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Sandia National Laboratories

Carlsbad Programs Group

Waste Isolation Pilot Plant

Task 3 of AP-114
Evaluation of Alternatives to the Southwestern No-Flow Boundary Condition
(AP-114: Analysis Plan for Evaluation and Recalibration of Culebra Transmissivity Fields)

Revision 0

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Introduction

The Waste Isolation Pilot Plant (WIPP) is located in southeastern New Mexico and has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth at Title 40 of the Code of Federal Regulations. The DOE demonstrates compliance with the containment requirements in the regulations by means of performance assessment (PA) calculations.

PA calculations were included in DOE's 1996 WIPP Compliance Certification Application (CCA, U.S. DOE, 1996), and in a subsequent Performance Assessment Verification Test (PAVT, MacKinnon and Freeze, 1997a, 1997b, 1997c). Based, in part, on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the containment criteria in the regulations and was approved for disposal of transuranic waste in May 1998. PA calculations were also an integral part of DOE's 2004 WIPP Compliance Recertification Application (CRA-2004, U.S. DOE, 2004). The CRA-2004 (referred to as 'CRA' is this document) is currently being reviewed by the EPA.

WIPP PA calculations estimate the probability and consequence of radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. For the purposes of WIPP PA, the accessible environment is considered to be the ground surface and/or the lateral limits of subsurface within the WIPP land withdrawal boundary (LWB). Among other release mechanisms, WIPP PA assesses the probability and consequence of radionuclide releases from the repository to the accessible environment due to the movement of radionuclide-contaminated brines moving up a (sealed) shaft or oil/gas exploration borehole, and migrating laterally to the LWB in the Culebra Dolomite Member of the Rustler Formation.

Background

The WIPP repository is located approximately 26 miles (42 kilometers) southeast of Carlsbad, New Mexico. The disposal horizon of the WIPP is approximately 2,150 feet (655 meters) below the ground surface in the Salado Formation of the Delaware Basin. The Salado is regionally extensive, consisting predominantly of halite, a low-permeability evaporite (Powers et al., 1978).

The Rustler Formation is located above the Salado and is of particular importance in estimating the potential for radionuclide releases from the WIPP because it contains the most transmissive units above the repository. In the vicinity of the WIPP, the Rustler consists of evaporite units interbedded with carbonates and siliciclastic units (Vine, 1963; Holt and Powers, 1988). The Culebra Dolomite Member has been identified as the most transmissive unit in the Rustler and consequently the most likely pathway for subsurface transport of radionuclides.

The Culebra model domain is oriented with the compass directions and is 30.6 km in the north-south direction and 22.3 km in the east-west direction. The corners of the Culebra model domain are given in Table 1. These coordinates define the center of 100X100-m^2 model cells at the four corners of the model domain.

Table 1. The UTM coordinates of the corners of the numerical model domain.

Domain Corner	X Coordinate (meters)	Y Coordinate (meters)
Northeast	624,000	3,597,100
Northwest	601,700	3,597,100
Southeast	624,000	3,566,500
Southwest	601,700	3,566,500

The WIPP land-withdrawal boundary, or the "WIPP site boundary", is an approximately 6.4 X 6.4 km area near the center of the model domain. The boundary of the WIPP site is defined by the coordinates shown in Table 2. For the calculations described in this report, the coordinates shown in Table 2 are used to determine when and where the particle tracks leave the WIPP site.

Table 2. The UTM coordinates of the WIPP site boundary.

WIPP Site 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

To estimate radionuclide transport through the Culebra, McKenna and Hart (2003a) constructed calibrated geostatistical realizations of Culebra hydraulic transmissivity fields (T-fields) for the CRA. The calibrated T-fields are a function of base T-fields, head measurements from both steady-state and transient responses to various hydraulic tests over a period of 11 years, and prescribed initial and boundary conditions, all briefly described below.

Base T-fields (Holt and Yarbrough, 2003) are based on multiple regression and therefore only fit the transmissivity measurements in the mean sense. Also reflected in the base T-fields are a high-transmissivity zone down the western side of the model connecting the northern and southern boundaries and a low-transmissivity zone along the east side of the domain.

The 2000 steady-state head data were compiled by Beauheim (2002). For the 2000 time period, there are a total of 35 well locations with steady-state head measurements. The wells, their locations, and the heads measured in the 2000 time period are given in Table 3. Responses to seven different hydraulic tests are employed in the transient portion of the calibration (Table 4). Details on the original sources of the data shown in Table 4 are given in Beauheim and Fox (2003). Hydraulic responses for each of the seven tests were monitored in three to ten different observation wells depending on the hydraulic test.

The boundary and initial conditions used in the CRA calculations are described fully in McKenna and Hart (2003a). The estimation of the initial and boundary heads is done by kriging of head measurements within the model domain. The prescribed boundary conditions used in the CRA consist of a no-flow boundary along Nash Draw and fixed-head boundaries estimated on the rest of the model domain boundary based on kriging results.

Table 3. Well names and locations of the 35 steady-state data obtained during the 2000 measurement period and used in the simultaneous steady-state and transient calibrations.

Measurement Number	Well Name	Easting (X) Coordinate (m)	Easting (Y) Coordinate (m)	2000 Measured Head (m)
1	AEC-7	621126	3589381	933.19
2	DOE-1	615203	3580333	916.55
3	DOE-2	613683	3585294	940.03
4	ERDA-9	613696	3581958	921.59
5	H-1	613423	3581684	927.19
6	H-2b2	612661	3581649	926.62
7	H-3b2	613701	3580906	917.16
8	H-4b	612380	3578483	915.55
9	H-5b	616872	3584801	936.26
10	H-6b	610594	3585008	934.20
11	H-7b1	608124	3574648	913.86
12	H-11b4	615301	3579131	915.47
13	H-12	617023	3575452	914.66
14	H-14	612341	3580354	920.24
15	H-15	615315	3581859	919.87
16	H-17	615718	3577513	915.37
17	H-18	612264	3583166	937.22
18	H-19b0	614514	3580716	917.13
19	P-17	613926	3577466	915.20
20	WIPP-12	613710	3583524	935.30
21	WIPP-13	612644	3584247	935.17
22	WIPP-18	613735	3583179	936.08
23	WIPP-19	613739	3582782	932.66
24	WIPP-21	613743	3582319	927.00
25	WIPP-22	613739	3582653	930.96
26	WIPP-25	606385	3584028	932.70
27	WIPP-26	604014	3581162	921.06
28	WIPP-30	613721	3589701	936.88
29	WQSP-1	612561	3583427	935.64
30	WQSP-2	613776	3583973	938.82
31	WQSP-3	614686	3583518	935.89
32	WQSP-4	614728	3580766	917.49
33	WQSP-5	613668	3580353	917.22
34	WQSP-6	612605	3580736	920.02
35	H-9b	613989	3568261	911.57

Table 4. Transient hydraulic test and observation wells for the drawdown data.

Stress Point	Observation Well	Observation Start	Observation End	Observation Type
H-3b2	DOE-1	10/15/1985	3/18/1986	Drawdown
	H-1	10/15/1985	4/14/1986	Drawdown
	H-2b2	10/15/1985	4/2/1986	Drawdown
	H-11b1	10/15/1985	4/21/1986	Drawdown
WIPP-13	DOE-2	1/12/1987	5/15/1987	Drawdown
	H-2b2	1/12/1987	5/15/1987	Drawdown
	H-6b	1/12/1987	5/15/1987	Drawdown
	P-14	1/12/1987	5/15/1987	Drawdown
	WIPP-12	1/12/1987	5/15/1987	Drawdown
	WIPP-18	1/12/1987	5/15/1987	Drawdown
	WIPP-19	1/12/1987	5/15/1987	Drawdown
	WIPP-25	1/12/1987	4/2/1987	Drawdown
	WIPP-30	1/12/1987	5/15/1987	Drawdown
P-14	D-268	2/14/1989	3/7/1989	Drawdown
	H-6b	2/14/1989	3/10/1989	Drawdown
	H-18	2/14/1989	3/10/1989	Drawdown
	WIPP-25	2/14/1989	3/7/1989	Drawdown
	WIPP-26	2/14/1989	3/7/1989	Drawdown
H-11b1	H-4b	2/7/1996	12/11/1996	Drawdown
	H-12	2/6/1996	12/10/1996	Drawdown
	H-17	2/6/1986	12/10/1996	Drawdown
	P-17	2/7/1996	12/10/1996	Drawdown
H-19b0	DOE-1	12/15/1995	12/10/1996	Drawdown
	ERDA-9	12/15/1995	12/10/1996	Drawdown
	H-1	12/15/1995	12/10/1996	Drawdown
	H-14	2/7/1996	12/10/1996	Drawdown
	H-15	12/12/1995	12/10/1996	Drawdown
	H-2b2	2/7/1996	12/10/1996	Drawdown
	H-3b2	12/15/1995	12/10/1996	Drawdown
	WIPP-21	1/18/1996	12/9/1996	Drawdown
	WQSP-4	1/1/1996	12/10/1996	Drawdown
	WQSP-5	1/18/1996	12/10/1996	Drawdown
WQSP-1	H-18	1/25/1996	2/20/1996	Drawdown
	WIPP-13	1/25/1996	2/20/1996	Drawdown
	WQSP-3	1/15/1996	2/20/1996	Zero Response
WQSP-2	DOE-2	2/20/1996	3/28/1996	Drawdown
	H-18	2/20/1996	3/28/1996	Drawdown
	WIPP-13	2/20/1996	3/28/1996	Drawdown
	WQSP-1	2/20/1996	3/24/1996	Drawdown
	WQSP-3	2/20/1996	3/24/1996	Zero Response

Purpose

Previous modeling results (Corbet and Knupp, 1996) and water-level measurements show a groundwater divide in the Culebra southwest of the WIPP site. Calibration of T-fields for the CRA are based on boundary conditions that represent the groundwater divide as a flow line that extended southeast from the potash tailings pond in Nash Draw. This flow line continues south on the west side of the high-transmissivity boundary (Figure 1). An alternate conceptualization of this groundwater divide is a groundwater mound resulting from infiltration into the Culebra in areas where it is unconfined. This study introduces two alternative conceptualizations of the groundwater divide. The first alternate conceptualization uses fixed heads along the boundary of Nash Draw (which coincides with the margin of upper Salado dissolution) in the southwest region; the second conceptualization moves the boundary to the west in order to include recharge where the Culebra is unconfined. The purpose of this task is to assess the influence of boundary conditions in the southwest region of the WIPP model domain using the two alternate boundary conditions.

This analysis report describes results of Task 3 of AP-114, "Analysis Plan for Evaluation and Recalibration of Culebra Transmissivity Fields" (Beauheim, 2004a). Task 3 was developed to explore the effect of alternate boundary conditions of the southwest model domain. This document describes the methods and results of evaluating two alternatives to the southwestern no-flow boundary conditions used in the CRA. The evaluation compares T-field calibration, particle tracking, and travel times resulting from the southwest boundary used in the CRA with two alternative SW boundary conditions.

Results from AP-114 Task 1B and Task 1D were not used in this Task 3 study. Task 1B identifies possible areas of recharge to the Culebra based on photos and field surveys of areas west and south of the WIPP site. The study is currently underway and results will be added to the continuing Task 3 study once Task 1B is complete. Task 1D collects current and historic information on water levels and fluid density in potash tailings ponds within the Culebra modeling domain. No changes to the head at the tailings pond on the western model boundary were made to simplify comparison of the results of this study to the CRA results.

Model Approach

For each change in boundary conditions, stochastic inverse calibration of the Culebra T-fields to both steady-state heads obtained during calendar year 2000 and to a series of transient responses to various hydraulic tests over a period of 11 years is carried out. MODFLOW 2000, v. 1.6 (Harbaugh et al., 2000) and PEST, v. 5.51 (Doherty, 2002) are used for the calibration. The final calibrated T-field is used as the basis for the calculation of travel time from a point above the center of the repository to the WIPP boundary. Travel time is calculated using DTRKMF v 1.0 (Rudeen, 2003). T-field calibration and travel times are calculated using 15 realizations of the base T-field. The CRA calibrations of three of these base T-fields represent the 5^{th}, 50^{th}, and 95^{th} ranking travel times for the CRA calculations. The remaining 12 T-fields cover a variety of calibration responses in the CRA calculations (Table 6). Results from the alternate southwest boundary conditions are then compared to results from the CRA calculations.

The computational cost of calibrating to the multiple transient events is significant. Due to these long run times, two separate parallel PC clusters were employed. Each of these clusters consists of 16 computational nodes. One cluster is located in Albuquerque and the other is in the Sandia office in Carlsbad. Both clusters use the Linux operating system. Average calibration time for one T-field to all transient events is approximately 36 hours. All T-field calibrations and particle-tracking simulations are carried out by use of the Arcons – Archived Run-CONtrol System. Run control scripts written for this task specify the checkout of files from the CVS repository, execution of simulations, and check in of files. The project directory for this task is located in /h/WIPPcvs/AP114/Task3 on lylin102, the Linux cluster in Albuquerque. Details of run control used in this task can be found in Appendix A. Run control files are detailed in Appendix B.

BOUNDARY CONDITIONS

Boundary conditions used in this model are either fixed-head or no-flow boundaries. Fixed-head boundaries are estimated from kriging based on the head measurements within the model domain. The measured heads from the 2000 data set are used in this model. Initial heads are a result of kriged residuals added back to a bivariate trend model. The initial head field was provided by McKenna and Hart (2003b). The initial heads estimated at the constant-head boundary locations are held fixed throughout the groundwater flow modeling. The current southwest boundary is defined as a no-flow boundary, representing a flow line.

Within MODFLOW 2000, cells are defined as active, inactive, or constant-head and are controlled by an array of integers called the IBND array. No-flow boundary cells are assigned an IBND value of "0", which defines them as inactive. Fixed-head cells are assigned an IBND value of "-1", setting each head constant. Active cells receive an IBND value of "1".

Alternate conceptualizations of the southwest groundwater divide include:

1. **Alternate SW boundary #1 (SW1):** Reposition the CRA southwestern boundary to coincide (roughly) with the edge of Nash Draw, which reflects the margin of upper Salado dissolution and demarcates the area where the Culebra is confined (as assumed by the model) from where it may potentially be unconfined, and convert it from a no-flow boundary to a fixed-head boundary. This alternate boundary extends from the potash tailings pond in Nash Draw to WIPP-26 to H-9.

2. **Alternate SW boundary #2 (SW2):** Reposition the CRA southwestern no-flow boundary in order to be able to include recharge where the Culebra is unconfined. This study is limited to a modification of the boundary location; recharge will be added at a later date. This alternate boundary extends from the southern extent of a series of connected potash tailings and brine ponds in Nash Draw through USGS-4 to the south boundary. The boundary is represented by a fixed-head boundary along the ponds and a no-flow boundary from the southern extent of the ponds along (or near) a Culebra topographic high through USGS-4 to the south model boundary.

Changes to the southwest boundary condition are listed in Table 5. Figure 1 illustrates the alternate boundary condition locations. Figure 2 shows the boundary conditions in relation to the top elevation of the Culebra and the initial head field.

Table 5. Alternate southwest boundary locations.

	Description, location in UTM, m
Alternate SW boundary #1 (SW1)	From potash tailings pond in Nash Draw (601700, 3581300) through WIPP-26 (604014, 3581162) and H-9 (613989, 3568261), to the south boundary (615351, 3566500)
Alternate SW boundary #2 (SW2)	From potash tailings pond in Nash Draw (601700, 3581300) to the southern extent of ponds (601700, 3577400), through USGS-4 (605841, 3569887), to the south boundary (607708, 3566500)

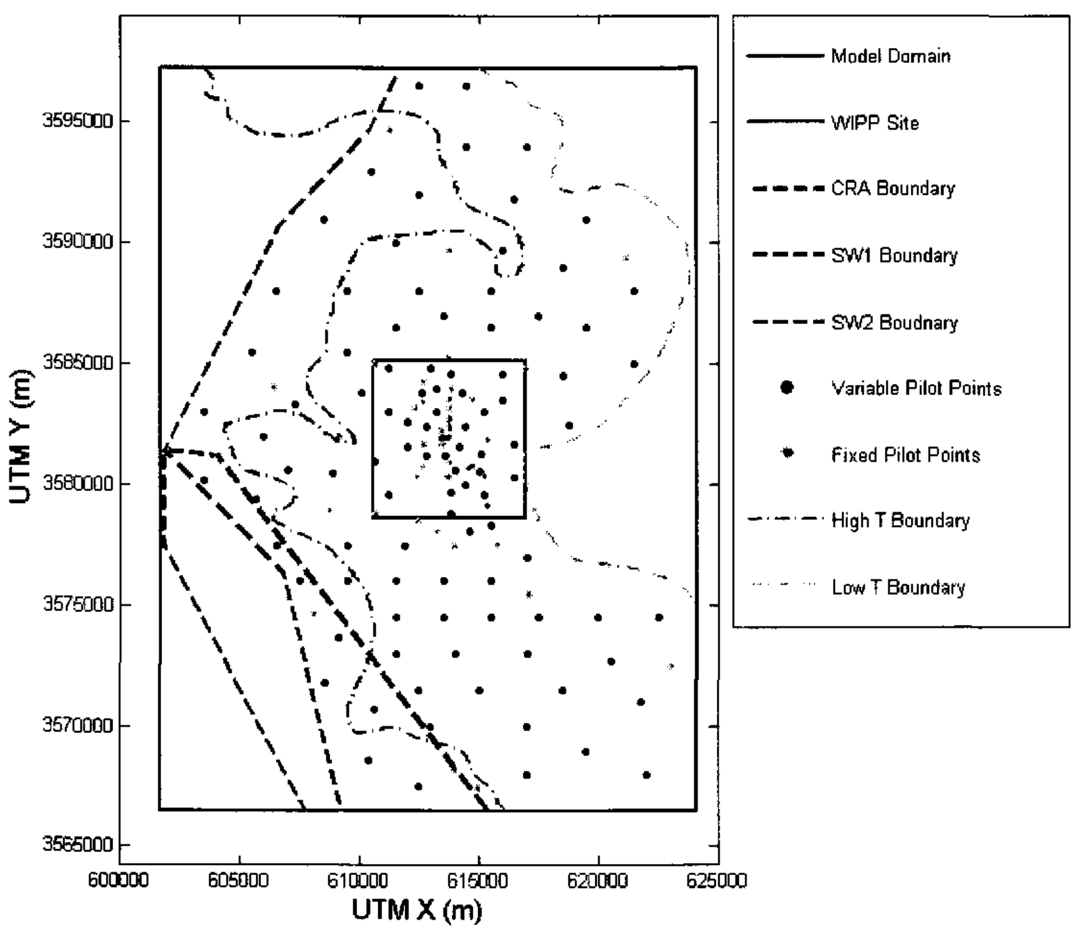

Figure 1. Locations of CRA SW boundary, SW boundary alternative #1 (SW1), SW boundary alternative #2 (SW2), pilot points (fixed and variable), and high- and low-T boundaries with respect to the WIPP site.

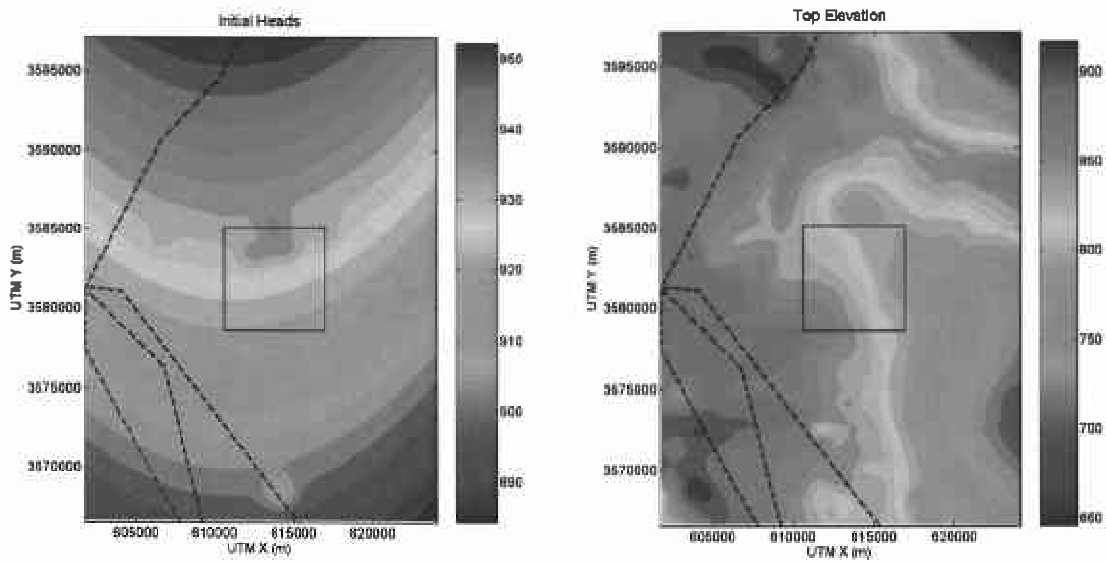

Figure 2. SW boundary (Original, SW1, and SW2) over initial head field and Culebra top elevation.

Pilot Point Calibration

Calibration of T-fields is carried out in the same manner as the calibration described by McKenna and Hart (2003a). The calibration creates a residual field that when added to the base T-field reproduces the measured transmissivity values at 43 measurement locations. Using PEST, 99 variable pilot points (Figure 1) are adjusted to update the residual field such that when the updated residual field is added to the base T-field, the fit to the observed head and drawdown data is improved relative to previous iterations of the model. The objective function (phi) to be minimized by PEST is the weighted sum of the squared errors (SSE) between the observed heads/drawdowns and the model-predicted heads/drawdowns. For the transient calibration process, a single steady-state solution is calculated for each iteration and then multiple calls to **MF2K** are made. This combined set of steady-state and transient runs allows for the simultaneous calibration of the T-field to the steady-state heads observed in 2000 as well as to multiple pumping tests.

Particle Tracking

Particle-tracking calculations use a single particle starting from the center of the repository footprint (location X = 613602 meters, Y = 3581425 meters), tracking the particle until it exits the WIPP site boundary. The starting location is the same location used to start particles in the CCA calculations. The coordinates of the corner points defining the WIPP site boundary are given in Table 2. Particle-tracking calculations use a constant porosity of 0.16 (McKenna and Hart, 2003b).

Transmissivity Fields

Calibrations are carried out for the T-fields with the 5th, 50th and 95th ranking travel time under CRA conditions along with 12 additional realizations of the base T-field used in the CRA. The

12 additional fields represent a range of T-fields based on calibration statistics (Beauheim, 2004b). These statistics include pilot point bounds and the objective function (phi) (Table 6). For the high- and low-transmissivity zones on the western and eastern sides of the model domain, respectively, the bounds on the possible pilot point value changes are set to –1.0 and +1.0 $\log_{10}$ T, and for the middle transmissivity zone, the bounds are set to –3.0 and +3.0 $\log_{10}$ T. The objective function to be minimized by PEST is the weighted SSE between the observed heads/drawdowns and the model-predicted heads/drawdowns. T-fields are named d##r## and are based on the original base T-field naming convention of Holt and Yarbrough (2002).

Table 6. T-fields.

T-Field		Description
5th, 50th, 95th ranking travel time	d08r01	5% ranking travel time to WIPP boundary
	d12r07	50% ranking travel time to WIPP boundary
	d10r09	95% ranking travel time to WIPP boundary
Additional 12 T-fields	d01r07	3rd most pilot points hitting bounds
	d02r02	most pilot points hitting bounds (total and lower)
	d03r03	Worst field (transient and total phi)
	d04r02	4th most pilot points hitting bounds
	d06r07	Best combined phi
	d07r06	2nd worst field (total phi)
	d09r05	Good field with many pilot points hitting bounds
	d11r08	Best transient phi
	d12r06	Best steady-state phi
	d13r08	Good field; most pilot points hitting upper bound
	d21r02	2nd most pilot points hitting bound
	d22r04	Worst steady-state phi

Results

Of the 100 T-fields used in the CRA calculations, 15 were selected to analyze how changes to the SW boundary condition impact pilot point calibration, particle tracking, and travel time. While the 15 T-fields chosen are intended to span the range of travel times calculated in the CRA simulations, they are not guaranteed to span the range of travel times that calibration of all 100 base T-fields using alternate SW boundary conditions would produce. While results are useful to check the calibration, particle tracking, and travel time dependency on the SW boundary condition, the subset might not represent a full investigation where an increased number of base T-fields are used.

Pilot Point Calibration

Pilot point calibration minimizes the weighted SSE between the observed heads/drawdowns and the model-predicted heads/drawdowns. Based on the initial base T-field and boundary conditions used, the resulting calibrated T-fields can vary greatly. Figure 3 details the differences in d08r01-based T-fields calibrated using the CRA, SW1, and SW2 boundary conditions. As compared to the CRA, the SW2 boundary condition produces more area of high transmissivity in the SW region of the modeling domain. A lesser change is noted in the T-field calibrated using the SW1 boundary condition.

A graphical representation of the difference in pilot point calibration between the CRA and the two alternate boundary conditions is shown in Figure 4 and Figure 5. These plots show the range and mean change in pilot point calibration for all 99 pilot points across each of the 15 T-fields. While changes to the SW boundary condition create a wide range of changes to pilot point calibration, the mean change to pilot point calibration remains small. The largest changes to pilot point calibration occur south of the WIPP site, namely with the SW2 boundary condition changes (Figure 6).

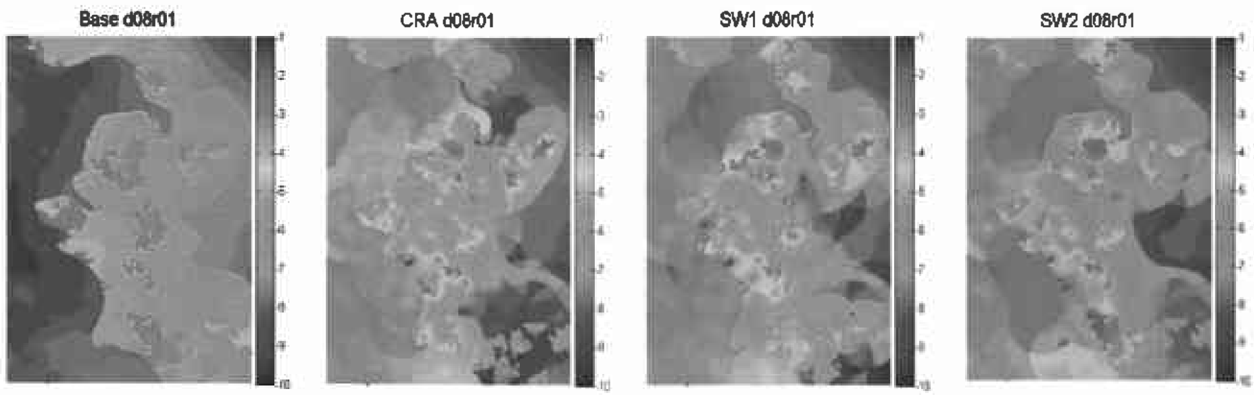

Figure 3. Base T-field and calibrated T-field for CRA, SW1, and SW2 boundary conditions using d08r01 ($log_{10}(T)$).

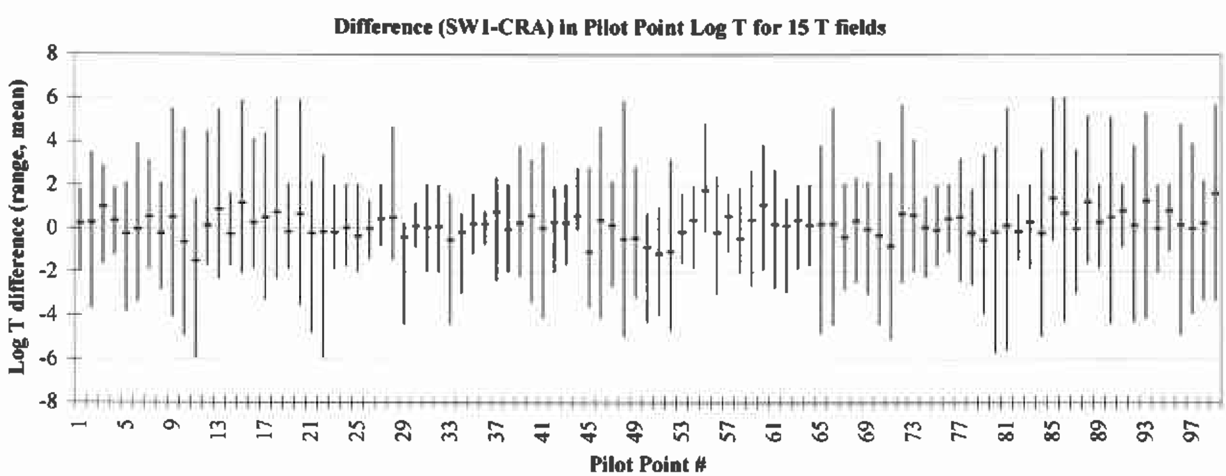

Figure 4. Difference between SW1 and CRA pilot point calibrations for all 15 T-fields. Range (blue line) and mean (black dash) calculated for each pilot point. In general, pilot points are numbered in increasing order from south to north.

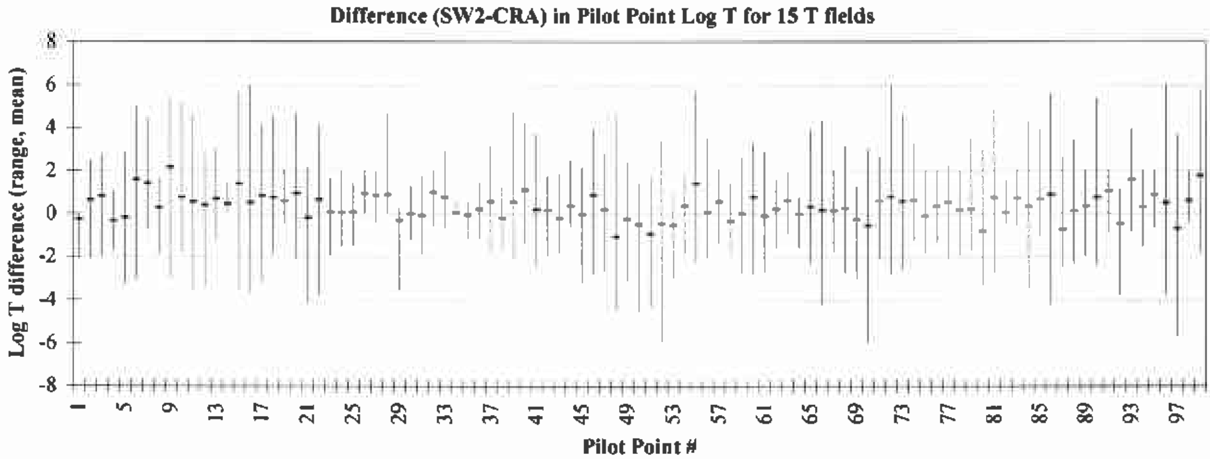

Figure 5. Difference between SW2 and CRA pilot point calibrations for all 15 T-fields. Range (blue line) and mean (black dash) calculated for each pilot point. In general, pilot points are numbered in increasing order from south to north.

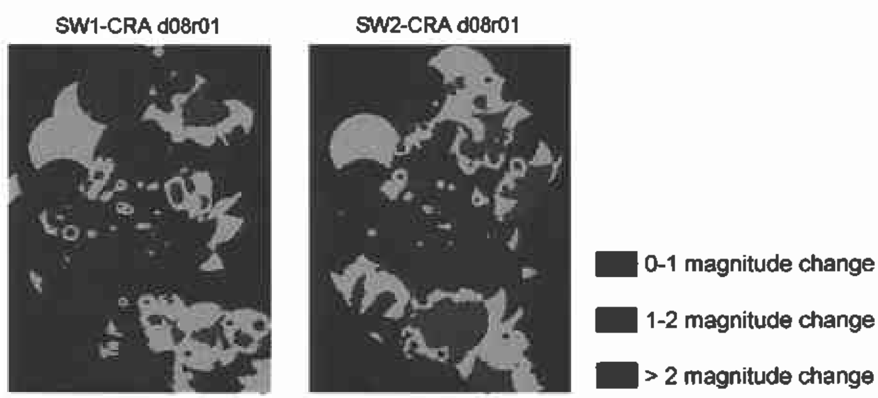

Figure 6. Absolute value of change in transmissivity calibration from CRA to SW1 and SW2 for d08r01.

Particle Tracking

Changes to the SW boundary condition do not greatly alter the family of particle-tracking paths from above the center of the repository to the WIPP site boundary (Figure 7). The locations at which particles leave the WIPP site boundary remain relatively stable between the CRA and the alternate SW boundary condition simulations (Figure 8). However, larger changes are noted in particle tracking to the model boundary (Figure 9). Since the SW1 boundary condition is a fixed-head boundary condition that runs through the relatively high initial head in the lower portion of the model, particles are likely to leave the model at that point. The larger area of high transmissivity in Nash Draw included in the SW2 scenario effectively pushes particles to the southeastern portion of the model domain. Figure 10 shows the impact that the alternate boundary conditions have on the steady-state heads used to calculate particle tracking for the d08r01 base T-field. The high-transmissivity zone in the SW2 case lowers the head drop across the SW portion of the model.

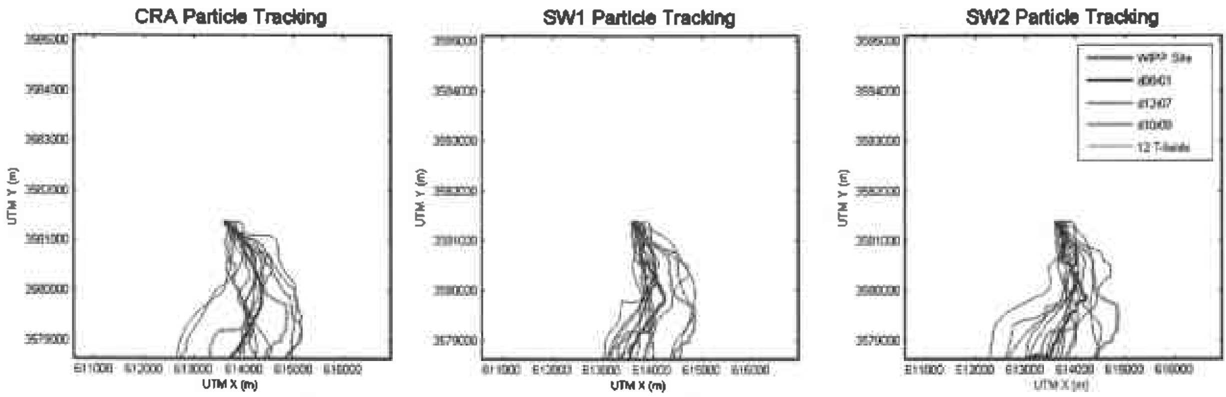

Figure 7. Particle tracking to WIPP site boundary.

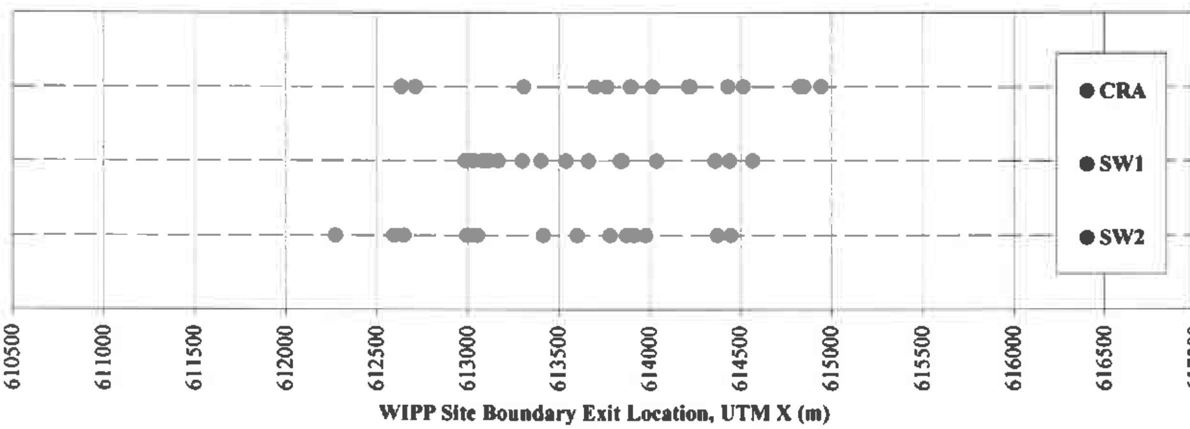

Figure 8. Particle tracking exit location at the WIPP site boundary.

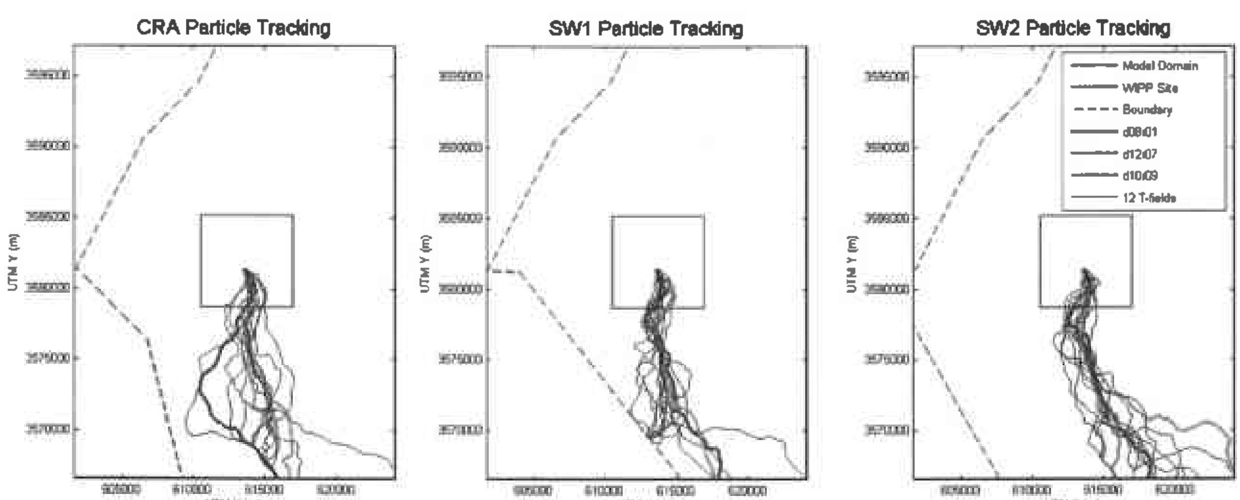

Figure 9. Particle tracking to model boundary.

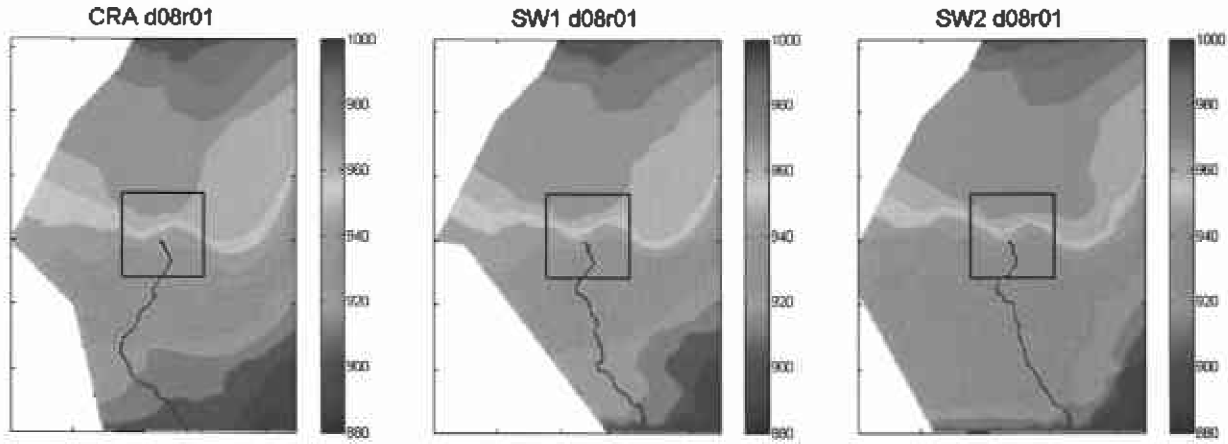

Figure 10. Particle tracking to model boundary overlain on steady-state heads for CRA, SW1, and SW2 simulations for the d08r01 T-field.

TRAVEL TIME

It is important to keep in mind that this study does not include an extensive set of base T-fields from which to draw conclusions of the effects on the travel time of the SW boundary of the WIPP groundwater model. Travel time results of the 15 selected T-fields are therefore compared to the travel time distribution from the 100 T-fields calibrated in the CRA study (McKenna and Hart, 2003b) (Figure 11). The CDF of travel times for the 15 T-fields closely approximates the CDF for the complete CRA study because the 5th, 50th and 95th ranking T-fields were specifically selected. It cannot be certain, however, that the CDF for 15 fields in the SW1 and SW2 scenarios will resemble a CDF using a larger number of base T-fields. Generally, travel time to the WIPP site boundary is decreased using the SW1 and SW2 boundary conditions, although not enough to be significant in radionuclide transport calculations that include matrix diffusion and sorption as retardation mechanisms. Travel time to the model boundary is largely unchanged by changes to the boundary condition.

Travel time statistics are shown in Table 7 and Table 8. The accompanying histogram for each table (Figures 12 and 13) show that changes to the SW boundary condition do not preserve the travel time ranking in the CRA study. This means that T-fields that result in long travel times using the CRA boundary condition do not necessarily result in long travel times using the SW1 or SW2 boundary condition. As only 15 T-fields are used in this study, it cannot be assumed that the 5th, 50th, and 95th ranking T-fields of the CRA study will produce a comparable travel time range in the SW1 and SW2 boundary condition simulations.

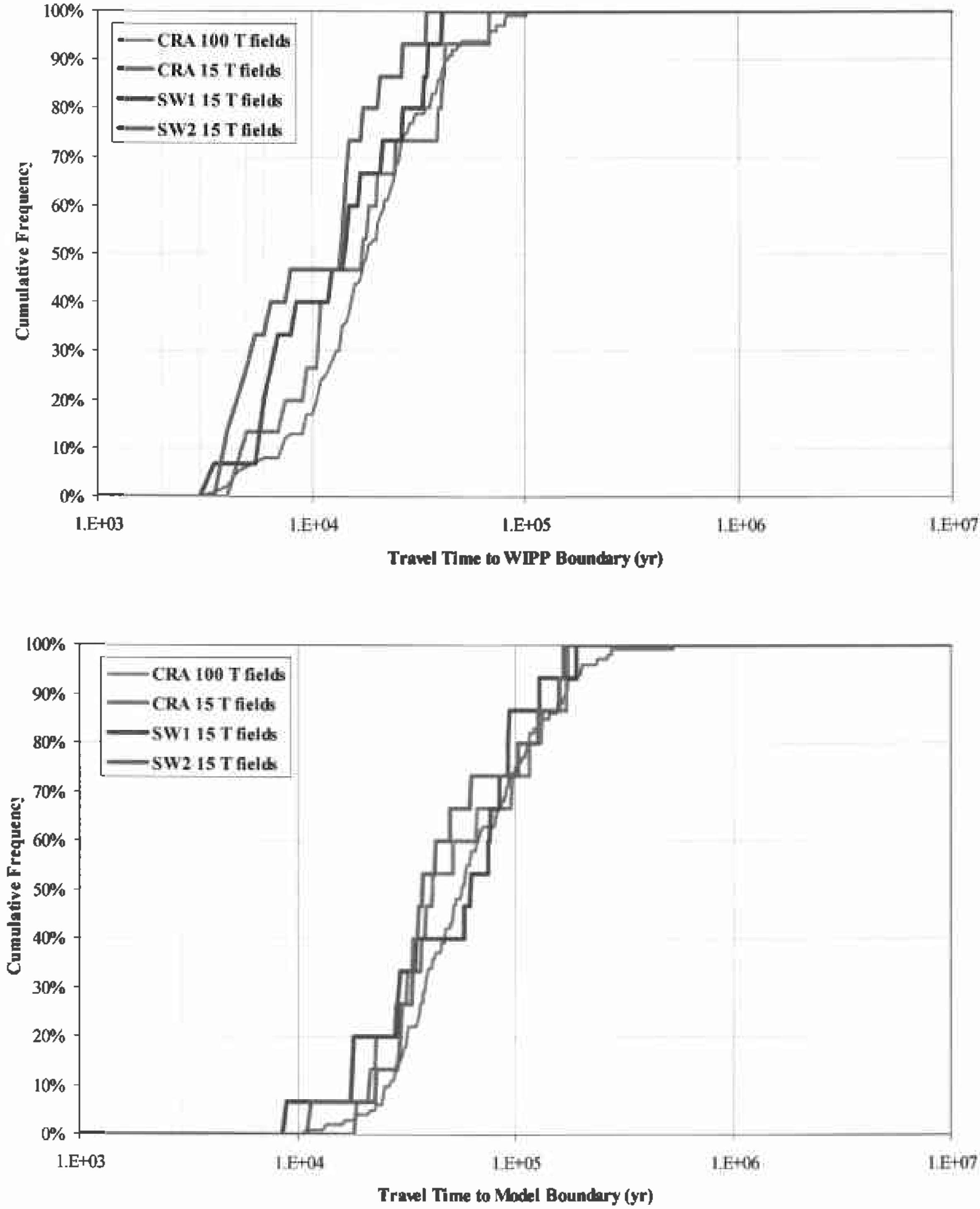

Figure 11. Travel time to WIPP site boundary and model boundary.

Table 7. Travel time to WIPP site boundary.

T-Field		Time to WIPP boundary (yr) CRA	SW1	SW2
5% ranking travel time to WIPP boundary (CRA)	d08r01	4388.3	14795.1	14601.5
50% ranking travel time to WIPP boundary (CRA)	d12r07	18283.4	6026.2	14105.7
95% ranking travel time to WIPP boundary (CRA)	d10r09	68051.7	33100.1	5133.8
Additional 12 T-fields	d01r07	42123.0	16501.3	20781.9
	d02r02	17217.0	8434.4	34787.4
	d03r03	7170.6	14275.6	6129.0
	d04r02	40593.2	35240.5	17481.1
	d06r07	12035.3	6845.3	13666.8
	d07r06	24641.1	5596.7	4695.6
	d09r05	10726.3	26970.8	14415.4
	d11r08	4520.4	3318.6	3583.2
	d12r06	39398.5	21040.4	7670.7
	d13r08	20313.1	40692.2	26985.9
	d21r02	9023.4	12199.7	3604.9
	d22r04	10536.7	5599.1	4429.0
STATS				
Minimum		4388.3	3318.6	3583.2
Maximum		68051.7	40692.2	34787.4
Median		17217.0	14275.6	13666.8
Mean		21934.8	16709.1	12804.8
Standard Deviation		18091.8	12093.1	9310.0

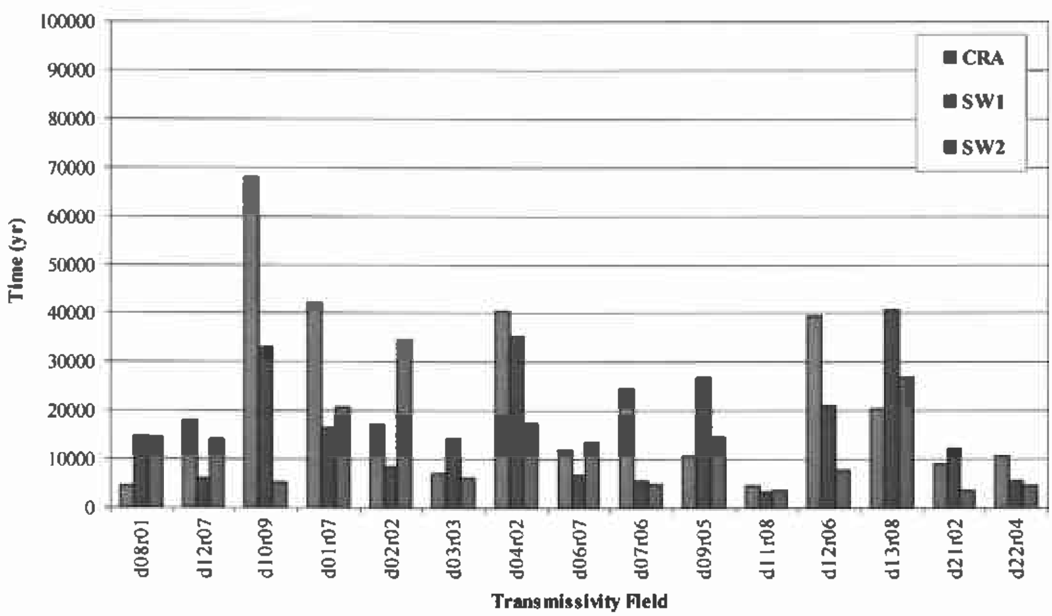

Figure 12. Histogram of travel time to WIPP site boundary by T-field.

Table 8. Travel time to model boundary.

		Time to model boundary (yr)		
T-Field		CRA	SW1	SW2
5% ranking travel time to WIPP boundary (CRA)	d08r01	22662.7	189736.2	42569.9
50% ranking travel time to WIPP boundary (CRA)	d12r07	96115.2	17520.4	29711.4
95% ranking travel time to WIPP boundary (CRA)	d10r09	131965.1	75135.3	29397.5
Additional 12 T-fields	d01r07	170937.1	58034.5	158803.5
	d02r02	41726.8	28825.0	127138.4
	d03r03	51836.6	92891.4	35819.1
	d04r02	116261.6	129641.9	102633.9
	d06r07	28199.8	29106.3	50151.1
	d07r06	38884.3	8671.8	11315.7
	d09r05	31575.1	76542.3	165866.5
	d11r08	18036.3	34655.3	37284.2
	d12r06	174326.5	62394.8	33744.6
	d13r08	66137.8	84584.6	62414.6
	d21r02	36981.9	93291.0	33666.7
	d22r04	21196.7	17866.0	22659.1
STATS				
Minimum		18036.3	8671.8	11315.7
Maximum		174326.5	189736.2	165866.5
Median		41726.8	62394.8	37284.2
Mean		69789.6	66593.1	62878.4
Standard Deviation		54433.8	48638.1	50482.9

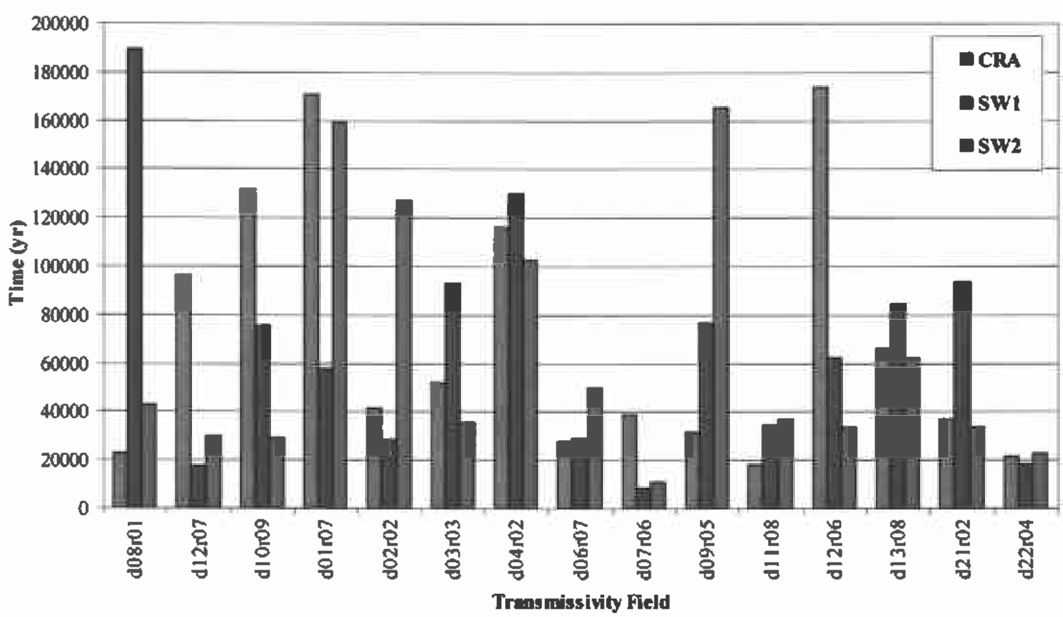

Figure 13. Histogram of travel time to model boundary by T-field.

Discussion

The two alternate conceptualizations to the SW boundary condition used in this study do not result in significantly different exit locations (Figure 8) for particle tracks crossing the WIPP site boundary compared to the CRA results, but the individual particle track locations (Figure 7) and travel times (Table 7) show more variation.

A T-test was run to determine statistical differences between the mean travel time for the CRA and SW1, and the CRA and SW2 scenarios. This analysis uses the mean, standard deviation, and sample size of two subsets to calculate the difference in means of two corresponding populations (Hines and Montgomery, 1990: Equation 10-37). The equation reads as follows:

$$\bar{X}_1 - \bar{X}_2 - t_{\alpha/2,v}\sqrt{S_1^{\,2}/n_1 + S_2^{\,2}/n_2} \le \mu_1 - \mu_2 \le \bar{X}_1 - \bar{X}_2 + t_{\alpha/2,v}\sqrt{S_1^{\,2}/n_1 + S_2^{\,2}/n_2}$$

$$v = \frac{\left(S_1^{\,2}/n_1 + S_2^{\,2}/n_2\right)^2}{\frac{\left(S_1^{\,2}/n_1\right)^2}{n_1+1} + \frac{\left(S_2^{\,2}/n_2\right)^2}{n_2+1}} - 2$$

where X_1 = CRA sample mean (15 T-fields)
X_2 = SW1 or SW2 sample mean (15 T-fields)
S_1 = CRA sample standard deviation (15 T-fields)
S_2 = SW1 or SW2 standard deviation (15 T-fields)
n_1 = sample size for CRA (15)
n_2 = sample size for SW1 or SW2 (15)
μ_1 = CRA population mean (100 T-field)
μ_2 = SW1 or SW2 population mean (100 T-field), unknown
t = t statistic, function of v and α
v = degrees of freedom
α = confidence level (.05 for a 95% confidence interval)

The T-test does not assume equal variance between the CRA and SW1 or SW2 travel time distributions. A 95% confidence interval is used to establish the difference in means between the CRA and SW1 simulations and the difference in means between the CRA and SW2 simulations. Using the population mean of the CRA (100 T-field study), the population mean for the SW1 and SW2 scenarios with 95% confidence is calculated. The results show that using 15 T-fields to predict the population mean for the SW1 and SW2 scenarios is difficult. The 95% confidence interval for the travel time to the WIPP boundary using the SW1 boundary condition is between 6555 and 28960 years, while the interval using the SW2 boundary condition is between 3307 and 25299 years (Figure 14). The large range suggests that the mean travel time cannot be predicted, with a high level of confidence, using the 15 T-fields. The results do suggest, however, that the mean travel times using the alternate boundary conditions are statistically different from the CRA results.

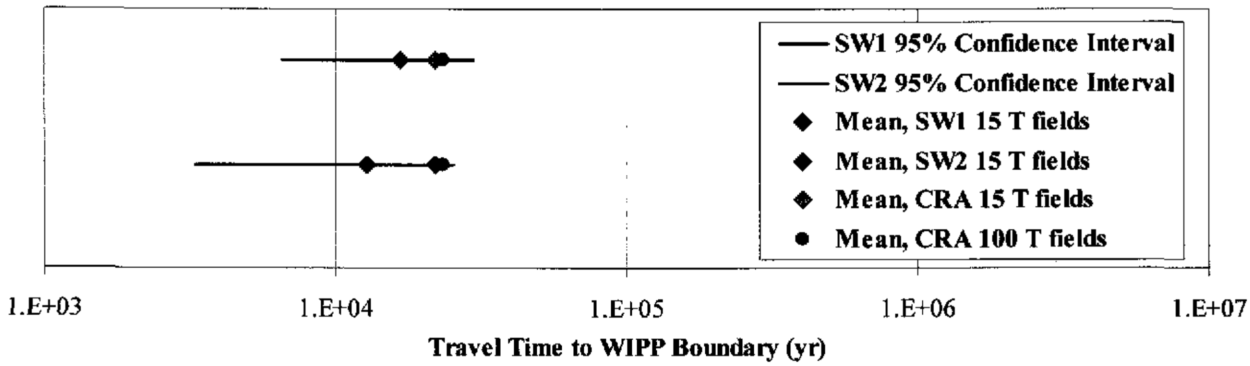

Figure 14. 95% confidence for the population mean travel time for the SW1 and SW2 scenarios based on results from 15 T-fields and CRA results.

Summary

This study uses a subset of CRA base T-fields to investigate the impact that the SW boundary condition has on pilot point calibration, particle tracking, and travel time. By recalibrating 15 base T-fields using two alternatives to the SW boundary condition, this study concludes the following:

- Pilot point calibration is highly sensitive to the SW boundary condition with changes to pilot point transmissivity up to 6 orders of magnitude. However, the average change over the 15 fields is generally low. The largest change to pilot point calibration occurs south of the WIPP site using the SW2 boundary condition.

- The family of travel paths from above the center of the WIPP repository to the WIPP site boundary is largely unchanged using the two alternate boundary conditions compared to the CRA results, although the locations of individual particle tracks vary. The distributions of particle exit locations from the WIPP site boundary from the CRA, SW1, and SW2 simulations are roughly equal.

- Travel times to the WIPP site boundary are decreased due to changes in the SW boundary condition. Generally, SW1 travel times are less than the CRA travel times, and SW2 travel times are less than the SW1 travel times. Travel times to the model boundary are largely unaffected by the changes to the SW boundary.

- Changing the SW boundary condition does not preserve the travel time ranking from the CRA study.

It is stressed that the above conclusions are based on a small subset of the CRA T-fields. Analyses based on the difference between two means shows that the 15 sampled T-fields for each boundary condition are not enough to statistically determine, with a high level of confidence, the magnitude of change of the mean travel time for the SW1 and SW2 scenarios as compared to the CRA results. However, the results suggest that changes to the boundary condition do result in a mean that is statistically different from that of the CRA.

Using the SW2 boundary condition, further study will include the effect of adding recharge to the Culebra groundwater model. The rate and location of possible recharge into the Culebra are based on air photos and field observations.

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Appendix A: Run Control

ARCONS: ARCHIVED RUN-CONTROL SYSTEM

All files used in the calibration, with the exception of task specific boundary condition files (described below) are the same as the CRA simulations. These files are located in the WIPPcvs directory.
- /h/WIPPcvs/bin (MF2K, DTRKMF, and PEST files)
- /h/WIPPcvs/src (script files)
- /h/WIPPcvs/trans (base T-files)

Task-specific files are located in /h/WIPPcvs/AP114/Task3/import. These files include:
- culebra_full.bot,v
- culebra_full.ihd,v
- culebra_full.top,v
- SW1.ibd,v
- SW2.ibd,v
- transient_SW1.pst,v

For this task, full model domain specification of culebra top elevation, bottom elevation, and initial heads are needed. culebra_full.bot and culebra_full.top were created from culebra_top.xls, while culebra_full.ihd was created from heads_00.xls (Excel sheets also located in /h/WIPPcvs/AP114/Task3/import). Files defining the new southwest boundary definitions were created based on the specification for the SW1 and SW2 boundaries. These files (SW1.ibd and SW2.ibd) replace culebra.ibd in the simulations. The location of the SW1 boundary requires that the weight of H-7b1 be changed to 0 for the purpose of calibration. H-7b1 is outside the active domain when using the SW1 boundary condition. This update is made in the file transient_SW1.pst, where transient_SW1.pst replaces transient.pst in the SW1 simulations.

Run control files are located in /h/WIPPcvs/AP114/Task3/control. These files include:
- pmaster,v
- pslave1,v
- pslave2,v
- pslave3,v
- pslave4,v
- pslave5,v
- pslave6,v
- pslave7,v
- SW1_template.checkin,v
- SW1_template.checkout,v
- SW1_template.execute,v
- SW1_template.rctl,v
- SW1_setup,v
- SW2_template.checkin,v

- SW2_template.checkout,v
- SW2_template.execute,v
- SW2_template.rctl,v
- SW2_setup,v

Run control files for specific base T-fields are created by running SW1_setup and SW2_setup with the desired base T-fields (d##r##) specified in the setup file. Using the template files, the resulting files (SW1_d##r##.checkin, SW1_ d##r##.checkout, SW1_ d##r##.execute, SW1_ d##r##.rctl, SW2_d##r##.checkin, SW2_ d##r##.checkout, SW2_ d##r##.execute, and SW2_ d##r##.rctl) are used to run each T-field calibration. See Appendix B for file format.

EXAMPLE ARCONS RUN

Table A-1 lists the steps necessary to run the AP114/Task3 simulations in a local directory. The example is for the SW1 boundary condition using the d08r01 base T-field.

Table A-1. Example Arcons run.

Description	Command from local directory
1. Setup CVS root directory	`export CVSROOT=/h/WIPPcvs`

2. Create a local copy of *SW1_setup*, *SW1_template.checkin*, *SW1_template.checkout*, *SW1_template.execute*, and *SW1_template.rctl*.
 	
Files are located in h/WIPPcvs/AP114/Task3/control.
	`cp $CVSROOT/AP114/Task3/control/SW1_setup,v SW1_setup`
	
	`cp $CVSROOT/AP114/Task3/control/ SW1_template.checkin,v SW1_template.checkin`
	
	`cp $CVSROOT/AP114/Task3/control/ SW1_template.checkout,v SW1_template.checkout`
	
	`cp $CVSROOT/AP114/Task3/control/ SW1_template.execute,v SW1_template.execute`
	
	`cp $CVSROOT/AP114/Task3/control/ SW1_template.rctl,v SW1_template.rctl`

3. Run *SW1_setup* with T-field "d08r01". Before running make sure *SW1_setup* has TFIELDS="d08r01" This creates *SW1_d08r01.checkin*, *SW1_d08r01.checkout*, *SW1_d08r01.execute*, and *SW1_d08r01.rctl*.	`SW1_setup`
4. Check in all project specific files (*SW1_d08r01.checkin*, *SW1_d08r01.checkout*, *SW1_d08r01.execute*, and	`cvs import AP114/Task3/control wipp control`

SW1_d08r01.rctl) To exit cvs import log, type 'shift-Z'	
5. Start run control The '-test' option keeps a local copy of the result files.	`arcons AP114/Task3/control/SW1_d08r01.rctl -test`

Note: Steps 3 and 4 can be complete for multiple T-fields by adding additional names to TFIELDS in the setup file (i.e. TFIELDS = "d08r01 d12r07 d10r09 d01r07 d02r02 d03r03 d04r02 d06r07 d07r06 d09r05 d11r08 d12r06 d13r08 d21r02 d22r04").

File Naming Convention

Programs, shells, and files needed to accomplish each T-field calibration are listed and described in Table A-2 and follow the convention in McKenna and Hart (2003b). Each T-field calibration is completed within its own subdirectory. Additional intermediate files (e.g., each drawdown output array at each time step from MODFLOW-2000) and intermediate subdirectories (e.g., the PEST slave subdirectories) are deleted at the end of the calibration process and are not included in the table.

Table A-2. File listing and descriptions within a calibration subdirectory.

File Prefix/Suffix	File Definition
d##r##.mod	The final calibrated T-field values in MODFLOW format.
d##r##T.out	Original base T-field in 4 column ARC-INFO format (input to base2mod program)
d##r##.par	The final values of the estimated pilot points (output from PEST)
d##r##.rec	Output record file from PEST
d##r##.res	Residuals output file from PEST
**.ba6*	MODFLOW input basic package file
**.bc6*	MODFLOW input block centered-flow package file
base2mod.set	Input control file for the base2mod program
**.bud*	MODFLOW cell by cell budget output file
combine.set	Input control file for the combine program
control.inp	DTRKMF input control file for particle track to model domain
culebra.bot	Elevations of the bottom of the Culebra in MODFLOW format (input to MODFLOW)
culebra.ibd	MODFLOW input ibound array
culebra.ihd	MODFLOW input initial heads
culebra.spc	PEST utilities grid specification file (input to PEST utilities)
culebra.top	Elevations of the top of the Culebra in MODFLOW format (input to MODFLOW)
d##r##.pts.dat	Current value of pilot points in residual space (also includes

	X,Y coordinates and zone number). Same file as points.dat
**.dis*	MODFLOW discretization input file
dtrk.dbg	DTRKMF debugging information file
fac2real.in	fac2real input file
files.fig	PEST utilities file name specification file (input)
**.hed*	MODFLOW output head files
*in_mod2obs.**	Input parameter file for the *mod2obs* code
**.inf*	Inputs to ppk2fac defining the lower and upper bounds of the residual field and the zone values (all in MODFLOW matrix format)
jacob.runs	PEST output record of the Jacobian calculations
**.lmg*	MODFLOW multigrid solver input file
**.log.mod*	Log10 space transmissivity or residual field values in MODFLOW format.
**.lst*	File containing the MODFLOW screen output
*measured.**	The measured heads at a location (output). These files contain four columns: the observation well name, date, time, and modeled head and there is one file for each hydraulic test period.
*modeled.**	The modeled heads at a location (output). These files contain four columns: the observation well name, date, time, and modeled head.
modeled..parsed*	The same as the modeled.* files but with the first 3 columns (Well ID, Date and Time) removed.
**.mtt*	PEST output file containing the statistical matrices
**.nam*	MODFLOW name file (input)
*obs_wells.**	Listing of the observation wells for each pumping test (input)
**.oc*	MODFLOW output control file (input)
**.old*	Results of the DTRKMF particle tracking with the incorrect starting point coordinates(not part of final results)
pcf.bot	Bottom portion of the PEST control file that does not change
pcf.top	Top portion of the PEST control file that does not change
pest.fnn	PEST intermediate output file (not used in calibration)
pest..ins*	PEST instruction files that hold the PEST identification for each observation
pest.stp	PEST intermediate output file that tells current run status of PEST
points.dat	Current value of pilot points in residual space (also includes X,Y coordinates and zone number)
points.tpl	PEST input template file identifying the names, locations and zones for each pilot point
ppk2fac.in	ppk2fac input file
ppoints.nodes	Listing of the pilot point locations in vector notation (input to getSgsimParams shell).
ppoints.pcf_add	File created by getSgsimParams that contains the initial values

	of the residual field at the pilot points
ppoints.zones	Vector listing of zones for each pilot point (used as input to getSgsimParams shell)
reg.out	PEST regularization output
resid_ns.dat	Input data file for sgsim
sd.dat	Ppk2fac binary output file containing kriging variance information (not used in calibration process)
settings.fig	PEST utility input file specifying data column/row and date format
sgsim.console	Screen capture of the output generated while running sgsim
sgsim.dbg	Sgsim debug information file
sgsim.out	Sgsim output file containing the initial simulated residual field
sgsim.par	Sgsim input parameter file
sgsim.par.tpl	Template file used as the basis for each sgsim.par file created
sgsim.trn	Sgsim output containing the raw residual data and the normal-score transform data (not used in calibration process).
tolerance.log	Record of the MODFLOW lmg solver tolerance values used to achieve solutions.
transient.jac	PEST Jacobian matrix saved for restart (binary)
transient.jco	PEST Jacobian matrix for best parameters (binary
transient.jst	PEST Jacobian matrix from the previous iteration (binary)
tupdate.mod	The final calibrated T-field values in MODFLOW format (same file as d##r##.mod)
transient.par	Final pilot point values estimated by PEST (same file as d##r##.par).
transient.pst	PEST control file (input driver file for PEST)
transient.rec	Output record file from PEST (same file as d##r##.rec)
transient.res	Residuals output file from PEST (same file as d##r##.res)
transient.rmf	The parallel PEST run management file (input)
transient.rmr	The parallel PEST run management record (output)
transient.rst	PEST intermediate output file that stores restart information at the beginning of each optimization iteration
transient.sen	PEST output file containing the parameter sensitivities
transient.seo	PEST output containing the observation sensitivities
**.trk*	Results of the DTRKMF particle tracking
variogram.str	Input file to ppk2fac program that contains variogram model specifications
**.wel*	MODFLOW well definition input file
wells.crd	Listing of well names and X,Y coordinates
wippctrl.inp	DTRKMF input control file for particle track to WIPP site boundary
YYMMDD_####.out	Screen capture of calibration run output. The file name contains the date and the batch queue job number
zones.inf	Input zone definition file for PEST

Appendix B: Run Control Files

SW1 Run Control Files

SW1_setup

```
#!/bin/bash
TFIELDS="d08r01 d12r07 d10r09 d01r07 d02r02 d03r03 d04r02 d06r07 d07r06 d09r05
d11r08 d12r06 d13r08 d21r02 d22r04"

for Tfield in $TFIELDS
do
   sed -e 's/d--r--/'$Tfield'/g' SW1_template.checkin > SW1_$Tfield.checkin
   sed -e 's/d--r--/'$Tfield'/g' SW1_template.checkout > SW1_$Tfield.checkout
   sed -e 's/d--r--/'$Tfield'/g' SW1_template.execute > SW1_$Tfield.execute
   sed -e 's/d--r--/'$Tfield'/g' SW1_template.rctl > SW1_$Tfield.rctl

   chmod +x SW1_$Tfield.checkin
   chmod +x SW1_$Tfield.checkout
   chmod +x SW1_$Tfield.execute
   chmod +x SW1_$Tfield.rctl
done
```

SW1_template.checkin

```
REPOSITORY=/h/WIPPcvs
PROJECT=AP114/Task3/output/SW1_d--r--
CVS_FLAGS=-kb
transient.trk
transient-wipp.trk
transient.par
transient.rec
transient.res
steady.bud
points.dat
Tupdate.mod
```

SW1_template. checkout

```
REPOSITORY=/h/WIPPcvs
DESTINATION=.
CVS_FLAGS=-kb

PROJECT=bin/mf2k
mf2k_1.6.release

PROJECT=bin/dtrkmf
```

```
dtrkmf_v0100

PROJECT=bin/pest
ppest_5.51_release
pslave_5.51_release
tempchek_5.5_release
inschek_5.5_release

PROJECT=bin/pest-util
fac2mf2k_release
fac2real_release
mod2obs_release
ppk2fac_release
ppkreg_release

PROJECT=bin/sgsim
sgsim_release

PROJECT=src/scripts
base2mod
getSgsimParams
pslave.sh
pmaster.sh
combine
adjH19.pl
adjP14.pl
adjW13.pl
adjH11.pl
adjWqsp1.pl
adjWqsp2.pl

PROJECT=trans/realizations
d--r--T.out

DESTINATION=.
PROJECT=AP114/Task3/inputs
SW1.ibd
culebra_full.top
culebra_full.bot
culebra_full.ihd
transient_SW1.pst

PROJECT=trans/LoosePP/execution_scripts
model.sh

DESTINATION=.
```

```
PROJECT=trans
settings
modflow

DESTINATION=slave1
PROJECT=trans
settings
modflow

DESTINATION=slave2
PROJECT=trans
settings
modflow

DESTINATION=slave3
PROJECT=trans
settings
modflow

DESTINATION=slave4
PROJECT=trans
settings
modflow

DESTINATION=slave5
PROJECT=trans
settings
modflow

DESTINATION=slave6
PROJECT=trans
settings
modflow

DESTINATION=slave7
PROJECT=trans
settings
modflow

DESTINATION=slave8
PROJECT=trans
settings
modflow
```

SW1_template. execute

```
#!/bin/bash -l
```

```
echo "s%/h/WIPP/pest/bin%$PWD%g" > sedscr
echo "s%/h/WIPP/sgsim/bin%$PWD%g" >> sedscr
echo "s%/h/WIPP/modflow/bin%$PWD%g" >> sedscr
echo "s%/h/WIPP/dtrkmf/bin%$PWD%g" >> sedscr
echo "s%/h/WIPP/pest-util/bin%$PWD%g" >> sedscr
echo "s%/h/wipp/bin%$PWD%g" >> sedscr
runsed model.sh
runsed getSgsimParams
runsed base2mod
./base2mod d--r--T.out
./getSgsimParams > sgsim.console
cat pcf.top > transient.pst
cat ppoints.pcf_add >> transient.pst
cat pcf.bot >> transient.pst
# This is only for the SW1 case
cp transient_SW1.pst transient.pst
cp SW1.ibd culebra.ibd
cp culebra_full.top culebra.top
cp culebra_full.bot culebra.bot
cp culebra_full.ihd culebra.ihd
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave1
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave2
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave3
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave4
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave5
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave6
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave7
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave8
```

SW1_template. rctl

```
RUNNAME=AP114/Task3/control/SW1_d--r--
RUNFILES_FROM_REPOSITORY=/h/WIPPcvs
RUNFILES_TO_REPOSITORY=/h/WIPPcvs
NO_GLOBAL_FILE
RUN_NAME=SW1 d--r--
RUN_INFO=
AUTHOR=K.A.Klise
EMAIL=kaklise@sandia.gov
CLUSTER_TYPE=pbs
SLAVE_SCRIPT=pslave1
SLAVE_SCRIPT=pslave2
SLAVE_SCRIPT=pslave3
SLAVE_SCRIPT=pslave4
SLAVE_SCRIPT=pslave5
SLAVE_SCRIPT=pslave6
SLAVE_SCRIPT=pslave7
```

```
MASTER_SCRIPT=pmaster
```

SW2 Run Control Files

SW2_setup

```
#!/bin/bash
TFIELDS=" d08r01 d12r07 d10r09 d01r07 d02r02 d03r03 d04r02 d06r07 d07r06 d09r05
d11r08 d12r06 d13r08 d21r02 d22r04"

for Tfield in $TFIELDS
do
   sed -e 's/d--r--/'$Tfield'/g' SW2_template.checkin > SW2_$Tfield.checkin
   sed -e 's/d--r--/'$Tfield'/g' SW2_template.checkout > SW2_$Tfield.checkout
   sed -e 's/d--r--/'$Tfield'/g' SW2_template.execute > SW2_$Tfield.execute
   sed -e 's/d--r--/'$Tfield'/g' SW2_template.rctl > SW2_$Tfield.rctl

   chmod +x SW2_$Tfield.checkin
   chmod +x SW2_$Tfield.checkout
   chmod +x SW2_$Tfield.execute
   chmod +x SW2_$Tfield.rctl
done
```

SW2_template.checkin

```
REPOSITORY=/h/WIPPcvs
PROJECT=AP114/Task3/output/SW2_d--r--
CVS_FLAGS=-kb
transient.trk
transient-wipp.trk
transient.par
transient.rec
transient.res
steady.bud
points.dat
Tupdate.mod
```

SW2_template. checkout

```
REPOSITORY=/h/WIPPcvs
DESTINATION=.
CVS_FLAGS=-kb

PROJECT=bin/mf2k
mf2k_1.6.release

PROJECT=bin/dtrkmf
```

```
dtrkmf_v0100

PROJECT=bin/pest
ppest_5.51_release
pslave_5.51_release
tempchek_5.5_release
inschek_5.5_release

PROJECT=bin/pest-util
fac2mf2k_release
fac2real_release
mod2obs_release
ppk2fac_release
ppkreg_release

PROJECT=bin/sgsim
sgsim_release

PROJECT=src/scripts
base2mod
getSgsimParams
pslave.sh
pmaster.sh
combine
adjH19.pl
adjP14.pl
adjW13.pl
adjH11.pl
adjWqsp1.pl
adjWqsp2.pl

PROJECT=trans/realizations
d--r--T.out

DESTINATION=.
PROJECT=AP114/Task3/inputs
SW2.ibd
culebra_full.top
culebra_full.bot
culebra_full.ihd

PROJECT=trans/LoosePP/execution_scripts
model.sh

DESTINATION=.
PROJECT=trans
```

```
settings
modflow

DESTINATION=slave1
PROJECT=trans
settings
modflow

DESTINATION=slave2
PROJECT=trans
settings
modflow

DESTINATION=slave3
PROJECT=trans
settings
modflow

DESTINATION=slave4
PROJECT=trans
settings
modflow

DESTINATION=slave5
PROJECT=trans
settings
modflow

DESTINATION=slave6
PROJECT=trans
settings
modflow

DESTINATION=slave7
PROJECT=trans
settings
modflow

DESTINATION=slave8
PROJECT=trans
settings
modflow
```

SW2_template. execute

```
#!/bin/bash -l
echo "s%/h/WIPP/pest/bin%$PWD%g" > sedscr
```

```
echo "s%/h/WIPP/sgsim/bin%$PWD%g" >> sedscr
echo "s%/h/WIPP/modflow/bin%$PWD%g" >> sedscr
echo "s%/h/WIPP/dtrkmf/bin%$PWD%g" >> sedscr
echo "s%/h/WIPP/pest-util/bin%$PWD%g" >> sedscr
echo "s%/h/wipp/bin%$PWD%g" >> sedscr
runsed model.sh
runsed getSgsimParams
runsed base2mod
./base2mod d--r--T.out
./getSgsimParams > sgsim.console
cat pcf.top > transient.pst
cat ppoints.pcf_add >> transient.pst
cat pcf.bot >> transient.pst
cp SW2.ibd culebra.ibd
cp culebra_full.top culebra.top
cp culebra_full.bot culebra.bot
cp culebra_full.ihd culebra.ihd
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave1
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave2
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave3
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave4
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave5
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave6
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave7
cp meanT.log.mod culebra.ibd culebra.top culebra.bot culebra.ihd slave8
```

SW2_template. rctl

```
RUNNAME=AP114/Task3/control/SW2_d--r--
RUNFILES_FROM_REPOSITORY=/h/WIPPcvs
RUNFILES_TO_REPOSITORY=/h/WIPPcvs
NO_GLOBAL_FILE
RUN_NAME=SW2 d--r--
RUN_INFO=
AUTHOR=K.A.Klise
EMAIL=kaklise@sandia.gov
CLUSTER_TYPE=pbs
SLAVE_SCRIPT=pslave1
SLAVE_SCRIPT=pslave2
SLAVE_SCRIPT=pslave3
SLAVE_SCRIPT=pslave4
SLAVE_SCRIPT=pslave5
SLAVE_SCRIPT=pslave6
SLAVE_SCRIPT=pslave7
MASTER_SCRIPT=pmaster
```

PMASTER AND PSLAVE FILES

pmaster

```
cd slave8
../pslave_5.51_release <<EOT &
../model.sh > /dev/null
EOT
cd ..
./ppest_5.51_release transient
./tempchek_5.5_release points.tpl points.dat transient.par
./model.sh
ln culebra.top fort.33
ln culebra.bot fort.34
./dtrkmf_v0100 control.inp steady.bud transient.trk dtrk.dbg
./dtrkmf_v0100 wippctrl.inp steady.bud transient-wipp.trk dtrk.dbg
```

pslave1

```
CWD=`pwd`
DIR=${CWD##/*/}
echo $DIR
cd slave1
../pslave_5.51_release <<EOF
../model.sh > /dev/null
EOF
```

pslave2*

```
cd slave2
../pslave_5.51_release <<EOF
../model.sh > /dev/null
EOF
```

* pslave3, pslave4, psalve5, pslave6, and pslave7 are the same as pslave2