MT3DMS Utilities

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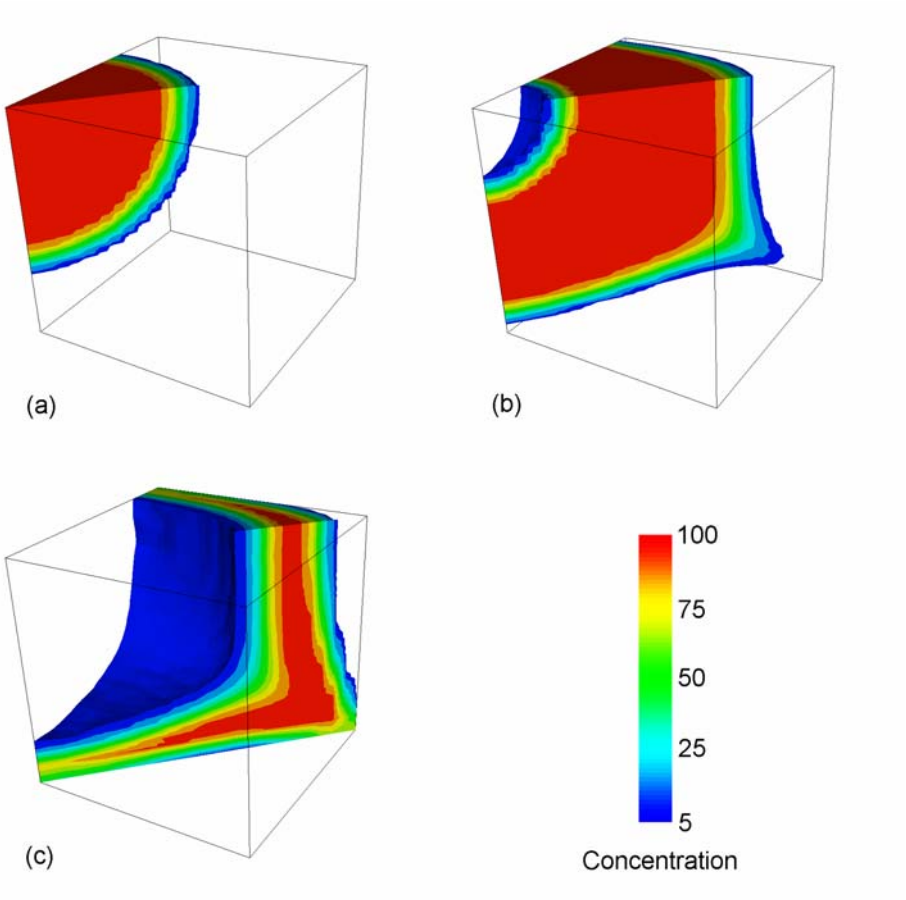

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I. PostMT3DMS (PM)

INTRODUCTION

PM is a utility program that can be used to extract the calculated heads/concentrations from the unformatted (binary) head/concentration files saved by MODFLOW/MT3DMS within a user-specified window along a model layer or cross section (2D), or within a user-specified volume (3D) at a particular time. The heads/concentrations within the specified window or volume are saved in such formats that they can be used by any available graphical packages to generate 2- or 3-D contour maps and other types of graphics. The source code in Fortran 90 was compiled to run in the command prompt mode under various Microsoft Windows operating systems.

Executable codes: `pm.exe`
Source code: `pm.for`
Example input files: `mt3d001.ucn`
`mt3d.cnf`
`pm.ini` `[response file]`

To use PM, two input files are required. The first is the unformatted head/concentration file saved by MODFLOW/MT3DMS after appropriate output control options have been set. PM has been compiled by Lahey LF95 Fortran compiler to accept a structured unformatted file saved in the style of LF95 and Compaq/HP Visual Fortran or a non-structured true binary file compatible with different compilers. The second is a text file which contains information on the spatial configuration of the model grid, referred to as the model configuration file. For output, PM generates data files either in the POINT format where the spatial coordinates of a nodal point are saved along with the data value at the nodal point, or in the ARRAY format that is directly readable by Golden Software's 2D contouring package Surfer©. In addition, the data files saved in the POINT format can include an optional header which is compatible with Amtec Engineering's 2D and 3D visualization package Tecplot©.

INPUT INSTRUCTIONS

Unformatted Head/Concentration File

The unformatted (binary) head (also drawdown) file saved by MODFLOW is of the following structure and contents:

For each time step saved:
For each layer of the three-dimensional head array:
Record 1: `KSTP,KPER,PERTIM,TOTIM,TEXT,NCOL,NROW,ILAY`
Record 2: `((HNEW(J,I,ILAY),J=1,NCOL),I=1, NROW)`

where

KSTP	is the time step at which the head is saved;
KPER	is the stress period at which the head is saved;
PERTIM	is the elapsed time within the current stress period;
TOTIM	is the total elapsed time from the beginning of simulation;
TEXT	is a character string (character*16) set equal to "HEAD";
NCOL	is the total number of columns;
NROW	is the total number of rows;
ILAY	is the layer for which the head is saved; and
HNEW	is the calculated head.

For MT3DMS, one unformatted (binary) concentration file is saved for each chemical species, with the default name MT3D`nnn`.UCN where `nnn` is the species index number as in MT3D`001`.UCN, MT3D`002`.UCN, and so on. The structure and contents of unformatted concentration files are as follows:

For each transport step saved:
For each layer of the three-dimensional concentration array:
Record 1: `NTRANS,KSTP,KPER,TOTIM,TEXT,NCOL,NROW,ILAY`
Record 2: `((CNEW(J,I,ILAY),J=1,NCOL),I=1,NROW)`

where

NTRANS	is the transport step at which the concentration is saved;
KSTP	is the time step at which the concentration is saved;
KPER	is the stress period at which the concentration is saved;
TOTIM	is the total elapsed time since the beginning of simulation;
TEXT	is a character string (character*16) set equal to "CONCENTRATION";
NCOL	is the total number of columns;
NROW	is the total number of rows;
ILAY	is the layer for which the concentration is saved; and
CNEW	is the calculated concentration.

Depending on which FORTRAN compiler was used to compile the MODFLOW and MT3DMS executables, the style of the unformatted (binary) head/concentration files may be different. PM supports either 'unformatted' or so-called 'true binary' style. See Section III for more information.

Model Configuration File

An input file is needed to provide PM with information on the spatial configuration of the model grid. This input file, referred to as the model configuration file, is saved automatically by MT3DMS. If PM is used to process the unformatted head or drawdown file saved by MODFLOW before MT3DMS is used, the user needs to create the model configuration file manually using a text editor. The structure and contents of the model configuration file are shown below:

Record 1:	`NLAY, NROW, NCOL`
Record 2:	`(DELR(J), J=1,NCOL)`
Record 3:	`(DELC(I),I=1,NROW)`
Record 4:	`((HTOP(J,I),J=1,NCOL),I=1,NROW)`
Record 5:	`(((DZ(J,I,K), J=1,NCOL),I=1,NROW),K=1,NLAY)`
Record 6:	`CINACT, CDRY`

where

NLAY	is the total number of layers;
DELR	is the width of columns (along the rows or x axis);
DELC	is the width of rows (along the columns or y axis);
HTOP	is a 2D array defining the top elevation of the first model layer;
DZ	is a 3D array defining the thickness of each model cell;
CINACT	is the value used in the model for indicating inactive cells;
CDRY	is the value used in the model for indicating cells gone dry.

The values in the model configuration file are arranged in list-directed (or free) format. Therefore, each record should begin at a new line and a record can occupy as many lines as needed. Either blank space or comma can be used to separate values within a record. In addition, input by free format permits the use of a repeat count in the form, *n*d,* where *n* is an unsigned-non-zero integer constant, and the input *n*d* causes n consecutive values of *d* to be entered. HTOP is a 2D array and its values should be arranged in the order of column first, sweeping from column 1 to column NCOL along the first row; then continuing onto row 2, row 3, ..., until row NROW. DZ is a 3D array and its values for each layer should be arranged similarly to those for HTOP, starting from the first layer, then continuing onto layer 2, layer 3, ..., until layer NLAY. Note that if one is only interested in creating data files for certain layers in plan view, then HTOP and DZ are never used, and thus may be entered as some dummy numbers with the use of repeat counts.

RUNNING PM

PM can be run in either interactive or batch mode. To run it interactively, simply type the name of the executable file at the command prompt:

```
C:\MT3DMS4\Bin\pm
```

where `C:\MT3DMS4\Bin` is the name of the subdirectory where the PM executable program resides. Alternatively, under folder view click on the program name to run. The program will prompt the user for the various input items and the user responds to the input requests directly from the keyboard. To run PM in batch mode, write all responses in the order required by PM to a text file and then re-direct PM to get responses from the response file instead of keyboard by issuing a command such as

```
C:\MT3DMS4\Bin\pm < pm.ini
```

where `pm.ini` is the name of a text file containing all responses to PM which the user would otherwise type in from the keyboard.

The user can select the concentrations, heads, or drawdowns at a desired time by specifying either a) the numbers of transport step, time step and stress period, or b) the total elapsed time, whichever is more convenient. (Note that transport step is used for MT3DMS only, not for MODFLOW.) The value of `-1` may be entered to obtain the results at the final step stored in the unformatted file. The user can also define a 2D window or 3D volume within which the graphical data files are desired by specifying the **starting** and **ending** column (J), row (I) and layer (K) indices of the window.

For example, to generate a data file for a cross sectional contour map along the 5th column, from row 20 to row 40 and from layer 1 to 10, enter the starting (J, I, K) indices as 5, 20, 1, and the ending (J, I, K) indices as 5, 40, 10. Similarly, to generate a data file for a cross sectional contour map along the 5th row, from column 20 to column 40 and from layer 1 to 10, enter the starting (J, I, K) indices as 20, 5, 1, and the ending indices as 40, 5, 10. Moreover, to generate a data file for a contour map on the 5th layer, from column 20 to column 40 and from row 1 to row 10, enter the starting (J, I, K) indices as 20, 1, 5 and at the lower right corner as 40, 10, 5. Finally, to generate a 3D data file within a volume defined from column 1 to column 40, from row 1 to row 20, and from layer 1 to layer 5, enter the starting (J, I, K) indices as 1, 1, 1, and the ending indices as 40, 20, 5. It is also possible to generate a data file for a contour map on the water table, i.e., the cells in the uppermost active layers instead of a specific layer, say, from column 20 to column 40 and from row 1 to row 10, enter the starting (J, I, K) indices as 20, 1, 0 and the ending indices as 40, 10, 0.

It should be pointed out that in MT3DMS/MODFLOW, the origin of the internal coordinate system (O_m) is set at the upper, top, left corner of the cell in the first column, first row and first layer, i.e., cell (1, 1, 1) and the positive x, y and z coordinates are in the directions of increasing column, row, and layer indices, respectively (Figure 1). However, in the output files generated by PM, the origin (O) is transformed to the lower, bottom, left corner of cell in the first column, last row and last layer, i.e., cell (1, NROW, NLAY) (Figure 1), as is customary in most graphical packages. As a result, the y and z axes used in MT3DMS/MODFLOW are reversed by PM whereas the x axis remains the same.

Therefore, if the contour map is on a layer or water table (i.e., the x-y plane), the horizontal axis of the map is along the direction of increasing column (J) indices, and the vertical axis is along the direction of decreasing row (I) indices. If the contour map is on a cross section along a row (i.e., the x-z plane), the horizontal axis of the map is along the

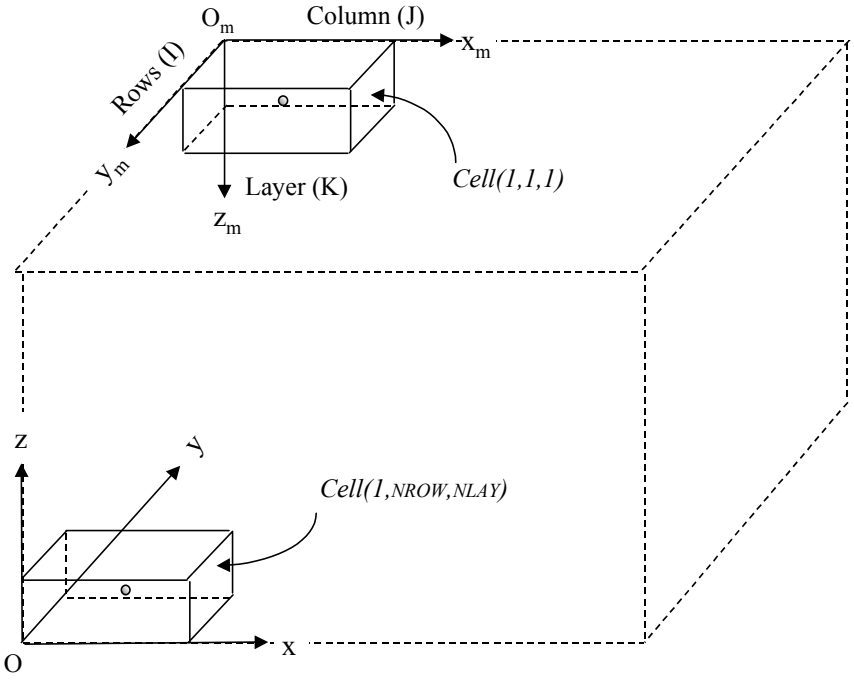

Figure 1. Transformation from the model internal coordinate system to the coordinate system used by the PM program for plotting purposes.

direction of increasing column (J) indices, and the vertical axis is along the direction of decreasing layer (K) indices. If the contour map is on a cross section along a column (i.e., the y-z plane), the horizontal axis of the map is along the direction of decreasing (I) indices, and the vertical axis is along the direction of decreasing layer (K) indices. All the necessary transformations are done by PM automatically. As an option, PM also allows the user to add an offset in the x, y and z directions to the map's origin for the convenience of posting data points on the map.

OUTPUT FILES

For output, PM writes data files in one of the two formats, referred to as the ARRAY format (with the file extension .GRD**)** and the POINT format (with the file extension .DAT**)**. The ARRAY format as listed below follows the convention used by Golden Software's Surfer© graphical contouring package. It saves the concentrations, heads, or drawdowns within a user-defined window of *regular* model mesh spacing to the output file, directly usable for generating contour maps by Surfer©. Note that if concentrations, heads, or drawdowns in an *irregular* portion of the model mesh is written to a ".GRD" file, no interpolation is performed and the contour map is thus deformed. The POINT format as listed below saves concentration, head, or drawdown at each nodal point along with the nodal coordinates within the user-defined 2D window or 3D volume

to the output file. This format is useful for generating data files of *irregular* model mesh spacing to be used by interpolation routines included in any standard contouring packages. It is also useful for generating plots of concentrations, heads, or drawdowns versus distances along a column, row or layer at a selected time. An optional header can be added to a ".DAT" file so that the file can be used directly by Amtec Engineering's 2D and 3D visualization package Tecplot©. The ARRAY and POINT formats are listed below for reference:

1. ARRAY(Surfer© GRD) File Format (free format):

DSAA
NX, NY, XMIN, XMAX, YMIN, YMAX, CMIN, CMAX
CWIN(NX,NY)

where

DSAA is the character keyword required by Surfer©.
NX is the number of nodal points in the horizontal direction of the window;
NY is the number of nodal points in the vertical direction of the window;
XMIN is the minimum nodal coordinate in the horizontal direction of the window;
XMAX is the maximum nodal coordinate in the horizontal direction of the window;
YMIN is the minimum nodal coordinate in the vertical direction of the window;
YMAX is the maximum nodal coordinate in the vertical direction of the window;
CMIN is the minimum concentration value within the window;
CMAX is the maximum concentration value within the window; and
CWIN is a 2D array containing all the calculated concentrations or heads within the window.

2. POINT (DAT) File Format without Header (free format):

For each active cell inside the specified 2D window or 3D volume:
X, Y, Z, CXYZ

where

X is the nodal coordinate in the x axis (along the rows);
Y is the nodal coordinate in the y axis (along the columns);
Z is the nodal coordinate in the z axis (along the layers); and
CXYZ is the calculated concentration or head at the nodal point defined by coordinates (X,Y,Z).

Note that for data files defined in a 2D window, one of the coordinates will be constant. In using an interpolation routine for gridding purposes, make sure to specify appropriate columns. For example, to create a contour map in a x-z cross section, the y column should either be deleted or skipped.

3. POINT (DAT) File Format with Header (free format):

This file format is identical to type 2 except the addition of a Tecplot©-compatible header consisting of the following information:

VARIABLES="X" "Y" "Z" "DATA"
ZONE I=NX **J**=NY **K**=NZ **F**=**POINT**

where

VARIABLES, **ZONE**, **I**, **J**, **K**, **F**, **POINT** are keywords used by Tecplot©;
NX is the number of columns within the user-specified 2D window or 3D volume;
NY is the number of rows within the user-specified 2D window or 3D volume;
NZ is the number of layers within the user-specified 2D window or 3D volume;
X, Y, Z and DATA are character labels for the four data columns saved in the file.

II. SaveLast

If it is necessary to continue a simulation from the end of a preceding run, the concentrations from the final step of the preceding run can be used as the starting concentrations for the continuation run. The dissolved-phased concentrations for species #nnn, are saved in the default unformatted concentration file, MT3Dnnn.UCN, and the sorbed- or immobile phase concentrations for species #nnn, are saved in a corresponding file, MT3DnnnS.UCN. Either file is directly readable by the array reader RARRAY. If there is more than one step of concentration saved in MT3Dnnn.UCN and/or MT3DnnnS.UCN, then SaveLast can be used to extract the concentrations of the final transport step and save them in separate unformatted files for a restart run. To run SaveLast, simply type SaveLast at the command prompt and enter the names of input and output files from the monitor screen. SaveLast has been compiled by Lahey LF95 Fortran compiler to accept a structured unformatted file saved in the style of LF95 and Compaq/HP Visual Fortran or a non-structured true binary file compatible with different compilers.

III. Unformatted File Converters

INTRODUCTION

Unformatted (binary) files used by MODFLOW, MT3DMS, and other related programs often have different, incompatible styles depending on which FORTRAN compilers have been used to compile these programs. This section contains a brief description of several file converters that can be used to convert an unformatted (binary) file from one style to another. All programs documented in this section were compiled to run in the command prompt mode under various Microsoft Windows operating systems.

PROGRAM DESCRIPTION

LF90to95[1]

This program converts an unformatted file (head, concentration, or flow-transport link file) in the style used by the Lahey LF90 FORTRAN compiler to that used by the Lahey LF95 compiler. The LF95 style is also compatible with that of Compaq/HP Visual FORTRAN (formerly Digital Visual FORTRAN). To run `LF90to95`, click on the program name under folder view, or enter the following command from the command prompt:

```
C:\MT3DMS4\Bin\LF90to95  LF90-inputfile  LF95-outputfile
```

where `C:\MT3DMS4\Bin` indicates the name of the subdirectory where the `LF90to95` program is located, `LF90-inputfile` is the LF90-style unformatted input file, and `LF95-outputfile` is the LF95-style unformatted output file after the conversion. If the input/output file names are not provided in the command line, the program will prompt the user for the file names.

LF95to90

This program performs the reverse function of `LF90to95`. It converts an unformatted file in the style used by the Lahey LF95 FORTRAN compiler (or Compaq Visual FORTRAN) to that used by the Lahey LF90 compiler. To run `LF95to90`, click on the program name under folder view, or enter the following command from the command prompt:

```
C:\MT3DMS4\Bin\LF95to90  LF95-inputfile  LF90-outputfile
```

where `LF95-inputfile` is the LF95(VF)-style unformatted input file, and `LF90-outputfile` is the LF90-style unformatted output file after the conversion. If the

[1] LF90to95 and LF90to95 are based on the utility programs, sequnf.f90 and unfseq.f90, distributed as part of the Lahey LF95 FORTRAN compiler.

input/output file names are not provided in the command line, the program will prompt the user for the file names.

UNFtoBIN

This program converts an unformatted file (head or concentration) in the style used by the Lahey LF95 FORTRAN compiler (and Compaq Visual FORTRAN) to the 'True Binary'-style that is exchangeable among various compilers, including LF90, LF95 and VF. To run `UNFtoBIN`, click on the program name under folder view, or enter the following command from the command prompt:

```
C:\MT3DMS4\Bin\UNFtoBIN  LF95-inputfile  TrueBinary-outputfile
```

where `LF95-inputfile` is the LF95(VF)-style unformatted input file, and `TrueBinary-outputfile` is the 'true binary'-style output file after the conversion. If the input/output file names are not provided in the command line, the program will prompt the user for the file names.

BINtoUNF

This program performs the reverse function of `UNFtoBIN`. This program converts a 'true binary'-style unformatted file to the LF95(VF)-style unformatted file. To run `BINtoUNF`, click on the program name under folder view, or enter the following command from the command prompt:

```
C:\MT3DMS4\Bin\BINtoUNF  TrueBinary-inputfile  LF95-outputfile
```

where `TrueBinary-inputfile` is the 'true binary'-style input file and `LF95-outputfile` is the LF95(VF)-style unformatted output file after the conversion. If the input/output file names are not provided in the command line, the program will prompt the user for the file names.

IV. Using Model Viewer

The U.S. Geological Survey's visualization software package, known as Model Viewer (Hsieh and Winston, 2002[2]) can be used to visualize and animate simulation results obtained with several flow and transport models, including MODFLOW, MT3DMS, MOC3D, and SUTRA. The software and user guide can be downloaded from the USGS ground-water software site:
http://water.usgs.gov/nrp/gwsoftware/modelviewer/ModelViewer.html

Zheng et al. (2000[3]) provide brief instructions on how to use Model Viewer with MT3DMS. When set up to display results from MT3DMS, Model Viewer obtains data from two output files from MT3DMS, the model configuration (CNF) file and the unformatted concentration (UCN) file. (In addition, the flow-transport link file saved by MODFLOW for MT3DMS can be read to display velocity vectors and model features.) The UCN and CNF files are saved by MT3DMS when the output control option for saving concentrations to unformatted files (SAVUCN) is set to T (for True) in the input file of the MT3DMS Basic Transport (BTN) Package. By default, MT3DMS names the model configuration file 'MT3D.CNF' and the unformatted concentration files 'MT3Dnnn.UCN' where nnn is the species index number such as 001 for species 1 and 002 for species 2. Because the UCN files for different species are structurally identical, the simulation results can be visualized one species at a time by selecting MT3D001.UCN, MT3D002.UCN, and so on in Model Viewer.

Depending on which Fortran compiler was used to compile the MT3DMS executable, the structure of the unformatted (binary) concentration file may be different. It is thus necessary to specify a correct data structure for the UCN file to be read properly by Model Viewer. Four types of the unformatted file structure supported by Model Viewer are:

(1) Binary (unstructured, non-formatted),
(2) Unformatted (Visual Fortran and Lahey Fortran LF95),
(3) Unformatted (Lahey Fortran LF90), and
(4) Big Endian - Unix

The standard executable code 'mt3dms4s.exe' included with the MT3DMS distribution files supports the second option, while the second executable 'mt3dms4b.exe' supports the first option. The unformatted file converters described previously can be used to convert unformatted head/concentration files from one style to another.

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[2] Hsieh, P.A., and Winston, R.B., 2002, *User's Guide To Model Viewer, A Program For Three-Dimensional Visualization of Ground-water Model Results:* U.S. Geological Survey Open-File Report 02-106, 18 p.
[3] Zheng, C., Hill, M.C. and Hsieh P.A., 2001, *MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model-User Guide to the LMT6 Package, The Linkage with MT3DMS for Multi-Species Mass Transport:* U.S. Geological Survey Open-File Report 01-82, 44 p.