydrogeologic features. The second type of boundary conditions consists of constant head cells along the southern, southwestern, and northern boundaries of the model domain; Figure 1 shows these boundaries in red. PEST adjusts the hydraulic heads assigned to the second type of boundary conditions during the calibration process.

In the MODFLOW-2000 groundwater model, the distinction between the two types of constant head boundaries is made using the boundary_types.py script. This distinction helps PEST recognize the boundary conditions to adjust during calibration. The constant head cells of the first type are not adjusted, and this is specified by setting the IBOUND array value to -1. The constant head cells of the second type are adjusted, and this is specified by setting the IBOUND array value to -2. The surface_02_extrapolate.py uses the output file generated by the boundary_types.py. The surface_02_extrapolate.py computes the initial head at active model cells (IBOUND=1) and the constant head at adjustable boundary condition cells (IBOUND=-2), using parameter values for the surface to extrapolate.

2.5. Calibration of the averaged MODFLOW-2000 model

To run the calibration in PEST, three main inputs are required: the forward model, the PEST input files, and the calibration targets. The forward model comprises the PA MODFLOW-2000 model and the necessary pre-/post-processing utilities. PEST runs the forward model iteratively to estimate sensitivities of model outputs to model inputs. The PEST configuration files specify the list of parameters and observation groups, the observation weights, and which parameters in the MODFLOW-2000 model need to be adjusted in the inverse simulation. The calibration targets correspond to November 2022 measured hydraulic head values. Table 1 provides a list of the wells along with their specific gravity. Note that wells H-9bR, H-12R, H-16, SNL-6, and SNL-15 were not used in the calibration.

The run_02_model Bash script is used to run the forward model. When the run_02_model script is called, the surface_02_extarpolate.py, the MODFLOW-2000 executable, and the PEST utility mod2obs are executed respectively. The surface_02_extrapolate.py script computes the starting heads of the MODFLOW-2000 domain, using a parametric surface to extrapolate the hydraulic head from the adjusted constant head boundary conditions. The use of the parametric surface also helps minimize the number of estimated parameters, and ensure smoothness of the constant head boundary condition values. The parametric surface used in this analysis is identical to the one used in the AP-114 Task 7 (Hart et al., 2009):

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$$h(x,y) = A + B(y + Dsign(y)abs(y)^{\alpha}) + C(Ex^3 + Fx^2 - x) \qquad (1)$$

where *abs(y)* is the absolute, *sign(y)* is the function returning 1 for $y>0$, -1 for $y<0$ and 0 for $y=0$, and x and y are coordinates scaled to the range $-1 \leq \{x, y\} \leq 1$. The initial values of these variables come from Hart et al., (2009): A=928.0, B=8.0, C=1.2, D=1.0, α=0.5, E=1.0 and F=-1.0. During model calibration, PEST adjusts the values of A, B, C, D, α, E, and F to provide a best fit with the measured heads. The surface_02_extarpolate.py script is then used to estimate the starting heads of the MODFLOW-2000 domain, based on the adjusted values of A-F and α. Once the surface_02_extrapolate.py and the MODFLOW-2000 executable are executed successfully, the mod2obs utility extracts simulated hydraulic heads at the observation wells.

The create_pest_02_input.py script generates the PEST input files. PEST requires three types of input files: instruction, template, and control files. The instruction file specifies how PEST reads the MODFLOW-2000 output files while the template file specifies the format to write MODFLOW-2000 input files. The PEST control file lists the adjustable parameters as well as their initial value and range. The PEST control file also includes the measured heads at the observation wells along with their weight. The observation weights used in this analysis come from expert knowledge of WIPP hydrology and trial-and-error simulations. Wells inside the WIPP LWB get higher observation weights (2.5). Lower observation weights (0.4) are assigned to wells distant from the WIPP site. Wells near the WIPP LWB get intermediate observation weight (1.0). Additional observations representing the average heads north and south of the LWB are used to prevent over-smoothing of the estimated results across the LWB. The additional observations and weights are assigned to improve the fit in the area of interest (inside the WIPP LWB), possibly at the expense of a somewhat poorer fit far from the WIPP LWB and closer to the boundary conditions.

2.6. Particle Tracking

The boundary conditions from the PEST calibration are used to run the MODFLOW-2000 model in "predictions" mode. The output cell-by-cell flow budget is used to simulate a particle pathway from the waste handling shaft to the WIPP LWB. Particle tracking stops once the particle exits the WIPP LWB. The convert_dtrkmf_output_for_surfer.py converts the MODFLOW-2000 cell-indexed results of DTRKMF into a UTM X and Y coordinate system, and saves the results in the Surfer blanking file format to facilitate plotting results. The head_bin2ascii.py converts the binary MODFLOW-2000 head output file to an ASCII matrix file format.

The simulated particle pathway and contours of modeled heads are plotted using the plot-contour-maps.py for the area including the WIPP LWB and the Annual Site Environmental Report domain. The merge_observed_modeled_heads.py script combines the modeled and observed heads into a single file. The plot-results-bar-charts.py script uses the output file of merge_observed_modeled_heads.py to perform a statistical comparison between observed and modeled heads.

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3. Results

3.1. 2022 Equivalent Freshwater Head Contours

Figures 2 and 3 show the hydraulic head contours within and around the WIPP LWB. Hydraulic head contours in the central portion of the map are east-west trending and closely spaced, which suggests a low transmissivity zone. The 2022 freshwater water contours are quite similar to the 2021 contour map (Akara, 2022). The general east-west trending head contours suggests a north-south groundwater flow direction, as shown with the black arrows in Figures 2 and 3. Hydraulic head contours are not drawn for the eastern region of the model domain. This region corresponds to the portion of the Culebra bounded by the Anhydrite of the Tamarisk Member and the Mudstone/Halite of the Los Medanos Member. The eastern region is considered a no-flow boundary because of its low transmissivity.

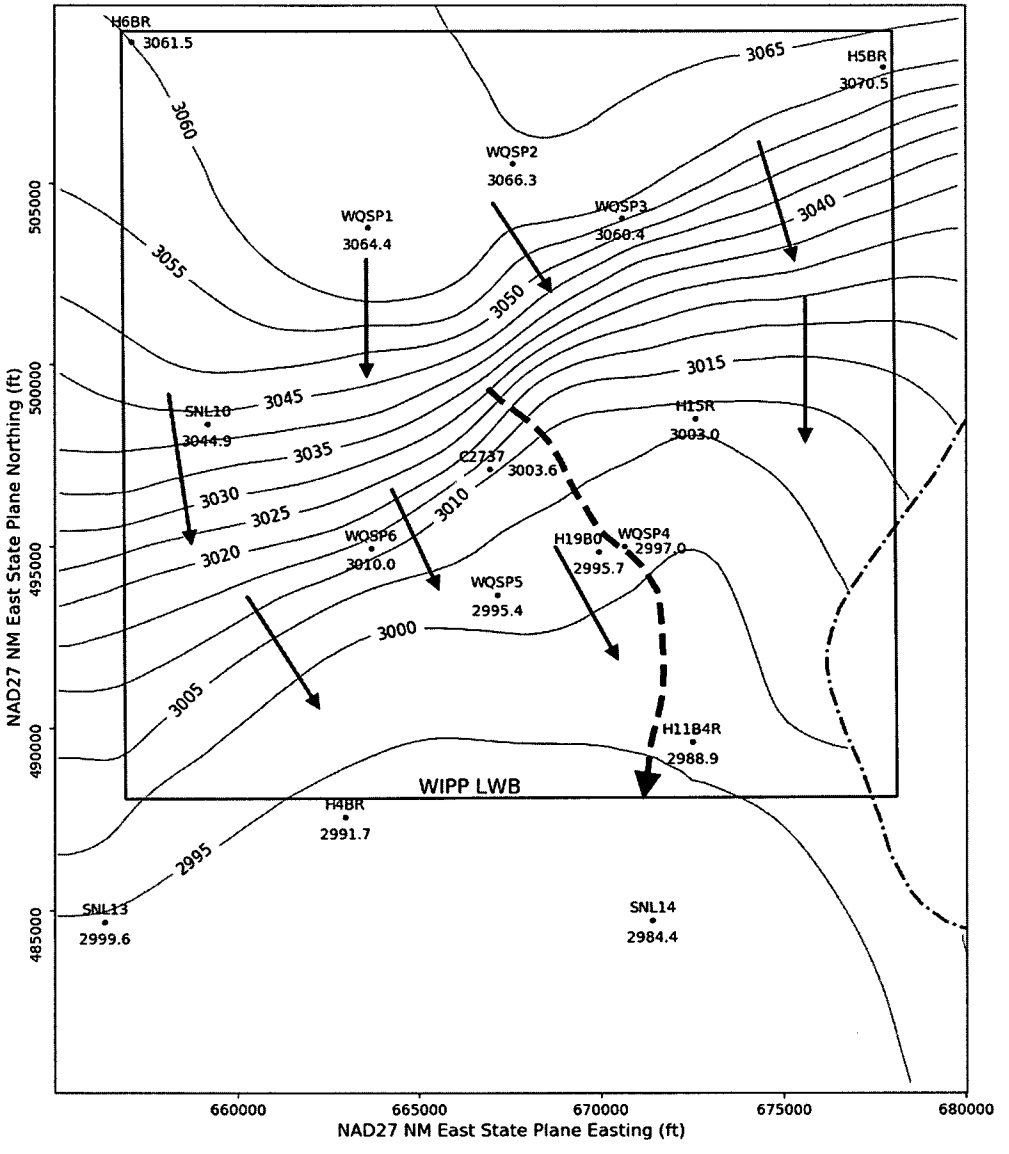


Figure 2: 2022 simulated freshwater head contours with measured freshwater heads (ft. AMSL) listed at each well (5-foot contour interval). The dashed line represents the DTRKMF simulated

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particle pathway from the waste handling shaft to the WIPP LWB. The black arrows indicate the groundwater flow direction inside the WIPP LWB.

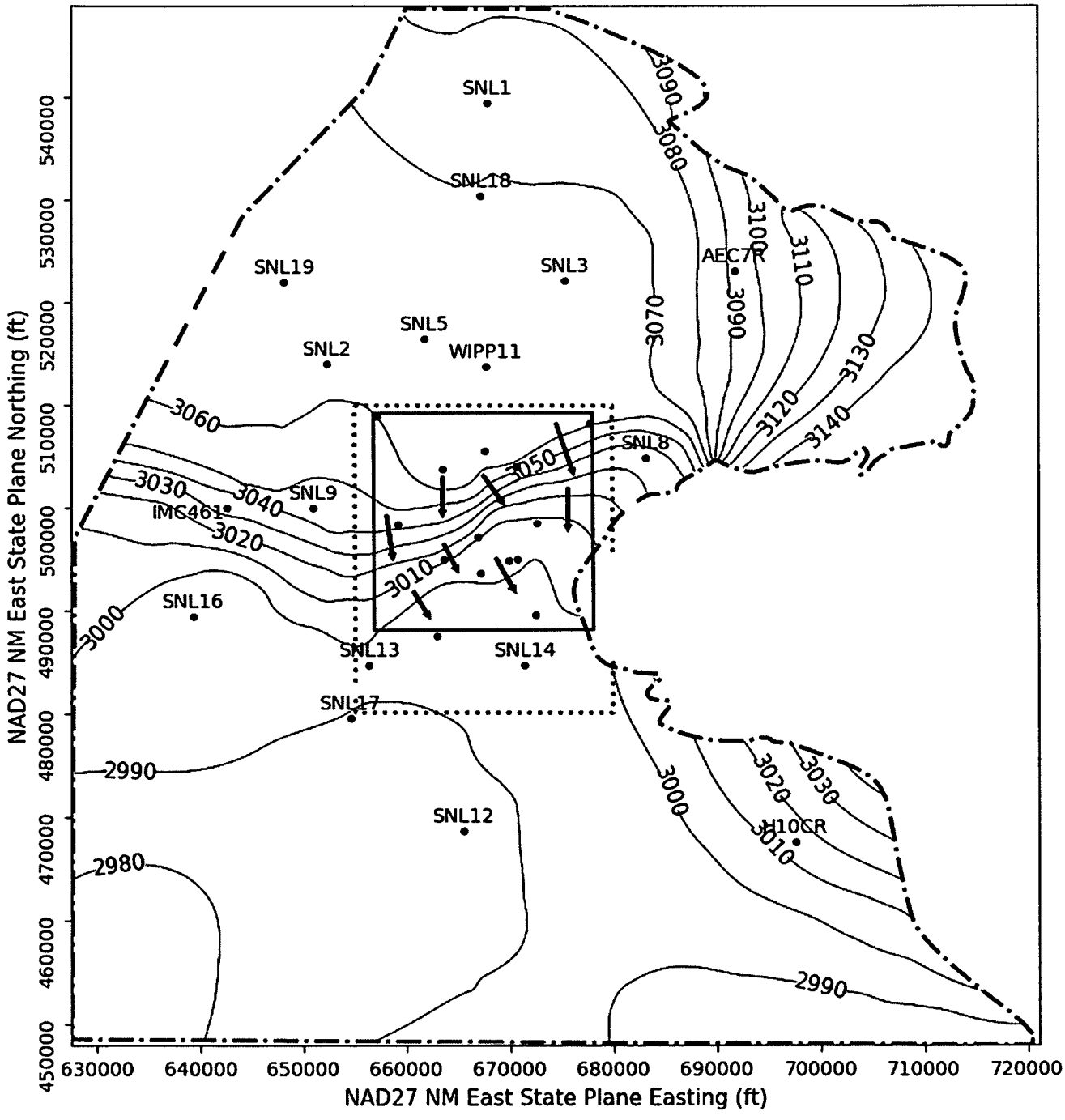


Figure 3: 2022 simulated freshwater head contours for the entire model domain (10-foot contour interval). The dash-dotted line indicates the active MODFLOW-2000 boundary. The dotted rectangle corresponds to the region contoured in Figure 2. The black square corresponds to the WIPP LWB. Wells inside the WIPP LWB are not labeled; refer to Figure 2 for identification of these wells. The black arrows indicate the groundwater flow direction inside the WIPP LWB.

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3.2. 2022 Particle Pathway

The black dashed line in Figure 2 corresponds to the DTRKMF-simulated pathway that a particle would take from the WIPP waste handling shaft to the WIPP LWB (a path length of 4091 m). The DTRKMF output assumes that the transmissive portion of the Culebra is 4 m thick (as opposed to the entire thickness of the aquifer at 7.5 m) and has a constant porosity of 16%. The Culebra thickness is reduced to 4 m to focus all flow through the lower and most permeable portion of the Culebra (Holt, 1997). The DTRKMF-simulated pathway indicates a travel time of 5582 years, which corresponds to an average velocity of 0.73 m/yr. The 2022 velocity is 9% higher than that of 2021, likely due to an increase in hydraulic gradient from December 2021 to November 2022.

3.3. 2022 Measured vs. Modeled Fit

Figure 4 presents the measured vs. simulated hydraulic heads for all wells used in the calibration process. These wells are divided into three groups, based on their proximity to the WIPP LWB. Wells inside the WIPP LWB are represented by circles, wells outside but within 3 km of the LWB are shown with the squares, all other wells are indicated by the stars. Figure 4 also shows the 1:1 line and the ±1m misfit lines. Note that only wells with a misfit greater than 1.5 m are labeled in Figure 4. The average hydraulic heads of wells north of the LWB and south of the LWB are used as calibration targets to prevent over-smoothing of the simulated heads across the LWB. In addition, these targets allowed PEST to reduce the misfit between simulated and observed hydraulic heads inside the area contoured in Figure 2, at the expense of fitting wells closer to the boundary conditions. The optimal values of Equation 1 parameters are as follows: A=924.46, B=8.44, C=1.44, D=0.83, α=1.83, E=3.08, and F=-2.74. *A, B, C,* and *D* are within ±20% of their initial values; *E, F,* and α are greater than their initial values by a factor of 2 to 3.

The simulated hydraulic heads are in good agreement with the observed heads; 71% of simulated heads are within ±1.5 m of observations (Figures 4, 5, and 7). Of all wells inside in the WIPP LWB, H-5bR has the highest residual, likely due to its low transmissivity. The r^2 values presented in Table 3 indicate a strong correlation between observed and simulated hydraulic heads. Similarly, the root mean square error (RMSE) and the normalized RMSE are 9.1 ft. and 4%, respectively. Table 3 also indicates that the strongest correlation between simulated and observed heads corresponds to wells inside the WIPP LWB (Figure 6). This is particularly important, given that the WIPP LWB is the primary region of interest in this analysis.

Table 3: Measured vs. modeled correlation coefficients

	Dataset	Measured vs. Modeled R^2
Uncalibrated	wells inside WIPP LWB	0.9933
	wells < 3km from WIPP LWB	0.9675
	all wells	0.9273
Calibrated	wells inside WIPP LWB	0.9935
	wells < 3km from WIPP LWB	0.9660
	all wells	0.9286

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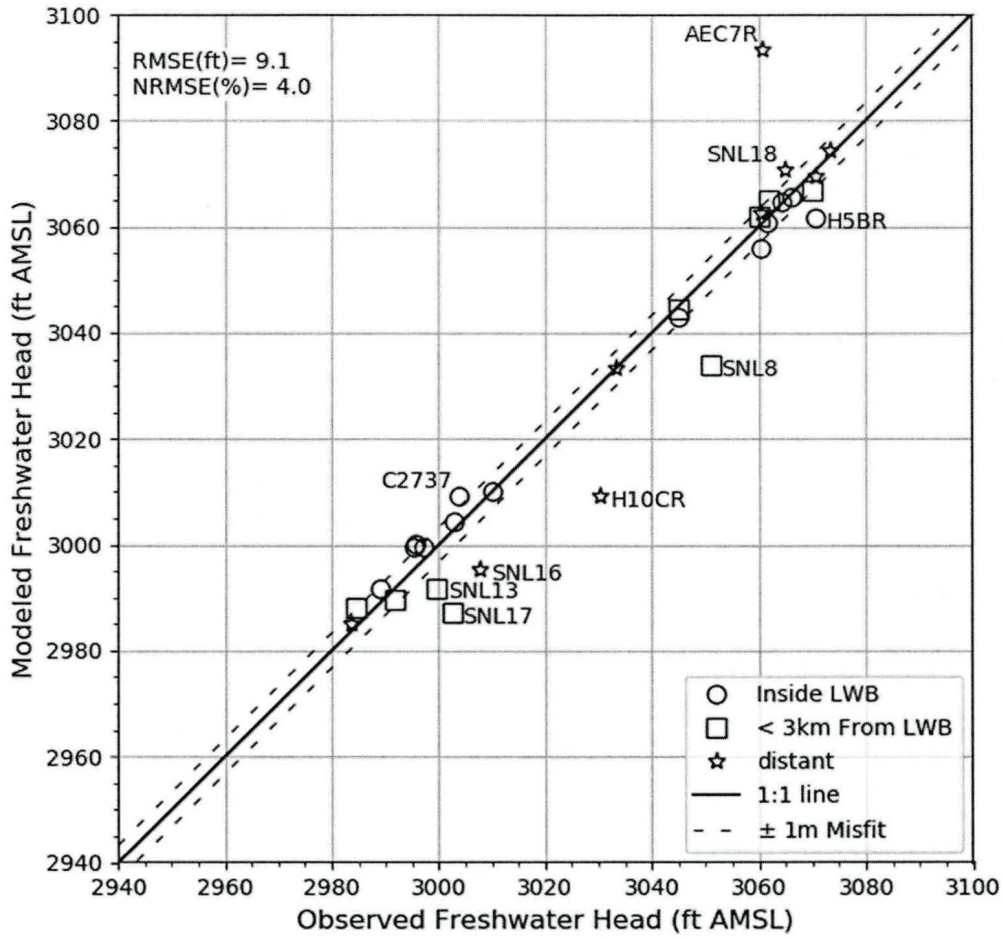
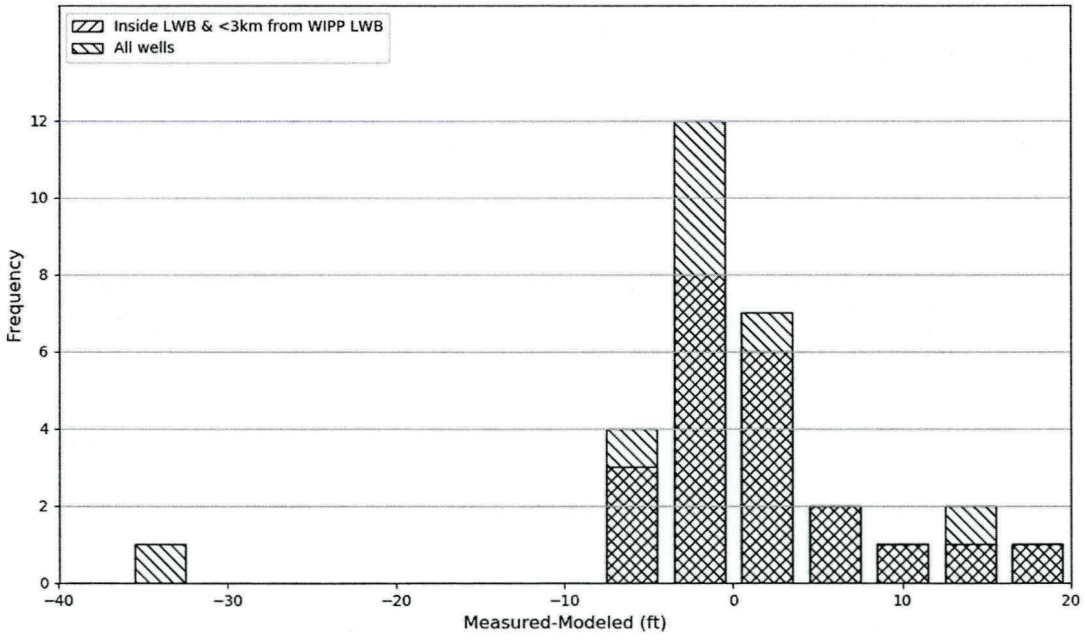


Figure 4: Scatter plot showing the modeled vs. the observed heads. The root mean square error (RMSE) and the normalized root mean square error (NRMSE) are also shown.



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Figure 5: Histogram of the measured−modeled heads.

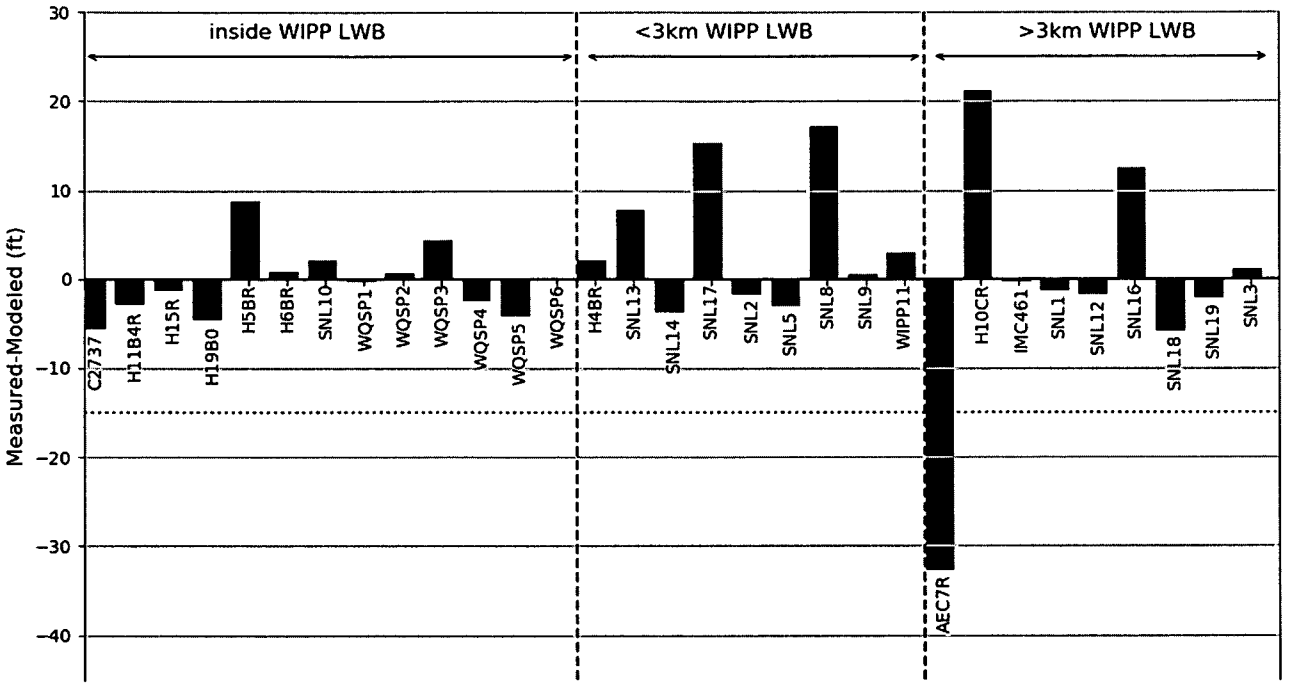


Figure 6: Measured−modeled heads for all calibration wells.

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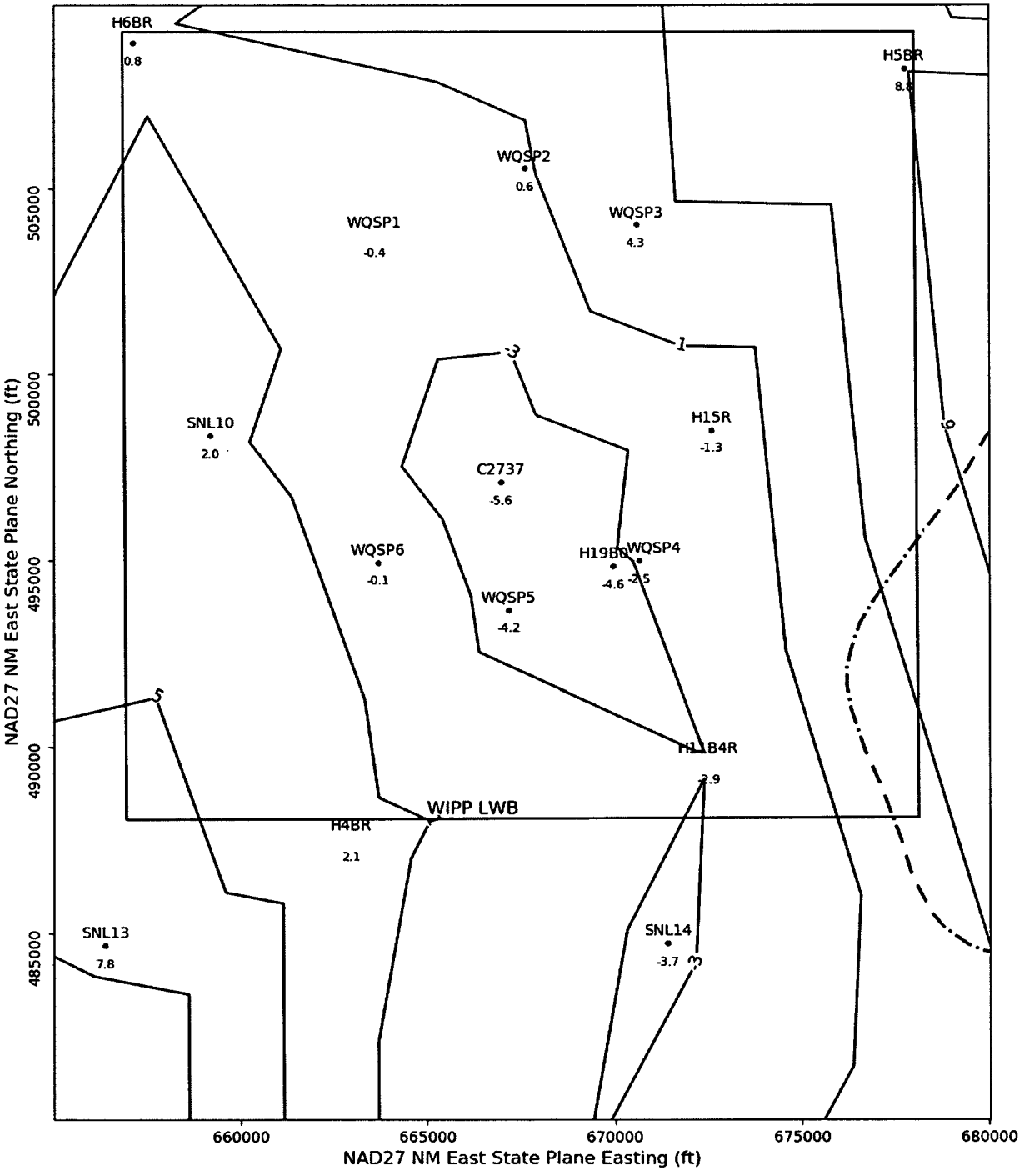


Figure 7: Triangulated contours of measured−modeled heads. The contour labels represent the difference between measured and modeled heads.

4. Conclusions

The 2022 Culebra potentiometric surface map was generated as required by the New Mexico Environment Department, and following the SP 9-9 Activity/Project Specific Procedure. Flow

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simulations presented in this report are based on the CRA-2009 calibrated parameter fields and measured hydraulic heads of November 2022. Overall, the 2022 Culebra potentiometric surface map does not show significant deviations from the 2021 map, especially within the WIPP LWB. Similar to previous years, the hydraulic head contours are east-west trending with a north-south groundwater flow direction. The 2022 particle path length and travel time are 4091 m and 5582 years, respectively. This corresponds to an average particle velocity of 0.73 m/yr.

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6. Run Control Narrative

This section is a narrative describing the calculation process mentioned in the text, which produced the provided figures. All the steps presented in this narrative are identical to those used by Hayes, 2021 and Kuhlman, 2012.

Figure 8 gives an overview of the driver script checkout_average_run_modflow.sh (§A-4.1); this Bash shell script (listed in Section 6.1) first exports the 4 parameter fields used in the TFIELDS calibration process (transmissivity (T), anisotropy (A), recharge (R), and storativity (S)) from CVS version control for each of the 100 realizations of MODFLOW, listed in the file keepers (see lines 17-26 of script). In the steady-state simulations done for this report, the S field is not used. Some of the realizations are inside the Update or Update2 subdirectories in CVS, which complicates the directory structure. An equivalent list included in keepers_short is made from keepers, and the directories are moved to match the flat directory structure (lines 31-53). At this point, the directory structure has been modified but the MODFLOW-2000 input files checked out from CVS are unchanged.

Python script average_realizations.py (§A-4.2) is called, which first reads in the keepers_short list, then reads in each of the 400 input files and computes the geometric average at each cell across the 100 realizations. The 400 input files are each saved as flattened matrices, in row-major order. The average result is saved into 4 parameter files, each with the extension.avg instead of .mod. A single value from each file, corresponding to either the cell in the southeast comer of the domain (input file row 87188 = model row 307, model column 284 for K [hydraulic conductivity - what is actually used by MODFLOW] and A) or on the west edge of the domain (input file row 45157 = model row 161, model column 1 for R and S) is saved in the text file parameter _representative_ values.txt to allow checking the calculation in Excel, comparing the results to the value given at the same row of the .avg file. The value in the right column of Table 4 can be found by taking the geometric average of the values in the text file, which are the values from the indicated line of each of the 100 realizations.

The input files used by this analysis and the output files from this analysis (including the plotting scripts) are checked into the WIPP version control system (CVS) under the repository $CVSLIB/ Analyses/SP9 _9.

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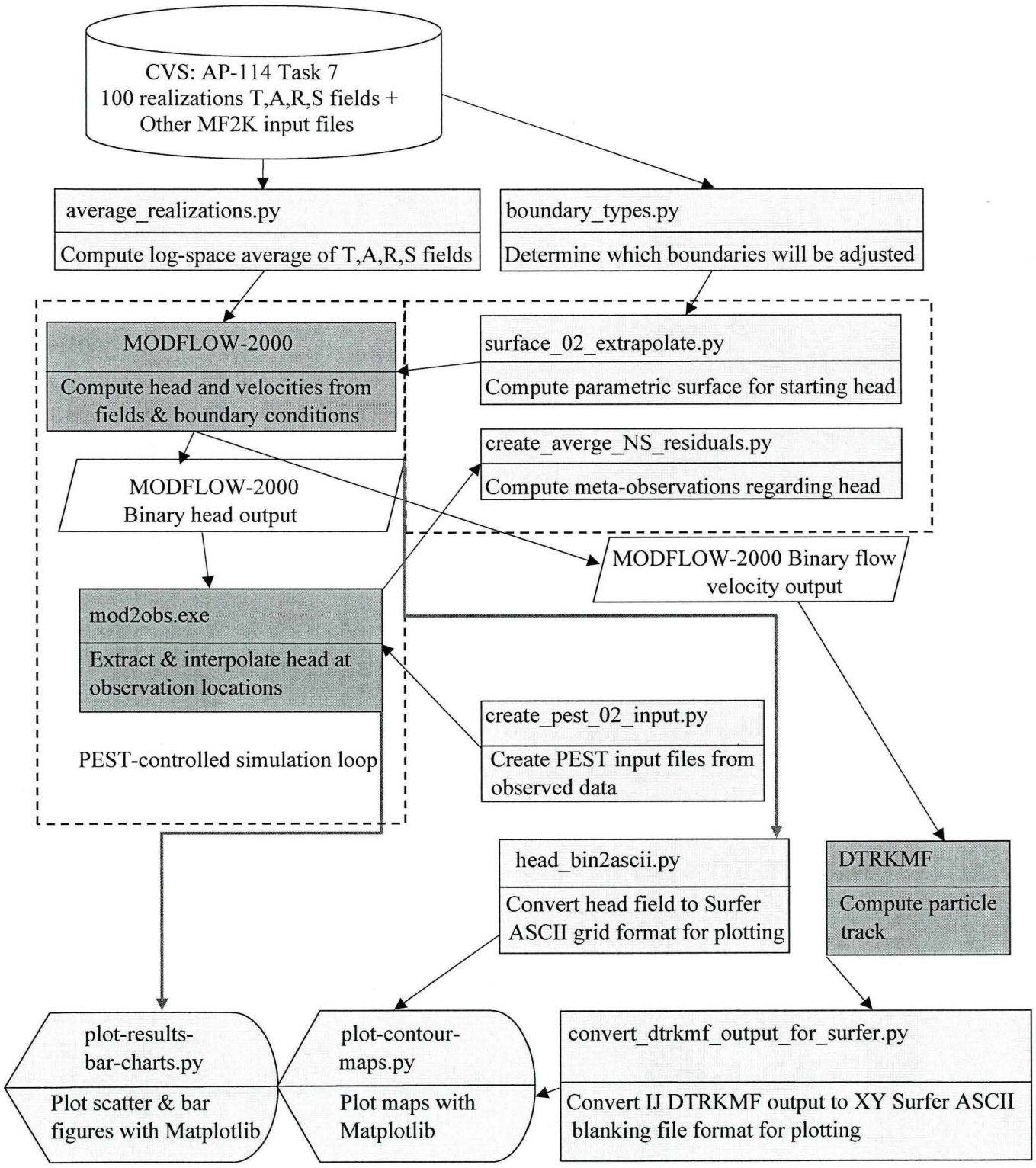


Figure 8: Analysis workflow. Qualified programs in dark gray; python scripts in light gray

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Table 4: Average values for selected model cells

Field	Input file row	Model row	Model column	Geometric average
K	87188	307	284	9.2583577E-09
A	87188	307	284	9.6317478E-01
R	45157	161	1	1.4970689E-19
S	45157	161	1	4.0388352E-03

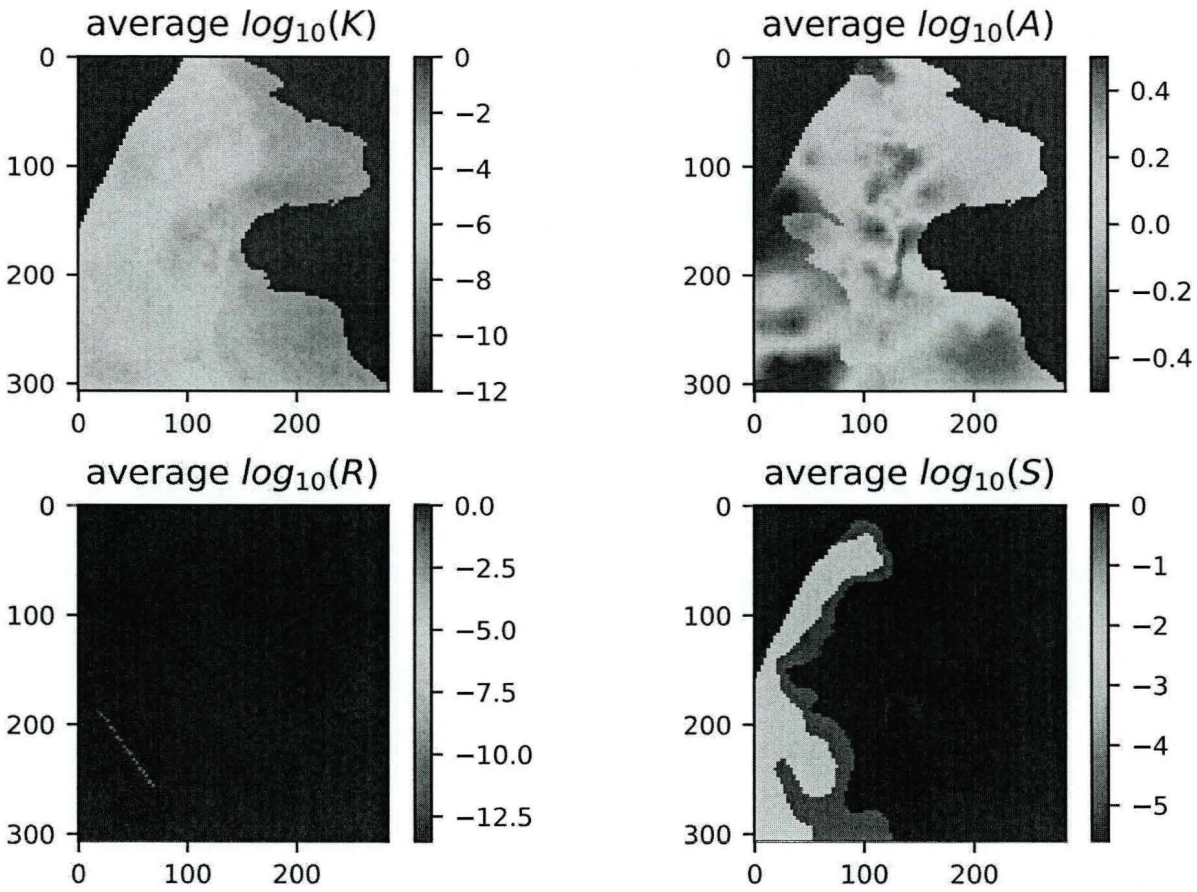


Figure 9: Average of parameter fields; rows and columns are labeled on edges of figure.

A subdirectory is created, and the averaged MODFLOW-2000 model is run without any modifications by PEST. Subsequently, another directory is created where PEST is run to improve the fit of the model to observed heads at well locations.

The next portion of the driving script checkout_average_run_modflow.sh links copies the input files needed to run MODFLOW-2000 and DTRKMF into the original_average run directory. Then MODFLOW-2000 is run with the name file mf2k_head.nam, producing binary head (modeled_head.bin) and binary cell-by-cell flow budget (modeled_flow.bud) files, as well as a text listing file (modeled_head.lst). DTRKMF is then run with the input files dtrkrnf.in and wippctrl.inp, which utilizes the cell-by-cell budget file written by MODFLOW-2000 to generate a particle track output file, dtrk.out. The input file wippctrl.inp specifies the starting location of

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the particle in DTRKMF face-centered cell coordinates, the porosity of the aquifer (here 16%), and the coordinates of the corners of the WIPP LWB, since the calculation stops when the particle reaches the LWB.

The Python script head_bin2ascii.py (§A-4.7) converts the MODFLOW-2000 binary head file, which includes the steady-state head at every element in the flow model domain (307 rows × 284 columns) into a Surfer ASCII grid file format. This file is simply contoured in Python using matplotlib, no interpolation or gridding is needed. The Python script convert_dtrkrnf_output_for_surfer.py (§A-4.9) reads the DTRKMF output file dtrk.out and does two things. First it converts the row, column format of this output file to an x, y format suitable for plotting, and second it converts the effective thickness of the Culebra from 7.75 m to 4 m. Table 5 shows the first 10 lines of the dtrk.out and the corresponding output of the Python script dtrk_output_original_average.bln. The first three columns of dtrk.out (top half of Table 5) after the header are cumulative time (red), column (blue), and row (green). The three columns in the blanking file (second half of Table 5) after the header are UTM NAD27 X (blue), UTM NAD27 Y (green), and adjusted cumulative time (red, which is faster than the original cumulative travel time by the factor 7.75/4=1.9375). The conversion from row, column to x,y is

$$X = 601700 + 100 * \text{column},$$

$$Y = 3597100 - 100 * \text{row}$$

since the I,J origin is the northwest comer of the model domain (601700, 3597100), while the X, Y origin is the southwest comer of the domain. The blanking file is plotted directly in Python using matplotlib, since it now has the same coordinates as the ASCII head file.

Table 5: Comparison of the first 10 lines of DTRKMF output and converted Surfer blanking file

	1	159							
0.00000000E+00	118.79	150.21	1.18790000E+04	1.50210000E+04	0.00000000E+00	1.89421272E-01	1.60000000E-01	1.00000000E+00	
5.43061113E+01	118.86	150.29	1.18859869E+04	1.50285482E+04	1.02855451E+01	1.89378188E-01	1.60000000E-01	1.00000000E+00	
1.08612223E+02	118.93	150.36	1.18929939E+04	1.50360747E+04	2.05688354E+01	1.89338229E-01	1.60000000E-01	1.00000000E+00	
1.62755578E+02	119.00	150.44	1.19000000E+04	1.50435570E+04	3.08192307E+01	1.89301503E-01	1.60000000E-01	1.00000000E+00	
3.20465684E+02	119.21	150.63	1.19205264E+04	1.50625551E+04	5.87881775E+01	1.77406841E-01	1.60000000E-01	1.00000000E+00	
4.78175791E+02	119.41	150.81	1.19412334E+04	1.50813875E+04	8.67781827E+01	1.77553926E-01	1.60000000E-01	1.00000000E+00	
6.35413239E+02	119.62	151.00	1.19620598E+04	1.51000000E+04	1.14709519E+02	1.77727552E-01	1.60000000E-01	1.00000000E+00	
7.23758137E+02	119.75	151.10	1.19746974E+04	1.51104027E+04	1.31077938E+02	1.85307751E-01	1.60000000E-01	1.00000000E+00	
8.12103034E+02	119.87	151.21	1.19873568E+04	1.51207870E+04	1.47451536E+02	1.85366919E-01	1.60000000E-01	1.00000000E+00	

159,1		
613579.0,	3582079.0,	0.00000000E+00
613586.0,	3582071.0,	2.80289607E+01
613593.0,	3582064.0,	5.60579215E+01
613600.0,	3582056.0,	8.40028790E+01
613621.0,	3582037.0,	1.65401643E+02
613641.0,	3582019.0,	2.46800408E+02
613662.0,	3582000.0,	3.27955220E+02
613675.0,	3581990.0,	3.73552587E+02
613687.0,	3581979.0,	4.19149953E+02

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The PEST utility script mod2obs.exe is run to extract and interpolate the model-predicted heads at observation locations. The input files for mod2obs.exe were taken from AP-114 Task 7 in CVS. The observed head file has the wells and freshwater heads, but is otherwise the same as that used in the model calibration in AP-114 (Hart et al., 2009). The Python script merge_observed_modeled_heads.py (§A-4.9) simply puts the results from mod2obs.exe and the original observed heads in a single file together for easier plotting and later analysis.

A similar process to that described so far in this narrative is carried out in a new directory called pest_02 (beginning line 146 of the driver script). The PEST calibration is carried out there, to keep it separate from the original_average simulation. The Python script boundary_types.py (§A-4.3) is also run, to create a new MODFLOW-2000 IBOUND array, where the two different types of boundary conditions are differentiated. This Python script uses the MODFLOW-2000 IBOUND array (init_bnds_orig.inf, first 1/3 of Table 6) and the initial head array (init_head_orig.mod middle 1/3 of Table 6) as inputs, and writes a new MODFLOW-2000 IBOUND array (init_bnds.inf bottom 1/3 of Table 6) with constant head nodes indicated in red in Figure 1 marked as -2 and other constant head nodes remaining as -1 as output. The script differentiates between these two types of boundary conditions by checking if the starting head is <1000m. Starting heads >1000m are associated with the constant head areas to the east of the halite margins (lighter gray areas in Figure 1).

Table 6: Input IBOUND, starting head, and output IBOUND array data corresponding to first row of MODFLOW-2000 model.

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1																											

943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943	943
944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944
944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944
944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944
944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944
944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944
944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	944	1087	1085	1085	1082	1081	1080	1079	1078	1078					
1077	1077	1077	1077	1077	1077	1078	1078	1077	1078	1079	1081	1083	1084	1086	1086	1088	1090	1092	1095	1096	1098	1099	1099	1100						
1100	1100	1101	1101	1101	1102	1104	1104	1104	1104	1104	1104	1105	1105	1105	1105	1106	1106	1106	1107	1107	1109	1110	1110	1112						
1113	1113	1114	1114	1115	1115	1115	1116	1116	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1127	1129	1129	1130						
1131	1132	1132	1133	1133	1134	1135	1136	1137	1137	1138	1139	1139	1140	1140	1140	1141	1142	1142	1142	1142	1142	1143	1143	1144						
1144	1144	1145	1145	1146	1147	1147	1147	1147	1148	1148	1147	1146	1144	1143	1143	1145	1147	1148	1149	1150	1149	1149	1148	1149						
1149	1151	1151	1151	1150	1152	1153	1154	1155																						

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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2	-2	-2	-2	-2	-2	-2
-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2
-2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1																													

Table 6 shows the data corresponding to the northernmost row of the MODFLOW-2000 model domain (284 entries long) for the two input files and one output file. In the top IBOUND array, the values are either 0 or -1, indicating either inactive (the region northwest of the no-flow area shown in dark gray in Figure 1) or constant head (both red and light gray cells in Figure 1). The first 284 values from the initial head file (reformatted from scientific notation to integers to facilitate printing) show a jump from approximately 944 (in blue) to >1000 (in red). These same cells are colored in the output, showing how the initial head value is used to distinguish between the two types of constant head boundaries. MODFLOW-2000 treats any cells that have an IBOUND entry < 0 as constant head, so both -2 and -1 are the same to MODFLOW, but allow distinguishing between them in the Python script which extrapolates the heads to the boundaries.

The required PEST input files are created by the Python script create_pest_02_input.py (§A-4.4). This script writes 1) the PEST instruction file (modeled_head.ins), which shows PEST how to extract the model-predicted heads from the mod2obs.exe output; 2) the PEST template file (surface_par_params.ptf), which shows PEST how to write the input file for the surface extrapolation script; 3) the PEST parameter file (surface_par_params.par), which lists the starting parameter values to use when checking the PEST input; 4) the PEST control file (bc_adjust_2022ASER.pst), which has PEST-related parameters, definitions of extrapolation surface parameters, and the observations and weights that PEST is adjusting the model inputs to fit. The observed heads are read as an input file in the PEST borehole sample file format (meas_head_2022ASER.smp), and the weights are read in from the input file (obs_loc_2022ASER.dat).

PEST runs the "forward model" many times, adjusting inputs and reading the resulting outputs using the instruction and template files created above. The forward model actually consists of a Bash shell script (run_02_model) that simply calls a pre-processing Python script surface_02_extrapolate.py (§A-4.5), the MODFLOW-2000 executable, the Python script create_average_NS_residuals.py, and the PEST utility mod2obs.exe as a post-processing step. The script redirects the output of each step to /dev/null to minimize screen output while running PEST, since PEST runs the forward model many dozens of times.

The Python script create_average_NS_residuals.py takes the output from the PEST utility mod2obs and creates a meta-observation that consists of the average residual between measured and model-prediction, only averaged across the northern or southern WIPP wells (the wells in the center of the WIPP site are not included in either group). This was done to minimize

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cancelation of the errors north (where the model tended to underestimate heads) and south (where the model tended to overestimate heads) of the WIPP. The results of this script are read directly by PEST and incorporated as four additional observations (mean and median errors, both north and south of WIPP).

The pre-processing Python script surface_02_extrapolate.py reads the new IBOUND array created in a previous step (with -2 now indicating which constant head boundaries should be modified), the initial head file used in AP-114 Task 7 (init_head_orig.mod), two files listing the relative X and Y coordinates of the model cells (rel_x,y_coord.dat), and an input file listing the coefficients of the parametric equation used to define the initial head surface. This script then cycles over the elements in the domain, writing the original starting head value if the IBOUND value is -1 or 0, and writing the value corresponding to the parametric equation if the IBOUND value is -2 or 1. Using the parameters corresponding to those used in AP-114 Task 7, the output starting head file should be identical to that used in AP-114 Task 7.

After PEST has converged to the optimum solution for the given observed heads and weights, it runs the forward model one more time with the optimum parameters. The post-processing Python scripts for creating the Surfer ASCII grid file and Surfer blanking file from the MOD FLOW and DTRKMF output are run and the results are plotted using additional Python scripts that utilize the plotting and map coordinate projection functionality of the matplotlib library.

These two plotting scripts (plot-contour-maps.py and plot-results-bar-charts.py) are included in the Section 6.2 for completeness, but only draw the figures included in this report, which are passed on to the Site Management & Operations Contractor for the ASER.

6.1. Input Files

Bytes	File Type	Description	File Name
1.4K	Python script	average 100 realizations	average_realizations.py
2K	Python script	distinguish different BC types	boundary_types.py
6.4K	Bash script	main routine: checkout files, run MODFLOW-2000, run PEST, call Python scripts	checkout_average_run_modflow.sh
632	Python script	convert DTRKMF IJ output to Surfer X, Y blanking format	convert_dtrkmf_output_for_surfer.py
2.8K	Python script	create meta observations of average head	create_average_NS_residuals.py
3.5K	Python script	create PEST input files from observed data	create_pest_02_input.py
48	input listing	responses to DTRKMF prompts	dtrkmf.in
4.2K	Python script	convert MODFLOW-2000 binary output to Surfer ASCII grid format	head_bin2ascii.py

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Bytes	File Type	Description	File Name
1.1K	input	listing of 100 realizations from CVS	keepers
1.1K	input	observed November 2022 heads in mod2obs bore sample file format	meas_head_2022ASER.smp
1K	Python script	paste observed head and model generated heads into one file	merge_observed_modeled_heads.py
76	file listing	files needed to run mod2obs	mod2obs_files.dat
138	input listing	responses to mod2obs prompts	mod2obs_head.in
76	file listing	files needed to run MODFLOW2000	modflow_files.dat
330	input	listing of wells and geographic groupings	obs_loc_2022ASER.dat
215	file listing	files needed to run PEST	pest_02_files.dat
2.3M	input	relative coordinate $-1 \leq x \leq 1$	rel_x_coord.dat
2.3M	input	relative coordinate $-1 \leq y \leq 1$	rel_y_coord.dat
490	Bash script	PEST model: execute MODFLOW2000 and do pre- and post-processing	run_02_model
26	input	mod2obs input file	settings.fig
47	input	mod2obs input file	spec_domain.spc
1.7K	input	mod2obs input file	spec_wells.crd
2.4K	Python script	compute starting head from parameter and coordinate inputs	surface_02_extrapolate.py
506	input	DTRKMF input file	wippctrl.inp

6.2. Output Files

Bytes	File Type	Description	File Name
19K	DTRKMF output	particle track results	dtrk.out
16K	DTRKMF output	particle track debug	drtk.dbg
1.6K	script output	heads at well locations	modeled_vs_observed_head_pest_02.txt
1.1M	script output	formatted MODFLOW-2000 heads	modeled_head_pest_02.grd
5.3K	script output	formatted DTRKMF particle	dtrk_output_pest_02.bln
14.2K	PEST output	matrix condition numbers	bc_adjust_2022ASER.cnd
2.3K	PEST output	binary intermediate file	bc_adjust_2022ASER.drf
6.3K	PEST output	binary intermediate file	bc_adjust_2022ASER.jac

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Bytes	File Type	Description	File Name
6.4K	PEST output	binary intermediate file	bc_adjust_2022ASER.jco
8.5K	PEST output	binary intermediate file	bc_ adjust_ 2022ASER.jst
3.7K	PEST output	parameter statistical matrices	bc_adjust_2022ASER.mtt
477	PEST output	parameter file	bc_adjust_2022ASER.par
59.1K	PEST output	optimization record	bc_adjust_2022ASER.rec
3.9K	PEST output	model outputs for last iteration	bc_adjust_2022ASER.rei
7.1K	PEST output	summary of residuals	bc_adjust_2022ASER.res
28	PEST output	binary restart file	bc_adjust_2022ASER.rst
23.1K	PEST output	relative parameter sensitivities	bc_adjust_2022ASER.sen
3.3K	PEST output	absolute parameter sensitivities	bc_adjust_2022ASER.seo
214K	png image	matplotlib plot (Fig 2)	aser-area-contour-map2022.png
195K	png image	matplotlib plot (Fig 3)	large-area-contour-map2022.png
116K	png image	matplotlib plot (Fig 7)	aser-area-modobs-contour-map2022.png
29.5K	png image	matplotlib plot (Fig 5)	model-error-histogram2022.png
54K	png image	matplotlib plot (Fig 6)	model-error-residuals2022.png
85K	png image	matplotlib plot (Fig 4)	scatter_pest_ 02_2022.png

Information Only