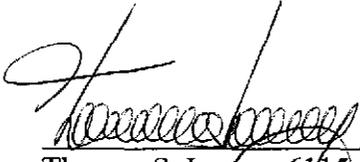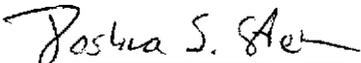# Analysis Report
## Task 2 of AP-110
## Evaluation of Water-Level Rise in the Culebra Due to Recharge from Refining Process Water Discharged onto Potash Tailings Piles

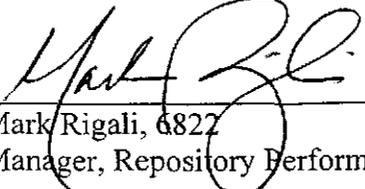### (AP-110: Analysis Plan for Evaluation of Culebra Water-Level-Rise Scenarios)

### Task Number 1.4.1.1

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# 1 Introduction

This analysis report describes the activities of Task 2 of AP-110, "Analysis Plan for Evaluation of Culebra Water-Level-Rise Scenarios" (Beauheim, 2003a). The purpose of this Task is to evaluate the likelihood that observed rising water levels in the Culebra Dolomite Member of the Rustler Formation near the Waste Isolation Pilot Plant (WIPP) are due to leakage from refining process water discharged onto potash tailings piles.

## 1.1 *Background*

The Culebra flow model used in performance assessment (PA) calculations for the WIPP Compliance Certification Application (CCA; DOE, 1996) was calibrated to heads assumed to represent steady-state conditions as well as to transient heads arising from hydraulic testing and shaft activities. In the assessment of compliance monitoring parameters (COMP's) for the year 2000 (SNL, 2001), freshwater heads were compared to trigger value ranges established for 28 of the 32 wells (Figure 1) used in generation of the CCA Culebra transmissivity ($T$) fields (water levels in the other four wells could not be determined because the wells had been removed from the monitoring network, i.e., plugged and abandoned, or converted to monitor units other than the Culebra). Of these 28 measurements, freshwater heads in 21 wells appeared to be outside the trigger value ranges, 20 higher and one lower than expected. Head changes in four of the wells could be explained by problems with well casings and/or leaking packers, leaving 17 wells with unexpectedly high freshwater heads. Exceeding trigger values does not mean that continued compliance is in jeopardy, but that further action must be taken to evaluate the cause(s) and consequences of exceeding the trigger value.

Based on requirements for further investigations when trigger values are exceeded and concerns expressed by the Environmental Protection Agency (EPA, 2002) and Environmental Evaluation Group (EEG, 2002), investigative studies were defined to explore possible scenarios that could explain the water-level changes (SNL, 2003).

## 1.2 *Water-Level Rise*

Water-level records (hydrographs) from the WIPP wells reveal a variety of changes since monitoring began in the earliest wells in 1977. Hydrographs from the wells within the 16 square miles of the WIPP site typically show myriad effects because of the extensive well testing and shaft activities that occurred in the 1980's. Hydrographs from wells in Nash Draw and P-14 (Figure 2) typically do not show responses to tests conducted on the WIPP site, but nevertheless show broad rising and falling trends over periods of several years. Since 1989, a general long-term rise has been observed in both Culebra and Magenta water levels (Figure 3) over a broad area including Nash Draw. At the time of the CCA, this long-term rise was recognized but was thought (outside of Nash Draw) to represent the recovery from the accumulation of tests and shaft leakage that had occurred at the WIPP site since the late 1970's. Changes in the amounts of potash mill effluent discharged onto tailings piles in or near to Nash Draw were considered the likely cause of water-level changes observed in wells in Nash Draw (e.g., Silva, 1996), but not at wells outside the draw. As the rise in water levels has continued over recent years, however, observed heads have exceeded the ranges of uncertainty established for the steady-state heads in most of the 32 wells used in calibration of the T fields for the CCA, throwing into question hypothesized explanations for the changes.

In light of these questions, three new scenarios have been postulated that may account for the long-term water-level rise. The scenarios are: 1) leakage into the Culebra of refining process water discharged onto potash tailings piles, probably through subsidence-induced fractures and/or leaky boreholes; 2) leakage into the Culebra of water from units above the Culebra (Magenta and/or Dewey Lake) or below the Culebra (e.g., Salado, Bell Canyon) through poorly plugged and abandoned boreholes; and 3) leakage into the Culebra of water being injected at depth (e.g., into the Bell Canyon Formation) through leaky boreholes. Conceptually, each one of these scenarios is plausible. Thus, each scenario must be qualitatively evaluated, through the use of numerical flow models, to demonstrate which, if any, are likely to explain the observed water-level changes. This report examines the first scenario by simulating a recharge source from the Mississippi East tailings pile north of the WIPP site due to the application of refining process water.
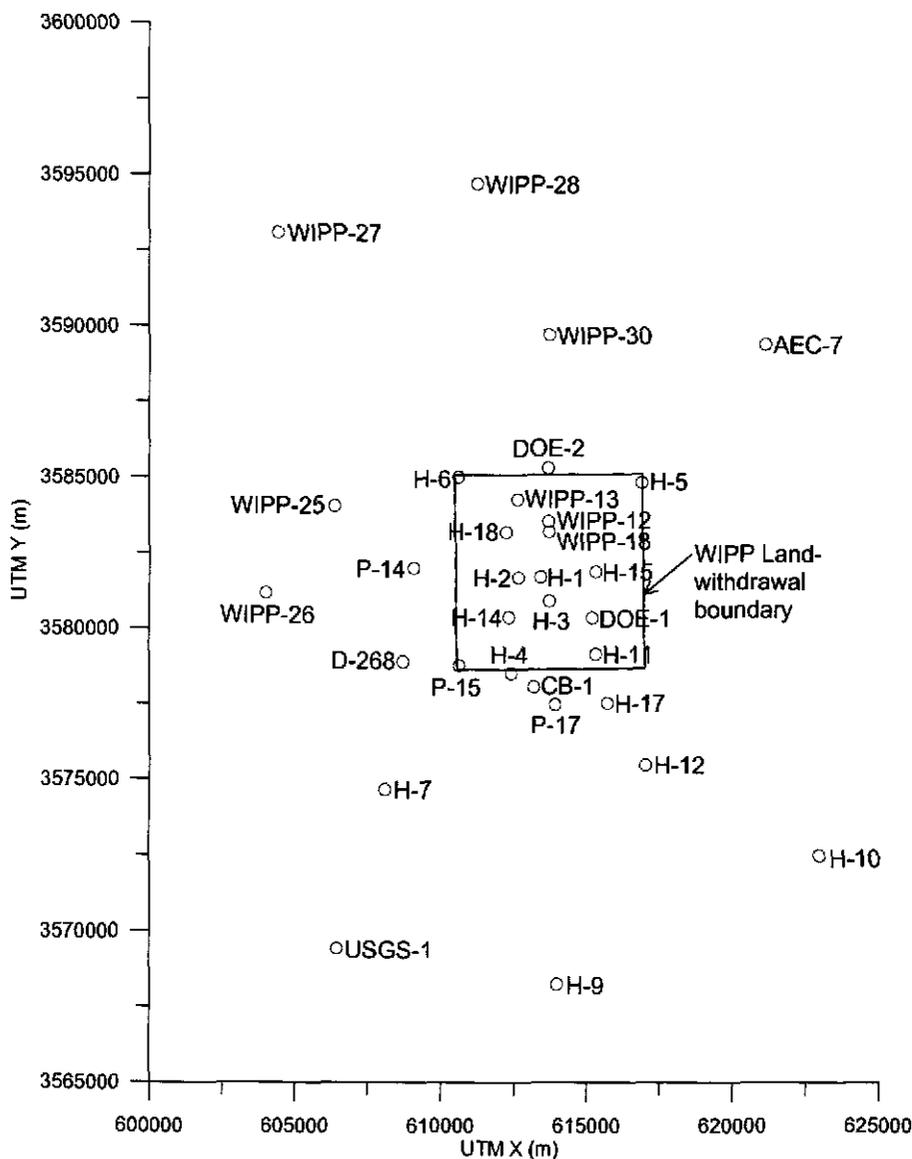


**Figure 1 - Locations of Culebra wells used in CCA modeling.**
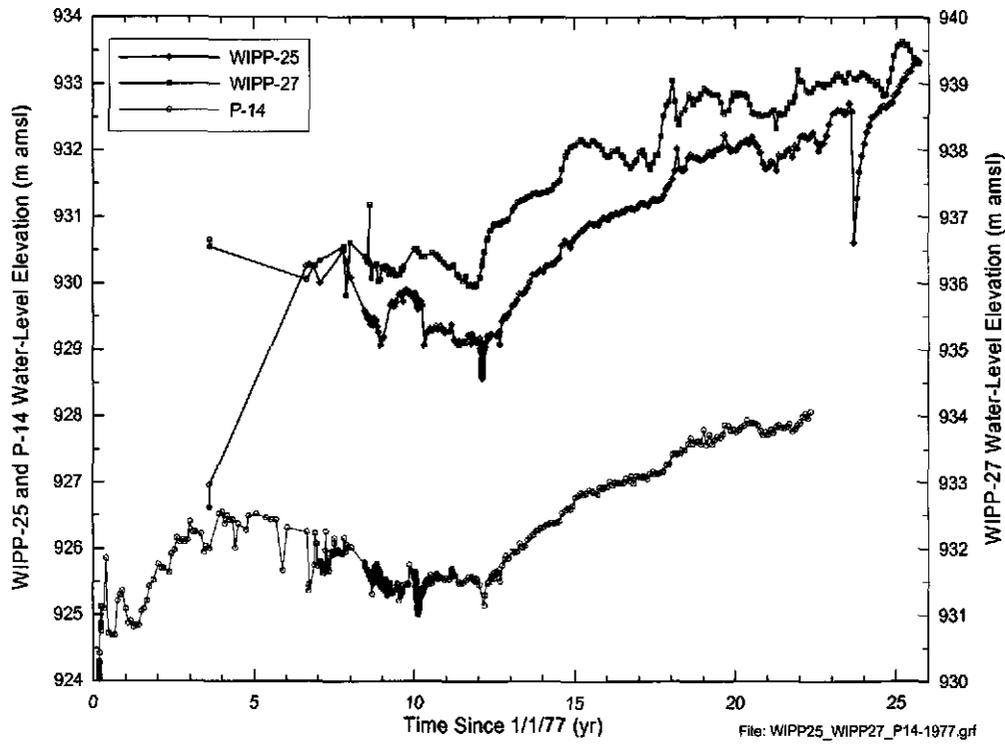
**Figure 2 - Water-level trends in Nash Draw wells and P-14.**
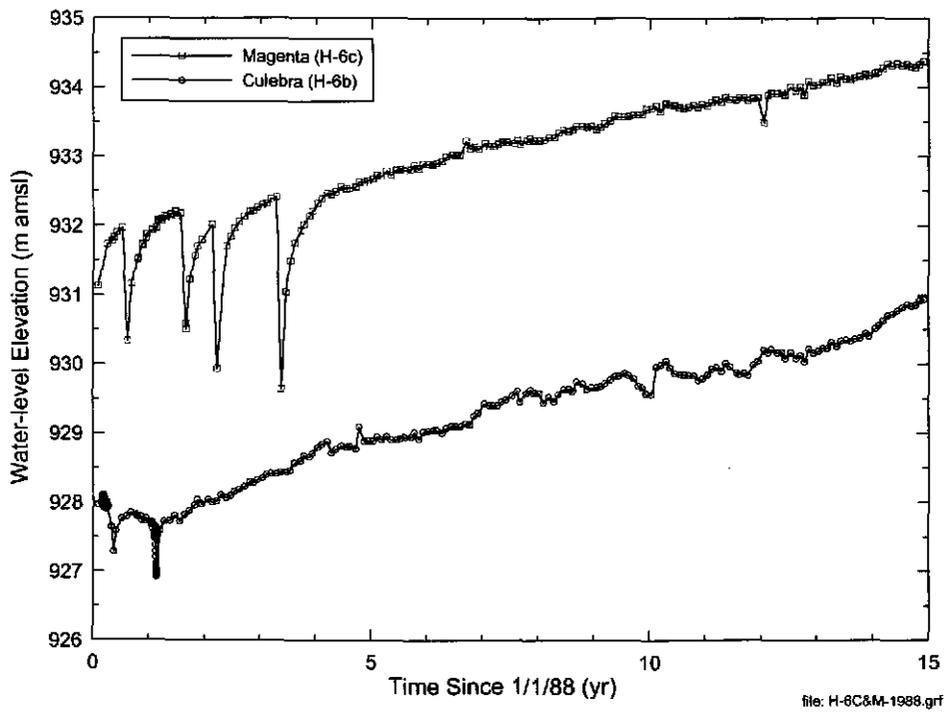


**Figure 3 - Rising Culebra and Magenta water levels at H-6.**

## *1.3  Outline*

This report documents the data, methods, and summary results of the work done as Task 2 of Analysis Plan 110 (Beauheim, 2003a). The sections of this report and a brief description of each subsection are:

**Section 2: Approach**

> **2.1: Overview;** Provides an overview and summary of the modeling approach.
>
> **2.2: Software;** Describes the software usage and information flow between programs.
>
> **2.3: File-Naming Convention;** Describes the file-naming conventions and the input and output files for each program.
>
> **2.4: Execution;** Discusses the data flow and program execution sequence.
>
> **2.5: Model Domain and Discretization, Boundary and Initial Conditions;** Outlines the computational grid, modeling domain, and boundary and initial conditions in terms of regional-scale coordinates.

**Section 3: Data;** Describes the well data used in the calibration procedure.

**Section 4: Modeling Assumptions and Parameters**

> **4.1: Assumptions;** Describes the major assumptions used in the modeling process.
>
> **4.2: Parameters;** Describes the main modeling parameters and the basis for the values used in the model simulations.

**Section 5: Results;** Presents results from the Task 2 tailings pile recharge scenario.

**Section 6: Discussion;** Discusses the implications and results with regard to the objective of this analysis and recommends future work.

**Section 7: Summary;** Presents a summary of this entire report.

# 2 Approach

## 2.1 Overview

For this analysis, the observed water-level rise in wells in and around the WIPP site is hypothesized to be the result of potash refining process water being discharged onto above-ground tailings piles. Specifically, it looks at the Mississippi East tailings pile located 10 to 12 km due north of the WIPP site (Figure 4). Disposal of mine tailings and refining-process effluent at that location began in 1965. Records obtained from the New Mexico State Engineer show how much water has been pumped from local aquifers (Ogallala or Capitan) each year since 1973 for use in the potash-refining process (Figure 5). Since 1973, an average of 2400 acre-feet of water per year has been pumped. Geohydrology Associates (1978) estimated that approximately 90% of this water is discharged onto the tailings pile, and of that, approximately half seeps into the ground while the remainder evaporates. Therefore, on average, approximately 1100 acre-ft of brine may be infiltrating each year. Brine from this tailings pile may enter the Culebra through leaky boreholes and/or by first moving laterally into Nash Draw and then downward through subsidence fractures that have opened over potash mine workings.

The groundwater flow model of the Culebra developed under AP-088 (Beauheim, 2002) is used in this analysis. The model domain, which runs in **MODFLOW-2000 (MF2K** – Harbaugh et al., 2000), is shown in Figure 6. One hundred instances of the model were run using calibrated T-fields from McKenna and Hart (2003). McKenna and Hart (2003) calibrated 137 different realizations of the Culebra T-field to heads measured in late 2000 (treated as "steady-state" heads) and to transient heads associated with seven pumping tests. Beauheim (2003b) developed and applied acceptance criteria to identify the 100 realizations that were used for performance assessment calculations for the WIPP Compliance Recertification Application (CRA; U.S. DOE, 2004). The 100 realizations from Beauheim (2003b) are used in this analysis.

Each model run was recalibrated using **Parallel PEST (PEST v5.51** – Doherty, 2002) coupled with **MF2K** to the slopes of observed drawdowns in 13 monitoring wells using three calibration parameters: specific storage ($S_s$) in the Nash Draw area, $S_s$ outside the Nash Draw area, and a constant leakage or recharge rate from the Mississippi East tailings pile to the Culebra. The two zones of $S_s$ are determined from Figure 4. Everything to the west of the Nash Draw line is calibrated with the $S_s$ Nash Draw value. Where the Nash Draw line is not present in the active portion of the model domain in the southwest, the Salado dissolution line is used. The calibration was transient using a simulation time of 27 years. The simulation time was determined from the length of the data records and was tested prior to the calibration runs to insure a long-term response was evident in all the wells. The slopes of the drawdowns are calculated by fitting a line to the data using linear-regression. Recalling that the general equation for a line is $y = at + b$, where $y$ would be the drawdown and $t$ is time. The slope is the time variable coefficient, '$a$', and '$b$' represents the $y$-intercept. Drawdowns for a water-level rise are negative.

# WIPP SITE AND SURROUNDING AREAS

*With Proposed Wells. Geological Overlays of Salado Dissolution and Rustler Halite Units Extents*
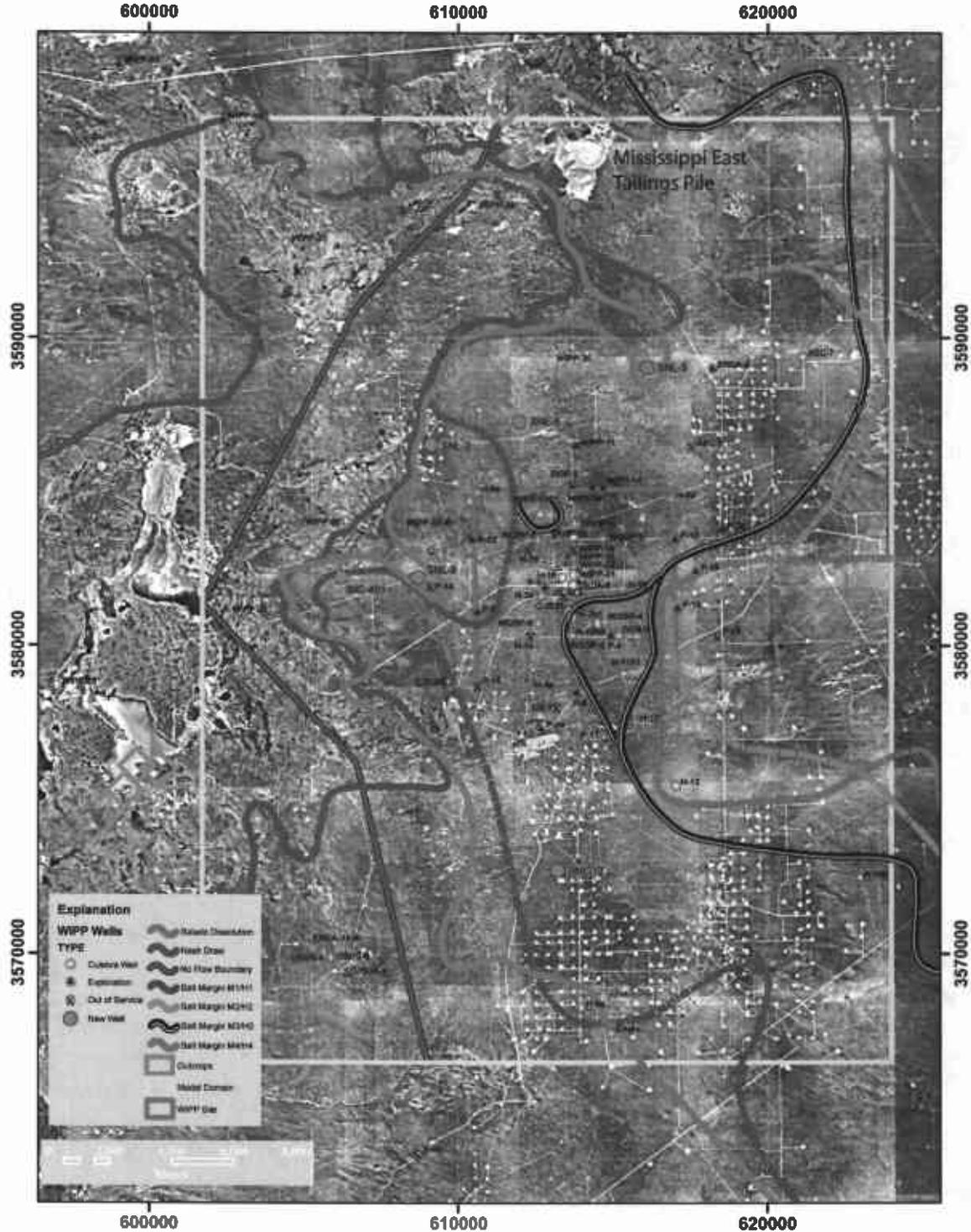


**Figure 4 - WIPP area showing the Mississippi East tailings pile (white area at the top of the figure).**
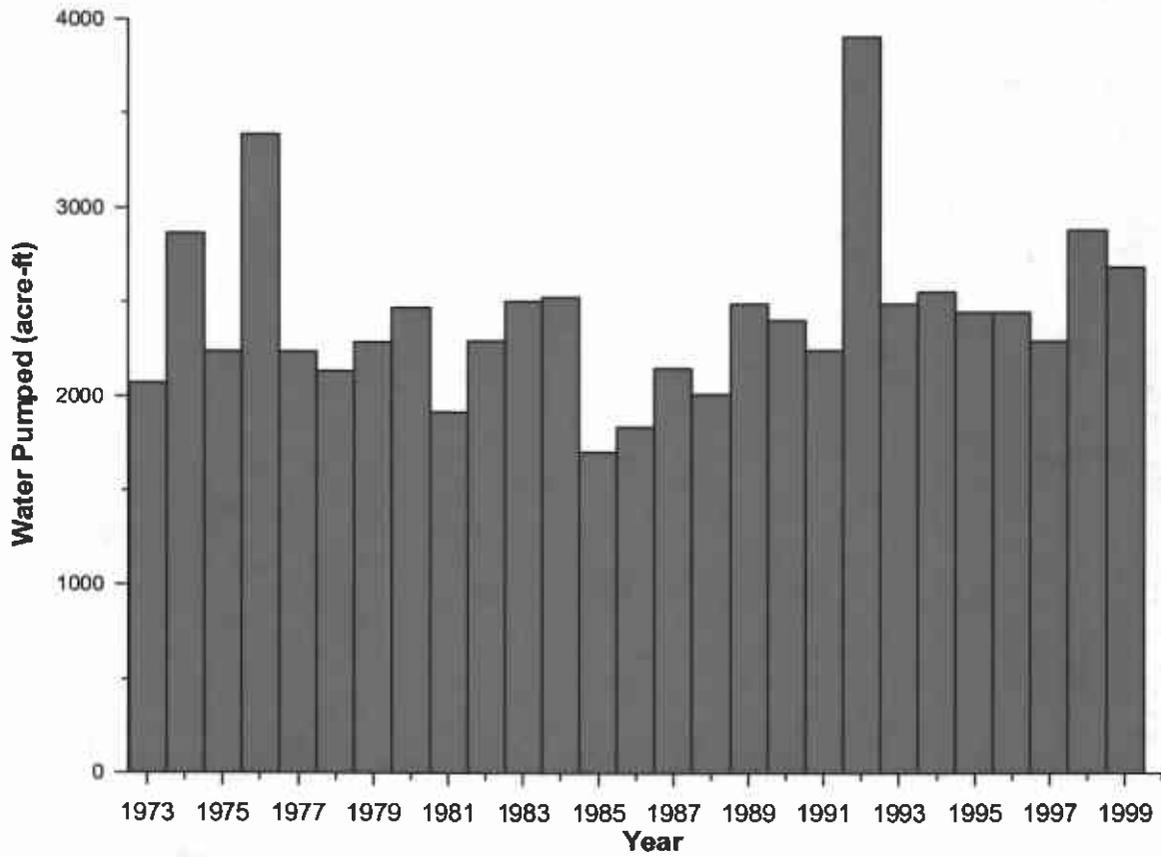
**Figure 5 - Annual water pumpage at Mississippi East potash mill location. Data source:
New Mexico Office of the State Engineer.**
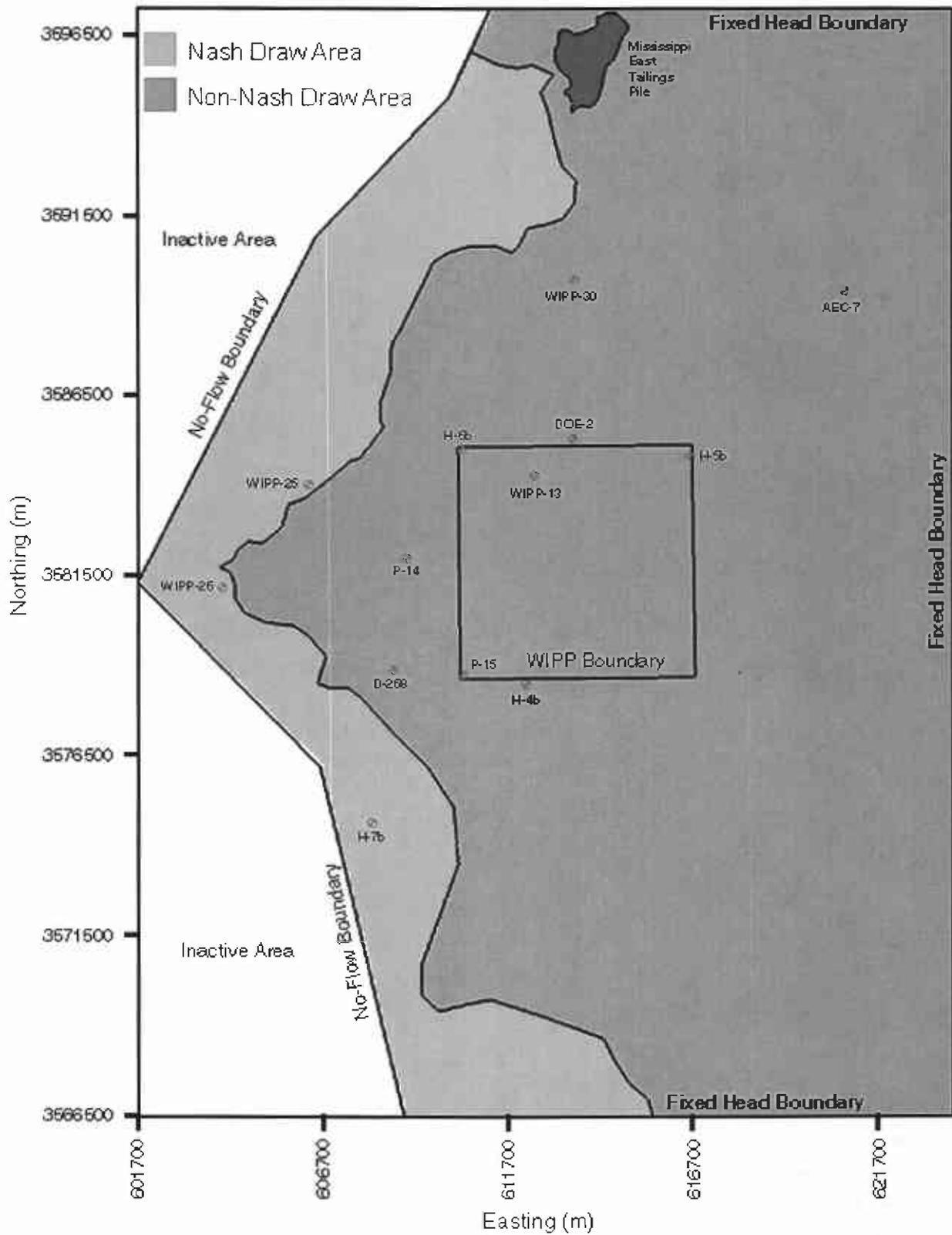
**Figure 6 - Modeling domain showing boundary features, well locations, Mississippi East tailings pile, Nash Draw area, and WIPP boundary.**

## 2.2 *Software*

The flow modeling was performed using **MODFLOW 2000 (MF2K)**, version 1.6 (Harbaugh et al., 2000). **MF2K** is a modular, finite-difference code for solving the groundwater flow equation on a two- or three-dimensional rectilinear grid. For calibration, the parallel version of **PEST** (version 5.51) was used. **PEST v5.51** is a parameter-estimation program that systematically changes parameter input values to fit a set of observations. The advantage of **PEST v5.51** over the non-parallel version of **PEST** is that **PEST v5.51** is designed to run each **MF2K** simulation simultaneously on a different computer, allowing for parallel processing over a networked system. The combination of **PEST v5.51** and **MF2K** is the same software package used to calibrate the T-fields in McKenna and Hart (2003). The programs are listed, with their respective ERMS #'s, in Table 1.

**Table 1 - Major codes used for this analysis.**

| Code Name | Description | ERMS # |
|---|---|---|
| **MODFLOW 2000**, v1.6 | Groundwater Flow Model | 523867 |
| **PEST**, v5.51 | Parameter Estimation Code | 527057 |

Several FORTRAN utility codes are used for data conversion purposes. These codes are, **T_Field.f90, Get_heads.f90, mfrun.f90, mfrch.f90**, and **exhdsdrw_scratch.f90**. The first, **T_Field.f90**, is used to read in each T-field from McKenna and Hart (2003) and write that to a **MF2K** layer-property flow (LPF) input file. **Get_heads.f90** is used to extract final results from a **MF2K** steady-state run, and re-write the final heads to a **MF2K** basic input file as the starting heads for the transient calibration. The code **mfrun.f90** is used to extract the calibrated specific storage values and write a **MF2K** LPF input file with the new values. Likewise, **mfrch.f90** extracts the calibrated recharge rate from the Mississippi East tailings pile and writes a new **MF2K** recharge package input file with the new value.

In order for **PEST v5.51** to calibrate to the slopes of the drawdowns at each well, the drawdowns must be extracted from the **MF2K** results file. This is done by **exhdsdrw_scratch.f90**, which reads the **MF2K** output files, extracts the heads and drawdowns at each well location, and outputs those values to a separate file. Finally, **cut.f90** is used to gather the calibrated drawdown at each well at each time step for each T-field and write the values to an output file that is suitable for plotting in MS Excel. The executable name for each FORTRAN utility code is the prefix of the FORTRAN file name (e.g., the executable of **T_Field.f90** is **T_Field**), with the exception of **cut.f90**, whose executable is named **ctout** to prevent conflicts with the intrinsic Linux command, 'cut'. The FORTRAN utility codes are reproduced in Appendices D through I. Each code is verified via visual inspection.

The Department of Defense Groundwater Modeling System (**GMS**, version 5.0) software is used for visualization and plotting purposes (GMS, 2004). **GMS** is a groundwater modeling and geo-statistical software package that provides a graphical user interface to numerous groundwater modeling codes. **GMS** is not used to perform any calculations or data conversions.

In addition, several Linux shell scripts are used to control the data flow and program execution and to automate the simulation over all 100 T-field realizations. Those scripts are **Ppest_run.sh**,

**clean.sh, mf_steady.sh, runpest.sh, setup.sh, pslave.cque, pmaster.cque,** and **mfrun.sh.** **Ppest_run.sh** is the parent script to all other scripts and provides the run control sequence for the entire simulation. All other scripts are called from within **Ppest_run.sh** or from another script that is called from within **Ppest_run.sh**. The script **clean.sh** is called by **Ppest_run.sh** and is used to delete unneeded files from previous **PEST v5.51** runs. Second in the series called by **Ppest_run.sh** is **mf_steady.sh**, which copies the appropriate files to the appropriate directories and runs **MF2K** in steady-state mode without recharge to calculate the starting heads for each T-field realization (this is described in more detail below). Third is **runpest.sh** that calls three additional scripts (**setup.sh, plsave.cque, pmaster.cque**) and controls the setup sequence for each **PEST v5.51** run. The first script called by **runpest.sh** is **setup.sh**, which creates directories for each slave computer and copies the appropriate files to each directory. The other two, **pslave.cque** and **pmaster.cque,** are used to initiate the slave computers and to start **PEST v5.51**. The final script that is called by **Ppest_run.sh, mfrun.sh**, is used to set up a final **MF2K** run using the calibrated values from **PEST v5.51**. The shell scripts are reproduced in Appendices J through Q.

## 2.3  File-Naming Convention

All calculations were performed on the Sandia 6115 Linux cluster (lylin102) and were completed in a common directory. To run **PEST v5.51**, each slave computer writes its output to a separate directory. At the end of the **PEST v5.51** calibration, the final results are accumulated in a single file called *stor.out* that lists the T-field name, the calibrated value of $S_s$ within the Nash Draw area, $S_s$ outside the Nash Draw area, and the recharge rate from the Mississippi East tailings pile. Once all the **PEST v5.51** calibrations are done, a separate directory for each T-field is created and **MF2K** is run in each directory using the calibrated values for each T-field. The general path for the simulation base directory, the directory that holds the final results file, as well as the set-up files, scripts, and programs is:

*/home3/tslowry/wipp/wtrlvl*

The general path for the T-field directories is:

*/home3/tslowry/wipp/wtrlvl/d##r##*

where *d##r##* is the original base transmissivity field naming convention as described in McKenna and Hart (2003). The ##'s next to *'d'* range from 01 to 22 and next to the *'r'* range from 01 to 10. The common directory from where the **PEST** runs are executed is:

*/home3/tslowry/wipp/wtrlvl/ppest1.*

In addition, a data directory that contains all the T-fields is located at:

*/home3/tslowry/wipp/Tfields*

where each T-field file has the format of *d##r##.mod.*

To help conserve hard disk space and computer memory, all input and output files for each calibration are deleted once the final results are written to *stor.out*. Templates of all input files, which are copied and re-written with the appropriate simulation values for each **PEST v5.51** run to the **PEST v5.51** common directory, are kept in the simulation base directory. The directory structure is shown in Figure 7 and the input and output files that will remain archived in the directories are listed in Table 2.

```
/home3/tslowry/wipp/
│
├─ /Tfields
│
├─ /wtrlvl
│   │
│   │
│   ├─ /ppest1
│   │   │
│   │   ├─ /slave1
│   │   │
│   │   ├─ /slave2
│   │   │   ⋮
│   │
│   ├─ /d01r02
│   │
│   ├─ /d01r04
│   │
│   ├─ /d01r06
│           ⋮
```
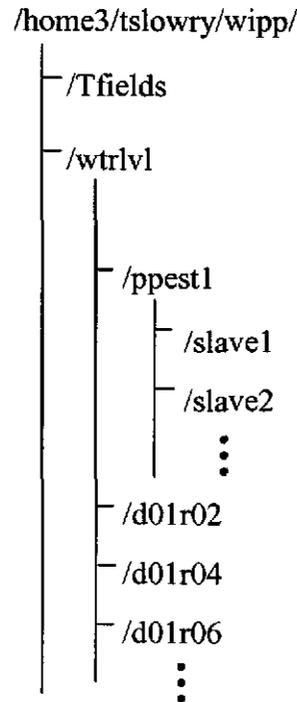
**Figure 7 - Directory structure for archived data and execution files.**

## 2.4 Execution

In order to perform a full **PEST v5.51** run, which consists of multiple **MF2K** runs, each with slightly different values for $S_s$ and recharge, a steady-state run that does not include recharge from the tailings pile must first be executed. The steady-state run assumes conditions before the tailings pile was in place (no recharge) and is used to set the initial head for the transient simulations that include recharge. This insures that the drawdown calculated at each well is due only to the added recharge and not an invalid starting condition.

Figure 8 is a flow chart showing the execution order and primary action of the major programs and scripts used in the full calibration process. As mentioned above, the script **Ppest_run.sh** controls the run sequence. This script starts by cleaning up the previous calibration's input and output files that exist in the */home3/tslowry/wipp/wtrlvl/ppest1* directory. Secondly, it calls the FORTRAN program **T_Field**. **T_Field** reads in a transmissivity field from the files located in */home3/tslowry/wipp/Tfields* and writes them to *Pest4.lpf*. It then reads in $S_s$ values from the **MF2K** LPF input file, *Pest4_old.lpf*. Within *Pest4_old.lpf*, two arbitrary $S_s$ values are assigned for specific storage, one value for cells within the Nash Draw area and another for cells outside the Nash Draw area. The values of $S_s$ within *Pest4_old.lpf* are meaningless in terms of their relevance to the problem, but were used as a test case to insure the files were set up correctly and that **MF2K** could execute properly. These values are also written to *Pest4.lpf*. **T_Field** then reads the file *Pest4.tmp*, which is a **PEST v5.51** input template file that tells **PEST v5.51** what parameters are eligible for adjustment between each **MF2K** simulation. *Pest4.tmp* is identical to the **MF2K** LPF input file, with the exception that rather than numerical values for $S_s$, placeholder characters are used. Finally, **T_Field** writes out the conductivity and the $S_s$ placeholders to *Pest4_new.tmp*.

**Table 2 - Input and output data files used for Task 2. Each directory is listed as its relation to */home3/tslowry/wipp*.**

| Directory | File | Description |
|---|---|---|
| */Tfields* | d##r##.mod | List of good T-fields in *d##r##* format |
| */wtrlvl* | Goodruns.txt | List of 100 T-field data files |
| | filelist.master | List of files necessary for **PEST v5.51** simulation |
| | filelist.slave | List of files for **PEST v5.51** slave execution |
| | filelist.modflow | List of files necessary for **MF2K** execution |
| | Pest4.ba6 | **MF2K** basic input file |
| | Pest4.lpf | **MF2K** layer property flow input file |
| | Pest4.nam | **MF2K** naming file used in **PEST v5.51** simulations |
| | Pest4_home.nam | **MF2K** naming file used in final calibrated run |
| | Pest4_steady.nam | **MF2K** naming file for steady-state runs |
| | Pest4.dis | **MF2K** discretization input file |
| | Pest4_steady.dis | **MF2K** discretization input file for steady-state runs |
| | Pest4.lmg | **MF2K** AMG1R5 solver input file |
| | Pest4.oc | **MF2K** output control file |
| | Pest4.rch | **MF2K** recharge package input file |
| | Pest4_new.ins | **PEST v5.51** instruction file |
| | Pest4_old.ba6 | **MF2K** basic input file template |
| | Pest4_old.lpf | **MF2K** layer property flow input file template |
| | Pest4.pst | **PEST v5.51** control file |
| | Pest4_rch.tmp | Recharge template file |
| | Pest4.rmf | **PEST v5.51** run management file |
| | Pest4_run.in | **PEST v5.51** executable input file |
| | Pest4.tmp | **PEST v5.51** template file for specific storage values |
| | Rech.tmp | Placeholder file for recharge values |
| | stor.out | Output of calibrated specific storage and recharge |
| | wellobs.txt | Time series output of calibrated drawdown |
| | Y_Int.txt | Holding file for initial condition at each well |
| */wtrlvl/ppest1* | * | **PEST v5.51** run directory (contains no data files) |
| */wtrlvl/d##r##* | Pest4.glo | **MF2K** global output file |
| | Pest4.hed | **MF2K** head output file |
| | Pest4.ccf | **MF2K** cell-by-cell output file |
| | Pest4.drw | **MF2K** drawdown output file |
| | wellobs.txt | Time series output of calibrated drawdown |

Controls run-time execution          **Ppest_run.sh**

Sets up **MF2K** LP file for
steady-state run as well as the          **T_Field.f90**
LPF and RCH template files for
the **PEST v5.51** run

Runs **MF2K** in steady-state          **mf_steady.sh**

Extracts solution heads from
**MF2K** steady-state solution and
writes to a **MF2K** BA6 file as          **Get_heads.f90**
the starting heads for the
transient calibration

                                                              **setup.sh**                    Copies input files
                                                                                              to appropriate slave
                                                                                              directories

Runs setup scripts and starts                                                                 Copies input files to
**PEST v5.51**          **run_pest.sh**  →  **pslave.cque**        each client and
                                                                                              starts **pslave**

Extracts calibrated $S_s$ and                              **pmaster.cque**          Copies input files to
recharge values, recreates                                                                    the master slave,
**MF2K** input files using those                                                              starts **pslave** for the
values, runs **MF2K** in steady-                                                              master, and then
state mode to get starting heads,          **mfrun.sh**                                       starts **PEST v5.51**
and then runs **MF2K** again in
transient mode.

**Figure 8 - Flow chart showing execution order and primary actions of the major programs
and/or scripts.**

**Ppest_run.sh** then queues the shell script **mf_steady.sh**. This script calls **MF2K** to execute the steady-state run. The input and output files for the steady-state run are kept in the simulation base directory, */home3/tslowry/wipp/wtrlvl*. **Ppest_run.sh** waits for the steady-state **MF2K** run to finish and then executes the FORTRAN program **Get_heads**. **Get_heads** reads in the head values for the grid from the output of the steady-state run, and then writes those values to a new **MF2K** basic input file called *Pest4_new.ba6* as the initial head values for the upcoming transient run. It also outputs the starting heads at each well location to a separate file called *Y_Int.txt* for use in later calculations of the drawdown at each well. To help with debugging and tracking problems during simulation, **Ppest_run.sh** moves the basic input file from the previous run, *Pest4.ba6*, to *Pest4_old.ba6*, and the newly generated basic input file from **Get_heads**, *Pest4_new.ba6* to *Pest4.ba6*.

Next, **Ppest_run.sh** runs the shell script **runpest.sh**. This short script, which is located in the **PPEST** common directory */home3/tslowry/wipp/wtrlvl/ppest1*, runs the setup script, **setup.sh**, which creates each slave subdirectory and populates those directories with files listed in *filelist.slave*. In addition, **setup.sh** populates the **PEST v5.51** common directory with the files listed in *filelist.master*. Following the setup, **runpest.sh** switches to each slave directory, copies the appropriate data files to each slave's hard drive, and initializes each slave with the **PEST v5.51** subprogram, **pslave**. It then calls **pmaster.cque**, which switches to the primary slave directory (slave1), starts **pslave** for the master slave, and then starts **PEST v5.51**. This starts the **PEST v5.51** run, which takes 40-60 minutes for complete execution using 14 slaves. Once **PEST v5.51** has finished executing, **Ppest_run.sh** reads the output file, *Pest4.sen*, and extracts the calibrated $S_s$ and recharge values and writes them to a list file called *stor.out* located in the simulation base directory. Finally, **Ppest_run.sh** calls the script, **mfrun.sh**, which creates a directory in the simulation base directory for each T-field, copies the appropriate **MF2K** input files into each of the directories, and then runs **MF2K** twice, once in steady-state mode to calculate the starting heads for each T-field, and once in transient mode using the calibrated $S_s$ and recharge values from the **PEST v5.51** calibration. The final step for **mfrun.sh** is to call the FORTRAN program **exhdsdrw** to extract the heads and drawdowns at each well from the **MF2K** output files and write the values to a separate file. The final FORTRAN utility, **ctout**, is run outside the scripts at the end of all **PEST v5.51** and **MF2K** simulations in order to compile the calibrated drawdowns at each well for each T-field into a single file called *wellobs.txt* that is useful for plotting in MS Excel.

## 2.5 Model Domain and Discretization

The modeling domain is the same as that of McKenna and Hart (2003) and consists of 224 cells in the east-west direction (x-direction) and 307 cells in the north-south direction (y-direction). Each cell is of uniform 100-m size on all sides making the modeling domain 22.4 km wide by 30.7 km tall (Figure 6). The discretization of the flow model domain into 100x100 meter cells leads to a total of 68,768 cells with 14,999 (21.8%) of the cells inactive to the west of the no-flow boundary and 53,769 active cells. The corner coordinates of the modeling domain and the WIPP land withdrawal boundary (LWB) in UTM NAD 27 (Zone 13) coordinates are given in Table 3 and Table 4.

**Table 3 - The coordinates of the corners of the numerical model domain in UTM NAD27 coordinates.**

| Domain Corner | X Coordinate (meters) | Y Coordinate (meters) |
|---|---|---|
| Northeast | 624,100 | 3,597,200 |
| Northwest | 601,700 | 3,597,200 |
| Southeast | 624,100 | 3,566,500 |
| Southwest | 601,700 | 3,566,500 |

**Table 4 - The coordinates of the corners of the WIPP land withdrawal boundary (LWB) in UTM NAD27 coordinates.**

| LWB Corner | X Coordinate (meters) | Y Coordinate (meters) |
|---|---|---|
| Northeast | 616,941 | 3,585,109 |
| Northwest | 610,495 | 3,585,068 |
| Southeast | 617,015 | 3,578,681 |
| Southwest | 610,567 | 3,578,623 |

## 2.6 Boundary and Initial Conditions

The initial conditions are the same as those used in McKenna and Hart (2003). As a summary, field head data from the year 2000 consisting of 37 head measurements across the modeling domain are interpolated to the computational grid using kriging. A five-parameter Gaussian function is used to de-trend the head data at which point a Gaussian variogram model is used to describe the variability of the head residuals with distance. The variogram model is used to estimate the residuals at each node in the grid. The final step is to add the regional trend back to the estimated residuals using the five-parameter Gaussian function.

The model boundaries along the north, east, and south edges of the domain are considered fixed-head boundaries (Figure 6). The kriged head values used to determine the initial heads are assigned to each constant-head cell and kept fixed for all simulations. The irregular western boundary is considered a no-flow boundary and falls roughly along the groundwater divide associated with Nash Draw. Nash Draw is interpreted as a regional groundwater divide, draining the Rustler units to the east and north (and also by implication via discharge symmetry, to the west). Since the parameter of interest is the drawdown at each well over the simulation time, the interior starting heads for each T-field must be computed. To do this, a steady-state simulation is run, using the fixed-head boundary values as discussed above, for each T-field. The results of the steady-state simulation are then used as the starting heads for the transient calibration and final calibrated simulations.

# 3 Data

Observed water levels in Culebra wells provide both the motivation for this study and the basic data to which the modeling results will be compared. Culebra water levels have been measured and reported by a number of different organizations since well installation for the WIPP project began. Data collected by the U.S. Geological Survey (USGS) have been reported by Mercer and Orr (1979) and Richey (1986; 1987a,b). Data collected by or on behalf of Sandia National Laboratories are reported in Hydro Geo Chem (1985), Intera Technologies and Hydro Geo Chem (1985), Intera Technologies (1986), Saulnier et al. (1987), and Stensrud et al. (1987; 1988a,b; 1990). Data collected by the WIPP Management and Operating Contractor (MOC), now known as Washington TRU Solutions (WTS), are reported in Kehrman (2002a).

Most of the well monitoring data show a variety of fluctuations with a general increasing water-level trend over time. Some of the fluctuations are known to be due to human-induced influences (e.g., pumping tests, mining operations, etc.), while the cause(s) of others are unknown. Simulating all of the fluctuations in head measurements in each well over time is beyond the scope of this model because of uncertainties in the distribution of hydraulic properties and the lack of detailed knowledge about potential rates, timing, and locations of mining-related recharge.

Rather than calibrate to the variable head levels in each well, calibration was based on the average slopes of the water-level rises in 13 wells over time (Table 5). The wells selected are those closest to the Mississippi East tailings pile and/or to Nash Draw. To determine the slope of the water-level change at each well over time, the time-series data were fit with a linear regression model. The raw data and fitted model for each well are shown in Appendix A. In all but one case (H-7b1), the raw data: 1) exhibited highly variable behavior for part of the time sequence, 2) did not show a rising trend until later in the time sequence, or 3) contained outliers that were clearly anomalous. In those cases, the linear regression was performed on a subset of the raw data. The data that were not included in the regression are plotted in red in Appendix A. Each well, its UTM NAD27 coordinates, and slope of the observed heads are listed in Table 5.

**Table 5 - Well coordinates in UTM NAD27, and the calculated slope of the water-level rise.**

| Well Name | Easting (m) | Northing (m) | Slope (m/yr) |
|---|---|---|---|
| AEC-7 | 621126 | 3589381 | -0.113568 |
| D-268 | 608702 | 3578877 | -0.126283 |
| DOE-2 | 613683 | 3585294 | -0.014003 |
| H-4b | 612380 | 3578483 | -0.198349 |
| H-5b | 616872 | 3584801 | -0.175516 |
| H-6b | 610594 | 3585008 | -0.201408 |
| H-7b1 | 608124 | 3574648 | -0.072852 |
| P-14 | 609084 | 3581976 | -0.229142 |
| P-15 | 610624 | 3578747 | -0.194967 |
| WIPP-13 | 612644 | 3584247 | -0.097052 |
| WIPP-25 | 606385 | 3584028 | -0.227839 |
| WIPP-26 | 604014 | 3581162 | -0.148470 |
| WIPP-30 | 613721 | 3589701 | -0.184103 |
|  |  |  |  |

# 4 Modeling Assumptions and Parameters

## 4.1 Assumptions

Besides assumptions inherent in all modeling exercises (e.g., physical processes can be adequately parameterized and estimated on a numerical grid), several other assumptions are specific and important to this Task. Those assumptions are as follows:

1.  It is assumed that the boundary conditions along the model domain boundary are known and are independent of the T-field being used. This is valid because each T-field was calibrated under the same boundary conditions.

2.  It is assumed that two values of $S_s$, one value for cells in the Nash Draw region (Figure 6), and another for areas outside the Nash Draw region, are adequate to describe the spatial variation of $S_s$ across the domain. This simplification is needed because little data exist that describe the spatial variation of $S_s$ within the modeling area.

3.  It is assumed that specific storage values in the Nash Draw area are higher than in other areas due to a higher frequency of open fractures from subsidence and collapse of the aquifer material. Filtering of the final results is set to honor this assumption.

4.  It is assumed that leakage from the Mississippi East tailings pile can be adequately represented by a constant recharge rate for the duration of the simulation.

5.  It is assumed that changing values of $S_s$ would not significantly change the magnitude or distribution of T in each calibrated T-field (each T-field was calibrated using a single value of $S_s$ for the entire domain). This assumption is discussed in the next section.

## 4.2 Parameters

The conceptual model assumes that the boundary conditions are known, and that each T-field is an equally likely possible T-field. Thus, the only unknown and consequently adjustable parameter values are the two $S_s$ values and the recharge flux from the tailings pile.

For the recharge flux, a base value was calculated from the recharge rate of 1100 acre-ft/yr. The area of the tailings pile was digitized from the map titled, 'WIPP Site and Surrounding Areas, With Proposed Wells, Geological Overlays of Salado Dissolution and Rustler Halite Units Extent', dated September 2002. Using the model domain and discretization, the gridded tailings pile area is 3,490,000 $m^2$, which gives a recharge flux rate of $1.23 \times 10^{-8}$ m/s. The minimum and maximum values for the **PEST v5.51** calibration were set to $1 \times 10^{-12}$ and $1 \times 10^{-7}$ m/s, respectively. The upper limit is an order of magnitude larger than the total possible recharge rate as determined from the average pumping rate of 2400 acre-feet per year. As will be shown below, calibrations never approached this value. The maximum was purposely set high to provide a 'degree of badness' in case calibration values were unreasonable.

McKenna and Hart (2003) calibrated the T-fields used in this Task with a single value of $S_s$ across the entire domain. In reality, $S_s$ varies across the region. Storativity is related to specific storage by the following equation:

$$S = S_s b \qquad (1)$$

where $S$ is the storativity, $S_s$ is the specific storage, and $b$ is the aquifer thickness. Beauheim (2003c) gives a range of storativity values in the WIPP area based on several pumping tests of $5.1 \times 10^{-6}$ (log = -5.29) to $7.3 \times 10^{-5}$ (log = -4.14). Given the aquifer thickness of 7.75 m (Beauheim, 1996), the corresponding values of $S_s$ range from $6.58 \times 10^{-7}$ m$^{-1}$ (log = -6.18) to $9.42 \times 10^{-6}$ m$^{-1}$ (log = -5.03).

Preliminary hand calibrations of $S_s$ to the drawdown data using a range of recharge rates prior to running **PEST v5.51** showed that given the conceptual model that included recharge from the tailings pile, the values given above were too small. Thus, for the **PEST v5.51** calibration runs, both values of specific storage (inside and outside the Nash Draw area) were given the same initial value of $1 \times 10^{-4}$ m$^{-1}$, with minimum and maximum values of $1 \times 10^{-8}$ m$^{-1}$ and $1 \times 10^{-1}$ m$^{-1}$, respectively.

# 5 Results

Inverse modeling using **PEST v5.51** only guarantees that an objective function reaches a minimum value. It does not guarantee that the calibrated values will reflect reality or other observations that are not included in the calibration process. Thus, each calibration run was filtered using the following criteria:

1. If the calibrated value of any of the parameters was its maximum or minimum, or if the total recharge was greater than the amount applied to the tailings pile, the run was not included

2. If the value for specific storage in the Nash Draw area was lower than that elsewhere in the model domain, the run was not included

Filtering of the 100 original T-fields resulted in 53 left for analysis.

The calibrated recharge flux through the Mississippi East tailings pile to the Culebra ranged from $4.20 \times 10^{-9}$ to $6.23 \times 10^{-11}$ m/s, with a mean value of $8.24 \times 10^{-10}$ m/s (73.55 acre-ft/yr), which is approximately 6.7% of the 1100 acre-ft/yr estimated to be infiltrating from the tailings pile. This may indicate that the majority of the infiltrating water may be reaching only shallower strata, such as the Dewey Lake and/or Magenta. The calibrated mean specific storage value for the Nash Draw area ranged from $2.13 \times 10^{-4}$ to $9.43 \times 10^{-6}$ m$^{-1}$ (log = -3.67 to -5.03), with a mean of $5.24 \times 10^{-5}$ m$^{-1}$ (log = -4.28). For the area outside Nash Draw, the range is $5.09 \times 10^{-5}$ to $2.40 \times 10^{-7}$ m$^{-1}$ (log -4.29 to -6.62) with a mean of $9.25 \times 10^{-6}$ m$^{-1}$ (log = -5.03). Corresponding mean storativities are $4.06 \times 10^{-4}$ (log = -3.39) within Nash Draw and $7.17 \times 10^{-5}$ (log = -4.14) outside of Nash Draw. The value for storativity outside the Nash Draw area falls within the range given in Beauheim (2003c). However, the value for storativity in the Nash Draw region is higher than the range indicates. This is not surprising because the values quoted in Beauheim (2003c) are from a limited number of pumping tests, none of which were conducted in Nash Draw. The calibrated value within the Nash Draw area reflects a value that is specific only to Nash Draw, while the pumping tests provide an averaged value across the area outside of Nash Draw (Beauheim, 2003c). Plots of the filtered drawdowns at each well as compared to the slopes calculated from the data are shown in Appendix B. Appendix C lists the raw calibration results for each filtered T-field.

Examination of the plots in Appendix B shows that the calculated rates of drawdown at the 13 wells declined with time, an expected transient result. Some of the well hydrographs presented in Appendix A also show rates declining with time. However, rather than trying to match the transient declines in the rates of water-level change, the calibration sought to match the average simulated rate to the average observed rate. This approach is considered sufficiently accurate to determine the feasibility of infiltration from the tailings pile causing the observed water-level rises.

In order to compare the relative fits among the T-fields, the average of the squares of the differences between the modeled slopes and the slopes of the data from Table 5 was calculated for each T-field. This average is given by the formula:

$$\varepsilon = \frac{\sum_{i=1}^{N}(D_i^d - D_i^m)(D_i^d - D_i^m)}{N} \tag{2}$$

where $\varepsilon$ is the relative error, $D^m$ is the modeled drawdown, $D^d$ is the data drawdown, and $N$ is the number of wells (13). Those T-fields with the lowest $\varepsilon$ were determined to provide the best fit, while those with the highest $\varepsilon$ were determined to have the worst fit. The relative error ranged from 2.99 x $10^{-3}$ to 9.10 x $10^{-3}$, with d22r09 being the best and d08r01 being the worst. Each T-field with its corresponding $\varepsilon$ value is shown in Table 6. A plot of the simulated drawdown slopes versus the observed drawdown slopes for T-field d22r09 is shown in Figure 9.

**Table 6 - Relative error, $\varepsilon$, of each T-field sorted by best (d22r09) to worst (d08r01).**

| T-field | $\varepsilon$ | T-field | $\varepsilon$ | T-field | $\varepsilon$ | T-field | $\varepsilon$ |
|---|---|---|---|---|---|---|---|
| d22r09 | 2.99E-03 | d12r09 | 5.69E-03 | d11r07 | 6.36E-03 | D01r08 | 7.81E-03 |
| d12r08 | 3.34E-03 | d04r07 | 5.76E-03 | d03r07 | 6.36E-03 | d09r05 | 7.83E-03 |
| d02r10 | 3.73E-03 | d04r03 | 5.83E-03 | d21r06 | 6.44E-03 | d11r01 | 8.07E-03 |
| d13r09 | 4.01E-03 | d21r10 | 5.83E-03 | d22r04 | 6.52E-03 | d08r05 | 8.10E-03 |
| d06r04 | 5.07E-03 | d05r02 | 5.86E-03 | d06r03 | 6.58E-03 | d21r05 | 8.17E-03 |
| d09r02 | 5.07E-03 | d07r10 | 5.98E-03 | d03r03 | 6.62E-03 | d03r10 | 8.21E-03 |
| d01r02 | 5.07E-03 | d07r05 | 6.09E-03 | d10r02 | 6.69E-03 | d01r04 | 8.56E-03 |
| d13r05 | 5.14E-03 | d12r07 | 6.12E-03 | d10r08 | 6.69E-03 | d08r01 | 9.10E-03 |
| d12r01 | 5.22E-03 | d03r06 | 6.15E-03 | d13r03 | 6.87E-03 | | |
| d22r10 | 5.29E-03 | d21r02 | 6.15E-03 | d07r09 | 6.88E-03 | | |
| d10r03 | 5.30E-03 | d13r08 | 6.19E-03 | d11r06 | 6.90E-03 | | |
| d05r05 | 5.32E-03 | d21r07 | 6.30E-03 | d07r07 | 6.97E-03 | | |
| d05r01 | 5.39E-03 | d06r06 | 6.33E-03 | d22r08 | 7.27E-03 | | |
| d13r01 | 5.59E-03 | d04r05 | 6.34E-03 | d12r06 | 7.47E-03 | | |
| d08r09 | 5.62E-03 | d04r06 | 6.34E-03 | d07r08 | 7.74E-03 | | |

Looking at a side-by-side comparison of the best- and worst-fit T-fields (Figure 10 – plotted as $\text{Log}_{10}$ T), the d22r09 T-field has higher values of T in the Nash Draw area and around the tailings pile, and more connected areas of high T. Visual examination of other T-fields with a low $\varepsilon$ score (not shown) reveals this same characteristic. This characteristic may be necessary for recharge from the tailings pile to have adequate influence across the domain.

**Modeled Slope (d22r09) vs. Data Slope**
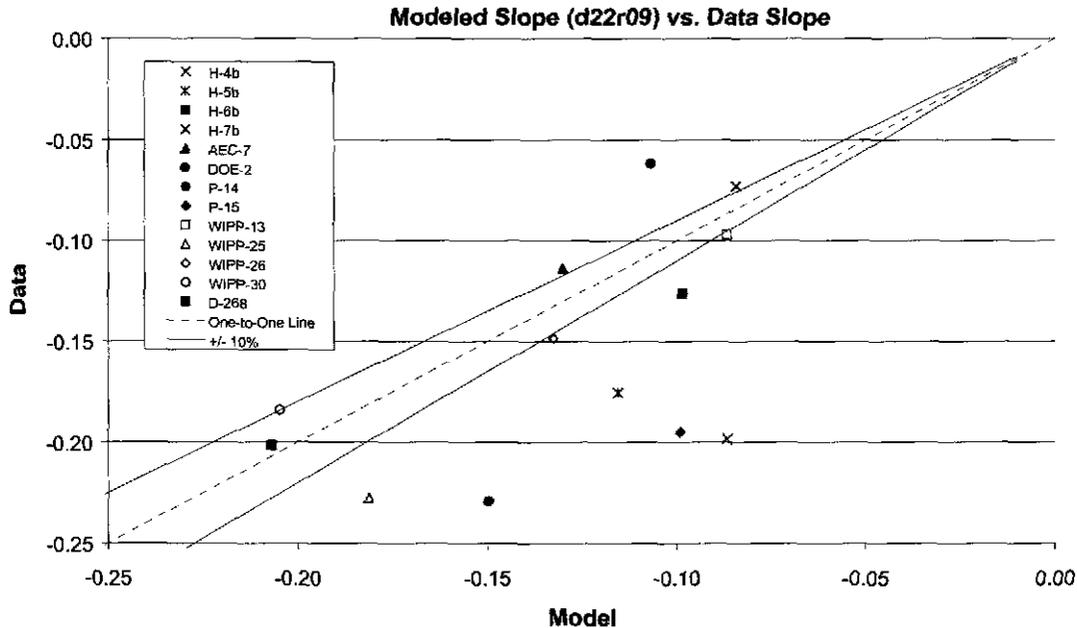


Figure 9 - Modeled slopes for T-field d22r09 versus slopes calculated from data. Data points in red indicate modeled slopes that are less than 90% of the data slopes, blue indicates modeled slopes greater than 110% of data, and green indicates slopes within ±10%.

Comparing the percentage contribution of each well to $\varepsilon$ (Table 7) for each T-field shows that wells H-4b, P-15, P-14, and WIPP-25 contribute 69.5% to the average total error. For the best-fit T-field (d22r09), those four wells contribute 80.1% of the total error. This could indicate that the T characterization around those four wells may be suspect. To further examine this, we compare T-field d13r05 and d12r08, which are the T-fields that fit well pairs H-4b/P-15 and P-14/WIPP-25, respectively, the best. Wells H-4b and P-15 contribute 27.5% of the total error for T-field d13r05 and wells P-14 and WIPP-25 contribute 8.3% of the total error for T-field d12r08. T-field d12r08 is the second-best overall fit across all wells and fits all other wells besides H-4b and P-15 better than T-field d22r09. The fact that for even their best fit, wells H-4b and P-15 contribute over 27% to the total error, and considering that they are relatively close to each other (both are located in the southwest corner of the WIPP site, see Figure 4) indicates that the suspect characterization may be localized around those wells. The other unique feature of wells H-4b and P-15 is that none of the 53 calibrated and filtered T-fields could match the magnitude of the drawdown shown by the data at each well (Appendix B). This may indicate that the modeled T-field and/or $S_s$ characterization in that area does not reflect the true conditions or that the water-level rise in the area to the west and southwest of the WIPP site is due to another water source other than (or in addition to) the Mississippi East tailings pile (such as the IMC tailings pile that is at the "apex" of the no-flow boundary on the western model domain boundary (Figure 4)). To visualize this, Figure 11 shows the relative error as spatially varying across the domain. For each T-field, the error terms at each well are normalized (with respect to the maximum error of the average field), plotted, kriged, and then contoured to get the spatial variability. The difficult area around wells H-4b and P-15 is clearly visible for each instance.

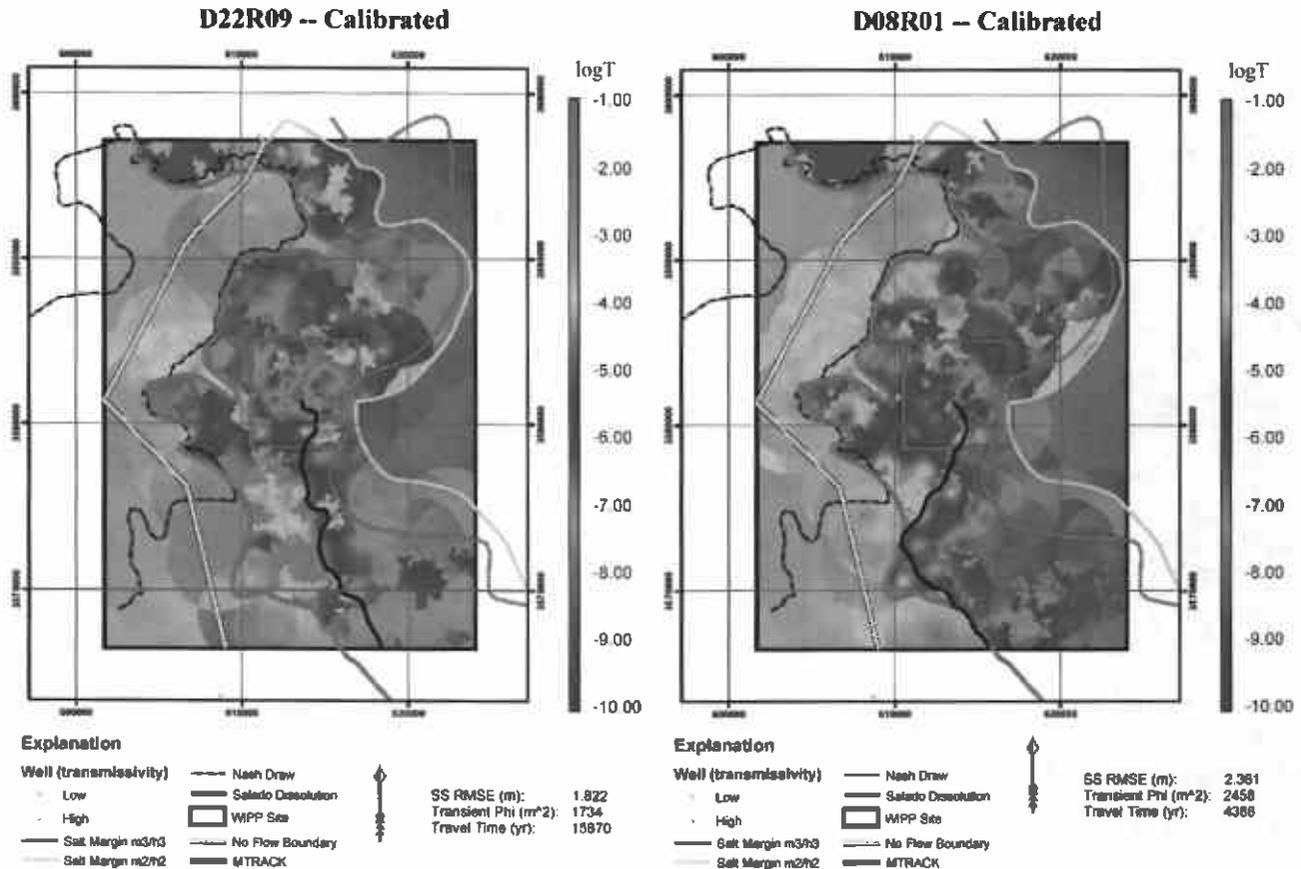D22R09 -- Calibrated      D08R01 -- Calibrated



Figure 10 - Comparison of the best-fit T-field (d22r09) and the worst-fit T-field (d08r01).

Table 7 – Percentage contribution of each well to the total error for the average case, T-field d22r09 (best fit), T-field d13r05 (fits wells H-4b and P-15 the best), and T-field d12r08 (fits wells P-14 and WIPP-25 the best).

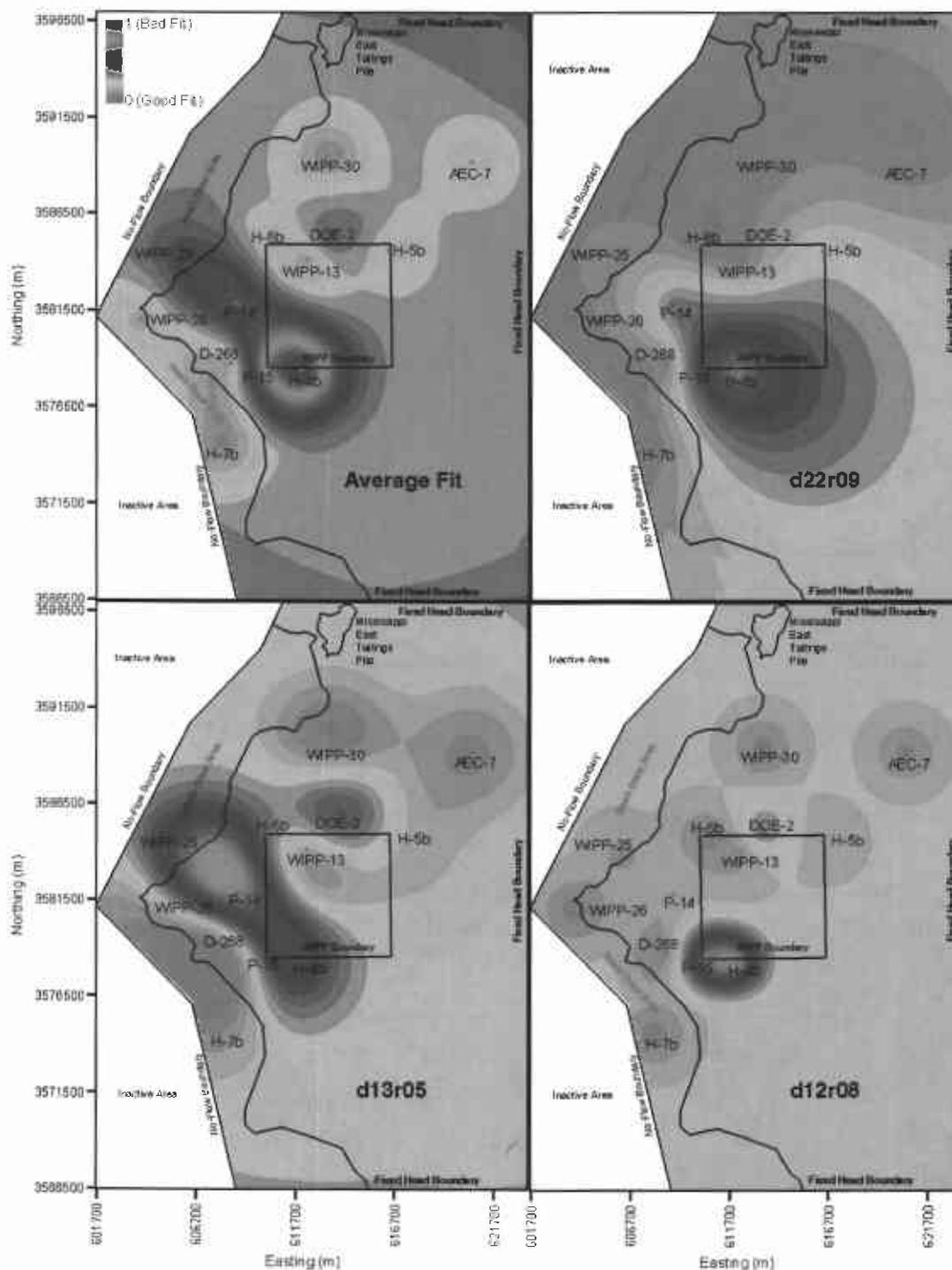| Well # | Average | d22r09 | d13r05 | d12r08 |
|--------|---------|--------|--------|--------|
| AEC-7 | 3.21% | 0.40% | 0.85% | 0.79% |
| D-268 | 3.30% | 2.45% | 0.58% | 2.83% |
| DOE-2 | 8.87% | 4.35% | 9.80% | 13.83% |
| **H-4b** | **24.00%** | **33.75%** | **14.78%** | **34.12%** |
| H-5b | 4.25% | 10.48% | 5.39% | 4.20% |
| H-6b | 4.21% | 0.02% | 9.68% | 1.17% |
| H-7b1 | 0.48% | 0.21% | 1.34% | 0.10% |
| **P-14** | **14.22%** | **16.69%** | **20.27%** | **5.08%** |
| **P-15** | **19.74%** | **25.17%** | **12.75%** | **30.07%** |
| WIPP-13 | 2.74% | 0.48% | 3.02% | 3.61% |
| **WIPP-25** | **11.52%** | **4.51%** | **18.67%** | **3.24%** |
| WIPP-26 | 2.62% | 0.74% | 2.34% | 0.26% |
| WIPP-30 | 0.84% | 0.74% | 0.53% | 0.71% |

Figure 11 - Plot of normalized relative error for each well for three selected T-fields, and the average case. Using equation (2), T-field d22r09 provides the best overall fit to all wells, d13r05 is the best fit to wells H-4b and P-15, and d12r08 is the best fit for wells P-14 and WIPP-25. The relative errors shown here are normalized with respect to the maximum error of the average field such that the areas with the lowest error values receive a value of 0 (red) and the areas with the highest error values receive a value of 1 (blue).

# 6 Discussion

While the results of this analysis support the initial hypothesis that the Mississippi East tailings pile may be responsible for the observed water-level rise in the Culebra across the WIPP area, a conclusive determination is not possible. This is due to limitations in the available data as well as limitations in the modeling approach. Firmer conclusions would require the following:

1. Simultaneous calibration of transmissivity, storativity, and recharge from the tailings pile. Transmissivity and storativity would be treated as spatially variable across the domain and possibly correlated to one another. Additional storativity values from the field, using a wider spatial distribution of pumping tests with responses observed across the majority of the model domain, would provide the needed data to narrow storativity values adequately across the domain. This exercise would preserve the physical relationship between storativity, transmissivity, and the water-level data in the wells.

2. Improve model boundary conditions. The boundary conditions of the current model are determined through interpolation and extrapolation of measured head levels across the WIPP area. However, no data are available along the boundary to verify this characterization. This issue becomes important with respect to the Mississippi East tailings pile, which lies relatively close to the northern boundary of the model. The boundary condition in that area does not account for water flux from the tailings pile. Changes in this boundary condition may have large impacts on the calibrated recharge rates from the tailings pile. To supplement the data collection and for use as an interim measure prior to sufficient boundary data becoming available, a basin-wide model could be constructed that would help establish boundary conditions for the WIPP-area model.

3. Use the data from Figure 5 to add time-varying rates of recharge from the tailings pile. In addition, other possible recharge sources (e.g., other tailings piles in the area such as the Mississippi West and IMC tailings piles) should also be identified and added to the model. The mild temporal fluctuation shown in Figure 5 may help in the calibration of $S_s$ because it would introduce transient responses for water-level rises across the domain. However, incorporating temporal fluctuations in the infiltration rate would require estimation of how the water discharged onto the tailings pile(s) is buffered (retarded) by the pile and along whatever route it takes from the pile to the Culebra.

4. Using historical water-level data, determine a more realistic initial condition than the 2000 head levels used in this modeling exercise. This point is similar to point 2 but addresses the conditions at the beginning of the simulation rather than current boundary conditions. A link between well data in the modeling domain and data collected on the boundary would need to be established for this to be possible. Coupled with points 1, 2, and 3, this would allow for calibration to the actual data, and not to the slope of the drawdown. Understanding the initial conditions would help insure that the model is capturing important temporal dynamics that may otherwise be lost.

Each of these points, individually or in any combination, would enhance the current understanding of the water-level rise and help to demonstrate its origin.

# 7 Summary

This analysis report describes the activities of Task 2 of AP-110, "Analysis Plan for Evaluation of Culebra Water-Level-Rise Scenarios" (Beauheim, 2003a). The purpose of this Task is to evaluate the likelihood that observed rising water levels in the Culebra Dolomite Member of the Rustler Formation near the Waste Isolation Pilot Plant (WIPP) are due to leakage from refining process water discharged onto the Mississippi East tailings pile, which lies 10 to 12 km north of the WIPP site.

The basis of this analysis relies on a numerical model of the WIPP area, with the same grid layout and boundary conditions as that used in McKenna and Hart (2003). Data from 13 wells in the WIPP area, which were first converted to drawdown slopes over time (rising water levels equate to negative drawdowns), were used to calibrate two zones of specific storage and the recharge rate from the tailings pile to the Culebra simultaneously. The two zones of specific storage correspond to the Nash Draw area and the balance of the model domain. One hundred calibrations were completed, each using a different T-field generated from separate calibrations in McKenna and Hart (2003). The calibration results were filtered to insure that specific storage values in the Nash Draw area were higher than outside that area, and that none of the calibration parameters calibrated to their respective maximum or minimum value as given in the input files.

Of the 100 T-fields used for the calibration process, 53 were determined to provide adequate fits to the data with realistic values for specific storage and recharge. The mean calibrated value of recharge from the Mississippi East tailings pile is $8.24 \times 10^{-10}$ m/s (73.55 acre-ft/yr), which is approximately 6.7% of the 1100 acre-ft/yr infiltration value derived from Geohydrology Associates (1978). This may indicate that the majority of the infiltrating water may be reaching only shallower strata, such as the Dewey Lake and/or Magenta. The mean specific storage value for the Nash Draw area is $5.24 \times 10^{-5}$ m$^{-1}$ (log = -4.28) and for the area outside Nash Draw it is $9.25 \times 10^{-6}$ m$^{-1}$ (log = -5.03), corresponding to storativities of $4.06 \times 10^{-4}$ (log = -3.39) and $7.17 \times 10^{-5}$ (log = -4.14), respectively.

Given the uncertainties and limitations in the model and available data, we conclude that recharge originating from the Mississippi East tailings pile is a plausible explanation for the observed water-level changes in and around the WIPP site.

Uncertainty could be reduced and the model improved by:

1. Determining the spatial variability of storativity through additional pumping tests and simultaneous model calibration of transmissivity, storativity, and recharge from the tailings pile.

2. Improving the model constant-head boundary estimation.

3. Adding in time-varying rates of recharge, as well as other possible recharge sources (e.g., other tailings piles in the area).

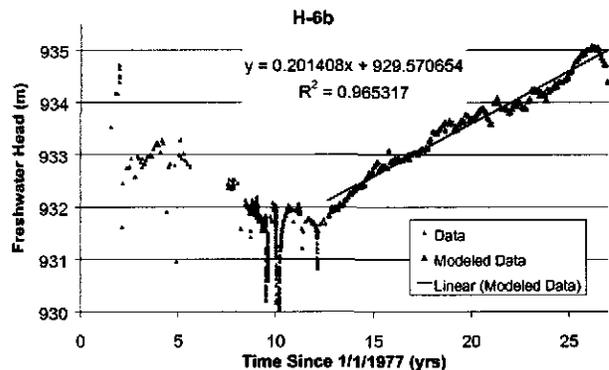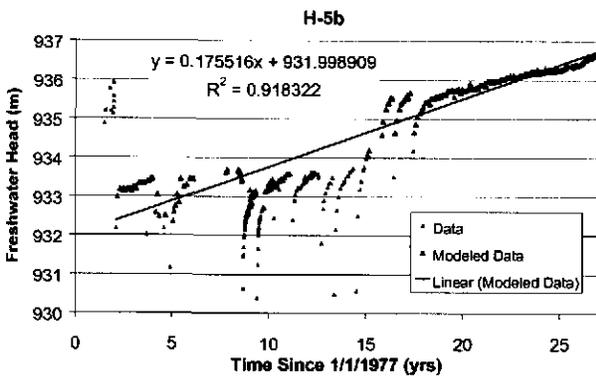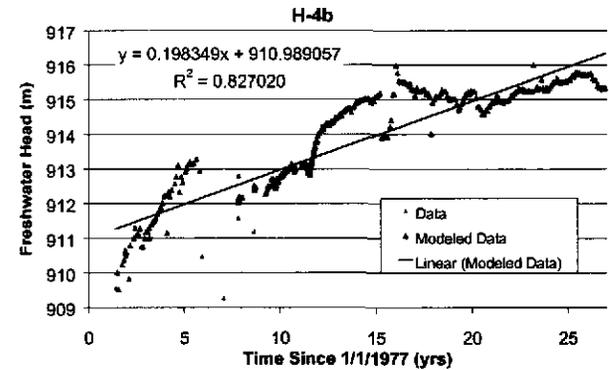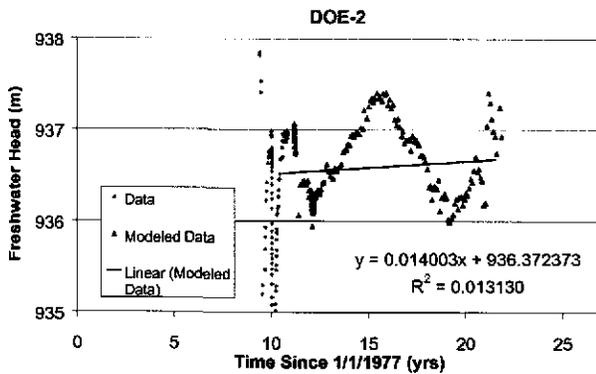4. Improving the estimation of the initial conditions.

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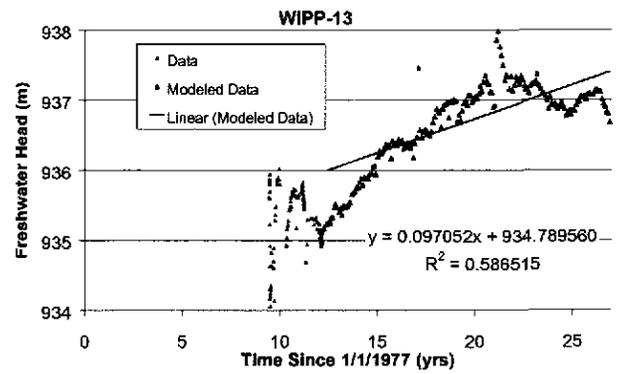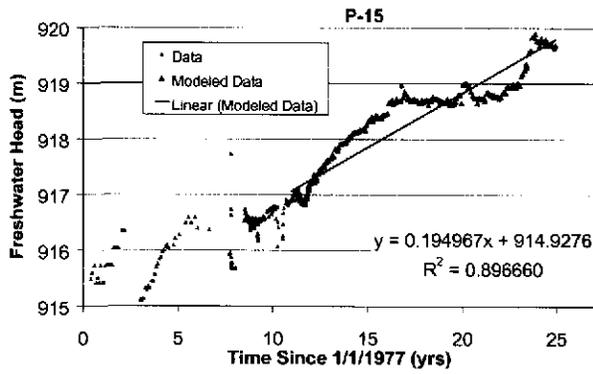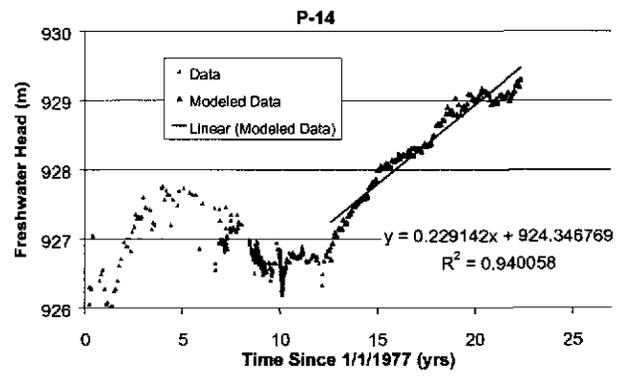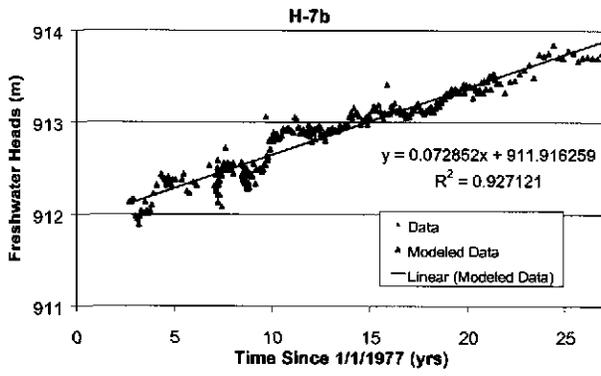EPA (U.S. Environmental Protection Agency). 2002. Letter from Frank Marcinowski, Director, Radiation Protection Division, U.S. EPA, to Dr. Inés Triay, Manager, Carlsbad Field Office, DOE, dated August 6, 2002. Washington, DC: U.S. Environmental Protection Agency, Office of Air and Radiation.

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# Appendix A: Fitted Well Data for Calibration

Each chart shows the raw data for each well, the fitted trend line, the equation of the fitted line, and the $R^2$ value of the fitted line. Data that are excluded from the regression are plotted in red. Each plot is scaled to emphasize the portions of the data that are used in the linear regression.

H-7b

$y = 0.072852x + 911.916259$
$R^2 = 0.927121$



P-14

$y = 0.229142x + 924.346769$
$R^2 = 0.940058$



P-15

$y = 0.194967x + 914.9276$
$R^2 = 0.896660$



WIPP-13

$y = 0.097052x + 934.789560$
$R^2 = 0.586515$



WIPP-25

$y = 0.227839x + 928.118998$
$R^2 = 0.885034$



WIPP-26

$y = 0.148470x + 917.613523$
$R^2 = 0.923727$



WIPP-30

$y = 0.184103x + 932.778492$
$R^2 = 0.791492$



D-268

$y = 0.126283x + 913.664946$
$R^2 = 0.834885$
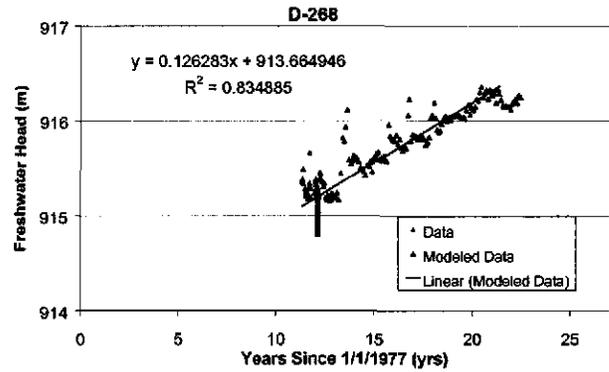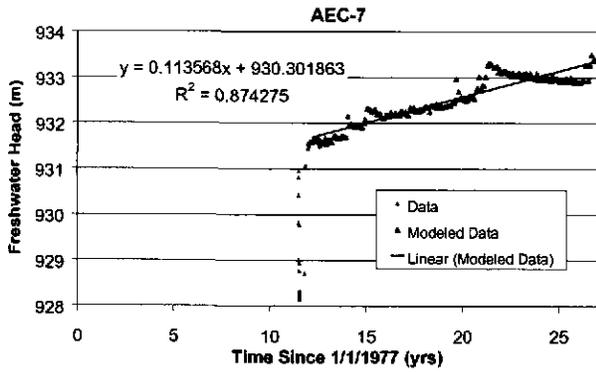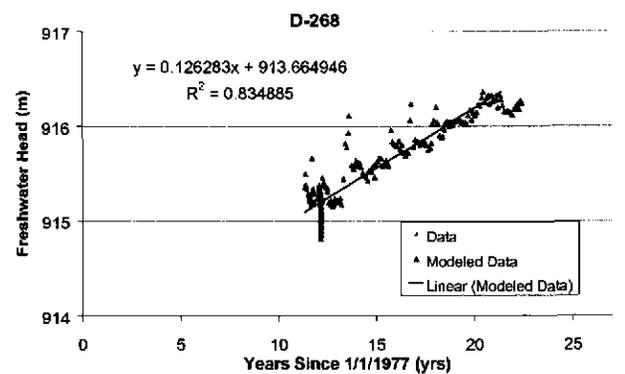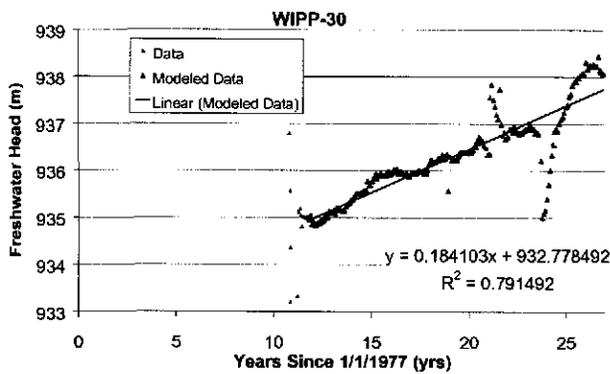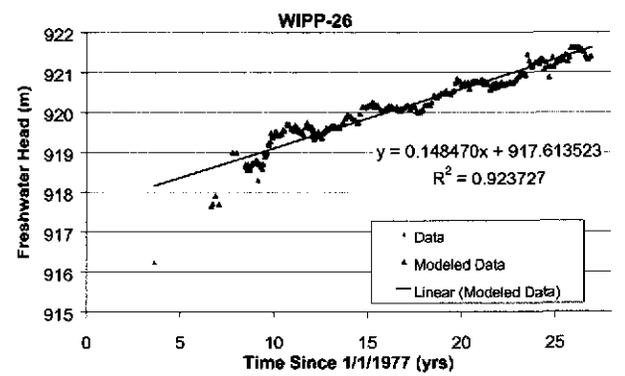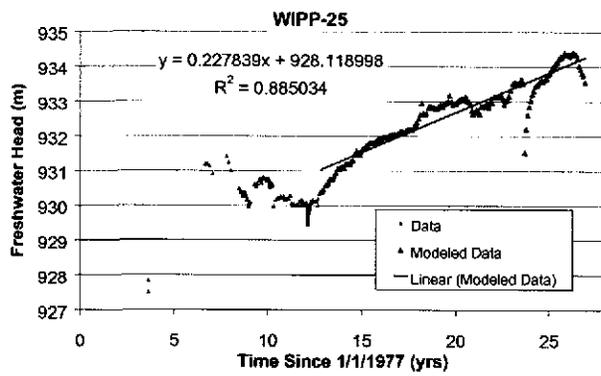
# Appendix B: Calibrated Filtered Drawdowns

Each plot shows the drawdown for each T-field using the calibrated parameters given in Appendix C. The thick red line in each plot represents the slope of the drawdown calculated from the data.
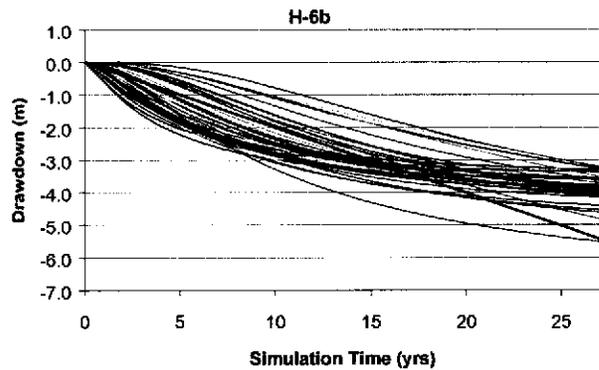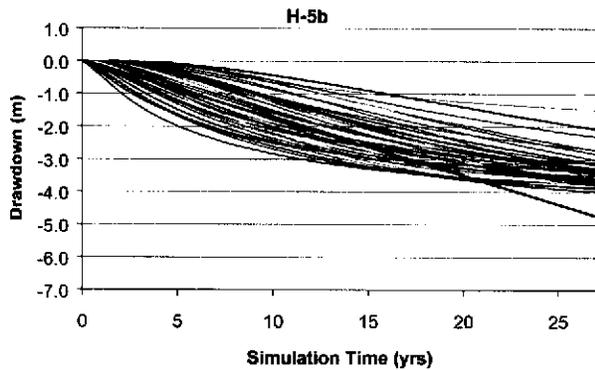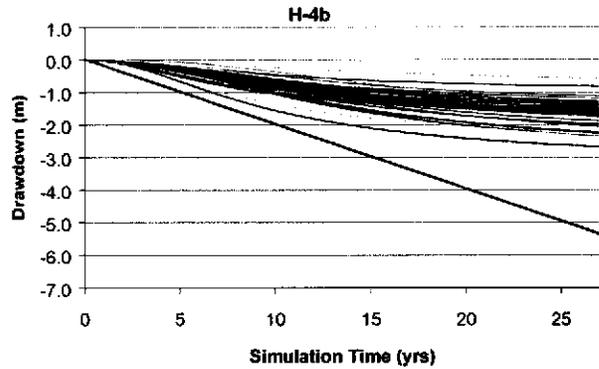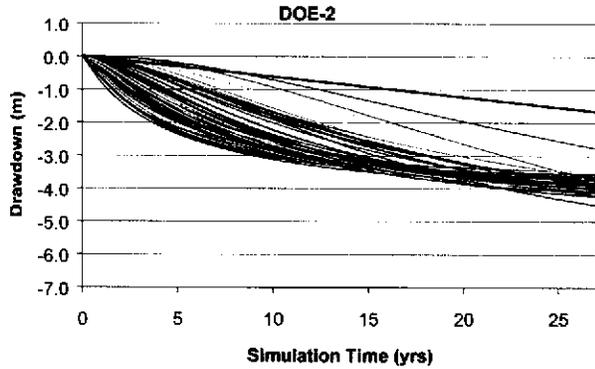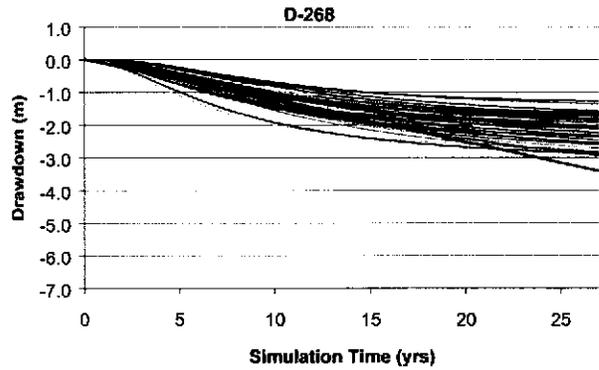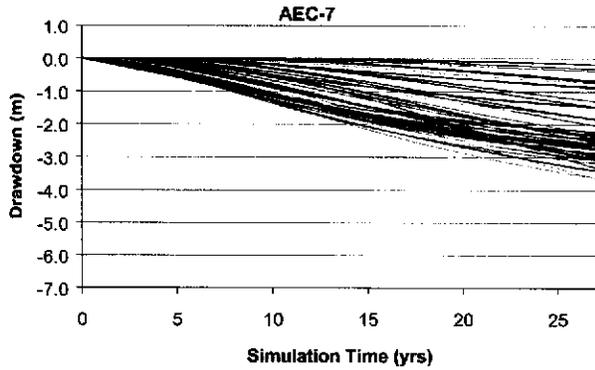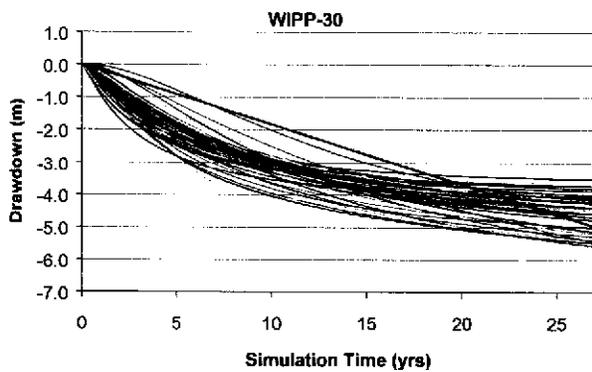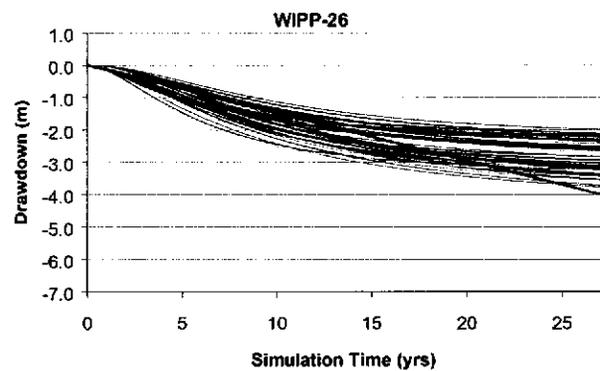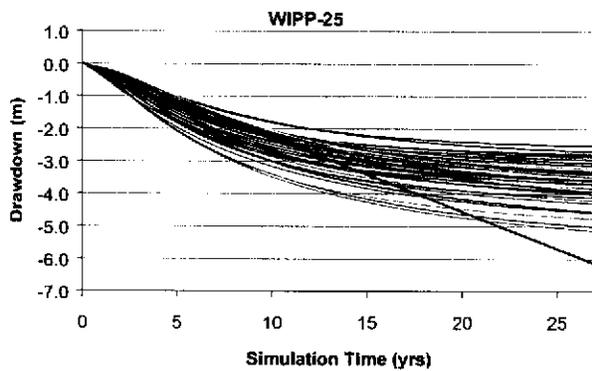
# Appendix C: Calibration Results

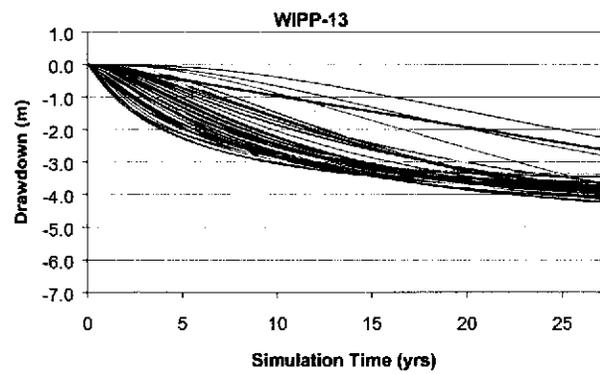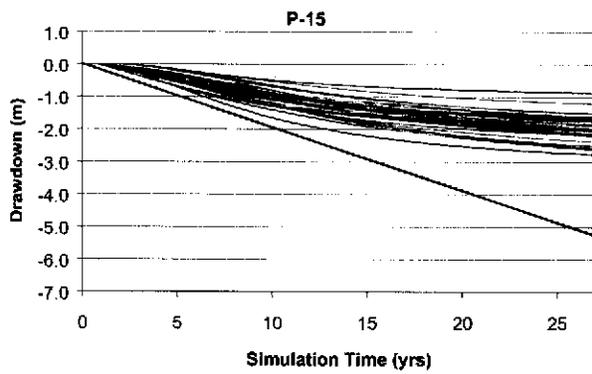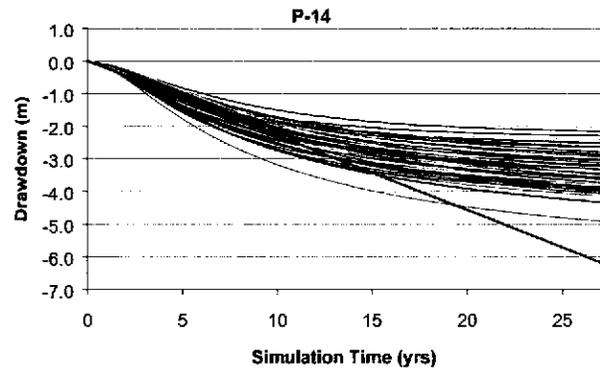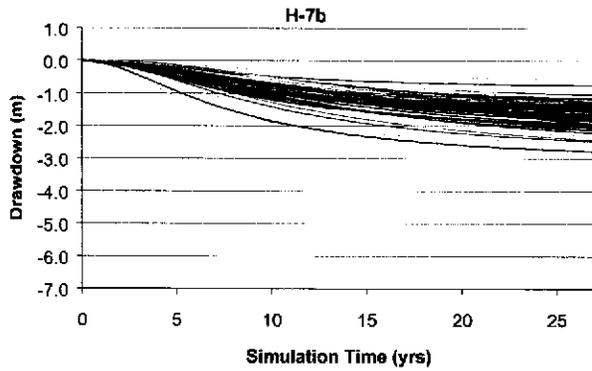| T-field | Actual Values | | | Log Values | | |
|---|---|---|---|---|---|---|
| | Recharge (m/s) | Specific Storage – Nash Draw Area $(m^{-1})$ | Specific Storage – Outside Nash Draw $(m^{-1})$ | Recharge (m/s) | Specific Storage – Nash Draw Area $(m^{-1})$ | Specific Storage – Outside Nash Draw $(m^{-1})$ |
| d01r02 | 6.23E-11 | 2.03E-05 | 2.25E-06 | -10.206 | -4.692 | -5.648 |
| d01r04 | 4.2E-09 | 0.000137 | 6.41E-06 | -8.377 | -3.862 | -5.193 |
| d01r08 | 7.44E-10 | 2.85E-05 | 6.47E-06 | -9.128 | -4.545 | -5.189 |
| d02r10 | 2.48E-10 | 1.82E-05 | 8.12E-06 | -9.605 | -4.741 | -5.090 |
| d03r03 | 3.51E-10 | 1.37E-05 | 6.24E-06 | -9.455 | -4.864 | -5.205 |
| d03r06 | 6.18E-10 | 4.73E-05 | 1.29E-05 | -9.209 | -4.325 | -4.891 |
| d03r07 | 1.93E-09 | 5.3E-05 | 5.19E-06 | -8.714 | -4.276 | -5.285 |
| d03r10 | 2E-09 | 5.31E-05 | 1.5E-05 | -8.699 | -4.275 | -4.823 |
| d04r03 | 2.5E-10 | 5.46E-05 | 2.23E-06 | -9.601 | -4.263 | -5.652 |
| d04r05 | 1.14E-09 | 6.11E-05 | 3.2E-05 | -8.943 | -4.214 | -4.495 |
| d04r06 | 1.34E-10 | 4.4E-05 | 3.52E-06 | -9.874 | -4.356 | -5.453 |
| d04r07 | 1.16E-09 | 6.73E-05 | 1.48E-05 | -8.934 | -4.172 | -4.830 |
| d05r01 | 4.53E-10 | 1.76E-05 | 1.15E-05 | -9.344 | -4.755 | -4.938 |
| d05r02 | 4.41E-10 | 9.94E-06 | 8.7E-06 | -9.356 | -5.003 | -5.061 |
| d05r05 | 6.02E-10 | 9.43E-06 | 3.97E-06 | -9.220 | -5.026 | -5.401 |
| d06r03 | 6.92E-10 | 0.000144 | 1.31E-06 | -9.160 | -3.841 | -5.883 |
| d06r04 | 4.48E-10 | 2.91E-05 | 1.52E-06 | -9.349 | -4.537 | -5.819 |
| d06r06 | 5.62E-10 | 7.12E-05 | 1.03E-05 | -9.250 | -4.148 | -4.987 |
| d07r05 | 1.17E-09 | 6.14E-05 | 8.03E-06 | -8.933 | -4.212 | -5.095 |
| d07r07 | 2.29E-09 | 3.73E-05 | 4.83E-06 | -8.640 | -4.429 | -5.316 |
| d07r08 | 9.7E-11 | 1.24E-05 | 5.29E-06 | -10.013 | -4.906 | -5.276 |
| d07r09 | 5.4E-10 | 5.11E-05 | 1.48E-06 | -9.268 | -4.291 | -5.829 |
| d07r10 | 5.87E-10 | 0.000156 | 1.59E-06 | -9.231 | -3.806 | -5.797 |
| d08r01 | 2.42E-10 | 1.74E-05 | 7.88E-06 | -9.616 | -4.759 | -5.104 |
| d08r05 | 2.07E-10 | 4.07E-05 | 1.3E-06 | -9.684 | -4.390 | -5.885 |
| d08r09 | 1.86E-10 | 1.71E-05 | 2.4E-06 | -9.730 | -4.766 | -5.620 |
| d09r02 | 5.59E-10 | 3.43E-05 | 1.7E-05 | -9.253 | -4.465 | -4.770 |
| d09r05 | 2.06E-10 | 4.3E-05 | 1.84E-06 | -9.687 | -4.366 | -5.736 |
| d10r02 | 1.13E-09 | 0.000213 | 3.03E-06 | -8.948 | -3.671 | -5.519 |
| d10r03 | 8.12E-10 | 7.6E-05 | 3.83E-05 | -9.090 | -4.119 | -4.416 |
| d10r08 | 3.2E-10 | 4.73E-05 | 1.59E-05 | -9.495 | -4.325 | -4.798 |
| d11r01 | 2.45E-10 | 2.62E-05 | 1.02E-06 | -9.611 | -4.581 | -5.993 |
| d11r06 | 1.76E-09 | 3.78E-05 | 3.35E-06 | -8.754 | -4.422 | -5.475 |
| d11r07 | 4.15E-10 | 5.66E-05 | 2.4E-07 | -9.382 | -4.247 | -6.619 |
| d12r01 | 3.05E-10 | 7.95E-05 | 7.29E-07 | -9.515 | -4.100 | -6.137 |
| d12r06 | 1.33E-10 | 3.11E-05 | 1.09E-06 | -9.877 | -4.507 | -5.963 |
| d12r07 | 5.18E-10 | 2.21E-05 | 1.81E-05 | -9.286 | -4.656 | -4.742 |
| d12r08 | 3.81E-09 | 5.22E-05 | 1.76E-05 | -8.419 | -4.282 | -4.755 |
| d12r09 | 8.1E-10 | 1.97E-05 | 9.91E-06 | -9.092 | -4.707 | -5.004 |
| d13r01 | 6.14E-10 | 5.36E-05 | 1.23E-05 | -9.212 | -4.271 | -4.912 |
| d13r03 | 8.37E-10 | 1.94E-05 | 4.85E-06 | -9.077 | -4.713 | -5.314 |
| d13r05 | 1.17E-09 | 1.9E-05 | 9.38E-06 | -8.933 | -4.722 | -5.028 |
| d13r08 | 3.28E-10 | 8.45E-05 | 1.13E-06 | -9.484 | -4.073 | -5.946 |
| d13r09 | 1.23E-09 | 8.06E-05 | 3.17E-05 | -8.910 | -4.094 | -4.498 |

| | | | | | | |
|---|---|---|---|---|---|---|
| d21r02 | 2.85E-10 | 4.92E-05 | 2.01E-06 | -9.545 | -4.308 | -5.696 |
| d21r05 | 8.7E-10 | 0.000105 | 2.75E-06 | -9.061 | -3.977 | -5.561 |
| d21r06 | 1.35E-09 | 5.53E-05 | 7.86E-06 | -8.871 | -4.257 | -5.104 |
| d21r07 | 6.28E-10 | 2.93E-05 | 6.03E-06 | -9.202 | -4.533 | -5.220 |
| d21r10 | 2.84E-10 | 2.66E-05 | 7.98E-06 | -9.546 | -4.575 | -5.098 |
| d22r04 | 2.33E-10 | 2.97E-05 | 3.39E-06 | -9.633 | -4.527 | -5.470 |
| d22r08 | 4.41E-10 | 2.19E-05 | 1.86E-05 | -9.356 | -4.660 | -4.731 |
| d22r09 | 8.11E-10 | 4.31E-05 | 1.79E-05 | -9.091 | -4.366 | -4.748 |
| d22r10 | 2.22E-09 | 0.000145 | 5.09E-05 | -8.653 | -3.839 | -4.293 |

# Appendix D: FORTRAN Utility Code - T_Field.f90

```fortran
!This program reads in the calibrated transmissivity values
!from AP-088 and writes them to an MODFLOW layer-property-flow
!file.  The transmissivities are converted to conductivities
!by dividing by the aquifer thickness.
!TSL - 2-19-04
INTEGER, PARAMETER :: ncol=224,nrow=307,nlay=1
REAL, PARAMETER :: thick=7.75
REAL*8 HkHet(ncol,nrow,nlay),xdum
REAL*8 stor(ncol,nrow,nlay)
CHARACTER runnum*6,TFile*10,path*30
CHARACTER pstor(ncol,nrow,nlay)*14
DATA path/'/home3/tslowry/wipp/Tfields'/

READ(*,*)runnum
TFile=runnum//'.mod'
OPEN(50,file=TRIM(ADJUSTL(path))//'/'//TFile,status='old')
DO j=1,nrow
    READ(50,*)(HkHet(i,j,1),i=1,ncol)
END DO

OPEN(60,file='Pest4_old.lpf',status='old')
! Layer-property flow package
READ(60,*)
READ(60,*)
READ(60,*)
READ(60,*)
READ(60,*)
READ(60,*)
READ(60,*)
DO j=1,nrow
    READ(60,*)
END DO
READ(60,*)
READ(60,*)
DO j=1,nrow
    READ(60,*)
END DO
READ(60,*)
DO j=1,nrow
    READ(60,*)(stor(i,j,1),i=1,ncol)
END DO

OPEN(70,file='Pest4.lpf',status='unknown')
WRITE(70,'(a15)')'15   -888.0    0'
WRITE(70,'(a1)')'0'
WRITE(70,'(a1)')'0'
WRITE(70,'(a4)')'-1.0'
WRITE(70,'(a1)')'1'
WRITE(70,'(a1)')'0'
WRITE(70,'(a23)')"INTERNAL 1 (75e20.11) 0"
DO j=1,nrow
    WRITE(70,'(75e20.11)')(HkHet(i,j,1)/thick,i=1,ncol)
END DO
WRITE(70,'(a13)')"CONSTANT  1.0"
```

```fortran
WRITE(70,'(a13)')"CONSTANT  1.0"
WRITE(70,'(a23)')"INTERNAL 1 (125e14.4) 0"
DO j=1,nrow
    WRITE(70,'(125e14.4)')(stor(i,j,1),i=1,ncol)
END DO

OPEN(80,file='Pest4.tmp',status='old')
! Pest template file
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
DO j=1,nrow
    READ(80,'(75e20.11)')(xdum,i=1,ncol)
END DO
READ(80,*)
READ(80,*)
READ(80,*)
DO j=1,nrow
    READ(80,'(125a14)')(pstor(i,j,1),i=1,ncol)
END DO
CLOSE(80)

OPEN(90,file='Pest4_new.tmp',status='unknown')
WRITE(90,'(a5)')'ptf #'
WRITE(90,'(a15)')'15   -888.0    0'
WRITE(90,'(a1)')'0'
WRITE(90,'(a1)')'0'
WRITE(90,'(a4)')'-1.0'
WRITE(90,'(a1)')'1'
WRITE(90,'(a1)')'0'
WRITE(90,'(a23)')"INTERNAL 1 (75e20.11) 0"
DO j=1,nrow
    WRITE(90,'(75e20.11)')(HkHet(i,j,1)/thick,i=1,ncol)
END DO
WRITE(90,'(a13)')"CONSTANT  1.0"
WRITE(90,'(a13)')"CONSTANT  1.0"
WRITE(90,'(a23)')"INTERNAL 1 (125e14.4) 0"
DO j=1,nrow
    WRITE(90,'(125a14)')(pstor(i,j,1),i=1,ncol)
END DO
CLOSE(90)

STOP
END
```

## Appendix E: FORTRAN Utility Code – Get_heads.f90

```
!This program reads in a MODFLOW *.hed file from a steady-state
!simulation, extracts the heads, and writes them to a new
!MODFLOW basic input file called Pest4_new.ba6 as the starting heads.
!The new basic input file will be used for the transient
!calibration runs.
!TSL - 2-19-04

REAL, PARAMETER :: tconv=86400*365
INTEGER, PARAMETER :: nx=224,ny=307
INTEGER, PARAMETER :: numwells=13

REAL*8 heads(nx,ny)
INTEGER ix(numwells),jy(numwells),ibound(nx,ny)
CHARACTER*80 hedFile,ba6File,outFile,yinFile

!Well locations by cell indices
!Well Name   i              j
!AEC-7              195          79
!D-268              71          184
!DOE-2              120         120
!H-4b        107         188
!H-5b        152         124
!H-6b        89          122
!H-7b1              65           226
!P-14        74          153
!P-15        90          185
!WIPP-13     110         130
!WIPP-25     47          132
!WIPP-26     24          161
!WIPP-30     121         75

DATA ix/195,71,120,107,152,89,65,74,90,110,47,24,121/
DATA jy/79,184,120,188,124,122,226,153,185,130,132,161,75/

hedFile="Pest4.hed"
ba6File="Pest4.ba6"
outFile="Pest4_new.ba6"
yinFile="Y_Int.txt"

OPEN(10,file=TRIM(ADJUSTL(hedFile)),status='old')
OPEN(15,file=TRIM(ADJUSTL(ba6File)),status='old')
OPEN(20,file=TRIM(ADJUSTL(outFile)),status='unknown')
OPEN(30,file=TRIM(ADJUSTL(yinFile)),status='unknown')

!Read in heads
READ(10,*)
DO j=1,ny
    READ(10,*)(heads(i,j),i=1,nx)
END DO
CLOSE(10)

!Get starting heads

!Skip header lines
```

```
DO i=1,4
    READ(15,*)
END DO


!READ IBOUND array
DO j=1,ny
    READ(15,*)(ibound(i,j),i=1,nx)
END DO
CLOSE(15)



!Write out ba6 file
WRITE(20,'(a22)')"#WIPP Water Level Rise"
WRITE(20,'(a16)')"#PEST Simulation"
WRITE(20,'(a4)')"FREE"
WRITE(20,'(a19)')"INTERNAL 1 (free) 0"
DO j=1,ny
    WRITE(20,'(224i3)')(ibound(i,j),i=1,nx)
END DO
WRITE(20,'(a11)')"-999.000000"
WRITE(20,'(a19)')"INTERNAL 1 (free) 0"
DO j=1,ny
    WRITE(20,'(224f8.2)')(heads(i,j),i=1,nx)
END DO
CLOSE(20)

!Write out y-intercepts (starting head at each well)
DO iw=1,numwells
    WRITE(30,'(f7.2)')heads(ix(iw),jy(iw))
END DO
CLOSE(30)

STOP
END
```

# Appendix F: FORTRAN Utility Code – mfrun.f90

```fortran
!This program reads the calibrated specific storage values from the compiled
!output file stor.out, and writes them to a MODFLOW LPF input file
!for use in the final calibrated MODFLOW run.
!TSL - 2-19-04
INTEGER, PARAMETER :: ncol=224,nrow=307,nlay=1
INTEGER, PARAMETER :: ivars=2,iruns=300
REAL, PARAMETER :: thick=7.75
REAL*8 HkHet(ncol,nrow,nlay),xdum
REAL*8 stor(ncol,nrow,nlay),str(iruns,ivars)
CHARACTER runnum*6,TFile*10,path*30
CHARACTER pstor(ncol,nrow,nlay)*14
CHARACTER arun(iruns,ivars)*6,adum*4
DATA path/'/home3/tslowry/wipp/Tfields'/

!Read in conductivity field
READ(*,*)runnum
TFile=runnum//'.mod'
OPEN(50,file=TRIM(ADJUSTL(path))//'/'//TFile,status='old')
DO j=1,nrow
    READ(50,*)(HkHet(i,j,1),i=1,ncol)
END DO

!Read in storage distribution array from PEST template file
OPEN(80,file='Pest4.tmp',status='old')
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
DO j=1,nrow
    READ(80,'(75e20.11)')(xdum,i=1,ncol)
END DO
READ(80,*)
READ(80,*)
READ(80,*)
DO j=1,nrow
    READ(80,'(125a14)')(pstor(i,j,1),i=1,ncol)
END DO
CLOSE(80)

!Get storage values from Pest output
OPEN(85,file='stor.out',status='old')
ip=1
DO i=1,iruns
    READ(85,*)str(ip),adum,arun(i,ip)
    IF(arun(i,ip).eq.runnum.and.ip.eq.1)THEN
        ip=ip+1
        READ(85,*)str(ip),adum,arun(i,ip)
        EXIT
    ENDIF
END DO
```

```
CLOSE(85)



!Assign values to appropriate nodes
stor=-999
DO i=1,ncol
    DO j=1,nrow
        IF(pstor(i,j,1)(6:9).eq."str1")THEN
            stor(i,j,1)=str(1)
        ELSEIF(pstor(i,j,1)(6:9).eq."str2")THEN
            stor(i,j,1)=str(2)
        ENDIF
    END DO
END DO

!Write new *.lpf file
OPEN(70,file='Pest4.lpf',status='unknown')
WRITE(70,'(a15)')'15   -888.0   0'
WRITE(70,'(a1)')'0'
WRITE(70,'(a1)')'0'
WRITE(70,'(a4)')'-1.0'
WRITE(70,'(a1)')'1'
WRITE(70,'(a1)')'0'
WRITE(70,'(a23)')"INTERNAL 1 (75e20.11) 0"
DO j=1,nrow
    WRITE(70,'(75e20.11)')(HkHet(i,j,1)/thick,i=1,ncol)
END DO
WRITE(70,'(a13)')"CONSTANT  1.0"
WRITE(70,'(a13)')"CONSTANT  1.0"
WRITE(70,'(a23)')"INTERNAL 1 (125e14.4) 0"
DO j=1,nrow
    WRITE(70,'(125e14.4)')(stor(i,j,1),i=1,ncol)
END DO

STOP
END
```

# Appendix G: FORTRAN Utility Code – mfrch.f90

```fortran
!This program reads the calibrated recharge value from the compiled
!output file stor.out, and writes them to a MODFLOW recharge input file
!for use in the final calibrated MODFLOW run.
!TSL - 2-19-04
INTEGER, PARAMETER :: ncol=224,nrow=307
INTEGER, PARAMETER :: iruns=300
REAL*8 rech(ncol,nrow),rch
CHARACTER runnum*6,TFile*10,path*30
CHARACTER arun(iruns)*6,adum*4

!Read in run number
READ(*,*)runnum

!Read in recharge distribution array from PEST template file
OPEN(80,file='Rech.tmp',status='old')
READ(80,*)
READ(80,*)
READ(80,*)
READ(80,*)
DO j=1,nrow
    READ(80,*)(rech(i,j),i=1,ncol)
END DO
CLOSE(80)

!Get storage values from Pest output
OPEN(85,file='stor.out',status='old')
DO i=1,iruns
    READ(85,*)str,adum,arun(i)
    IF(arun(i).eq.runnum)THEN
        READ(85,*)
        READ(85,*)rch
        EXIT
    ENDIF
END DO
CLOSE(85)

!Assign values to appropriate nodes
DO i=1,ncol
    DO j=1,nrow
        IF(rech(i,j).eq.1.0)rech(i,j)=rch
    END DO
END DO

!Write new *.rch file
OPEN(70,file='Pest4.rch',status='unknown')
WRITE(70,'(a4)')'1 15'
WRITE(70,'(a3)')'1 1'
WRITE(70,'(a23)')"INTERNAL 1 (free) 0"
DO j=1,nrow
    WRITE(70,'(10e14.5)')(rech(i,j),i=1,ncol)
END DO

STOP
END
```

# Appendix H: FORTRAN Utility Code – exhdsdrw_scratch.f90

```fortran
!This program reads in a MODFLOW *.hed and *.drw file and extracts the
!heads and drawdowns at selected nodes in the domain.  The MODFLOW
!output files must be located in the scratch/temp/pest directory of
!the executing slave computer.  It then writes the output to
!to an output file called wellhdsdrw.txt.  It will also calculate
!the root mean squared error between the simulated drawdowns and the
!observed drawdowns.  This program is called from the script,
!Pest4_run.sh, which executes MODFLOW within each PPEST calibration.
!TSL - 2-19-04

REAL, PARAMETER :: tconv=86400*365
INTEGER, PARAMETER :: nx=224,ny=307,nper=27
INTEGER, PARAMETER :: numwells=13

REAL*8 heads(nx,ny,nper),drw(nx,ny,nper)
REAL*8 sheads(numwells)
REAL*8 time(nper)
REAL slp(numwells),yint(numwells)
REAL resid(numwells,nper)
INTEGER ix(numwells),jy(numwells)
CHARACTER*7 wellname(numwells)
CHARACTER*80 hedFile,drwFile,ba6File,outFile,RSEFile,yinFile

!Well locations by cell indices
!Well Name  i            j
!AEC-7      195          79
!D-268      71           184
!DOE-2      120          120
!H-4b       107          188
!H-5b       152          124
!H-6b       89           122
!H-7b1      65           226
!P-14       74           153
!P-15       90           185
!WIPP-13    110          130
!WIPP-25    47           132
!WIPP-26    24           161
!WIPP-30    121          75

!Slopes from Data
! AEC-7     0.113568t + 930.301863
! D-268     0.126283t + 913.664946
! DOE-2     0.014003t + 936.372373
! H-4b      0.198349t + 910.989057
! H-5b      0.175516t + 931.998909
! H-6b      0.201408t + 929.570654
! H-7b      0.072852t + 911.916259
! P-14      0.229142t + 924.346769
! P-15      0.194967t + 914.927600
! Wipp-13   0.097052t + 934.789560
! Wipp-25   0.227839t + 928.118998
! Wipp-26   0.148470t + 917.613523
! WIPP-30   0.184103t + 932.778492

DATA ix/195,71,120,107,152,89,65,74,90,110,47,24,121/
```

```fortran
DATA jy/79,184,120,188,124,122,226,153,185,130,132,161,75/
DATA wellname/"AEC-7","D-268","DOE-2","H-4b","H-5b","H-6b",&
      "H-7b1","P-14","P-15","WIPP-13","WIPP-25","WIPP-26","WIPP-30"/
DATA slp/0.113568,0.126283,0.014003,0.198349,0.175516,0.201408,&
      0.072852,0.229142,0.194967,0.097052,0.227839,0.148470,0.184103/

hedFile="/home/scratch/temp/pest/Pest4.hed"
drwFile="/home/scratch/temp/pest/Pest4.drw"
ba6File="/home/scratch/temp/pest/Pest4.ba6"
outFile="wellhdsdrw.txt"
RSEFile="RSE.txt"
yinFile="../../Y_Int.txt"

OPEN(10,file=TRIM(ADJUSTL(hedFile)),status='old')
OPEN(15,file=TRIM(ADJUSTL(drwFile)),status='old')
OPEN(20,file=TRIM(ADJUSTL(outFile)),status='unknown')

DO ip=1,nper
    !Read in heads
    READ(10,*)i1,i2,time(ip)
    DO j=1,ny
        READ(10,*)(heads(i,j,ip),i=1,nx)
    END DO
END DO
CLOSE(10)

DO ip=1,nper
    !Read in drawdowns
    READ(15,*)
    DO j=1,ny
        READ(15,*)(drw(i,j,ip),i=1,nx)
    END DO
END DO
CLOSE(15)

!Output results
WRITE(20,'(14a10)')"Time (sec)",(wellname(iw),iw=1,numwells)
DO ip=1,nper

WRITE(20,'(e10.5,13f10.4)')time(ip),(heads(ix(iw),jy(iw),ip),iw=1,numwells)
END DO
WRITE(20,*)
DO ip=1,nper
    WRITE(20,'(e10.5,13f10.4)')time(ip),(drw(ix(iw),jy(iw),ip),iw=1,numwells)
END DO

CLOSE(20)

!Get starting heads
OPEN(30,file=TRIM(ADJUSTL(ba6file)),status='old')

!Skip header lines
DO i=1,4
      READ(30,*)
END DO

!Skip IBOUND array and starting head headers
```

```fortran
DO j=1,ny+2
      READ(30,*)
END DO

!Read in heads
DO j=1,ny
      READ(30,*)(heads(i,j,1),i=1,nx)
END DO
CLOSE(30)

!Get heads at each well
DO iw=1,numwells
    sheads(iw)=heads(ix(iw),jy(iw),1)
END DO

!Get y-intercept values (starting heads at each well)
OPEN(35,file=yinFile,status='old')
DO iw=1,numwells
    READ(35,*)yint(iw)
END DO
CLOSE(35)

!Calculate differences in drawdowns
rsum=0
DO ip=1,nper
    DO iw=1,numwells
        ddown=sheads(iw)-(slp(iw)*time(ip)/tconv+yint(iw))
        resid(iw,ip)=(ddown-drw(ix(iw),jy(iw),ip))*(ddown-
drw(ix(iw),jy(iw),ip))
        rsum=rsum+resid(iw,ip)
    END DO
END DO

RSE=rsum/(iw*ip)

OPEN(40,file=RSEFile,status='unknown')
WRITE(40,*)RSE
CLOSE(40)

STOP
END
```

# Appendix I: FORTRAN Utility Code – cut.f90

```fortran
!This program is run after the final MF2K calibrated run.  It succesively
!goes to each T-field directory and reads the output from exhdsdrw, called
!wellhdsdrw.txt.  It will read the output for all T-fields and then
!recompile it into a single file call wellobs.txt, located in the base
!simulation directory.  wellobs.txt is suitable for import to MS Excel for
!visualization.
INTEGER, PARAMETER :: numwells=13,nper=27,nobs=100
REAL*8 time(nper,nobs),heads(numwells,nper,nobs),drw(numwells,nper,nobs)
CHARACTER*10 head1,wellname(numwells,nobs)
CHARACTER file1*100,trun(nobs)*6

OPEN(10,file='Goodruns.txt',status='old')

DO io=1,nobs
   READ(10,*)trun(io)
   print *,trun(io),io
   file1='/home3/tslowry/wipp/wtrlvl/'//trun(io)//'/wellhdsdrw.txt'
   OPEN(20,file=TRIM(ADJUSTL(file1)),status='old')
   READ(20,'(14a10)')head1,(wellname(iw,io),iw=1,numwells)
   DO ip=1,nper
      READ(20,'(e10.5,13f10.4)')time(ip,io),(heads(iw,ip,io),iw=1,numwells)
   END DO
   READ(20,*)
   DO ip=1,nper
      READ(20,'(e10.5,13f10.4)')tdum,(drw(iw,ip,io),iw=1,numwells)
   END DO
   CLOSE(20)
END DO
CLOSE(10)

OPEN(30,file='wellobs.txt',status='unknown')

DO iw=1,numwells
   WRITE(30,'(a10)')wellname(iw)
   WRITE(30,'(a10,100a10)')"Time (sec)",(trun(io),io=1,nobs)
   WRITE(30,'(101a10)')("     0       ",io=1,nobs+1)
   DO ip=1,nper
      WRITE(30,'(e10.5,100f10.4)')time(ip,1),(drw(iw,ip,io),io=1,nobs)
   END DO
   WRITE(30,*)
END DO

STOP
END
```

# Appendix J: Linux Shell Script – Ppest_run.sh

```bash
#!/bin/bash
RUNS=`cat Goodruns.txt`
THISDIR=`pwd`

#This script controls the entire PPEST run sequence across
#all T-fields.

for Runs in $RUNS
do
#Clean up files from last run
    cd ppest1
    clean.sh
    cd $THISDIR

#Generate new *.lpf and *.tmp files
    echo $Runs | T_Field
    rm Pest4.tmp
    mv Pest4_new.tmp Pest4.tmp

#Run steady-state model
    CQue mf_steady.sh

#Wait for model run to complete
    sleep 60s
    rm 04*.out

#Extract new starting heads to new *.ba6 file
    Get_heads
    mv Pest4.ba6 Pest4_old.ba6
    mv Pest4_new.ba6 Pest4.ba6

#Setup and run PEST
    cd ppest1
    runpest.sh
    sleep 120s
    SlavesFree=`CFree | wc -1 | awk '{print $1}'`
    while [ $SlavesFree -lt  2 ]
    do
      sleep 150s
      SlavesFree=`CFree | wc -1 | awk '{print $1}'`
    done
    cd $THISDIR

#Get storage coefficients from PEST output file and write to new file
    echo `tail -31 ./ppest1/Pest4.sen | grep -i str1 | awk '{print $3}'` "
str1 " $Runs >> stor.out
    echo `tail -31 ./ppest1/Pest4.sen | grep -i str2 | awk '{print $3}'` "
str2 " $Runs >> stor.out
    echo `tail -31 ./ppest1/Pest4.sen | grep -i rch1 | awk '{print $3}'` "
rch1 " $Runs >> stor.out
    rm /home1/usr/bin/Que/*.*
done
#Run MODFLOW for each T-field using new storage coefficients
mfrun.sh
```

# Appendix K:  Linux Shell Script – clean.sh

```
rm -rf slave*
rm -f 04*.out
rm -f Pest4*.*
rm -f jacob.*
rm -f pest.*
rm -f pmaster.cque

#This script removes the directories, output, and temporary files
#from the previous PPEST simulation.
```

# Appendix L:  Linux Shell Script – mf_steady.sh

```
#!/bin/bash
#This script executes MF2K in steady-state mode
#with no recharge.

mf Pest4_steady.nam
```

# Appendix M: Linux Shell Script – runpest.sh

```
#!/bin/bash

#This script controls the setup sequence for the PPEST
#run.

setup.sh
TOPDIR=`pwd`
SLAVES=`ls -d slave* | grep -v slave1`

for Slave in $SLAVES
do
    cd $Slave
    CQue pslave.cque
    cd $TOPDIR
done
CQue pmaster.cque
```

# Appendix N: Linux Shell Script – setup.sh

```
#!/bin/bash
SLAVES="slave1 slave2 slave3 slave4 slave5 slave6 slave7 slave8 slave9
slave10 slave11 slave12 slave13 slave14"
THISDIR=`pwd`
FILES=`cat ../filelist.master`

#This script creates the slave directories and populates the directories
#with the appropriate files, listed in filelist.slave.

for File in $FILES
do
    cp ../$File $THISDIR
done
for Slave in $SLAVES
do
    mkdir $THISDIR/$Slave
    FILES=`cat ../filelist.slave`
    for File in $FILES
    do
        cp ../$File $THISDIR/$Slave
    done
done
cd $THISDIR
```

## Appendix O: Linux Shell Script – pslave.cque

```
#!/bin/bash
THISDIR=`pwd`
FILES=`cat ../../filelist.modflow`
cd /home/scratch
mkdir temp
cd temp
mkdir pest
cd $THISDIR
for File in $FILES
do
    cp ../../$File /home/scratch/temp/pest/
done
pslave < Pest4_run.in
rm -rf /home/scratch/temp
```

## Appendix P: Linux Shell Script – pmaster.cque

```
#!/bin/bash
MASTERDIR=`pwd`
FILES=`cat ../filelist.modflow`
cd /home/scratch
mkdir temp
cd temp
mkdir pest
cd $MASTERDIR/slave1
for File in $FILES
do
     cp ../../$File /home/scratch/temp/pest/
done
pslave < Pest4_run.in &> slave1.out &
cd $MASTERDIR
ppest Pest4
wait
rm -rf /home/scratch/temp
```

# Appendix Q: Linux Shell Script – mfrun.sh

```
#!/bin/sh
RUNS=`cat Goodruns.txt`
THISDIR=`pwd`

#This script sets up and runs the final calibrated MODFLOW
#run.  This occurs for all T-fields after all the PPEST
#calibrations are complete.

for Runs in $RUNS
do

#Set-up *.lpf file with calibrated storage values
    echo $Runs | mfrun

#Set-up *.rch file with calibrated recharge value
    echo $Runs | mfrch

#Make new directory and copy files
    mkdir $Runs
    cp Pest4.ba6 $Runs
    cp Pest4.lpf $Runs
    cp Pest4.oc $Runs
    cp Pest4.lmg $Runs
    cp Pest4_home.nam $Runs
    cp Pest4_steady.nam $Runs
    cp Pest4.dis $Runs
    cp Pest4_steady.dis $Runs
    cp Pest4.rch $Runs

#Create new que file
    runFile=$Runs.sh
    echo '#!/bin/sh' > ${runFile}
    echo ' ' >> ${runFile}
    echo '# Run steady-state model' >> ${runFile}
    echo 'mf Pest4_steady.nam' >> ${runFile}
    echo '# Re-write new starting heads' >> ${runFile}
    echo 'Get_heads' >> ${runFile}
    echo 'mv Pest4.ba6 Pest4_old.ba6' >> ${runFile}
    echo 'mv Pest4_new.ba6 Pest4.ba6' >> ${runFile}
    echo '# Run transient model' >> ${runFile}
    echo 'mf Pest4_home.nam' >> ${runFile}
    echo '# Get heads and drawdowns at each well location' >> ${runFile}
    echo 'exhdsdrw' >> ${runFile}
    mv $runFile $Runs
    cd $Runs
    chmod u+x $runFile

#Que run file
    CQue $runFile
    cd $THISDIR
done
```