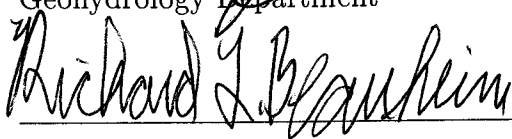# Analysis Report
Tasks 2 & 3 of AP-100: Grid Size Conversion and Generation of SECOTP2D Input
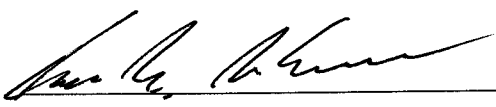
(AP-100: Analysis Plan for Calculations of Culebra
Flow and Transport: Compliance Recertification Application)

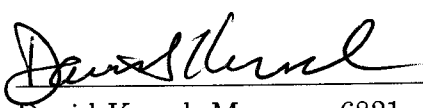Task Number 1.4.1.1, ERMS #531137

Report Date: October 13, 2003

Author: _____ Date: 10/13/03
Thomas S. Lowry, 6115
Geohydrology Department

Technical Review: _____ Date: 10/20/03
Richard L. Beauheim, 6822
Repository Performance Dept.

_____ Date: 10/13/03
Sean A. McKenna, 6115
Geohydrology Department

QA Review: _____ Date: 10/20/03
Mario Chavez, 6820
Carlsbad Programs Group

Management Review: _____ Date: 10/20/03
David Kessel, Manager 6821
Performance Assessment and Decision Analysis Dept.

WIPP:1.4.1.1:PA:QA-L:DPRP1:531035

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1 Introduction

This analysis report describes the activities of Tasks 2 and 3 of AP-100, "Analysis Plan for Calculation of Culebra Flow and Transport: Compliance Recertification Application" (Leigh et al., 2003).

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 re-certification every five years after the initial receipt of waste. The re-certification 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). The tasks outlined in this report are part of the CRA-PA.

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

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larger Salado Formation (Ramsey et al., 1996). It is hypothesized that subsidence of the Culebra due to mining extraction causes fracturing and unconsolidation 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.

AP-088 (Beauheim, 2002) develops calibrated transmissivity fields (T-fields) for the Culebra based on transient hydraulic-response data (Task 4 of AP-088) and examines the effects of potash mining on those T-fields (Task 5 of AP-088). The purpose of Tasks 2 and 3 of this report is to refine the 100x100 m uniform cell size grid used for AP-088 to a grid with a 50x50 m uniform cell size. Task 3 produces the mining-affected flow-fields on the refined grid for use in Tasks 4 through 6 of AP-100 (Task 4 extracts a subset of the refined flow field, Task 5 scales the results for climate change, and Task 6 performs radionuclide transport modeling in the Culebra using the modified flow-field).

1.3 Outline

This report documents the methods, software, input and output files used to complete Tasks 2 and 3 of AP-100. The sections of this report and a brief description of each subsection are:

Section 2: Approach
> Describes the methodology used in Tasks 2 and 3.
> > **2.1: Software;** Describes the software usage and information flow between programs.
> > **2.2: File Naming Convention;** Describes the file naming conventions and the input and output files for each program.

Section 3: Assumptions
> Summarizes the major assumptions of Tasks 2 and 3.

Section 4: Summary
> Presents a brief summary of this report.

2 Approach

To help with efficiency, the steps necessary to complete Tasks 2 and 3 are combined with those of Task 5 of AP-088 (Lowry, 2003). The purpose of

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Task 5/AP-088 is to evaluate the effects of future potash mining on flow and transport in the Culebra. Specifically, Task 5/AP-088 investigates two categories of transmissivity fields: one that limits mining to outside the land withdrawal boundary (LWB) and the other that includes mining both inside and outside the LWB (partial- and full-mining scenario's, respectively). The impacts of mining are accounted for by scaling each calibrated T-field from Task 4/AP-088 (McKenna and Hart, 2003) 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), for three replicates of mining factors, resulting in 600 simulations (there are 100 calibrated T-fields from Task 4/AP-088). These simulations are performed on a computational grid consisting of 307 cells in the north-south direction and 224 cells in the east-west direction. Each cell is uniformly dimensioned at 100x100 m. However the radionuclide transport simulations for Task 6 of AP-100 require a 50x50 m cell size, thus Tasks 2 and 3 are needed to convert the data from Task 5/AP-088 and create the flow-fields for use in Tasks 4-6 of AP-100.

The approach of Task 2 is to refine the mining-affected T-field from Task 5/AP-088 and format the output for input to MODFLOW 2000 (**MF2K**). The refinement involves an exact mapping of the 50x50 m cell grid onto the 100x100 m cell grid. This means that each 100x100 m cell grid is split into four 50x50 m cells, with each of the four smaller cells containing the same attributes as the original cell. An example of the cell mapping is illustrated in Figure (1). The refinement results in a computational grid that is 614 cells in the north-south direction and 448 cells in the east-west direction. The modeling boundary is the same as for Tasks 4 and 5 of AP-088. The refinement is done using a small FORTRAN utility program discussed in the next section. Task 3 runs **MF2K** with the refined grid and converts the binary flow-budget output file to ASCII format and ports the ASCII file to the Open VMS platform where Tasks 4-6 are completed.

In addition to the grid-size conversion of the T-fields from Task 5/AP-088, the **MF2K** input files are also converted. The converted data include the initial heads, the IBOUND array (the IBOUND array designates which cells are active, inactive, or constant head cells), and the top and bottom Culebra elevations. This is done in the same manner as the T-fields, using the same FORTRAN utility. The model domain consists of constant-head cells along the north, east, and south boundaries, as designated by the IBOUND array and initial heads (the initial heads are invariant throughout the sim-

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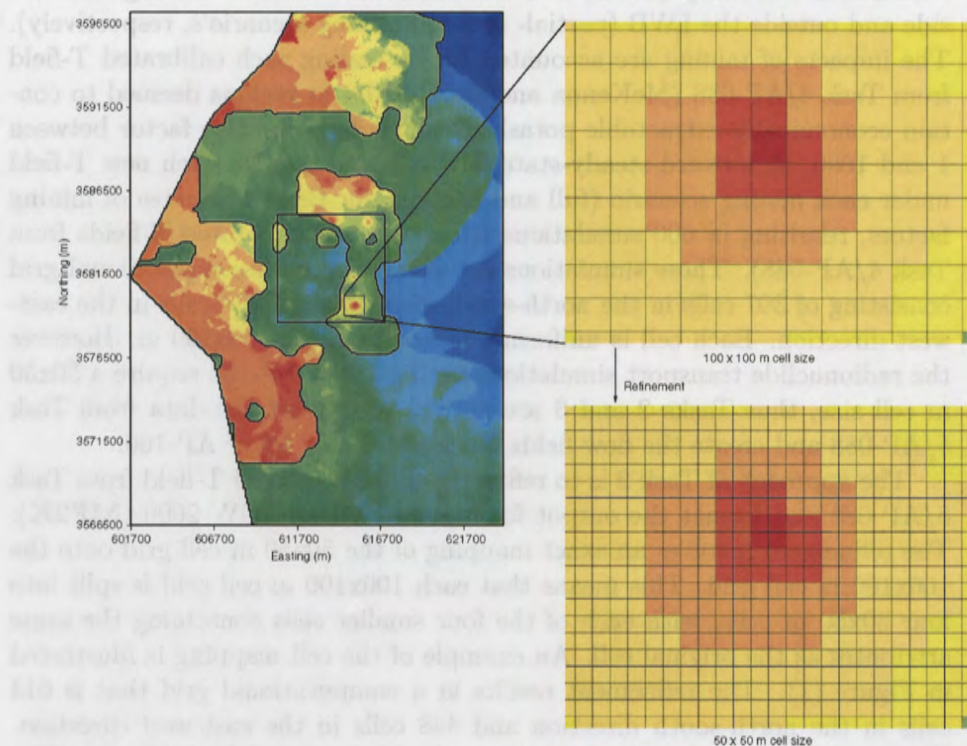
Figure 1: Large regional view on left shows the relative log-conductivity values for each cell. Upper close-up shows the cell mapping for a small portion of the 100 x 100 m cell sized grid. Lower close-up shows the same mapping for the 50 x 50 m cell sized grid. Each 100 x 100 m cell translates to four 50 x 50 m cells each with the same attributes as the original cell. The irregular black outline shows the active model domain and the mining zones for the full-mining case. The red box is the outline of the WIPP boundary.

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ulation along the constant-head boundary). To maintain consistency with the 100x100 m cell grid from AP-088, two rows of cells along the north and south boundaries and two columns of cells along the east boundary are designated as constant head in the refined grid. This preserves the 100-m-thick constant-head boundary from the coarser grid.

2.1 Software

Two FORTRAN utility codes are used to complete the Tasks of this report: **REFINE.F** and **BA.F**. The source codes are reproduced in the Appendices. **REFINE.F** converts the calibrated T-field from the 100x100 m uniform cell size that is used in Task 5/AP-088, to the 50x50 m uniform cell size that is used for the **SECOTP2D** simulations in Task 6 of AP-100. Output from **REFINE.F** is formatted for input to **MF2K**, which is run to provide the cell-by-cell flow budget file on the 50x50 m cell grid. Once **MF2K** is run on the refined grid, the output must be converted to ASCII text format since the **MF2K** runs are completed 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 **MF2K** binary output files are unable to be transferred directly between the two platforms. **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.

As mentioned above, the Tasks of this report are run in conjunction with the efforts of Task 5/AP-088 (Lowry, 2003). Several Linux shell scripts are used to help automate and coordinate the running of the programs. The scripts relating to the Tasks described here are **MINING.SH** and **POST-FLOW.SH**. **MINING.SH** is the main script that coordinates the running of each model, FORTRAN utility programs, and the other scripts in succession for Task 5/AP-088, and Tasks 2 and 3 of AP-100. Part of that sequence is running **REFINE.F** and **BA.F**. **POST-FLOW.SH** is used to gather and rename the ASCII budget files produced by **BA.F** into a single directory called /aff for easy uploading to the VMS machines. **MINING.SH** and **POST-FLOW.SH** are also reproduced in the Appendices. Figure (2) shows the software and information flow chart, with the output/input relationship between the different programs. Programs and scripts illustrated in Figure (2) that are not discussed here are detailed in Lowry (2003).

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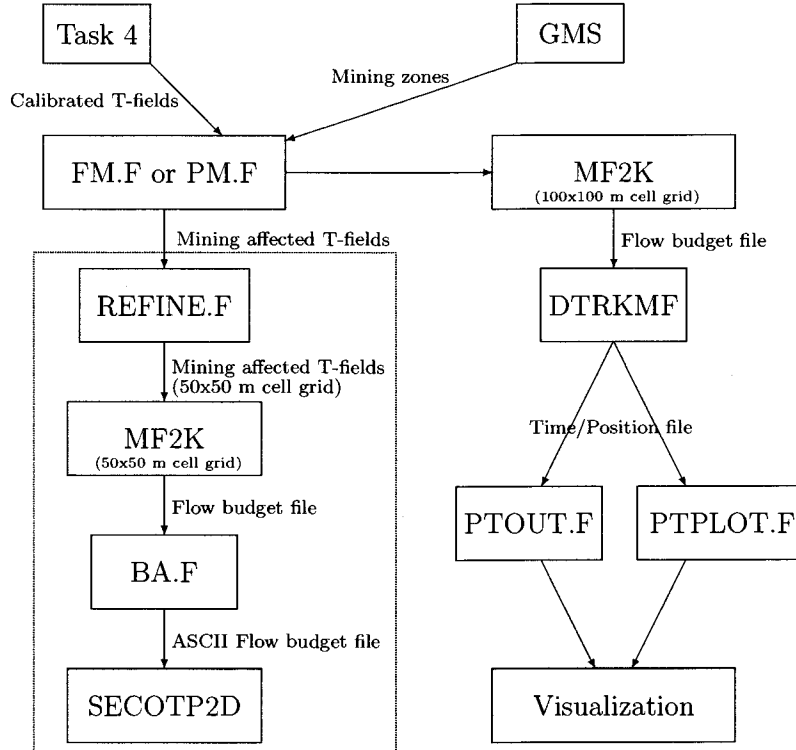
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Figure 2: Software and information flow-chart. The elements within the dashed box are pertinent to AP-100. All else refers to Task 5 of AP-088.

2.2 File Naming Convention

The file naming convention for Tasks 2 and 3 is kept consistent with that of Task 4 and Task 5 of AP-088, with the exception of adding a p or f and the replicate number (*R1, R2,* or *R3*) to the base filename. The p and f are used to distinguish between full- and partial-mining scenarios. The reason for the additions are that the file names in Task 5/AP-088 for each replicate/T-field/mining-scenario combination are identical, but are generated and kept under separate directories to maintain separation. When the files are collected into one directory, they need to be distinguishable from one another.

The calculations for Tasks 2 and 3 are performed on the 6115 Linux

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cluster and are performed in the same directory tree as the Task 5/AP-088 calculations. The general path for the T-field subdirectories is:

$$/home3/tslowry/wipp/mining/R*/[scenario]/d\#\#r\#\#$$

where, $R*$ is either $R1$, $R2$, or $R3$, depending on the mining factor replicate, [scenario] is either *full* or *partial*, depending on the 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 that qualifying criteria are used (Beauheim, 2003) to reduce the 137 calibrated fields to 100. Thus, the numbering of the $d\#\#r\#\#$ directories is not necessarily consecutive. Within each $d\#\#r\#\#$ directory, **BA.F** generates a file from the refined **MF2K** binary output called steady50x50_ascii.dat. The script **POST-FLOW.SH** copies this file to a directory called /home3/tslowry/wipp/mining/R*/aff, renaming the file with the format of $d\#\#r\#\#[s]R*.out$, where [s] is either p or f and the other symbols are explained above.

Also pertinent to the Tasks of this analysis report is a data directory (*50x50*) that contains the **MF2K** input files for the refined grid, and two directories (*scripts* and *source*) that contain backups of the shell scripts and the source code of the FORTRAN utility programs. The parent copy of the shell scripts and the FORTRAN executables are kept and run from /home3/tslowry/wipp/mining. A schematic of the directory tree is shown in Figure (3). The input and output files related to these Tasks that will remain archived in the directories are listed in Table (1). The details relating to Task 5/AP-088 can be found in Lowry (2003).

3 Assumptions

The main assumption incorporated into Tasks 2 and 3 concerns the exact mapping of the **MF2K** input data from the 100x100 m cell grid to the 50x50 m cell grid. The use of exact mapping maintains the exact input structure of the coarser grid, meaning that spatially varying model parameters (e.g. transmissivity, elevations, etc.) are constant within 100x100 m square areas on the 50x50 m grid. A more accurate method of mapping the coarse data

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```
/home3/tslowry/wipp/mining
    ├ /100x100
    ├ /50x50
    ├ /data
    ├ /R1
    │    ├ /aff
    │    ├ /full
    │    │     ├ /d01r02
    │    │     ├ /d01r04
    │    │           ⋮
    │    ├ /partial
    │    │     ├ /d01r02
    │    │     ├ /d01r04
    │    │           ⋮
    │    └ /ptout
    ├ /R2
    │    └ Same as R1
    │
    ├ /R3
    │    └ Same as R1
    ├ /scripts
    └ /source
```

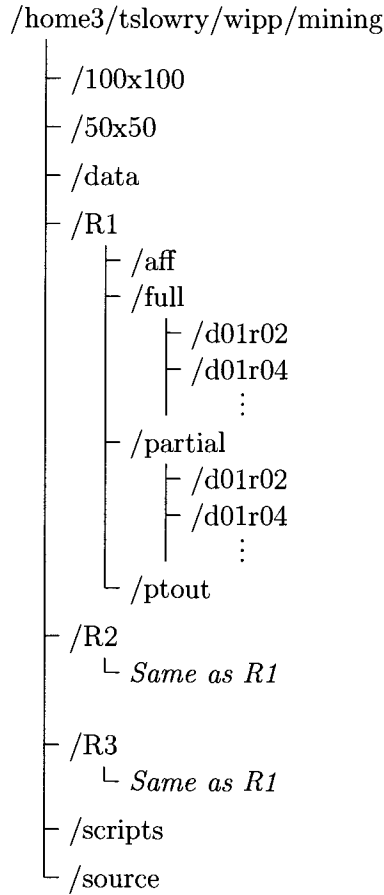Figure 3: Directory tree of Tasks 2 and 3 of AP-100 and Task 5 of AP-088. *Note that the subdirectories d01r02 and d01r04 appearing under the R*/full and R*/partial directories represent the first two of 100 subdirectories.*

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Table 1: Input and output files used for Tasks 2 and 3 of AP-100.

Directory	File	Description
/50x50	cNew.ibd	IBOUND file
	cNew.ihd	Initial heads
	cNew.top	Culebra top elevations
	cNew.bot	Culebra bottom elevations
	steady.ba6	**MF2K** basic input file
	steady.bc6	**MF2K** block-centered input file
	steady.nam	**MF2K** naming file
	steady.dis	**MF2K** discretization input file
	steady.oc	**MF2K** output control file
	steady.lmg	**MF2K** AMG1R5 solver input file
/R*/[scenario]/ d##r##/	steady50x50_ascii.dat	**BA.F** ASCII budget output
	steady50x50.bud	**MF2K** flow budget output
	steady50x50.hed	**MF2K** head output
	steady50x50.lst	**MF2K** listing file
	TNew.mod	Mining-altered T-field from **REFINE.F**
/R*/aff	d##r##[s]R*.out	Collected and renamed ASCII budget output file

to the refined grid would be to perform a scaling and/or interpolation to the finer grid. While this would allow for more accurate predictions on scales of a few hundred meters or less, the impact on the flow pattern at larger scales would be minimal. This is due to the fact that the groundwater flow equation as used in this simulation is described by the Laplace equation, which is a simple statement of water balance within each computational cell. Laplace's equation is dispersive in nature meaning the influence of small scale variations in the spatial parameters are 'smoothed' as part of the solution process. For this reason, the added complexity of interpolating or scaling the **MF2K** input data to the finer grid is not performed.

4   Summary

This analysis report describes the activities of Tasks 2 and 3 of AP-100: "Analysis Plan for Calculation of Culebra Flow and Transport: Compliance Recertification Application" (Leigh et al., 2003). The approach of Task 2 is to refine the mining-affected T-fields and **MF2K** input files from Task 5 of AP-088, and format the refined data to be re-run with **MF2K**. The refinement

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involves an exact mapping of the 50x50 m cell grid onto the 100x100 m cell grid. This means that each 100x100 m cell grid is split into four 50x50 m cells, with each of the four smaller cells containing the same attributes as the original cell. This is done using a small FORTRAN utility program called **REFINE.F**. Task 3 then runs **MF2K** with the refined grid and converts the binary flow-budget output file to ASCII format using a FORTRAN utility program called **BA.F**. The final step is transferring the ASCII flow-budget file via FTP to the VMS platform where Tasks 4-6 of AP-100 take place.

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WIPP_PA, 2003b. Analysis Report for the ES40 Regression Test. Sandia National Laboratories, ERMS # 525278.

WIPP_PA, 2003c. Analysis Report for the ES45 Regression Test. Sandia National Laboratories, ERMS # 525278.

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Appendix A: Grid Refinement Code, REFINE.F

```fortran
! 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 SECOTP.
! Program assumes original grid size is 100x100m.

    PARAMETER(nx=224,ny=307,nnx=448,nny=614,dOld=100,dNew=50)
    REAL tOld(nx,ny),tNew(nnx,nny)

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

    DATA file1/"CMine.mod"/
    DATA file2/"TNew.mod"/
    DATA file3/"Good_runs.txt"/
    DATA path1/"/h/wipp/data/runs/"/

!Get replicate number
    READ(*,*)rep

!Set base path
    path4="/home3/tslowry/wipp/mining/"//rep//"/"

!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

!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

!Goto 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,'(224e12.5)')(tOld(i,j),i=1,nx)
            END DO
            CLOSE(12)

!Transfer old values to new grid
            DO jn=1,nny
            DO in=1,nnx
                io=1+INT((in-1)*dNew/dOld)
                jo=1+INT((jn-1)*dNew/dOld)
```

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```
                tNew(in,jn)=tOld(io,jo)
            END DO
            END DO

!Output to new file
            OPEN(13,file=TRIM(path3)//TRIM(ADJUSTL(path2))//
      &          "/"//TRIM(ADJUSTL(file2)),status='unknown')
            DO jn=1,nny
            WRITE(13,'(448e12.5)')(tNew(in,jn),in=1,nnx)
            END DO
            CLOSE(13)
         END DO
      END DO
100   STOP
      END
```

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Appendix B: Binary to ASCII Conversion: BA.F

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

    PROGRAM AsciiBud
    PARAMETER(nx=448,ny=614,ndbmx=nx*ny)

    REAL qx(nx,ny),qy(nx,ny)
    REAL xdumb
    CHARACTER*40 file1,file2,file2a,file3,mine
    CHARACTER*68 path1,path2,path1f2a1,path1f2a3
    CHARACTER*16 text
    CHARACTER*2  rep(3)
    INTEGER kstp,kper,ncol,nrow,nlay,nlist,imeth
    REAL delt,pertim,totim

!Input file names
    DATA file1/"steady50x50.bud"/
    DATA file2/"Good_runs.txt"/
    DATA file3/"steady50x50_ascii.dat"/
    DATA path2/"/h/wipp/data/"/
    DATA rep/"R1","R2","R3"/

    DO ir=1,3

!Assign base path
        path1="/home3/tslowry/wipp/mining/"//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=5000)file2a
            mine="full/"
            DO imine=1,2
            IF(imine.eq.2)mine="partial/"
!Read in cell-by-cell flow file
            path1f2a1=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=path1f2a1,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 in=1,nlist
                         READ(13)xdumb
                     END DO
```

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```
            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
        path1f2a3=TRIM(path1)//TRIM(ADJUSTL(mine))//
    &           TRIM(ADJUSTL(file2a))//
    &           "/"//TRIM(ADJUSTL(file3))

        OPEN(15,file=path1f2a3,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(448e16.8)

    STOP
    END
```

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Appendix C: Linux Shell Script: MINING.SH

```
#For Task 5 of AP-088 and Tasks 2 and 3 of AP-100
#THISDIR is equal to: '/home3/tslowry/wipp/mining'
THISDIR=`pwd`
S1DIR=$THISDIR/100x100
S5DIR=$THISDIR/50x50
MODDIR=/home2/wipp/data
SCENARIO="full partial"
REPLICATE=`cat Replicate.txt`
FINISHED=`cat Good_runs.txt`

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

#Make directory and copy steady-state files
             mkdir ./$Run
             cd ./$Run
             cp $S1DIR/culebra.top ./fort.33
             cp $S1DIR/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

     cd ./$rep

#Loop through full and partial mining scenarios and
#run MODFLOW and DTRKMF for AP-088 and MODFLOW for AP-100

     for scn in $SCENARIO
     do
         cd ./$scn

         for Run in $FINISHED
         do
```

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```
            cd ./$Run
            mf2k $S1DIR/steady.nam
            echo 'Finished with MF2K 100x100 in' $rep/$scn/$Run
            dtrkmf < $S1DIR/dtrkmf.in
            echo 'Finished with DTRKMF in' $rep/$scn/$Run
            rm fort.33
            rm fort.34
            mf2k $S5DIR/steady.nam
            echo 'Finished with MF2K 50x50 in' $rep/$scn/$Run
            rm *.hed
            rm *.lst
            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 ptout'
ptout

#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!'
```

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Information Only

Appendix D: 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
```

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