Analysis Report
Task 5 of AP-088
Evaluation of Mining Scenarios

(AP-088: Analysis Plan for Evaluation of the Effects of Head Changes on Calibration of Culebra Transmissivity Fields)

Task Number 1.4.1.1, ERMS #531138

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1 Introduction

This analysis report describes the activities of Task 5 of AP-088, “Analysis Plan for Evaluation of the Effects of Head Changes on Calibration of Culebra Transmissivity Fields” (Beauheim, 2002). The purpose of this Task is to evaluate the effects of future potash mining on flow and transport in the Culebra.

1.1 Background

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 in Title 40 of the Code of Federal Regulations, Parts 191 and 194. The DOE demonstrates compliance with the containment requirements in the regulations by means of a performance assessment (PA), which estimates releases from the repository for the regulatory period of 10,000 years after closure.

In October 1996, DOE submitted the Compliance Certification Application (CCA) to the EPA, which included the results of extensive PA analysis and modeling. After an extensive review, in May 1998 the EPA certified that the WIPP met the criteria in the regulations and was approved for disposal of transuranic waste. The first shipment of waste arrived at the site in March 1999.

The results of the PA conducted for the CCA were subsequently summarized in a Sandia National Laboratories (SNL) report (Helton et al., 1998) and in refereed journal articles (Helton and Marietta, 2000).

The DOE is required to submit an application for recertification every five years after the initial receipt of waste. The recertification applications take into account any information or conditions that have changed since the original certification decision. Accordingly, the DOE is conducting a new PA in support of the Compliance Recertification Application (CRA).

1.2 Purpose

Potash mining in the WIPP area involves resource extraction below the Culebra dolomite in the underlying McNutt Potash zone, which is part of the
larger Salado Formation (Ramsey et al., 1996). It is hypothesized that subsi-
dence of the Culebra due to mining extraction causes fracturing and uncon-
solidation of the aquifer material that results in higher transmissivities. This
increase in transmissivity may significantly change the regional groundwater
flow pattern in the Culebra and additionally the transport of any nuclides
entering the aquifer from the underlying repository. The purpose of this anal-
ysis is to determine the impact of the increase in transmissivity in the Culebra
due to mining on groundwater flow direction and velocity. Specifically, this
task involves three subtasks:

1. Update from previous versions (Ramsey et al., 1996; Wallace, 1996),
   the potential areas of future potash mining that are within the model
domain and map those areas to the new computational grid

2. Modify the calibrated transmissivity fields (T-fields) from Task 4 of AP-
   088 and Task 1 of AP-100 to include mining effects and run steady-state
groundwater flow simulations to calculate the new flow-field

3. Perform particle tracking using the new mining-affected flow-fields to
determine travel times to the WIPP land-withdrawal boundary (LWB)

This analysis report highlights the differences and additions relative to the
"Analysis Package for the Culebra Flow and Transport Calculations (Task
3) of the Performance Assessment Analysis Supporting the Compliance Cer-
tification Application" (Ramsey et al., 1996) and the "Summary Memo of
Record for NS-11; Subsidence Associated with Mining Inside or Outside the
Controlled Area" (Wallace, 1996) that was required by the EPA pursuant to
40CFR Part 194, which contains the minimum specifications for incorporat-
ing potash-mining impacts upon the performance of the WIPP repository.
The Summary Memo of Record for NS-11 is the documentation of the efforts
to meet regulation 40CFR Part 194 as part of the 1996 certification of the
WIPP. The reader is encouraged to review those documents for background
information.

1.3 Outline

This report documents the data, methods and summary results of the work
done as Task 5 of Analysis Plan 088 (Beauheim, 2002). 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: Modeling Domain and Discretization; Outlines the computational grid and modeling domain in terms of regional scale coordinates.

2.5: Boundary and Initial Conditions; Describes the determination and justification for the boundary and initial modeling conditions.

2.6: Determination of Potential Mining Areas; Describes the methodology of determining the potential mining areas.

2.7: Use of Mining Zones in Forward Simulations; Describes how mining zones are applied to the flow model.

2.8: Particle Tracking using DTRKMF; Describes the use of the DTRKMF particle tracking code.

Section 3: Modeling Assumptions

Summarizes the major assumptions of Task 5.

Section 4: Results

Presents results from the Task 5 mining scenario simulations.

Section 5: Summary

Presents a summary of this entire report.

2 Approach

2.1 Overview

This analysis investigates two mining-altered scenarios. The first includes mining in all potential mining zones both inside and outside the land withdrawal boundary and is called the full-mining scenario. The second includes only the potential mining zones outside the IWB and is called the partial-mining scenario. The impacts are considered by scaling each calibrated T-field generated from Task 4 of AP-088 (McKenna and Hart, 2003b) and selected by Task 1 of AP-100 (Beauheim, 2003) in regions deemed to contain
economically-extractable potash resources by a random factor between 1 and 1000. The range of this factor is set by the EPA in regulation 40 CFR Part 194, p. 5229 (Federal Register/vol. 61, No. 28) and is reproduced in Wallace (1996). The scaling factor for each T-field is provided from Latin Hypercube Sampling (LHS).

A forward steady-state flow model is run for each new T-field under each mining scenario (full and partial), for three replicates of mining factors, resulting in 600 simulations (there are 100 qualified T-fields passed from Task 1 of AP-100, see Beauheim (2003)). Particle tracking is performed on the modified flow fields to determine the flow path and groundwater travel time from a point above the center of the WIPP disposal panels to the LWB. A cumulative probability distribution function (CDF) is produced for each mining scenario (as well as an undisturbed scenario generated from Task 4 of AP-088) that describes the probability of a conservative tracer reaching the LWB at a given time. Incorporated into the Task described here (Task 5, AP-088), are Tasks 2 and 3 of AP-100 (Leigh et al., 2003) that refine the modeling grid used here (Task 2) and generates a forward steady-state flow field on the refined grid (Task 3). The detailed steps involved in Tasks 2 and 3 of AP-100 can be found in Lowry (2003). Their inclusion in this report is only to provide context to the procedures and approach of Task 5.

2.2 Software

The forward steady-state flow modeling is performed using MODFLOW 2000 (MF2K), version 1.6 (Harbaugh et al., 2000). The same executable used for the Task 4 calibration is used in this analysis. MF2K is a modular, finite-difference code for solving the groundwater flow equation on a two- or three-dimensional rectilinear grid. The code DTRKMF (Rudeen, 2003) is used to perform the particle-tracking simulations. DTRKMF calculates particle tracks in 2-D or 3-D for steady-state and time-dependent, variably saturated flow fields. The particles are tracked cell-by-cell using a semi-analytical solution (WIPP-PA, 2003d). DTRKMF assumes that the velocities vary linearly between the cell faces as a function of the space coordinate and, for time-dependent cases, that the velocities at the faces vary linearly between time planes. It directly reads the cell-by-cell flow budget file from MF2K and uses those values to calculate the velocity field. The modeling codes for Task 5 are listed in Table (1).

Several FORTRAN utility codes are used for data conversion purposes.
Table 1: Modeling software for Task 5.

<table>
<thead>
<tr>
<th>Code Name</th>
<th>Description</th>
<th>ERMS #</th>
</tr>
</thead>
<tbody>
<tr>
<td>MODFLOW 2000, v1.6</td>
<td>Groundwater Flow Model</td>
<td>523867</td>
</tr>
<tr>
<td>DTRKMF</td>
<td>Particle-tracking model</td>
<td>523244</td>
</tr>
</tbody>
</table>

These codes are FM.F, PM.F, REFINE.F, BA.F, PTOUT.F, and PT- PLOT.F. Their source codes are reproduced in the Appendices. The first, FM.F is the full-mining scenario pre-processor. This code reads in the calibrated T-fields passed from Task 1 of AP-100, as well as the random mining multiplicative factor, multiplies the transmissivity value in the cells that lie within the mining zone areas by the random factor, and then outputs the modified T-field to a file. Likewise, PM.F performs the same task but for the partial-mining scenario. REFINE.F is specific to Task 2 of AP-100 (Leigh et al., 2003) and converts the calibrated T-field from the 100x100 m uniform cell size (see below) that is used here, to a 50x50 m uniform cell size that is used for Task 6 of AP-100. Task 6 of AP-100 performs the radionuclide transport calculations in the mining-affected flow fields using SECOTP2D. The grid conversion is a simple conversion, meaning each grid cell from the 100x100 m cell-sized grid becomes four 50x50 m sized cells, each with the same attributes as the original 100x100 m cell. The attributes include transmissivity, top and bottom elevations, initial head, and the IBOUND array (the IBOUND array designates the active/inactive/constant-head status for each cell). Output from REFINE.F is formatted for input to MF2K, which is then run to provide the cell-by-cell flow budget file on the 50x50 m cell grid. This step is Task 3 of AP-100. Since MF2K is run on a qualified multiple processor Linux cluster (SNL Dept. 6115) and SECOTP2D is run on ES-40, ES-45, and/or 8400 Compaq ALPHA computers running Open VMS Version 7.3-1 (WIPP_PA, 2003a,b,c), the binary files are unable to be transferred directly between the two platforms. Thus, BA.F is used to read in the binary budget file from MF2K and write it out in ASCII format. The ASCII text file is then transferred to the ALPHA computers via FTP. The other two codes, PTOUT.F and PTPL0T.F are data manipulation codes and are used to convert the DTRKMF output to a format that is suitable for summary and visualization.

The Department of Defense Groundwater Modeling System (GMS, ver-
sion 4.0) software is used for digitizing the mining zone areas onto the computa-
tional grid as well as for general visualization purposes (GMS, 2003). GMS is a groundwater modeling and geo-statistical software package that provides a graphical user interface to numerous groundwater modeling codes. Its strength lies in the ability to apply spatially varying data (e.g., the mining zones) to a discrete grid of any given size. GMS is not used to perform any calculations or data conversions. Its use in this Task is to provide visual aid in matching the computational grid to the mining zone map and to perform a coordinate conversion for the mining zone map (see below).

In addition, several Linux shell scripts are used to help automate and coordinate running the programs. Specifically, they are MINING.SH, POST.SH, and POST-FLOW.SH. MINING.SH is the main script that coordinates the running of each model and the other scripts in succession. Starting with each replicate directory, MINING.SH creates separate directories for the full and partial-mining scenarios, and then under each of those directories, a separate directory for each T-field. The naming convention of the files and T-fields is addressed in Section 2.3. With the directories set up, MINING.SH then calls FM.F, PM.F, and REFINE.F to produce the 100x100 m modified T-fields and the refined 50x50 m modified T-fields, MF2K to run the 100x100 m flow model, DTRKMF to perform the particle tracking, and then MF2K again to run the 50x50 m flow model. Finally, MINING.SH calls POST.SH to gather all the DTRKMF output into a single directory called ptout, PTOUT.F to combine all the DTRKMF output into two files (one each for the full and partial-mining scenarios), BA.F to convert the binary 50x50 m budget file to ASCII format, and POST-FLOW.SH to gather the ASCII budget files into a single directory called off. The shell scripts are reproduced in Appendices (G) to (I).

Figure (1) shows the software and information flow chart, with the output/input relationship between the different programs.

2.3 File Naming Convention

The file naming convention for this Task is kept consistent with that of Task 4 (McKenna and Hart, 2003b) to prevent confusion during comparisons. All calculations are performed on the 6115 Linux cluster and are done in a separate directory for each T-field. The general path for the T-field directories is:
Figure 1: Software and information flow-chart. Elements within the dashed box are part of AP-100.

\[ \text{AREA} / \text{task} / \text{scenario} / \text{d##r##} \]

where, R* is either R1, R2, or R3, depending on the mining factor replicate, /scenario/ is either ‘full’ or ‘partial’, depending on the mining scenario, and \(d##r##\) is the original base transmissivity field naming convention as described in Holt and Yarbrough (2003). The ##’s next to ‘d’ ranges from 01 to 22 and next to the ‘r’ it ranges from 01 to 10. In Task 4 of AP-088, 150 calibration runs were attempted, with 137 able to be calibrated. However, some of the calibrated T-fields can be a poor representation of the known field so that qualifying criteria are used (Beauheim, 2003) to reduce the 137 calibrated fields to 100. Thus for the naming convention, not all values of ## will appear as a directory. In addition, there are two data di-
rectories ('100x100' and '50x50') that contain the MF2K and DTRKMF input files for the 100x100 m and 50x50 m cell grid, respectively, and two directories ('scripts' and 'source') that contain backups of the shell scripts and the FORTRAN source files for the files described above. These directories are subdirectories of /home3/tslowry/wzpp/mining. The parent copy of the shell scripts and the FORTRAN executables are kept in and run from /home3/tslowry/wzpp/mining. A schematic of the directory tree is shown in Figure (2). The input and output files that will remain archived in the directories are listed in Table (2).

2.4 Model Domain and Discretization

The model domain used in Task 5 is the same as that used in Task 4. The original intent for Task 4 was to use 50x50 m cells, but due to computational constraints in the calibration process it was decided that the grid should be coarsened to the 100x100 m uniform cell grid. This change is discussed fully in McKenna and Hart (2003b). For the SECOTPSD input, model parameters from the Task 4 grid are exactly delineated onto a 50x50 m cell grid meaning each 100x100 m cell is split into four 50x50 m cells. Each of the four smaller cells is assigned the same attribute as the original cell. While this is not a true refinement from a data resolution point of view, it does provide the needed compatibility to the 50x50 m SECOTPD grid.

A general description of the modeling domain and grid-layout is given in McKenna and Hart (2003a) and is reproduced here for completeness:

The north-south and east-west extent of the model domain was specified by Richard Beaulieu, Robert Holt, and Sean McKenna. This determination considered several factors including: 1) hydrogeological features in the vicinity of the WIPP site that could serve as groundwater flow boundaries (e.g. Nash Draw); 2) the areas to the north of the WIPP site that might create additional recharge to the Culebra due to water applied to potash tailings pile; and 3) the limits imposed on the domain size by the available computational resources and the desired fine scale discretization of the domain within the groundwater model. The final model domain is rectangular and aligned with the north-south and east-west directions. The coordinates of each corner of the domain are given in Table 1 in UTM (NAD87) coordinates. A no-flow
Figure 2: Directory tree of Task 5 files and programs. Note that the subdirectories d01r02 and d01r04 appearing under the R*/full and R*/partial directories represent the first two of 100 subdirectories.
Table 2: Input and output files used for Task 5. File names in *italics* denote files associated with Tasks 2 and 3 of AP-100.

<table>
<thead>
<tr>
<th>Directory</th>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Good.runs.txt</td>
<td>List of good T-fields in d##r## format</td>
</tr>
<tr>
<td>/mining</td>
<td>mR*.txt</td>
<td>Mining factors (R* = R1, R2, or R3)</td>
</tr>
<tr>
<td></td>
<td>Replicate.txt</td>
<td>Replicate number input file</td>
</tr>
<tr>
<td></td>
<td>Full.mining.dat</td>
<td>Full-mining input file</td>
</tr>
<tr>
<td></td>
<td>Part.mining.dat</td>
<td>Partial-mining input file</td>
</tr>
<tr>
<td></td>
<td>culebra.iid</td>
<td>BOUND file</td>
</tr>
<tr>
<td></td>
<td>culebra.ihd</td>
<td>Initial heads</td>
</tr>
<tr>
<td></td>
<td>culebra.top</td>
<td>Culebra top elevations</td>
</tr>
<tr>
<td></td>
<td>culebra.bot</td>
<td>Culebra bottom elevations</td>
</tr>
<tr>
<td></td>
<td>steady.ba6</td>
<td>MF2K basic input file</td>
</tr>
<tr>
<td></td>
<td>steady.bc6</td>
<td>MF2K block-centered input file</td>
</tr>
<tr>
<td></td>
<td>steady.nam</td>
<td>MF2K naming file</td>
</tr>
<tr>
<td></td>
<td>steady.dis</td>
<td>MF2K discretization input file</td>
</tr>
<tr>
<td></td>
<td>steady.oc</td>
<td>MF2K output control file</td>
</tr>
<tr>
<td></td>
<td>steady.lmg</td>
<td>MF2K AMG1R5 solver input file</td>
</tr>
<tr>
<td></td>
<td>dtrkmf.in</td>
<td>D1RKM device file name input</td>
</tr>
<tr>
<td></td>
<td>wppctrl.imp</td>
<td>D1RKM device file input</td>
</tr>
<tr>
<td>/100x100</td>
<td>cNew.iid</td>
<td>BOUND file</td>
</tr>
<tr>
<td></td>
<td>cNew.ihd</td>
<td>Initial heads</td>
</tr>
<tr>
<td></td>
<td>cNew.top</td>
<td>Culebra top elevations</td>
</tr>
<tr>
<td></td>
<td>cNew.bot</td>
<td>Culebra bottom elevations</td>
</tr>
<tr>
<td></td>
<td>steady.ba6</td>
<td>MF2K basic input file</td>
</tr>
<tr>
<td></td>
<td>steady.bc6</td>
<td>MF2K block-centered input file</td>
</tr>
<tr>
<td></td>
<td>steady.nam</td>
<td>MF2K naming file</td>
</tr>
<tr>
<td></td>
<td>steady.dis</td>
<td>MF2K discretization input file</td>
</tr>
<tr>
<td></td>
<td>steady.oc</td>
<td>MF2K output control file</td>
</tr>
<tr>
<td></td>
<td>steady.lmg</td>
<td>MF2K AMG1R5 solver input file</td>
</tr>
<tr>
<td></td>
<td>CMine.mod</td>
<td>Mining-altered T-field from FM.F or PM.F</td>
</tr>
<tr>
<td></td>
<td>dtrk.dbg</td>
<td>D1RKM debug output file</td>
</tr>
<tr>
<td></td>
<td>dtrk.out</td>
<td>D1RKM output file</td>
</tr>
<tr>
<td></td>
<td>steady100x100.bud</td>
<td>MF2K budget output</td>
</tr>
<tr>
<td></td>
<td>steady100x100.hed</td>
<td>MF2K head output</td>
</tr>
<tr>
<td></td>
<td>steady100x100.lst</td>
<td>MF2K listing file</td>
</tr>
<tr>
<td></td>
<td>steady50x50.asci.dat</td>
<td>BAF ASCII budget output</td>
</tr>
<tr>
<td></td>
<td>steady50x50.bud</td>
<td>MF2K flow budget output</td>
</tr>
<tr>
<td></td>
<td>steady50x50.hed</td>
<td>MF2K head output</td>
</tr>
<tr>
<td></td>
<td>steady50x50.lst</td>
<td>MF2K listing file</td>
</tr>
<tr>
<td></td>
<td>TNew.mod</td>
<td>Mining-altered T-field from REFINE.F</td>
</tr>
</tbody>
</table>
boundary corresponding roughly to the center of Nash Draw is shown in Figure 1 [not shown] as a purple line extending from the northern to southern boundaries in the western one-third of the model domain. Model cells falling to the west of this boundary are considered to be inactive in the groundwater flow calculations.

Thus, for the mining field and DTRKMF simulations in Task 5, the modeling domain 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 3). 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. This number is nearly a factor of 5 larger than the 10,800 (108x100) cells used in the CCA calculations.

The corner coordinates of the modeling domain in UTM NAD 27 are given in Table (3). The current grid differs from the 1996 grid described in Wallace (1996) in that the previous grid was non-uniform and rotated clockwise approximately 38° from the north-south/east-west alignment. In addition, the previous grid used a non-uniform cell size across the domain with a minimum cell dimension of 100 m square over the LWB area and a maximum cell dimension of 800 m square cells at the corners. The model domains of the 1996 grid and the current grid for both the full- and partial-mining scenarios are shown in Figures (4) and (5), respectively.

For the DTRKMF particle tracking simulations, a single particle is tracked from the point $X = 613,597.5$, $Y = 3,581,385.2$ (UTM NAD 27) to the LWB for each T-field and replicate/scenario combination (Ramsey et al., 1996, p. 9). The coordinates of the LWB are shown in Table (4).

### 2.5 Boundary and Initial Conditions

Like the model domain and discretization, the boundary and initial conditions used in Task 5 for the groundwater flow modeling runs using MF2K are the same as those used in Task 4, and are described fully in McKenna and Hart (2003b). 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
Figure 3: Modeling domain and boundary conditions for the CRA grid configuration. The western no-flow boundary coincides with the groundwater divide underneath Nash draw.
Figure 4: 1996 modeling domain and outline of full-mining zones (red) overlayed on current full-mining zones and modeling domain.
Figure 5: 1996 modeling domain and outline of partial-mining zones (red) overlayed on current partial-mining zones and modeling domain.
Table 3: The coordinates of the corners of the numerical model domain in UTM NAD27 Coordinates.

<table>
<thead>
<tr>
<th>Domain Corner</th>
<th>X Coordinate (meters)</th>
<th>Y Coordinate (meters)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Northeast</td>
<td>624,100</td>
<td>3,597,200</td>
</tr>
<tr>
<td>Northwest</td>
<td>601,700</td>
<td>3,597,200</td>
</tr>
<tr>
<td>Southeast</td>
<td>624,100</td>
<td>3,566,500</td>
</tr>
<tr>
<td>Southwest</td>
<td>601,700</td>
<td>3,566,500</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Domain Corner</th>
<th>X Coordinate (meters)</th>
<th>Y Coordinate (meters)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Northeast</td>
<td>616,941</td>
<td>3,585,109</td>
</tr>
<tr>
<td>Northwest</td>
<td>610,495</td>
<td>3,585,068</td>
</tr>
<tr>
<td>Southeast</td>
<td>617,015</td>
<td>3,578,681</td>
</tr>
<tr>
<td>Southwest</td>
<td>610,567</td>
<td>3,578,623</td>
</tr>
</tbody>
</table>

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. The Kriged head values to determine the initial heads are assigned to each constant head cell and kept fixed throughout the simulation. Since all simulations for this Task are steady-state, determination of the initial heads are important only in relation to setting the fixed boundary conditions. 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). The initial head contours across the active modeling domain are shown in Figure (6).

Since the extent of possible potash mining extends well beyond the modeling domain, the effects of mining on the boundary conditions must be considered. Regional flow rates within the flow model are controlled by the
Figure 6: Initial heads across modeling domain.
boundary conditions and the hydraulic conductivity distribution. The regional gradient across the domain is approximately 0.0017, which is higher than the 0.001 quoted in Wallace (1996) for the CCA. It should be noted that the regional gradients are difficult to directly compare since the CCA grid is rotated approximately 35° clockwise from the CRA grid. Thus, for the CCA grid, the regional gradient is calculated by taking the difference of the highest constant head in the northern corner of the model and the lowest constant head in the southern end of the model, and dividing by the distance between these two points. For the current grid we average the constant heads along the northern boundary, subtract the average heads along the southern boundary, and then divide by the north-south model domain distance. Using only the cells with the highest and lowest constant heads and dividing by the distance between the two, as was done with the CCA grid, the regional gradient is calculated to be 0.0022, which overestimates the regional behavior. It is assumed that mining impacts would not significantly change this regional gradient and thus the boundary conditions for the mining scenarios are identical to those in Task 4. In addition, the CCA used the same conceptualization (keeping boundary conditions fixed between the mining and non-mining scenarios) and to allow for comparisons between the CCA and the CRA, the same conceptualization is maintained.

2.6 Subtask 1: Determination of Potential Mining Areas

An updated version of the 1993 BLM map, “Preliminary Map Showing Distribution of Potash Resources, Carlsbad Mining District, Eddy and Lea Counties, New Mexico” (BLM, 1993), was obtained directly from David Hughes of Washington Regulatory Environmental Services (WRES) as an Autocad DXF file (Figure 7). This map was originally developed for the CCA and is periodically updated as part of the "Delaware Basin Drilling Surveillance Program", which is performed by WRES.

The coordinates of the DXF file are in State Plane NAD 27, Region 3001 (New Mexico East), and thus required conversion to the UTM NAD 27 (zone 13) system used in this study. The coordinate conversion was done using the Department of Defense groundwater modeling software, GMS (GMS, 2003). After the coordinate conversion, three coverages were extracted from the DXF file, 'Leases inside the Basin', 'Possible Future Mining', and 'Mining Areas'.
Figure 7: Leased potash resources near the WIPP site. Coordinates are in UTM NAD 27.

boundaries'. The first coverage, 'Leases inside the Delaware Basin', delineates the areas that are leased to mining companies with no determination of whether potash exists in that area or not. However it does contain all areas that have been or are currently being mined. Consequently, this coverage was matched with the second coverage, 'Possible Future Mining' to determine the leased areas that have viable potash resources. The third coverage, 'Mining Boundaries' is a set of one-mile diameter circles around each well drilled for oil and gas exploration. These areas are under control of the oil and gas companies and thus are off limits to potash mining. This means the
Figure 8: Potential potash distribution within WIPP boundary (red). The repository structure is shown in the center. Coordinates are UTM NAD 27.
third coverage is subtracted from the joining of the first two. The result is a new composite coverage that shows the currently mined and future potential mining areas.

Since the potash mining area is located in the Salado Formation, below the Culebra, the areas disturbed by mining activities in the Culebra are larger than shown on the the BLM map due to subsidence-induced angle-of-draw effects. The rationale for determining the extent of these effects is described in Wallace (1996) with the final conclusion stating that an additional 253 m wide 'collar' was to be added to the mining-impacted areas. This is considered a conservative estimation of the angle-of-draw effects. The new delineation is then compared to the 1996 model mining zones to make sure there are no unexplainable differences. The main differences between the CCA map and the current CRA map created here are from recent oil and gas borehole explorations in the area that have ruled out extraction of potash resources. The current modeling domain and mining zones for the full-mining case are shown in comparison to the 1996 delineation in Figure (4). A closeup of the WIPP site and the associated mining zones is shown in Figure (8). The partial-mining case is shown in Figure (5).

The output of this delineation is a file that contains one value for each cell in the grid. A value of 0 is an inactive cell, a value of 1 means the cell lies within a potential mining zone, and a value of 2 means it lies outside a potential mining zone. One file for each scenario, full-mining and partial-mining, is generated, and used as input to the data conversion programs, FM.F and PM.F (Appendices A and B) respectively.

2.7 Subtask 2: Use of Mining Zones in Forward Simulations

The calibration process in Task 4 produces a transmissivity field that minimizes the error between the steady-state and transient head distributions and the calculated distributions using the calibrated field. Since the calibration process does not produce a unique solution, i.e. given a different set of starting transmissivities a different final set of transmissivities may be reached, multiple T-fields are produced and 100 are selected based on the criteria set forth in Beauheim (2003). Each selected T-field is multiplied by its own unique mining scaling factor in areas of potential mining, and MF2K is run to produce the mining-affected head distribution and the cell-by-cell flow budget files. The cell-by-cell flow budget file is used for input to Subtask 3.
To assure repeatability, three different sets of mining factors are used, each set forming a replicate. Thus, for this Task and for each mining scenario (full and partial), 3 sets of 100 mining-altered T-fields are produced. A list of the qualified runs and the corresponding random mining factor for each replicate is listed in Appendix (J).

2.8 Subtask 3: Particle Tracking using DTRKMF

As explained above in Section 2.4, a single particle is tracked from the point \( X = 613,597.5, \ Y = 3,581,385.2 \) (UTM NAD27) to the LWB for each T-field and replicate/scenario combination, using the code DTRKMF. Two outputs are generated from the suite of particle tracks. First are plots showing the individual tracks for all 100 T-fields in each scenario for each replicate (6 plots total). This allows for visual comparison of the prevailing flow directions for the full- and partial-mining scenarios and the qualitative comparison of the variability of the tracking direction. Secondly, cumulative distribution functions (CDF's) are constructed for each replicate and scenario. The CDF's describe the probability that a particle will cross the LWB in a given amount of time. The six plots and the CDF's are presented below in the results section.

3 Modeling Assumptions

Besides assumptions inherent in all modeling exercises (e.g. physical processes can be adequately parameterized and estimated on a numerical grid) there are several assumptions that 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 not dependent on mining. The reasoning for this assumption is described in Section 2.5.

2. It is assumed that the flow-field over the duration of the particle tracking and transport times can be adequately represented by steady-state conditions. This is related to the first assumption in that the boundary conditions are also assumed to remain constant over time. This assumption is necessary since data do not exist that can predict the transient conditions at the site over the time frames involved (>100,000 years).

3. It is assumed that the mining effects can be adequately represented with a single mining factor that increases the transmissivity uniformly
across the potential mining zones within the Culebra. This is directed by EPA regulation 40CFR Part 194, p. 5229 and is assumed adequate for this Task. The regulation is included as an appendix in Wallace (1996).

Other assumptions related to this Task can be found in McKenna and Hart (2003b).

4 Results

The effect of mining on transport in the Culebra is difficult to quantify given the high level of uncertainty in the overall conceptualization and the various input parameters. This uncertainty is addressed by the repetitive nature of the simulations: 100 T-fields are passed from Task 1 of AP-100, and 3 replicates across two different mining scenarios are examined for this Task. However, qualitative conclusions are useful in providing insight as to the impacts of mining and thus the results presented here will concentrate more on the qualitative conclusions of this Task rather than specific deductions.

4.1 Particle Travel Times

For both of the mining scenarios, travel times to the LWB are longer than for the non-mining cases; the median travel times across all 3 replicates for the full- and partial-mining scenarios are approximately 3.61 and 2.64 times greater than for the non-mining scenario, respectively. A plot of the cumulative distribution functions (CDFs) for the full-, partial-, and non-mining scenario's is shown in Figure (9).

Given the increase in transmissivity due to mining, the increase in travel time may seem counter-intuitive. However, upon examination of the head contours and flow patterns of the mining cases, the high transmissivity areas corresponding to the mining zones create preferential pathways through the system. Figure (10) shows the normalized velocity in each cell for the T-field/replicate averaged case for the full-mining scenario. The normalized velocity is the velocity magnitude in each cell divided by the maximum velocity magnitude across the domain. Since the velocity magnitudes are highly skewed, the color bands for Figure (10) are non-uniformly scaled at the high end (i.e. a wider range of velocity magnitudes is used to designate the orange and red bands). This allows for a better qualitative comparison of the
Figure 9: Cumulative distribution function plot of the full-, partial-, and non-mining scenarios for the CRA.

spatial distribution of high and low velocities. 'T-field/replicate averaged' means the transmissivity value for each cell is the average of the transmissivities across all T-field/replicate combinations for the full-mining scenario (300 T-fields in total). Not surprisingly, it is clear that the areas of high velocities correspond with the mining zones. The higher velocities and corresponding higher flow rates through the mining zone areas translate to slower velocities in the non-mining zone areas. In most cases, the particles for the mining-scenarios stay in the lower velocity zones along the entire pathway to the LWB, which accounts for the higher average travel times. A comparison of the median, maximum, and minimum values for the full-, partial-, and non-mining scenario travel times is presented in Table (5).

A comparison to the compliance certification application (CCA) results is useful to provide perspective on the impact of the changes between the CCA
Figure 10: Normalized pore velocities for the full-mining case. Red indicates zones of high velocity. The black lines show the full-mining zones and the red box is the WIPP LWB. The T-field used to produce the velocity profile is averaged across all T-field/replicate combinations for the full-mining scenario (300 T-fields in total).
and the CRA. Figures (11) and (12) show the full- and partial-mining scenarios, respectively, for all three replicates as compared to the CCA results. The CRA travel times are approximately 2.2 and 3.5 times longer for the full- and partial-mining scenarios, respectively, than for the CCA scenarios. This is mainly due to the difference in how the base T-fields are generated. The CCA fields use a categorical simulation technique to capture both high transmissivity (T) and low T regions. In contrast, the CRA fields incorporate more geological understanding, with regions to the west categorized as high T, regions to the east categorized as low T, and the area in between given high or low T on a stochastic basis. This results in significant differences in T in the southern part of the WIPP site. The CCA fields tend towards lower and more uniformly distributed T's in the southwestern portion of the WIPP site, and a high T channel down the southeastern part of the site that leads to shorter travel times than the CRA. The CRA fields show higher T's in the southwestern part of the WIPP site and tend not to have the high T channel in the southeast, causing travel times to increase.

Another interesting point illustrated by Figures (11) and (12) is the similarity between the 3 replicates for the CRA curves. This indicates that the use of 100 T-fields from Task 1 of AP-100 is adequate to capture the mean
Figure 11: Cumulative distribution function plot of the 3 full-mining scenario replicates as compared to the CCA full-mining scenario. An increase in travel time can be seen for the CRA scenarios.

behavior of the mining effects.

4.2 Travel Direction

The effects of mining also have an impact on the direction of transport, significantly changing where the particles cross the LWB. This is especially true of the full-mining scenario where mining within the LWB creates high head along the eastern boundary of the WIPP resulting in a general flow direction to the west-southwest. This is in contrast to the partial-mining scenario where the tracking direction is mainly towards the south, similar to the non-mining scenario. The particle track directions for the full- and
Figure 12: Cumulative distribution function plot of the 3 partial-mining scenario replicates as compared to the CCA partial-mining scenario. An increase in travel time can be seen for the CRA scenarios.

partial-mining scenarios are illustrated in Figures (13) to (18). There is a strong similarity within each replicate for each scenario. Individual tracks can be recognized from one replicate to the next, with some slight variations. This indicates that track directions are determined more by the spatial variation of the calibrated T-field than by the random mining factors. As long as there is some (see below) increase in the mining zone transmissivities over that of the non-mining areas, the tracks for each T-field will be similar from one replicate to the next.

The insensitivity of the track directions to the random mining factor also carries over to insensitivity of the travel time. Correlation analysis shows correlations between travel time and the random mining factor for the full and partial-mining scenarios as 0.091 and 0.151, respectively. Thus, like the
Figure 13: Particle tracks for replicate 1 for the full-mining scenario.

Figure 14: Particle tracks for replicate 2 for the full-mining scenario.
Figure 15: Particle tracks for replicate 3 for the full-mining scenario.

Figure 16: Particle tracks for replicate 1 for the partial-mining scenario.
Figure 17: Particle tracks for replicate 2 for the partial-mining scenario.

Figure 18: Particle tracks for replicate 3 for the partial-mining scenario.
track directions, travel times are not sensitive to the random mining factor but rather to the spatial structure of the calibrated T-field.

This insensitivity to the random mining factor can be explained by recalling that the factor is applied only to zones deemed as probable mining areas. This means that velocity and flow increases are limited to the mining zones, with little change in the non-mining areas (assuming gradients are somewhat constant). Conditions within the non-mining zones are affected most for cases where the mining zone transmissivities are close to the non-mining zone transmissivities. However, the mining factor ranges uniformly from 1-1000 meaning 99% of the T-field/replicate combinations will have multipliers greater than one order of magnitude (for the 300 combinations in this Task, only two have multipliers that are less then 10). This translates into small changes within the non-mining zones for relatively large changes in the mining zones. To illustrate this, Figure (19) shows the $\log_{10}$ travel times versus the random mining factor for the full- and partial-mining scenarios across all replicates. The high scatter in both the plots is due to the independence of travel time with regards to the mining factor. This conclusion supports the mining scenario conceptual model and the use of a random mining factor to model changes in transmissivity due to mining activities. It also indicates that the controlling parameters are the spatial distribution of the non-mining scenario T-field and the delineation of the mining and non-mining zones.

### 4.3 Extreme Values

Examination of the extreme travel time values, and the causes behind those values, is useful in quantifying the range of outcomes given the amount of uncertainty incorporated into the models. For the full-mining scenario, T-field d04r01 from replicate 2 had the longest travel time of 3,387,185 years. In contrast, T-field d01r07 from replicate 2 had the shortest travel time of 611 years. The median travel time (66,215 years) is best represented by T-field d10r09 in replicate 1. Figures 20 to 22 show the head contours for each of these cases along with the corresponding particle track. What distinguishes the plots is the head distribution across the regions. For the slow case (Figure (20)) the head contours to the west of the repository are spread far apart, indicating a low gradient and thus lower groundwater velocities. The fastest case (Figure (21)) shows a high-gradient band that originates along the no-flow boundary to the northwest and runs down the western side of the WIPP site. This high gradient corresponds to higher groundwater velocities. The
Figure 19: Correlation between the random mining factor and Log-travel time.
median case (Figure (22)) also shows this high-gradient band but it is not as extreme as in the fast case. In all cases, the mining-zone areas look very similar, with widely spaced head contours and higher velocities relative to the non-mining zones.

The partial-mining cases have similar characteristics to that of the full-mining cases (Figures 23 to 25) except that the band of high gradient to the northwest is more pronounced and persistent. The slowest partial-mining T-field is d04r01 (Figure (23)) from replicate 2 (531,136 years), the fastest is d08r01 (Figure (24)) from replicate 3 (4,603 years), and the median is best represented by d01r04 (Figure (25)) from replicate 1 (48,472 years). The particle tracking directions are more similar between each other in the partial-mining case than in the full-mining cases. Overall, for both the full and partial-mining scenarios, those T-fields that contain higher and more heterogeneous transmissivities in the non-mining areas produce the fastest travel times. However, the partial-mining scenario shows a smaller range of values due to the lack of the large mining zone in the WIPP area. This smaller range is clearly visible in Figure (19).
Figure 20: Head contours and particle track for the maximum travel time T-field (d04r01-R2) for the full-mining case. The WIPP boundary is the red box in the center of the figure and the particle track is the blue track originating from the approximate center of the WIPP.
Figure 21: Head contours and particle track for the minimum travel time T-field (d01r07-R2) for the full-mining case. The WIPP boundary is the red box in the center of the figure and the particle track is the blue track originating from the approximate center of the WIPP.
Figure 22: Head contours and particle track for the median travel time T-field (d10r09-R1) for the full-mining case. The WIPP boundary is the red box in the center of the figure and the particle track is the blue track originating from the approximate center of the WIPP.
Figure 23: Head contours and particle track for the maximum travel time T-field (d04r01-R2) for the partial-mining case. The WIPP boundary is the red box in the center of the figure and the particle track is the blue track originating from the approximate center of the WIPP.
Figure 24: Head contours and particle track for the minimum travel time T-field (d08r01-R3) for the partial-mining case. The WIPP boundary is the red box in the center of the figure and the particle track is the blue track originating from the approximate center of the WIPP.
Figure 25: Head contours and particle track for the median travel time T-field (d01r04-R1) for the partial-mining case. The WIPP boundary is the red box in the center of the figure and the particle track is the blue track originating from the approximate center of the WIPP.
5 Summary

This Task (Task 5) of AP-088, Analysis Plan for Evaluation of the Effects of Head Changes on Calibration of Culebra Transmissivity Fields, investigates the impact of the increase in transmissivity in the Culebra due to potash mining in and around the WIPP regional area. To accomplish this investigation, two categories of mining-impacted transmissivity fields are modeled: one with mining outside the land withdrawal boundary (LWB) only and the other with regions both inside and outside the LWB mined (partial and full-mining scenario's, respectively).

The impacts are modeled by scaling each calibrated T-field passed from Task 1 of AP-100 in regions deemed to contain economically-extractable potash resources by a random factor between 1 and 1000. A forward steady-state flow model is run for each new T-field under each mining scenario (full and partial) across three replicates, resulting in 600 simulations (there are 100 calibrated T-fields from Task 1 of AP-100). Particle tracking is performed on the modified flow fields to determine the flow path and groundwater travel time from a point above the center of the WIPP disposal panels to the LWB. Cumulative probability distribution functions (CDF) are produced for each mining scenario and compared to the undisturbed scenario generated from Task 4 of AP-088, as well as to the full- and partial-mining scenarios from the 1996 CCA. The CDF's describe the probability of a conservative tracer reaching the LWB at a given time. In addition to comparing travel times, particle tracking directions are also examined to determine the effect on the regional flow direction in the WIPP area due to mining. The flow fields generated from the mining scenarios are then refined and passed to Task 6 of AP-100 that performs radionuclide transport modeling in the Culebra.

Results show that for both the full- and partial-mining scenarios, the median particle travel times of 66,215 and 48,472 years are 3.61 and 2.64 times longer than for the non-disturbed case (18,289 years). The increase in transmissivity due to mining in the potential mining zones increases the relative flow rate through these zones, with a corresponding decrease in flow through the non-mining zones. This decrease in flow through the non-mining zones accounts for the longer travel times in the two mining scenarios. Comparing the full- and partial-mining scenarios from the CRA to the CCA, the median travel times are approximately 2.2 and 3.5 times longer, respectively, for the CRA scenarios. This is due to the difference in how the base T-fields are generated between the CCA and the CRA. The CCA fields use a categori-
cal simulation technique to capture both high transmissivity (T) and low T regions while the CRA fields incorporate more geological understanding and stochastic factoring of uncertainty. The net result is longer travel times to the LWB.

No correlation was found between the travel time or the flow direction to the random mining factor. This indicates that even small increases (≈2 - 5 times) in transmissivity in the mining zone areas are enough to shift the regional flow from a non-mining gradient to a mining gradient. As the mining factor is increased beyond that point (298 out of 300 mining factors are greater than 10) the flow rate and velocities in the mining zones also increase, but with little impact on the non-mining zones or the regional flow directions.
References


cation, AP-100, Revision 0. Carlsbad, NM: Sandia National Laboratories. ERMS # 530172.


Wallace, M. G., 1996. Record of FEP screening work, FEP ID# NS-11: Subsidence associated with mining inside or outside the controlled area. ERMS #240816.


Appendix A: Full Mining Conversion Code, FM.F

Conversion program for full mining case. This program reads two data sets:
1. Update.mod and full.mining.dat. Update.mod contains the calibrated t-fields
   from Task 4. Full.mining.dat is a digitized file consisting of a single integer
   for each cell in the grid: 0 - inactive, 1 - mining zone, 2 - non-mining zone.
   The transmissivities in the mining areas are then multiplied by a random number
   between 1 and 1000 to simulate the random increase in transmissivity caused by
   mining disturbance. The new t-field values are output to an ascii file for input
   to MODFLOW. Two other parameter files are read, Good_runs.txt and R*_.txt.
   Good_runs.txt contains the list of calibrated T-fields from Task 4 and
   R*_.txt contains the random mining factors for each replicate. R* is either
   R1, R2, or R3, depending on the replicate number.

Variable list:
- dx,dy = cell dimension in the x and y directions
- nx,ny = number of cells in the x and y directions
- imeine = input array of mining, non-mining, and inactive zones
- trans = input array of calibrated t-field from Task 4
- rnum = input variable of random mining multiplier
- file3a = name of mining zone input file
- file3b = name of replicate file
- file3 = name of finished run file
- file2a = name of finished run
- file5a = name of random mining factor input file
- file5 = name of t-field input file
- file6a = name of modified t-field output file
- path1 = name of local directory
- path2 = name of remote t-field directory
- path2a = path1 + "full" + "full" + "full" + file2a + file6
- path2a = path2 + file2a + file6

5/7/03 - Thomas S Lowery | Modified 6/27/03, 8/12/03 - TSL

PROGRAM FM_Main
PARAMETER(dx=100,dy=100,nx=224,ny=307)
INTEGER imein(nx,ny)
REAL trans(nx,ny),rnum(100)
REAL mio_mhd(nx,ny),mis_mhd(nx,ny)

CHARACTER=40 file1,file2,filo2a,filo3,filo6,filo6
CHARACTER+12 fname,fil2
CHARACTER=55 path1,path2,path1f2a,path22a
CHARACTER=2 rep

!Input file names
DATA filei/"Full.mining.dat"/
DATA file2/"Good_runs.txt"/
DATA file5/"Update.mod"/
DATA file6/"CMine.mod"/
DATA path2/"/home3/tsovy/wipp/data/"

!Get replicate number
READ(*,*)rep
file3=lat/"rep/".txt"

!Set base path
path1=lat/home3/tsovy/wipp/mining/"/rep/*"
!Open mining file and read mining zones
OPEN(i1,file=TRIM(file1),status='old')
DO j=1,ny
   READ(i1,*)((imine(i,j),i=1,nx)
END DO
CLOSE(i1)

!Open file of finished t-field calibration runs
OPEN(i2,file=TRIM(AJUSTL(file2)),status='old')

!Read random mining factor
OPEN(i3,file=TRIM(AJUSTL(file3)),status='old')
DO i=1,istop
   READ(i3,*)idmb,rnum(i)
END DO

!Read each finished t-field run, if end of file, go to end
DO ifinished=1,1000
   READ(12,'(a5)'),END=5000,FILE=file2a
   OPEN(i6,file=TRIM(AJUSTL(file2a)),status='old')
   DO j=1,ny
      READ(i6,11)(trans(i,j),i=1,nx)
   END DO
   CLOSE(i6)
   END DO

!Open calibrated t-field file and read in transmissivitias
!Note: cell counting is based on MODFLOW grid, i.e. x-direction
!is left to right and y-direction is top to bottom.
!Multiply transmissivity field within the mining zones by random coefficient
DO i=1,ny
   IF(imine(i,j).eq.1)THEN
      trans(i,j)=trans(i,j)*rnum(ifinished)
   ENDIF
END DO
END DO

!Output new transmissivity field
pathf2a6=TRIM(pathf2a6)//full"//TRIM(AJUSTL(file2a))""//TRIM(AJUSTL(file6))
OPEN(i6,file=pathf2a6,status='unknown')
DO j=1,ny
   WRITE(i6,41)(trans(i,j),i=1,nx)
END DO
CLOSE(i6)
END DO

!Format declarations
11 FORMAT(224e12.5)
FORMAT(23413)
FORMAT(234e12.5)
END
Appendix B: Partial Mining Conversion Code, PM.F

Conversion program for partial mining case. This program reads two data sets, Tupdate.mod and full_mining.dat. Tupdate.mod contains the calibrated t-fields from Task 4. Partial_mining.dat is a digitized file consisting of a single integer array for each cell in the grid: 0 - inactive, 1 - mining zone, 2 - non-mining zone. The transmissibilities in the mining areas are then multiplied by a random number between 1 and 1000 to simulate the random increase in transmissivity caused by mining disturbance. The new t-field values are output to an ascii file for input to MODFLOW. Two other parameter files are read, Good_runs.txt and mfr*.txt. Good_runs.txt contains the list of calibrated t-fields from Task 4 and mfr*.txt contains the random mining factors for each replicate. R* is either R1, R2, or R3, depending on the replicate number.

Variable list:

| dx, dy = cell dimension in the x and y directions |
| nx, ny = number of cells in the x and y directions |
| imine = input array of mining, non-mining, and inactive zones |
| trans = input array of calibrated t-field from Task 4 |
| rnum = input variable of random mining multiplier |
| file1 = name of mining zone input file |
| file2 = name of replicate file |
| file2a = name of finished run file |
| file3 = name of random mining factor input file |
| file4 = name of t-field input file |
| file5 = name of modified t-field output file |
| path1 = name of local directory |
| path2 = name of remote t-field directory |
| path2a5 = path1 + "full" + file2a + file6 |
| path2a5 = path2 + file2a + file6 |

6/7/03 - Thomas S Loury! Modified 6/27/03, 8/12/03 - TSL

PROGRAM PM_Main
PARAMETER(dx=100, dy=100, nx=224, ny=307)
INTEGER imine(nx,ny)
REAL trans(nx,ny), rnum(100)
REAL no_min(nx,ny), min_hd(nx,ny)
CHARACTER*40 file1, file2, file2a, file3, file5, file6
CHARACTER*12 fname, filz
CHARACTER*55 path1, path2, path2a5, path2a5
CHARACTER*3 realize
CHARACTER*2 rep

!Input file names
DATA file1/"Part_mining.dat"/
DATA file2/"Good_runs.txt"/
DATA file4/"Tupdate.mod"/
DATA file5/"Chine.mod"/
DATA path2/"/wipp/data/"

!Get replicate number
READ(*,*) rep
reada mũi*\"\"/rep\"\".txt

!Set base path
path1="/home3/tsloury/wipp/mining/"/rep/"/"
Open mining file and read mining zones
OPEN(11,FILE=TRIM(file1),STATUS='OLD')
DO j=1,ny
  READ(11,*) (imine(i,j),i=1,nx)
END DO
CLOSE(11)

Open file of finished t-field calibration runs
OPEN(12,FILE=TRIM(ADJUSTL(file2)),STATUS='OLD')

Read random mining factor
OPEN(13,FILE=file3,STATUS='OLD')
DO i=1,istop
  READ(13,*) idumb,rnum(i)
END DO

Read each finished t-field run, if end of file, go to end
DO ifinished=1,1000
  READ(12,'(A6)'),END=5000)file2a
END DO

Open calibrated t-field file and read in transmissivities
Note: cell counting is based on MODFLOW grid, i.e. x-direction
1s left to right and y-direction is top to bottom.
path22a5=TRIM(ADJUSTL(path2))/TRIM(ADJUSTL(file2a))//
&     TRIM(ADJUSTL(file5))
OPEN(15,FILE=path22a5,STATUS='OLD')
DO j=1,ny
  READ(15,11)(trans(i,j),i=1,nx)
END DO
CLOSE(15)

Multiply transmissivity field within the mining zones by random coefficient
DO j=1,ny
  DO i=1,nx
    IF(imine(i,j).EQ.1) THEN
      trans(i,j)*=trans(i,j)*rnum(ifinished)
    ENDIF
  END DO
END DO

Output new transmissivity field
path22a5=TRIM(path2)="/partial"/TRIM(ADJUSTL(file2a))//
&     TRIM(ADJUSTL(file5))
OPEN(16,FILE=path22a5,STATUS='UNKNOWN')
DO j=1,ny
  WRITE(16,41)(trans(i,j),i=1,nx)
END DO
CLOSE(16)

FORMAT declarations
11 FORMAT(224E12.5)
21 FORMAT(224F13)
41 FORMAT(224E12.5)
5000 STOP
END
Appendix C: Grid Refinement Code, REFINE.F

This program reads in calibrated t-field from Task 4 and refines the grid to 50x50m cell size. The new t-field is used as input for MODFLOW and subsequent input to SEGCNP.

Program assumes original grid size is 100x100m.

PARAMETER(nx=224, ny=307, nxn=448, any=614, dOld=100, dNew=50)
REAL tOld(nx,ny), tNew(mn,ny)

CHARACTER*40 file1,file2,file3,file4,file5
CHARACTER*12 frame,filz
CHARACTER*50 path1,path2,path3,path4,path5
CHARACTER*3 realize
CHARACTER*2 rap

! Get replicate number
READ(*,*) rap

! Set base path
path4='~/home3/tlowry/wipp/mining'/"rap/"/

! Open file of finished t-field calibration runs
OPEN(11,file=TRIM(ADJUSTL(file3)),status='old')

! Read each finished t-field run, if end of file, go to end
DO ifinished=1,1000
READ(11,'(a6)'),END=100)path2
END DO

! Extract realization number from directory naming convention
DO is=1,2
IF(is.eq.1)THEN
path3=TRIM(path4)/"full"/
ELSE
path3=TRIM(path4)/"partial"/
ENDIF

! Go to directory with finished t-field
OPEN(12,file=TRIM(path3)/TRIM(ADJUSTL(path2))/"/
& TRIM(ADJUSTL(file1)),status='old')

! Read in calibrated t-field
DO j=1,ny
READ(12,'(2(24E32.5*))')(tOld(i,j),i=1,nx)
END DO
CLOSE(12)

! Transfer old values to new grid
DO jm=1,ny
DO jin=1,nx
i=1+INT((jin-1)*dNew/dOld)
j=1+INT((jm-1)*dNew/dOld)

INFORMATION ONLY
thNew(in,jn)=Old(io,jn)
END DO
END DO

!'Output to new file
OPEN(13, file=TRIM(path3)//TRIM(AJUSTL(path2))//
  ""//TRIM(AJUSTL(file2)), status='unknown')
DO jn=1, nyn
  WRITE(13, '(44B102.5)') (thNew(in,jn), in=1, max)
END DO
CLOSE(13)
END DO
END DO
100 STOP
END
Appendix D: Binary to ASCII Conversion: BA.F

!Program to convert MODFLOW flow budget binary file to ASCII format.

PROGRAM AscllBud
PARAMETER (nx=648, ny=614, nsflx=mx*ny)

REAL qx(nx,ny), qy(nx,ny)
REAL xhumb
CHARACTER*40 file1, file2, file2a, file3, mine
CHARACTER*68 path1, path2, path2a, path2a3
CHARACTER*16 text
CHARACTER*2 rep(3)
INTEGER kstp, kper, ncol, nrow, nlay, nlist, imeth
REAL delt, pertim, totim

!Input file names
DATA filel//‘steady50x50.bud’/
DATA file2//‘Good.runs.trtm4’/
DATA file3//‘steady50x50.ascii.dat’/
DATA path2//‘/h/uipp/dat.’/
DATA rep//‘R1’, ‘R2’, ‘R3’/

DO ir=1,3

!Assign base path
path=’/home3/talowry/uipp/mineing’/’/rep(ir)’/

!Open file of finished t-field calibration runs
OPEN(2, file=TRIM(ADJUSTL(file2)), status=’old’)

!Read each finished t-field run, if end of file, go to end
DO ifinished=1,1000
READ(2, ’(a6)’, END=6000) file2a
mine=’full’
DO imine=1,2
IF(mine.eq.2)mine=’partial’/
!Read in cell-by-cell flow file
pathf2a=TRIM(path1))/TRIM(ADJUSTL(mine))//
& TRIM(ADJUSTL(file2a))//
& ’/’/TRIM(ADJUSTL(file1))

!Read volumetric flow field in m3/sec from MODFLOW *.ccf file.
!Flow across right face is the flow between cell i,j and i+1,j
!Flow across front face is the flow between cell i,j and i,j-1
!using column (i), row (j), counting in this model

OPEN(13, file=pathf2a, status=’old’, form=’unformatted’)
DO i=1,3
20 READ(13, END=25) kstp, kper, text, ncol, nrow, nlay
READ(13) itemp, delt, pertim, totim
IF(TRIM(ADJUSTL(text)).eq. ‘CONSTANT HEAD’) THEN
READ(13) nlist
DO im=1, nlist
READ(13) xhumb
END DO
END

INFORMATION ONLY
ELSEIF(TRIM(ADJUSTL(text)).eq."FLOW FRONT FACE")THEN
READ(13)qy
ELSEIF(TRIM(ADJUSTL(text)).eq."FLOW RIGHT FACE")THEN
READ(13)qx
ENDIF
END DO

!GOTO 20
25  CLOSE(13)

! Open file for ASCII output
pathif2a2=TRIM(path1)'/TRIM(ADJUSTL(mine))'/
 & TRIM(ADJUSTL(file2a2))/
 & '/TRIM(ADJUSTL(file3))
OPEN(15, file=pathif2a2, status='unknown')
DO j=1,ny
  WRITE(15,150)(qx(i,j),i=1,nx)
END DO
WRITE(15,*)
DO j=1,ny
  WRITE(15,150)(qy(i,j),i=1,nx)
END DO
CLOSE(15)
END DO
END DO
5000 CONTINUE
CLOSE(2)
END DO

150 FORMAT(4d8e16.8)
STOP
END
Appendix E: Particle Tracking Post-processing, PTOUT.F

The program reads in each DTRKHF output file and combines the results into one file for post processing in EXCEL. Output is two separate files, one for full mining case and the other the partial mining case.

16/16/03 - Thomas S Lowry

PROGRAM PTOUT_Half
PARAMETER(runs=200, times=1000)
REAL*8 dtimes(times,runs), xd(times,runs), yd(times,runs)
INTEGER etime(runs), xrc
CHARACTER*30 path
CHARACTER*18 finished(runs), file1
CHARACTER*6 fin
CHARACTER*7 mine
CHARACTER*2 rep(3)

DATA file1("Replicates.txt")/
DATA rep("R1","R2","R3")/

DO ir=1,3
!
  Set base path
  path1="/home/tslowry/wipp/mining"/rep(ir)="/\%ptout/

dtimes=999
xd=-998
yd=777
xrc=0

DO ip=1,2
!
    IF(ip.eq.1)THEN
    mine="full"
    ELSE
    mine="partial"
    ENDIF

    OPEN(1,FILE='Good-runs.txt',STATUS='OLD')

    DO jr=1,runs
      READ(1,*,END=100)fin
      xrc=xrc+1
      finished(xrc)=fin//"="//TRIM(ADJUST(etime))//"out"
      OPEN(3,FILE=path1//TRIM(ADJUST(finished(xrc))),
        STATUS='OLD')
      READ(3,*,END=1000)dtimes(1,xrc),tempx,tempy,
        xd(1,xrc),yd(1,xrc)

    END DO

200 CONTINUE
CLOSE(3)
END DO

100 CONTINUE
CLOSE(1)
END DO

OPEN(2,FILE=path1//"ptout.out",STATUS='UNKNOWN')
OPEN(13,FILE=path1//"times.out",STATUS='UNKNOWN')

INFORMATION ONLY
DO ip=1,2
   WRITE(2,20)(finished(j),j=(ip-1)*xrc/2+1,xrc/2+(ip-1)*xrc/2)
   DO i=1,times
      WRITE(2,21)(ctime(i,j),xd(i,j),yd(i,j),
                  j=(ip-1)*xrc/2+1,xrc/2+(ip-1)*xrc/2)
   END DO
   WRITE(2,=)
END DO

DO j=1,xrc
   DO i=1,times
      IF(ctime(i,j).lt.0)THEN
         WRITE(13,33)(finished(j),ctime(i-1,j))
         EXIT
      ENDIF
   END DO
END DO
END

20 FORMAT(100a48)
21 FORMAT(100(x16.6))
33 FORMAT(a13,f15.5)

5000 STOP
END
Appendix F: Particle Tracking Post-processing, PTPLOT.F

The program reads in each DYNOMF output file and combines the results into one file for post processing in EXCEL. Output is two separate files, one for the full mining case and the other the partial mining case.

16/16/03 - Thomas S Lowry

```fortran
PROGRAM PTPLOT_Main
PARAMETER(runs=200, times=1000)
REAL*8 xd(times, runs), yd(times, runs)
INTEGER itime, xrc
CHARACTER*36 path1
CHARACTER*18 finished(runs)
CHARACTER*6 fin
CHARACTER*7 mine
CHARACTER*2 rep(3)

DATA rep/'R1', 'R2', 'R3'/

DO ir=1,3
  ! Set base path
  path1='/home3/tslowry/app/mining/''rep(ir)/''/''ptout/''
  
  dtime=999
  xd=601700
  yd=3687200
  xrc=0

  DO ip=1,2
    IF(ip.eq.1)THEN
      mine='full'
    ELSE
      mine='partial'
    ENDIF
    DO j=1,runs
      READ(j,*)finished(xrc)+fin
      xrc=xrc+1
      OPEN(j,FILE='Good_runs.txt',STATUS='OLD')
      DO k=1,itime
        READ(k,*)tempo,itime
        READ(3,*)tempo,itime
    CONTINUE
    CLOSE(3)
    CONTINUE
  END DO

200 CONTINUE
CLOSE(3)
END DO

100 CONTINUE
CLOSE(1)
END DO

OPEN(2,FILE=path1//''plot.out'',STATUS='UNKNOWN')

DO ip=1,2
  WRITE(2,20)(finished(j), j=(ip-1)*xrc/2+1, xrc/2*(ip-1)*xrc/2)
END DO
```

62
DO i=1, times
  WRITE(2,21)(xd(i,j)+6e1700,3597200-ys(i,j)),
  j=(ip-1)*xrc/2+1,xrc/2+(ip-1)*xrc/2
END DO
WRITE(2,*)
END DO
END

20 FORMAT(100a32)
21 FORMAT(100(2f16.3))
5000 STOP
END
Appendix G: Linux Shell Script: MINING.SH

```bash
# For Task 5 of AP-088 and Tasks 2 and 3 of AP-100
# THISDIR is equal to: '/home3/tsworby/vipp/mining'
THISDIR='pwd'
SIDIR=THISDIR/100x100
SIDIR=THISDIR/50x50
MINDIR=/home2/vipp/data
SCENARIO="full partial"
REPLICAT='cat Replicate.txt'
FINISHED='cat Good_runs.txt'

# Loop through each replicate
for rep in $REPLICAT
    do
        cd ../$rep

        # Loop through the full and partial mining scenarios
        for scn in $SCENARIO
            do
                cd ../$scn
                echo 'Writing files to $rep/$scn directory.'

                # Loop through each realization
                for Run in $FINISHED
                    do
                        snake directory and copy steady-state files
                        mkdir ./Run
                        cd ./Run
                        cp $SIDIR/culebra.top ./fort.33
                        cp $SIDIR/culebra.bot ./fort.34
                        cd ..
                        done
                        cd $THISDIR/$rep
                    done
                    cd $THISDIR

                    echo 'Executing fm'
                    echo $rep | fm
                    echo 'Executing pm'
                    echo $rep | pm
                    echo 'Executing refine'
                    echo $rep | refine
                done
            done

        # Loop through full and partial mining scenarios and run MODFLOW and DTRKHF for AP-088 and MODFLOW for AP-100
        for scn in $SCENARIO
            do
                cd ../$scn

                for Run in $FINISHED
                    do
                        #...
                    done
            done
        done
```
cd ./$Run
mf2k $SIDIR/steady.nam
echo 'Finished with MF2K 100x100 in' $rep/$scn/$Run
dtrkmf < $SIDIR/dtrkmf.in
echo 'Finished with DTRKM in' $rep/$scn/$Run
rm fort.33
rm fort.54
mf2k $SIDIR/steady.nam
echo 'Finished with MF2K 50x50 in' $rep/$scn/$Run
rm *.bed
rm *.lat
cd ...
done
cd $THISDIR/$rep
done
cd $THISDIR
done
cd $THISDIR

#Move dtrkmf output files to common directory
sh post.sh
#Combine dtrkmf output to two separate files (full and part)
echo 'Running pout'
pout
#Put all X-Y Coordinate pairs into one file for plotting purposes
echo 'Running ptplot'
ptplot
#Create ASCII budget file from MODFLOW binary output
echo 'Executing ASCII conversion program: ba'
ba
#Move all ASCII budget files to one directory for easy ftp
sh post-flow.sh
#Finished!
echo 'Finished!'
Appendix H: Linux Shell Script: POST.SH

# This script is to collect the DTRKMF output for each realization into a single directory to allow for easier access when post-processing. Each replicate directory will contain a sub-directory called 'ptout' that holds all the files.

#THISDIR = '/home3/clevery/wipp/mining'

THISDIR='pwd'
SCENARIO="full partial"
REPLICATE='cat Replicate.txt'
FINISHED='cat Good_runs.txt'

# Loop through each replicate for rep in $REPLICATE do
# Make particle tracking output directory
mkdir ./$rep/ptout

# Loop through the full and partial mining scenarios for scn in $SCENARIO do
# Loop through each realization, get each particle tracking output, and copy to output directory
for Run in $FINISHED do
    cp ./$rep/$scn/$Run/dtrk.out ./$rep/ptout/$Run-$scn.out
done
done
Appendix I: Linux Shell Script: POST-FLOW.SH

#This script collects the ASCII flow budget file
#produced by ba.f within each realization directory
#and places them in a single directory called 'aff'.

THISDIR="pwd"
SCENARIO="f p"
REPLICATE="cat Replicate.txt"
FINISHED="cat Good_runs.txt"

for rep in $REPLICATE
  do
    #Make ASCII flow-file output directory
    mkdir ./rep/aff

    #Loop through the full and partial mining scenarios
    for scn in $SCENARIO
      do
        #Designate directory
        if test $scn = p
          then
            scdir=partial
          else
            scdir=full
          fi

        #Loop through each realization
        for Run in $FINISHED
          do
            #Get each particle tracking output and copy to output directory
            cp ./rep/$scdir/$Run/steady50x50_ascii.dat ./rep/aff/$Run$scn$rep.out
            rm ./rep/$scdir/$Run/steady50x50_ascii.dat
          done
      done
  done
## Appendix J: Qualified Runs and Random Mining Factors

Qualified runs and random mining factors for each replicate.

<table>
<thead>
<tr>
<th>Run</th>
<th>E1</th>
<th>E2</th>
<th>E3</th>
</tr>
</thead>
<tbody>
<tr>
<td>d01r02</td>
<td>905.50</td>
<td>31.85</td>
<td>12.54</td>
</tr>
<tr>
<td>d01r04</td>
<td>508.40</td>
<td>345.70</td>
<td>202.20</td>
</tr>
<tr>
<td>d01r07</td>
<td>340.30</td>
<td>696.60</td>
<td>936.30</td>
</tr>
<tr>
<td>d01r10</td>
<td>615.20</td>
<td>322.70</td>
<td>391.30</td>
</tr>
<tr>
<td>d02r02</td>
<td>675.30</td>
<td>579.30</td>
<td>306.80</td>
</tr>
<tr>
<td>d03r01</td>
<td>204.00</td>
<td>760.50</td>
<td>935.90</td>
</tr>
<tr>
<td>d03r03</td>
<td>94.90</td>
<td>514.90</td>
<td>77.79</td>
</tr>
<tr>
<td>d03r06</td>
<td>91.30</td>
<td>187.60</td>
<td>238.40</td>
</tr>
<tr>
<td>d03r07</td>
<td>630.50</td>
<td>567.10</td>
<td>725.20</td>
</tr>
<tr>
<td>d03r08</td>
<td>203.90</td>
<td>475.90</td>
<td>85.67</td>
</tr>
<tr>
<td>d03r09</td>
<td>769.30</td>
<td>750.00</td>
<td>647.80</td>
</tr>
<tr>
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<td>130.20</td>
<td>630.30</td>
<td>478.70</td>
</tr>
<tr>
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<td>351.90</td>
<td>483.30</td>
<td>996.70</td>
</tr>
<tr>
<td>d04r03</td>
<td>46.40</td>
<td>146.00</td>
<td>122.90</td>
</tr>
<tr>
<td>d04r04</td>
<td>149.60</td>
<td>487.90</td>
<td>217.30</td>
</tr>
<tr>
<td>d04r05</td>
<td>208.90</td>
<td>493.60</td>
<td>138.30</td>
</tr>
<tr>
<td>d04r06</td>
<td>264.40</td>
<td>584.00</td>
<td>895.30</td>
</tr>
<tr>
<td>d04r07</td>
<td>931.50</td>
<td>723.90</td>
<td>802.00</td>
</tr>
<tr>
<td>d04r08</td>
<td>897.30</td>
<td>51.00</td>
<td>96.80</td>
</tr>
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<td>d04r10</td>
<td>32.66</td>
<td>256.50</td>
<td>34.92</td>
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<td>364.10</td>
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<td>189.00</td>
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<td>908.20</td>
<td>525.90</td>
<td>145.50</td>
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<td>d06r02</td>
<td>790.00</td>
<td>679.40</td>
<td>856.70</td>
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<tr>
<td>d06r03</td>
<td>384.10</td>
<td>171.20</td>
<td>261.20</td>
</tr>
<tr>
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<td>265.50</td>
<td>856.00</td>
<td>293.90</td>
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<td>832.00</td>
<td>734.10</td>
<td>297.60</td>
</tr>
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<td>d06r06</td>
<td>10.02</td>
<td>653.20</td>
<td>172.50</td>
</tr>
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<td>d06r07</td>
<td>514.10</td>
<td>211.50</td>
<td>915.60</td>
</tr>
<tr>
<td>d06r10</td>
<td>262.90</td>
<td>70.11</td>
<td>861.40</td>
</tr>
<tr>
<td>d07r01</td>
<td>927.30</td>
<td>694.20</td>
<td>625.20</td>
</tr>
<tr>
<td>d07r02</td>
<td>621.30</td>
<td>894.30</td>
<td>737.80</td>
</tr>
<tr>
<td>d07r05</td>
<td>338.40</td>
<td>775.30</td>
<td>341.60</td>
</tr>
<tr>
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<td>450.20</td>
<td>591.70</td>
<td>848.70</td>
</tr>
<tr>
<td>d07r07</td>
<td>609.60</td>
<td>447.20</td>
<td>841.08</td>
</tr>
<tr>
<td>d07r08</td>
<td>557.70</td>
<td>942.30</td>
<td>349.00</td>
</tr>
<tr>
<td>d07r09</td>
<td>528.60</td>
<td>66.94</td>
<td>265.00</td>
</tr>
<tr>
<td>d07r10</td>
<td>715.80</td>
<td>370.60</td>
<td>187.30</td>
</tr>
<tr>
<td>d08r01</td>
<td>449.30</td>
<td>408.40</td>
<td>194.00</td>
</tr>
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<td>d08r02</td>
<td>569.70</td>
<td>789.70</td>
<td>983.70</td>
</tr>
<tr>
<td>d08r03</td>
<td>419.60</td>
<td>45.16</td>
<td>356.30</td>
</tr>
<tr>
<td>d08r04</td>
<td>100.00</td>
<td>684.00</td>
<td>887.00</td>
</tr>
<tr>
<td>d08r05</td>
<td>971.90</td>
<td>661.10</td>
<td>571.60</td>
</tr>
<tr>
<td>d08r06</td>
<td>118.60</td>
<td>588.90</td>
<td>743.26</td>
</tr>
<tr>
<td>d08r07</td>
<td>741.30</td>
<td>130.20</td>
<td>706.78</td>
</tr>
<tr>
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<td>729.70</td>
<td>497.00</td>
<td>429.30</td>
</tr>
<tr>
<td>d09r03</td>
<td>483.00</td>
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