

A Graphical-User Interface for MODFLOW and MT3D 1.5 Using Argus ONE

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Introduction

This report describes a graphical-user interface (GUI) for MT3D 1.5, a widely used solute-transport model developed by Chunmiao Zheng of the Department of Geology, University of Alabama. It is based on a similar, earlier version (MT3D 1.1) developed for the U.S. Environmental Protection Agency (Zheng, 1990). MT3D does not determine fluid flow but instead uses the output of a finite-difference flow model such as MODFLOW. Thus the GUI for MT3D also includes a GUI for MODFLOW. The GUI for MODFLOW is based on that developed by Shapiro and others (1997).

During installation, a 32-bit MT3D version 1.5 and a modified 32-bit version of MODFLOW-96 will be installed on your computer. These versions are compatible with the MODFLOW/MT3D PIE. The modifications required to make MODFLOW-96 suitable for use with the MODFLOW/MT3D PIE are described in Appendix 1.

Documentation and example input files for MT3D may be downloaded from the Environmental Protection Agency (EPA) <http://www.epa.gov/ada/models.html>. You can also get a version of MT3D there but it may not run on Pentium computers and is not the most recent version of MT3D. A better source for MT3D is <http://hydro.geo.ua.edu/mt3d/mt3d150d.htm>. Some, but not all, of the example input files for MODFLOW included with EPA version of MT3D will not work with the USGS version of MODFLOW. They were designed for a special version of MODFLOW that could read data in additional formats not supported by the USGS version of MODFLOW. If you wish to use those example-input files, you will need to revise the MODFLOW source code to conform to those requirements. A compiled version of MODFLOW-88 (and source code) that has these modifications can be downloaded from <http://hydro.geo.ua.edu/mt3d/mt3d150d.htm>. However, this version of MODFLOW is not compatible with the MODFLOW/MT3D PIE because it is a version of MODFLOW-88 rather than MODFLOW-96.

System Requirements and Installation

The pre- and post-processing GUI for MT3D 1.5 require Argus ONE version 4.0 or later operating on Windows 95, or Windows NT. To run MODFLOW models, you must have MODFLOW-96. To run MT3D 1.5 models you must have MT3D 1.5 and a version of MODFLOW-96 that creates the input files for MT3D. The version of MODFLOW distributed by the USGS does not create the MT3D input files. Suitable versions of MODFLOW and MT3D 1.5 can be downloaded from are installed with the PIE. The modifications to MODFLOW-96 to allow it to write the MT3D input files are described in Appendix 1.

If you already have the USGS MODFLOW PIE installed, you must first removing it by removing its files from the ArgusPIE directory or one of its subdirectories. At the time this was written, the default location of the USGS MODFLOW PIE was the mfgui1.41 subdirectory of the ArgusPIE directory. There is no need to retain the USGS MODFLOW PIE because MODFLOW/MT3D PIE can do everything the USGS MODFLOW PIE could do and can open files created by the USGS MODFLOW PIE. The USGS MODFLOW PIE can not open files created by the MODFLOW/MT3D PIE.

To install the PIE, download the PIE installer program and execute it. When prompted, select the directory in which Argus ONE is installed. The PIE will install files in subdirectories of the ArgusPIE and ArgusHELP directories and will create an install log in the directory in which Argus ONE is installed. **Do not select the ArgusPIE directory when choosing the**

directory in which to install the PIE. If you do, the PIE will not be installed correctly. If you install the PIE in the wrong directory, uninstall the PIE. You can uninstall it as you would any Windows 95 program.

If your version of Argus ONE is not installed in the default directory, you should change the default locations of MODFLOW and MT3D as described in the section "Changing Default locations of MODFLOW and MT3D".

Previously, the MODFLOW post-processing and preprocessing PIE's were packaged in two separate files. In the first version of the USGS MODFLOW PIE, these were named MFGUI_10.DLL and MFPOST10.DLL. In the MODFLOW/MT3D PIE, they have been combined in a single file; MODFLOW.DLL. In addition, online help for the PIE is provided in a series of linked web pages. These web pages are not required for the PIE to work but may prove helpful in using the PIE. If you do not require them, you may delete them by deleting the MF_Help subdirectory of the ArgusHelp directory.

Both MODFLOW and MT3D must be compiled with the same (or compatible) compilers for MT3D to read the flow file produced by MODFLOW. In addition, pm.dll used by MT3D post-processing utility must be compiled with the same (or compatible) compiler as MT3D and MODFLOW for it to be able to read the concentration file created by MT3D. It must also export functions in pm.for to PostMT3D.exe which was written using Borland Delphi 3.0. Pm.dll and the Argus versions of MODFLOW and MT3D were all compiled with the Lahey Fortran 90 version 4 compiler. Modflow.dll was written using Microsoft Visual C++ version 5.

Launching ArgusONE and the MODFLOW/MT3D PIE

For the PIE to function properly you must start Argus ONE through a 32 bit interface. For example, you can start it from the Start Menu, a shortcut on your desktop, or by double clicking ArgusONE.EXE or any ArgusONE project (*.mmb) from within Windows Explorer™. Launching Argus ONE from a 16-bit interface such as certain 16-bit toolbars may prevent you from accessing the online Help for MODFLOW. In this occurs, an error message will be displayed.

Changing Default locations of MODFLOW and MT3D

The default locations and files names for the MODFLOW-96 and MT3D are C:\Program Files\Argus Interware\ArgusPIE\Mt3d_gui\Modflw96_Argus32.exe and C:\Program Files\Argus Interware\ArgusPIE\Mt3d_gui\Mt3d15_Argus32.exe. To change the default location or file name, edit MODFLOW.VAL file with a text editor that can save files in ASCII format. Locate the lines containing "@MODFLOW_Path@" or "@MT3D_Path@". At present those lines read as follows.

```
@MODFLOW_Path@ C:\Program Files\Argus Interware\ArgusPIE\Mt3d_gui\Modflw96_Argus32.exe
@MT3D_Path@    C:\Program Files\Argus Interware\ArgusPIE\Mt3d_gui\Mt3d15_Argus32.exe
```

If you edit the file names or paths in these lines, the new paths and names will become the default values. You must include the full path and the path must be separated from @MODFLOW_Path@ or @MT3D_Path@ by one or more space or tab characters. For example, you could change the line containing @MT3D_Path@ to the following.

```
@MT3D_Path@    D:\MT3D\BIN\MT3D15.exe
```

This would change the path for MT3D from C:\Program Files\Argus Interware\ArgusPIE\Mt3d_gui\Mt3d15_Argus32.exe to D:\MT3D\BIN\ and would change the name of the executable from Mt3d15_Argus32.exe to MT3D15.exe.

MT3D Preprocessing: Non Spatial Data

If the MODFLOW/MT3D PIE is properly installed, “New MODFLOW Project...” will appear on the Argus ONE “PIEs” menu. Select this item to start the preprocessing of a new MODFLOW and MT3D project. When you do, the Project information dialog box will appear. It is used to edit non-spatial data and data that can not vary within a model layer. Initially, the dialog box will 9 tabs labeled:

About

Project

Geology

Misc. Controls

Stresses/Solvers

Time

Output Files

Output Controls

Solver (where *Solver* is one of the following, **PCG**, **SOR**, **DE4**, or **SIP**).

Most of these tabs are the same as those in the USGS MODFLOW PIE. The About tab, however, is new. It gives information about the PIE but is not used in running the PIE. There are two other obvious changes. On the Stresses/Solvers tab there is a check box for MT3D 1.5 and there is a “Help” button next to the OK and Cancel buttons. If the MT3D 1.5 check box is selected, additional tab pages related to MT3D 1.5 will appear. The additional MT3D-related tabs are labeled:

MT3D BAS

MT3D Adv1

MT3D Adv2

MT3D Disp/Chem

MT3D Out.

Not all of these tabs will appear when the MT3D 1.5 check box on the Stresses/Solvers tab is checked. Initially, only MT3D BAS and MT3D Out will appear. The others are related to specific MT3D packages and will appear only if the appropriate check boxes on the MT3D BAS tab are checked.

To accept changes in the Project Info dialog box, click the OK button. Click the Cancel button to reject changes. You can re-edit the information at any time by selecting “Edit Project Info” from the PIEs menu.

To access the online Help, select the Help button on the Project Info Dialog box, or the Run Modflow dialog box or by selecting “MODFLOW Help” from the PIE menu of a MODFLOW project. (In the future “MODFLOW Help” may appear under the “Help” menu.)

There have been a variety of other, minor changes to the MODFLOW interface in the PIE as described in the section " Differences between the USGS MODFLOW PIE (version 1.41) and the MODFLOW portion of the ARGUS MODFLOW/MT3D PIE".

MT3D BAS

MT3D BAS is used to specify data required by the MT3D Basic package. MT3D Heading, Lines 1 and 2 are exported to MT3D. You can set the concentration that MT3D will assign to inactive concentration cells by assigning a value to CINACT. This value should normally be negative and have a large absolute value. You can use whatever length and mass unit you wish in the model by assigning them on the MT3D BAS page but you must use consistent units throughout your model. If you choose to use one or more of the other MT3D Packages, use the check boxes for those packages on the MT3D BAS page. The other packages are the Advection, Dispersion, Sink and Source Mixing, and Chemical Reaction packages. The Sink and Source Mixing Package will be automatically selected and can not be unselected if any of the Stresses from the Stresses/Solvers are selected. It should also be selected if any prescribed heads with non-zero concentrations or time-varying constant concentrations are used in the model. You also set the transport step size and maximum number of transport steps per time steps for each stress period on the MT3D BAS tab. (To add or remove stress periods, you must change to the "Time" tab.)

MT3D Variable	Use
MT3D Heading, Line1	Set the text printed as the first line of the title in the MT3D output
MT3D Heading, Line2	Set the text printed as the second line of the title in the MT3D output
CINACT	In printouts, all inactive concentration cells will be assigned a concentration equal to CINACT so that they can be distinguished from active concentration cell.
LUNIT	Length unit of model. You must use consistent units throughout the model.
MUNIT	Mass unit of model. You must use consistent units throughout the model.
ADV	To use the advection package, check this box.
DSP	To use the dispersion package, check this box.
SSM	To use the source- and sink-mixing package, check this box. It will be automatically checked in many circumstances but you must check it manually if you use prescribed heads with non-zero concentrations or time-varying constant concentrations in the model.
RCT	To use the chemical reaction package, check this box.
DTO (Transport Step Size)	Set the transport step size for any stress period using this option
DTO (Use calculated transport step size)	To let MT3D automatically calculate the transport step size, check this box.
MXSTRN	Set the maximum number of transport steps per time step.

MT3D Adv1 and MT3D Adv2

MT3D Adv1 and MT3D Adv2 are used to set parameters associated with the advection package.

MT3D Variable	Use
MIXELM	Set the advection solution scheme. The MOC method works better than the MMOC method for cases with sharp concentration fronts but is slower and requires more memory. The hybrid method uses the MOC method near sharp concentration fronts and uses MMOC elsewhere. The choice of advection solution scheme determines which other data are required for the model. If data will not be used in a model, the edit boxes for those data will be disabled.
ITRACK	The first order Euler particle tracking algorithm is faster but less accurate than the Runge-Kutta method especially in areas of converging or diverging flow such as sources and sinks.
PERCEL	PERCEL is the Courant number or number of cells a particle can move in one transport step. Usually values of 0.5 to 1 are appropriate.
MXPART	MXPART is the maximum number of particles used in the MOC or hybrid MOC/MMOC scheme
WD	WD is a concentration weighting factor between 0 and 1. 0.5 is usually a good choice. You can adjust it to achieve a better mass balance. Advection becomes more dominant as WD increases.
DCEPS	DCEPS is the size of the concentration gradient that is considered negligible. DCEPS affects how many particles are used in each cell. (See NPL and NPH).
NPL	In cells in which the concentration gradient is less than DCEPS, NPL is the number of particles that will be placed in that cell.
NPH	In cells in which the concentration gradient is greater than DCEPS, NPH is the number of particles that will be placed in that cell.
NPLANE	The initial placement of moving particles can be either random or fixed.
Number of vertical planes of particles in each cell	If the fixed option is selected for NPLANE. You must specify the number of vertical planes of particles in each cell.
NPMIN	NPMIN is the minimum number of particles per cell. It can be 0 in relatively uniform flow fields. It generally doesn't need to be larger than 4. If the number of particles in a cell falls below NPMIN more particles will be added.
NPMAX	NPMAX is the maximum number of particles per cell. A value twice that of NPH is often appropriate. If the number of particles in a cell rises above NPMAX, particles will be removed.
SRMULT	SRMULT is the multiplier for the particle number at source cells. It should be ≥ 1

MT3D Variable	Use
INTERP	There is only one choice of interpolation method in MT3D 1.5 so you never set INTERP. This field is included to facilitate incorporating future changes in MT3D
NLSINK	The initial placement of moving particles in sink cells can be either random or fixed.
Number of vertical planes of particles in each sink cell	If the fixed option is selected for NLSINK. You must specify the number of vertical planes of particles in each sink cell.
NPSINK	NPSINK is the number of particles used to approximate sink cells in the MMOC scheme.
DCHMOC	DCHMOC is the critical relative concentration gradient for controlling the use of either the MOC or MMOC scheme in the hybrid MOC/MMOC scheme.

MT3D Disp/Chem

MT3D Disp/Chem is used to set parameters associated with the Dispersion and Chemical reaction packages.

MT3D Variable	Use
ISOTHM	ISOTHM is used to indicate which (if any) sorption type will be simulated. The choice of ISOTHM affects the meaning of SP1 and SP2.
IREACT	IREACT is used to indicate whether a first order chemical reaction is to be simulated (radioactive decay or biodegradation). RC1 and RC2 are only used if a first order reaction is simulated.
RHOB	RHOB is the bulk density of the porous medium M/L^3
SP1	SP1 is the first sorption constant. For linear sorption, SP1 is the distribution coefficient (K_d) (L^3/M) For Freundlich sorption, SP1 is the Freundlich sorption equilibrium constant (K_f) with units that depend on the Freundlich exponent α . For Langmuir sorption, SP1 is the Langmuir sorption equilibrium constant (K_l) (L^3/M).
SP2	SP2 is the second sorption constant. For linear sorption, SP2 is not used For Freundlich sorption, SP2 is the Freundlich exponent α . For Langmuir sorption, SP2 is total concentration of sorption sites available(S) (M/M).
RC1	RC1 is the first-order rate constant for the dissolved phase (1/T).
RC2	RC2 is the first-order rate constant for the sorbed phase (1/T). For radioactive decay RC1 should generally equal RC2. For some types of biodegradation RC1 may differ from RC2.
TRPT	TRPT is the ratio of horizontal transverse dispersivity (α_{TH}) to the longitudinal dispersivity (α_L)
TRPV	TRPV is the ratio of vertical transverse dispersivity (α_{TV}) to the longitudinal dispersivity (α_L). For an isotropic aquifer, TRPV can be set equal to TRPT.
DMCOEF	DMCOEF is the effective molecular diffusion coefficient (L^2/T). If molecular diffusion is considered unimportant set DMCOEF = 0.

MT3D Out

The MT3D Out tab is used to specify output options for MT3D.

MT3D Variable	Use
Print out Contents of Flow-Transport Link File for Checking	The "Flow-Transport Link File" is a binary file created by MODFLOW when the LKMT package is used. It lists the flows for each time step between each cell and its neighbors and boundary condition flows. If this check box is checked, the contents of the Flow-Transport Link File will be printed in the MT3D output.
Printout format	MT3D allows you to print the results in "wrap" or "strip" form. In wrap form, all the data for each row in the model will be printed before moving on to the next row. Thus you might have several lines of text in a table that are all from the same model row. In strip form, the model data are printed in a series of tables each of which will have 10-15 columns of data. This means that data for a single model row will not be split over several rows in the same table making it somewhat easier for humans to read. If the model output will be read by another computer program, wrap, rather than strip form might be better. Note that although you can change the format of the output, you can not change the format in which the input data are printed on the output file.
Numeric format	The output from MT3D can be printed in a variety of Fortran formats. Fortran formats can be read as followed: The first number represents how many numbers will be printed on each line of the output file. Thus 11G10.3 will have 11 digits per line. The letter For G is used to distinguish between the fixed and general formats. In fixed format, there will be a fixed number of digits to the right of the decimal point whereas the general format will put as many significant digits as possible within the available space. The number following F or G is the width of the field in which the number will be printed. 11G10.3 will be printed in 10 spaces. The number after the decimal point is the number of digits that will be printed to the right of the decimal point. Thus 15F7.1 will have one digit to the right of the decimal point.
IFMTCH	IFMTCH, IFMTRF, IFMTDP, and IFMTNP are used to specify whether or not the concentrations, retardation factors, dispersion coefficients and number of particles per cell should be printed in the MT3D output file. If you choose to print one or more of these items, the corresponding "Numeric format" drop-down list will be enabled so that you can specify the format in which it will be printed. All of these items will be printed in strip or wrap form depending on your choice of "Printout format".
IFMTRF	
IFMTDP	
IFMTNP	

MT3D Variable	Use
CHKMAS	If the CHKMAS checkbox is checked, a one-line summary of mass balance information for each transport step will be saved in MT3D.MAS for checking purposes. The mass balance can help you evaluate the accuracy of you simulation results. However, MT3D is not entirely based on mass conservation so large mass balance errors in the initial time steps may occur without this indicating a problem with the model. See section 4.7 of the MT3D documentation. Although, no Zheng gives no specific values for acceptable mass balance errors, in his last example, errors range from -12.7% for the first time step to a minimum of -2.8% on the last time step.
SAVUCN	If SAVUCN is checked, the concentration in each cell for specific time steps (as specified with NPRS and TIMPRS) will be saved in a file named MT3D.UCN and the grid configuration will be saved in MT3D.CNF. Both these files are required for debugging. (The CNF extension may not be visible in Windows Explorer™ because that extension is now used for other purposes by Windows 95. However, the file may still be used.)
Results printed (NPRS)	NPRS is used to indicate at what model times model results should be printed to file. If you choose to print model results, you can designate the times by the transport step or by elapsed time using the NPRS drop down list. If you select "Each N'th transport timestep within each flow timestep", the results will be printed every time the transport step is an even multiple of N. If you select "Specified times", the times entered will TIMPRS will determine at which transport steps results will be printed.
N	See "Results printed (NPRS)"
Printout times (TIMPRS)	If in " Results printed (NPRS)" you select "Specified times", TIMPRS will be a list of the model times at which output will be generated. Modify the list via " Printout time". The times listed in TIMPRS need not be in order. They will be sorted automatically when you click the OK button.
Printout time	When you select a value in TIMPRS, that time will be displayed in "Printout time" If you wish to change that time, edit the value and click the "Modify" button. To insert a new value before the selected value, click the "Insert" button on the dialog box. To delete the selected value, click the "Delete" button on the dialog box.

MT3D Layers

The MODFLOW/MT3D PIE creates a layer structure that reflects the stresses you have chosen to apply to your model. **You should not delete or rename any of the layers or parameters created by the PIE.** You may however, create new layers and parameters for your own use. In addition, **it is generally unwise to override the parameter expressions on the MODFLOW FD Grid layer** without thoroughly determining the effects of such an action by careful study of the export template (the modflow.met file).

MT3D Domain Outline

The MT3D model is not required to include the entire region modeled by MODFLOW model. To specify what region should be included in the MT3D model, outline the area with to be modeled on the MT3D Domain Outline layer with a closed contour. Assign a value other than 0 to the contour or else create an expression that links the MT3D Domain Outline to MODFLOW Domain Outline. You can also set the value of ICBUND Unit[i] or Active MT3D Cell Unit[i] of individual cells on the MODFLOW FD Grid layer. (However, any cells that are inactive MODFLOW cells will also be treated as inactive MT3D cells by MT3D.)

As with the MODFLOW Domain Outline, all areas outside the MT3D Domain Outline, will not be part of the model unless individual cells are set on the MODFLOW FD Grid layer. Unlike, the MT3D Domain Outline, the MT3D Domain Outline has no effect on the grid cell size. Use "Added MT3D Inactive Area Unit[i]" to inactivate an area within the MT3D Domain Outline for one particular geologic unit.

Added MT3D Inactive Area Unit[i]

To inactivate part of a layer in an MT3D model, outline the area on the "Added MT3D Inactive Area Unit[i]" layer with a closed contour and assign the contour a value of 0. By default, the "Added MT3D Inactive Area Unit[i]" layer is linked to the "Added Inactive Area Unit[i]" layer. Thus if no contours are placed on the layer and the MT3D Domain Outline is the same as the MODFLOW Domain Outline, the layer will have the same active area as the MODFLOW model. You should not change this layer to a data layer.

MT3D Porosity Unit[i]

The MT3D Porosity Unit[i] is used to assign the porosity of an individual layer. You can use closed contours to assign values to zone or you can change the interpolation method from the Exact Contour method to the Interpolation method and assign point contours. In the latter case, the value assigned to any particular cell will be determined by interpolation among the points assigned to the MT3D Porosity Unit[i] layer. If desired, you may change this layer to a data layer.

MT3D Observations Unit[i]

MT3D Observations Unit[i] is used to specify the location of observation cells. Any cell that intersects a point or open contour or whose center is inside a closed contour will be treated as an observation cell. The concentration will be saved in the file MT3D.OBS at every transport step. You should not change this layer to a data layer.

MT3D Point Constant Concentration Unit[i]

MT3D Point Constant Concentration Unit[i] is used to specify constant concentration point sources. If any Point Contours are on a MT3D Point Constant Concentration Unit[i] layer, the cell will be designated as a constant concentration cell with a concentration equal to the mass divided by the cell volume. If the unit has a vertical discretization greater than 1, the mass will be divided among all the cells in the geologic unit that contain the point contour. If a cell contains more than one point object, the one that is closest to the center of the cell will be used in setting the concentration of the cell. You should not change this layer to a data layer.

MT3D Area Constant Concentration Unit[i]

MT3D Area Constant Concentration Unit[i] is used to specify constant concentration sources that extend over several cells. Cells whose centers are enclosed by a closed contour on an MT3D Area Constant Concentration Unit[i] layer will be designated as a constant concentration cells with a concentration equal to the concentration specified on the MT3D Area Constant Concentration Unit[i] layer. Values specified on an MT3D Area Constant Concentration Unit[i] layer will be overridden by values specified on an MT3D Point Constant Concentration Unit[i] layer. If desired, you may change this layer to a data layer. However, if you do, the entire layer will be made up of constant concentration cells.

MT3D Point Time Varying Constant Concentration Unit[i]

In the earlier version of MT3D, (version 1.1), constant concentration cells retained the same concentration throughout the duration of the model. Version 1.5 of MT3D introduces a new type of boundary condition called "time-varying constant-concentration". A better name might be "time-varying specified-concentration" because the concentration does not remain constant. Instead, the user is allowed to change the specified concentration in each stress period. **A cell that has been designated as a "time-varying constant-concentration" cell can not revert back to a normal, active-cell.** If no concentration is specified for a particular stress period, the time-varying constant-concentration cell will be treated as a constant concentration cell with a concentration equal to that for the previous stress period. You should not change this layer to a data layer.

The MT3D Point Time Varying Constant Concentration Unit[i] is used to specify time varying constant concentration along a vertical line in a geologic unit. The concentration applied to a cell will be calculated from the mass specified in the Mass parameter, the top and bottom of the geologic unit and the values of the Top Elevation and Bottom Elevation parameters of an MT3D Point Time Varying Constant Concentration contour. The mass will be allocated according to the following formula

Mass fraction = (length of overlap between current layer thickness and vertical extent of the source) / (vertical extent of the source).

MT3D Area Time Varying Constant Concentration Unit[i]

See MT3D Point Time Varying Constant Concentration Unit[i] for a discussion of time varying constant concentration cells.

Any cells whose centers are enclosed in a closed contour on an MT3D Area Time Varying Constant Concentration Unit[i] layer will be treated as time varying constant concentration cells with a concentration equal to the concentration specified on the . MT3D Area Time Varying Constant Concentration Unit[i] layer. Values assigned on an MT3D Area Time

Varying Constant Concentration Unit[i] layer are overridden by those assigned on an MT3D Point Time Varying Constant Concentration Unit[i] layer. If desired, you may change this layer to a data layer. However, if you do, the entire layer will be made up of constant concentration cells.

MT3D Point Initial Concentration Unit[i]

MT3D Point Initial Concentration Unit[i] is used to specify point sources that do not maintain a constant concentration. If any Point Contours are on a MT3D Point Initial Concentration Unit[i] layer, the initial concentration of the cell will be set equal to the mass divided by the cell volume. If the unit has a vertical discretization greater than 1, the mass will be divided among all the cells in the geologic unit that contain the point contour. If a cell contains more than one point object, the one that is closest to the center of the cell will be used in setting the concentration of the cell. Values specified on an MT3D Point Initial Concentration Unit[i] layer will be overridden by values specified on an MT3D Point Constant Concentration Unit[i] layer or MT3D Area Constant Concentration Unit[i] layer. You should not change this layer to a data layer.

MT3D Area Initial Concentration Unit[i]

MT3D Area Initial Concentration Unit[i] is used to specify initial concentrations that are not specified elsewhere. Cells whose centers are enclosed by a closed contour on an MT3D Area Initial Concentration Unit[i] layer will be assigned an initial concentration equal to the concentration specified on the MT3D Area Initial Concentration Unit[i] layer. Values specified on an MT3D Area Initial Concentration Unit[i] layer will be overridden by values specified on an MT3D Point Constant Concentration Unit[i] layer, MT3D Area Constant Concentration Unit[i] layer, or MT3D Point Initial Concentration Unit[i] layer.

By default the Exact contour method is used to assign values on MT3D Area Initial Concentration Unit[i] layers. However, you can interpolate among point sources instead by changing to the interpolation method and using point contours or by changing an MT3D Area Initial Concentration Unit[i] layer from an information layer to a data layer and importing data points.

MT3D Parameters on MODFLOW Layers

Recharge, Evapotranspiration, Prescribed Head , Wells, Line River, Area River, Line Drain, Area Drain, Point General Head Boundary, Line General Head Boundary, Area General Head Boundary,

In an MT3D model, each of the potential sources or sinks for water has a parameter named MT3D Concentration[j] where j represents the stress period. On the Recharge and Evapotranspiration layers, the default concentration is 0. On the others, it is \$N/A. You only need to specify a concentration value for sources that have concentrations different than 0. All sources that are not explicitly set to a concentration different than 0 will be treated as having a concentration of 0 by MT3D. Except for evapotranspiration, MT3D does not use the concentrations of sink. If any of the MT3D concentrations are set to \$N/A, no data for that particular stress period will be exported for that object. MT3D will treat the source as having a concentration of 0. The units for the concentration must be the consistent with the units for the rest of the model.

Hydraulic Conductivity

Longitudinal dispersivity is set using the MT3D Longitudinal Dispersivity parameter on the Hydraulic Conductivity Unit[i] layer. Its units must be consistent with the units for the rest of the model.

Creating MT3D Input Files and Executing MT3D

The MODFLOW.MET file in the ArgusPIE directory is the export template used by the MODFLOW/MT3D PIE to create the MODFLOW and MT3D input files and to run MODFLOW or MT3D. To run a model, change to the MODFLOW FD Grid layer, and select Run MODFLOW/MT3D from the PIE directory. The "Run MODFLOW and MT3D" dialog box will be displayed. By default the dialog box will create the input files for MODFLOW and run MODFLOW model. You can choose which packages you wish to export by checking or unchecking the check boxes in the MODFLOW Output packages.

To create input files for MT3D or run MT3D, Select the "Create MT3D input files only" or "Create Input files and Run MT3D". When you do the MT3D Output packages check boxes will appear. You can choose which packages will be exported by checking or unchecking those check boxes. It is only possible to select one of the MT3D radio buttons if you have an MT3D model as specified in the Project Info Dialog box. MODFLOW will only create the flow file required by MT3D if you have selected the MT3D option is selected on the Stresses/Solvers tab of the Project Info dialog box. You can call up the Project Info Dialog box by selecting Edit Parameters. If you select the "Help" button, you will activate the on-line help.

When you have chosen which packages to export, click the OK button to begin exporting the input files for MT3D or MODFLOW. Because MT3D requires the flow file produced by MODFLOW. You must wait until MODFLOW has finished before starting MT3D.

To leave the "Run MODFLOW and MT3D" dialog box without creating input files or running a model, select Cancel. You can then select a directory that will in which the input files and output files will be created. This must be a directory containing the

The default names and locations of the MODFLOW and MT3D executables are shown in the MODFLOW-96 path or MT3D 1.5 path edit boxes. To change those names or paths, type them in the edit boxes or select them by pressing the "Browse" button.

Postprocessing

To view the results of an MT3D simulation, select "MT3D Post Proc..." from the PIE menu. This will start the MT3D Import Utility. Argus ONE will pass required information to import utility so you do not need to enter the information manually. You can select the sort of file from which you wish to import data and whether a logarithmic transformation will be applied to the data. By default, data will be imported from an MT3D concentration file. However, you can also import data from a MODFLOW binary head file or binary drawdown file. However, you must first run MT3D before importing data from the MODFLOW binary output files because the import utility uses the grid configuration file created by MT3D.

Once you have selected the type of data and whether or not a logarithmic transformation will be applied. Click the Import Data button. Then select the data source (a concentration file: MT3D.UCN; a binary head file: Rootname.BHD; or binary drawdown file: Rootname.BDN). Next select the grid configuration file (MT3D.CNF). You must next select the type of data to import to Argus ONE. You can import data along a single row, column or layer or from the water table. Then select the time or times for which you wish to import data. If they do not

already exist, Argus ONE will create two new layers named MT3D Data and MT3D Post Processing Charts. If "MT3D Post Processing Charts" already exists, a warning message will appear telling you that it already exists and giving you the choice of adding the chart to the existing charts or replacing the existing chart. The data that are imported will overwrite the existing data unless you change the name of the MT3D Data layer before importing the new data. Finally, you can choose whether to create a contour map, color map, 3D chart or cross section.

If a concentration is zero or negative and a logarithmic transformation has been applied, the concentrations will be assigned a value equal to one tenth the minimum absolute value of the concentration for that data set before applying the logarithmic transformation. The logarithmic transformations are calculated using base 10 logs rather than natural logs. Although a logarithmic transformation can be applied to head and drawdown data as well, this is not recommended because it is unlikely to make the data easier to understand.

You can run the MT3D Import Utility without calling it from Argus ONE. If you do, you can use it to create Surfer Grid or Dat files. The program is located in the ArgusPIE\MT3D_GUI directory.

Files created for MODFLOW and MT3D models.

Files Created by MODFLOW for MT3D Models

In addition to the files documented by Shapiro and others (1997) one additional file may be created by MODFLOW when used with the MODFLOW/MT3D PIE. If the MT3D option is selected on the Stresses/Solvers tab of the Project Info dialog box, a binary file named *Rootname.FLO* will be created where "Rootname" is the root name specified in the Output Files tab of the Project Info dialog box.

Whenever MODFLOW-96 runs from a batch file it creates a file named *modbatch.rpt*. It will list the name file(s) that was run followed by "Normal termination of simulation" if the program completed the model successfully. Abnormal terminations may occur if the model did not converge to a solution or for any of a number of other reasons. If the model does not terminate normally, you should examine the output to determine the cause of the problem. *modbatch.rpt*. *Modbatch.rpt* is also created when MODFLOW-96 is run from the USGS MODFLOW PIE but it was not listed in the PIE documentation.

Files Created for MT3D Simulations

Rootname.MTR is a response file for MT3D. It gives the names of the MT3D input files and a response to the query "Print out contents of Flow Transport Link File for Checking?"

Rootname.BTN is the input file for the MT3D Basic Transport Package.

Rootname.ADV is the input file for the MT3D Advection Package.

Rootname.DSP is the input file for the MT3D Dispersion Package.

Rootname.SSM is the input file for the MT3D Source and Sink Mixing Package.

Rootname.RCT is the input file for the MT3D Chemical Reaction Package.

Files Created by MT3D

Rootname.MLS is the MT3D Output file.

MT3D.MAS is a text file with a one-line summary of the mass balance for each transport step.

MT3D.CNF is the grid configuration file created by MT3D. The CNF extension may not be visible on some computers because Windows now uses that extension for another type of file.

MT3D.UCN is a binary file containing the concentration in every cell at each time step for which the user specified that output be written to file.

MT3D.OBS is an ASCII file containing the concentration at every observation point for every transport step. The location of each observation point in the table is indicated by the layer, row and column of the observation point above the column of concentrations.

Temporary Files

Several temporary files are created by the MODFLOW/MT3D PIE or by the post-processing utility. These include "MODFLOW-last.template", "LastExp.exp", "SelTimes.txt". These files will be created in the directory containing the MODFLOW/MT3D PIE. They can be safely deleted whenever you are not exporting data to MODFLOW or MT3D or importing data from MT3D.

New Expression for Initial Head

There are a number of differences between the USGS MODFLOW PIE and the MODFLOW portion of the ARGUS MODFLOW/MT3D PIE. Most require little discussion. However, the expressions for "Initial Heads Unit[i]" on the MODFLOW FD Grid layer requires more explanation. In the USGS PIE, the expression Initial Head on Unit1 was as follows.

```
If(((CountObjectsInBlock(Prescribed Head Unit1,1))>0|(CountObjectsInBlock(Prescribed Head Unit1,0)>0)|(Prescribed Head Unit1!=$N/A)),Interpolate(Prescribed Head Unit1),Initial Head Unit1)*Abs(MODFLOW FD Grid.IBOUND Unit1)
```

This formula interpolates to the center of a block from all the contours on the Prescribed Head Unit[i] layer and applies the interpolated value to a cell if the cell contains a contour or was inside a closed contour on the Prescribed Head Unit[i] layer or if a default value had been assigned to the layer. Thus the value assigned to a cell would not be exact value of the contour in the cell unless the contour was directly under the center of the cell. (It would, however, be close to that value.)

In the MODFLOW/MT3D PIE, you can choose to use a different expression for the initial head. In new models, the default expression for initial head has the following effect.

1. If there are any point objects on the Prescribed Head Unit[i] layer in a block, the block is assigned the average value of those point objects.
2. If there are no point objects on the Prescribed Head Unit[i] layer in a block but the block contains one or more open contours, the block is assigned the average value of the open contours.
3. If there are neither point objects nor open contours on the Prescribed Head Unit[i] layer in a block but the center of the block is at a location that has been assigned a value different from \$N/A on the Prescribed Head Unit[i] layer. The value assigned to the block comes from the Prescribed Head Unit[i] layer. (This happens if the center of a block is inside a closed contour on the Prescribed Head Unit[i] layer or the Prescribed Head Unit[i] layer has been assigned a default value different from \$N/A.)

4. If none of the above apply, the value assigned to a cell is taken from the Initial Head Unit[i] layer.

If you wish to use the new expression with old models and you have **not** overridden the expressions for any parameters on the MODFLOW FD Grid layer, it is easy to convert. Select the Customize tab in the Edit Project Dialog box and select "Use Point Contours First" for Initial Head Formula.

If you have overridden the default expression for a parameter on the MODFLOW FD Grid layer, create a new model with the same number of layers as your old model. Then copy the expressions for each parameter from the new model to the old model. To copy the expressions of the new model, open the layers dialog box (View|Layers...) and select the MODFLOW FD Grid in the top half of the dialog box. Next select the correct parameter in the lower half of the dialog box. In the "Lock" column, unselect "Lock Def Val". You will now be able edit the default value. An "f_x" button will appear under the Value column. Click it and the Expression editor will appear. Copy the formula in the upper half of the expression editor by selecting it and pressing Ctrl-C. Follow a similar set of steps to bring up the expression editor for the same parameter in the old model and paste the expression into it by pressing Ctrl-V. (In the old model, you will not need to unlock editing of the default value.)

You may wish to average the values of point and line contours in the Prescribed Head Unit1 layer to determine the value of the Initial Head Unit[i] layer. You can choose an expression that will do so by selecting "Average Points and Open Contours" on the Customize tab.

If you wish to use the old expression for initial head, select "Interpolate" on the Customize tab.

Differences between the USGS MODFLOW PIE (version 1.41) and the MODFLOW portion of the ARGUS MODFLOW/MT3D PIE.

- Formula for Initial Heads (see "New Expression for Initial Head")
 - USGS: Interpolated value
 - Argus: Choice of three formulas
- Default location of MODFLOW
 - USGS: C:\MODFLW96.3_1\BIN\MODFLW96.EXE
 - Argus: C:\Program Files\Argus Interware\ArgusPIE\Mt3d_gui\Modflw96_Argus32.exe
- Method of changing path of executable
 - USGS: Edit MODFLOW.MET file to change path.
 - Argus: Edit MODFLOW.VAL file to change default path or select a path from the Run MODFLOW dialog box.
- WSEED field of SIP tab
 - USGS: Always enabled.
 - Argus: Enabled only when used.
- Online help
 - No help for MODFLOW.
 - Help for MODFLOW available.

- Maximum number of geologic units
 - USGS: 100 geologic units; PIE causes Argus ONE to crash if the maximum is exceeded.
 - Argus: 100 geologic units; warning message is displayed if the user attempts to exceed the maximum. (To change this maximum, change the value of kMaxLayers in modflow_pie.h and recompile the PIE.)
- Maximum number of stress periods
 - USGS: 100 stress periods; PIE causes Argus ONE to crash if the maximum is exceeded.
 - Argus: 500 stress periods; warning message is displayed if the user attempts to exceed the maximum. (To change this maximum, change the value of kMaxStressPeriods in modflow_pie.h and recompile the PIE.)
- Maximum number of MODFLOW layers
 - USGS: does not check if the maximum number of layers allowed by the USGS version of MODFLOW is exceeded.
 - Argus: displays warning if the maximum number of layers allowed by the USGS version of MODFLOW is exceeded. (To change this maximum, change the value of kMaxMODFLOW_Layers in modflow_pie.h and recompile the PIE. You will also need to modify the maximum number of layers in MODFLOW itself.)
- Postprocessing
 - USGS: Grid rotation not supported. Contours and other post-processing objects truncated in long, narrow blocks. Postprocessing PIE separate from MODFLOW PIE
 - Argus: Grid rotation supported. Contours and other post-processing objects continuous across long, narrow blocks. Postprocessing PIE combined with MODFLOW/MT3D PIE
- Group Layers
 - USGS: Group layers are not used
 - Argus: Group layers are used to group together layers of the same geologic unit. (However, models created with the USGS MODFLOW PIE and opened with the MODFLOW/MT3D PIE will not have group layers added automatically.)
- MOC3D support
 - USGS: MOC3D support is incomplete so radio button for MOC3D is inactive.
 - Argus: MOC3D radio button has been changed to invisible.
- Hidden functions
 - USGS: All MODFLOW functions are hidden from the user.
 - Argus: Four MODFLOW/MT3D PIE functions that were previously hidden are now visible. These will probably be useful only to users who wish to create export templates for additional MODFLOW packages. These functions are:
 - MODFLOW_NLAY(): returns the number of geologic units.
 - MODFLOW_NDIV(Unit_Number): returns the number of MODFLOW model layers represented the geologic unit specified by Unit_Number.
 - MODFLOW_SIMUL(Unit_Number): returns 1 if the geologic unit specified by Unit_Number is a simulated unit, otherwise returns 0.
 - MODFLOW_NPER(): returns the number of stress periods.

- Precision
 - USGS: Non-spatial real numbers are saved in single-precision format. HCLOSE values less than 10^{-7} are exported as 0.0.
 - Argus: Non-spatial real numbers are saved in double-precision format. HCLOSE values less than 10^{-7} are exported correctly.
- MT3D Flow file
 - USGS: MT3D flow file is never created by MODFLOW.
 - Argus: MT3D flow file is created by MODFLOW if the link to MT3D is incorporated into MODFLOW as described in Appendix 1 and the MT3D option is checked on the Stresses/Solvers tab of the Project Info dialog box.
- Canceling running MODFLOW
 - USGS: An open-file dialog box appears after clicking the cancel button on the Run-MODFLOW dialog box.
 - Argus: An open-file dialog box does not appear after clicking the cancel button on the Run-MODFLOW dialog box.
- DAMP parameter in PCG2
 - USGS: Does not support using the DAMP parameter in PCG2.
 - Argus: Obsolete IPCGCD parameter replaced by DAMP.
- About tab
 - USGS: not present
 - Argus: present
- Rootname size
 - USGS: no limit
 - Argus: limited to eight characters (the limit of the MT3D executable).
- Locked layers and parameters size
 - USGS: not used
 - Argus: used where appropriate.
- Formula for MODFLOW FD Grid.Wetting Unit[i]
 - USGS: allows all inactive cells to become active not just cells that have gone dry
 - Argus: allows only cells that have gone dry to become reactivated.

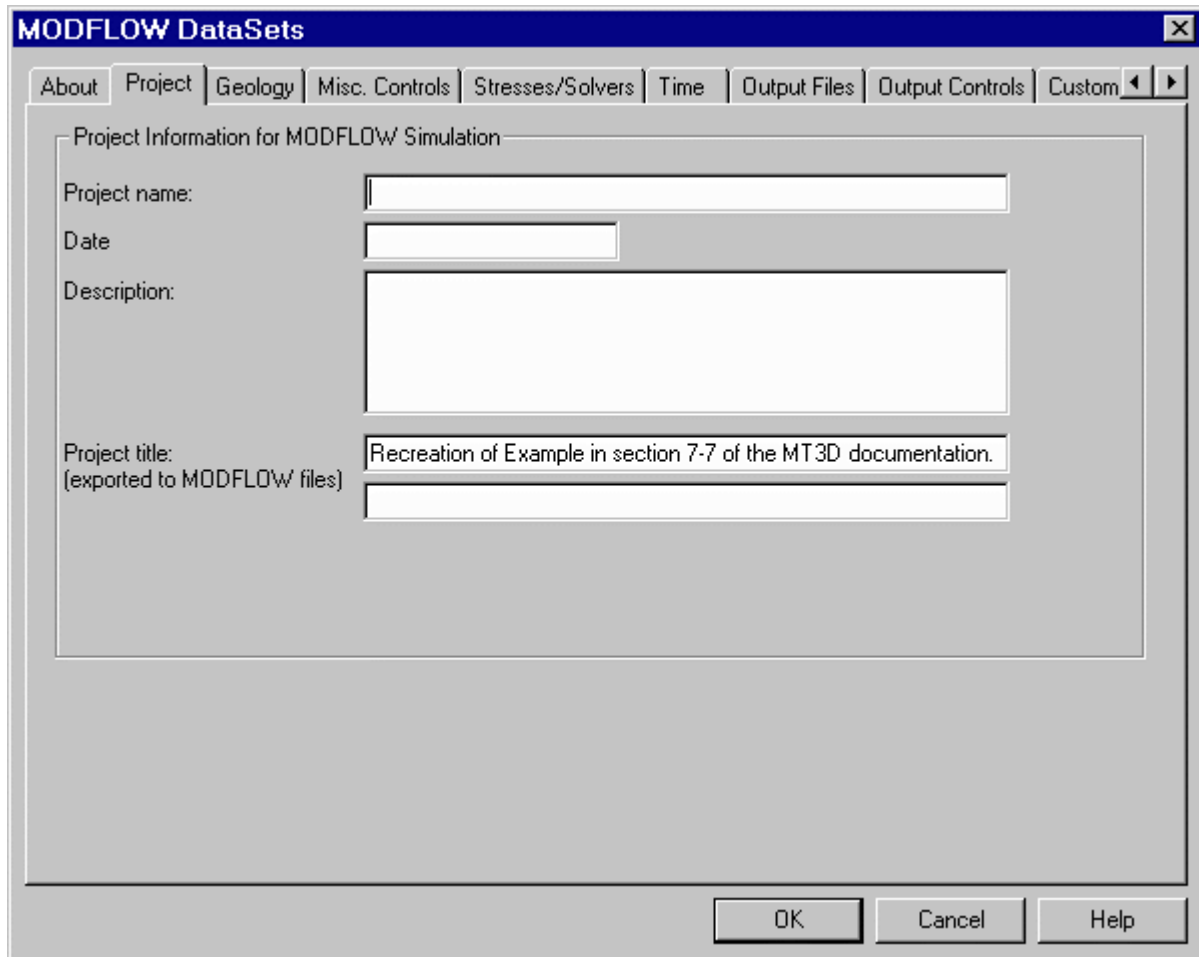
Example

The following example is based on the example in section 7.7 of the MT3D documentation (Zheng, 1990). I have not attempted to recreate his model exactly but instead have created a model similar to his based on the data in his report. In the cases where the data were insufficient to reproduce the model, I have used the original input data from the MT3D example. The original input files and documentation are available from <http://www.epa.gov/ada/models.html>.

MODFLOW Model

Non-Spatial Data

After installing Argus ONE and the MODFLOW/MT3D PIE, we start Argus ONE and select "New MODFLOW/MT3D Project..." from the PIE's menu. The MODFLOW Project Info Dialog box will appear. Assign an appropriate title (if desired) to the model.



The image shows a screenshot of the "MODFLOW DataSets" dialog box, specifically the "Project" tab. The dialog box has a title bar with the text "MODFLOW DataSets" and a close button (X). Below the title bar is a menu bar with the following items: "About", "Project", "Geology", "Misc. Controls", "Stresses/Solvers", "Time", "Output Files", "Output Controls", and "Custom" with left and right arrow buttons. The main area of the dialog is titled "Project Information for MODFLOW Simulation" and contains several input fields:

- "Project name:" followed by an empty text box.
- "Date" followed by an empty text box.
- "Description:" followed by a large empty text area.
- "Project title: (exported to MODFLOW files)" followed by a text box containing the text "Recreation of Example in section 7-7 of the MT3D documentation." and an empty text box below it.

At the bottom of the dialog box are three buttons: "OK", "Cancel", and "Help".

Figure 1. Example, MODFLOW Project Info

On the Geology Tab, we will delete or rename the Aquitard and create another model layer. You should end up with four model layers, all of which are simulated layers. The top layer should be unconfined. The other three should be confined. If you wish, You may also change the Interblock transmissivity of the top layer to "Arithmetic mean". This is appropriate for unconfined aquifers with uniform hydraulic conductivity. However, a harmonic average would also work well. When the original model was created, the harmonic mean was the only option available and so Cheng used the harmonic mean. Be sure all layers are simulated layers because that is a requirement of MT3D.

Details for Argus ONE novices:

To change the geologic structure displayed on the geology tab, select a layer from the table, The data from that layer will appear in the boxes below. Edit those boxes and click the Modify button. **Your changes do not take effect until you click the Modify button.** To insert a layer, select a layer and click the Insert button. A layer will be inserted above the one you selected. You can insert a layer below the bottom layer by selecting the blank field below the lowest layer and clicking the Insert button. To delete a layer, select it and click the Delete button.

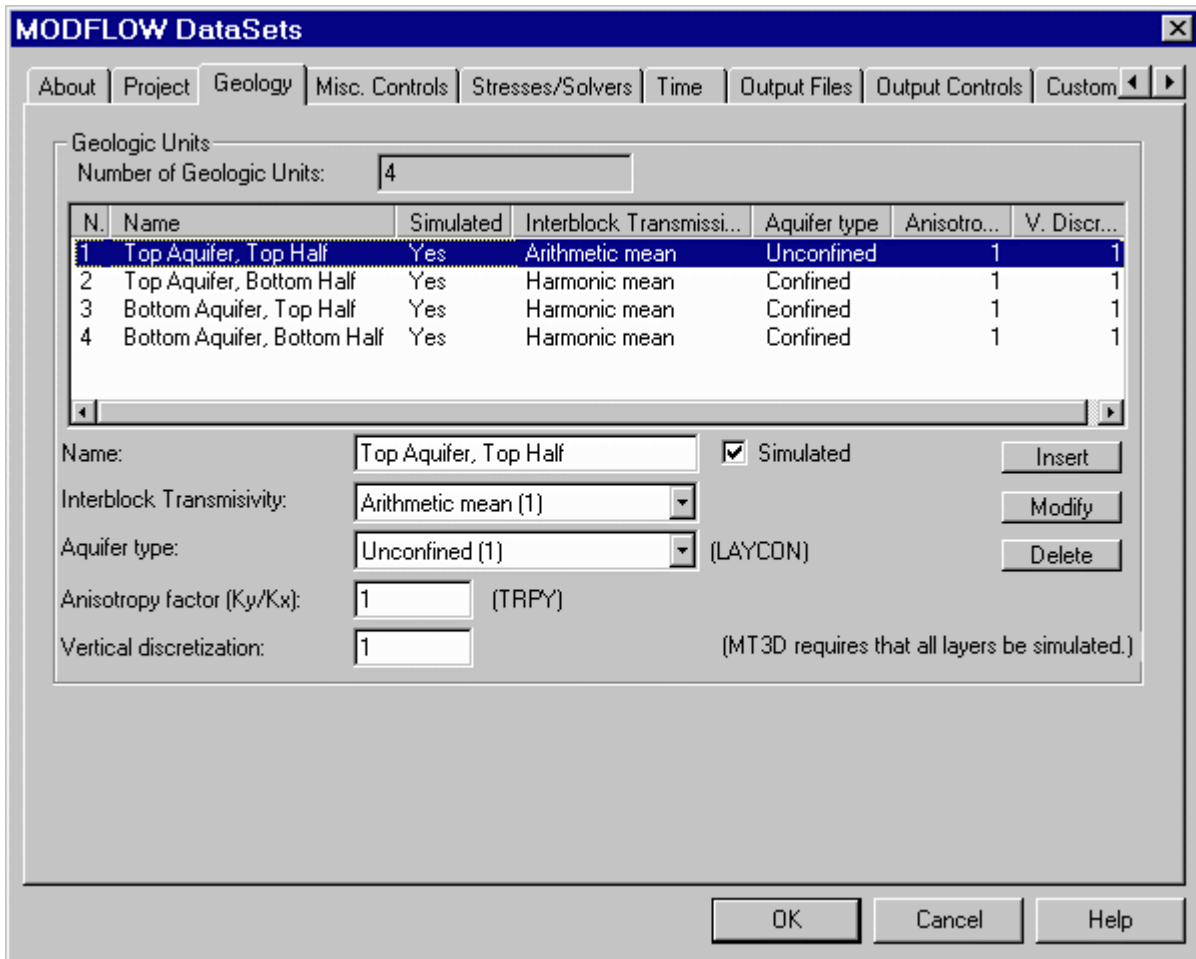


Figure 2. Example, MODFLOW Geology

We don't need to do anything on the Misc. Controls tab. On the Stress/Solvers tab we will select the Recharge, Well and MT3D 1.5 check boxes. This indicates that we will be using recharge and wells in the model and we will be creating an MT3D model. When you click on the MT3D check box, additional tabs will appear that you use to edit non-spatial data related to MT3D. We will be using steady stress and applying recharge to the top layer so we don't need to edit the drop down lists that are activated when the Recharge and Well check boxes are checked.

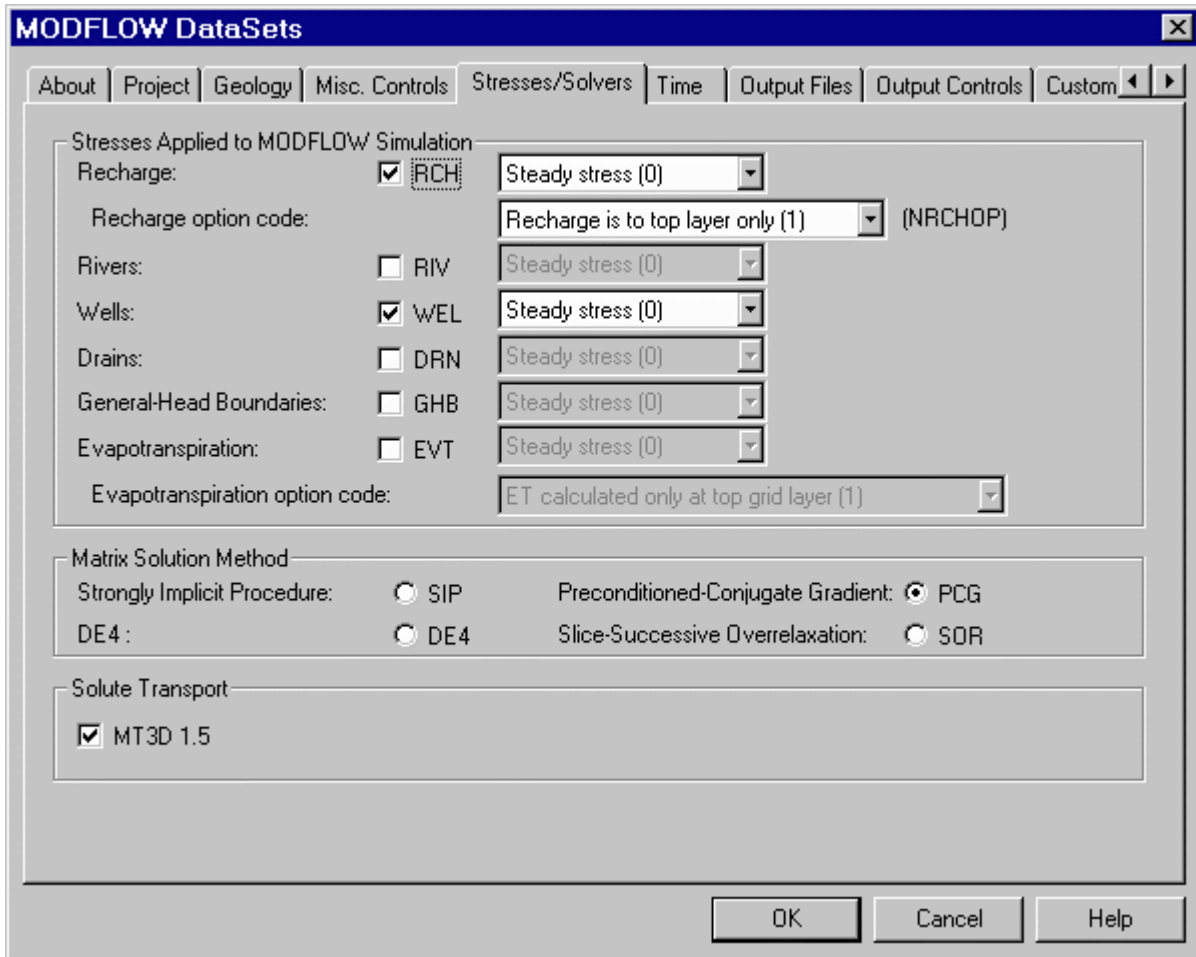


Figure 3. Example, MODFLOW stresses.

On the Time tab change the time units to Days (4) and the Length (Stress period length) to 1000.

Details for Argus ONE novices:

To change the stress period information displayed on the time tab, select a stress period from the table, The data from that stress period will appear in the boxes below. Edit those boxes and click the Modify button. **Your changes do not take effect until you click the Modify button.** To Insert a stress period, select a stress period and click the Insert button. A layer will be inserted before the one you selected. You can insert a stress period after the last stress period by selecting the blank field after the last stress period and clicking the Insert button. To delete a stress period, select it and click the Delete button.

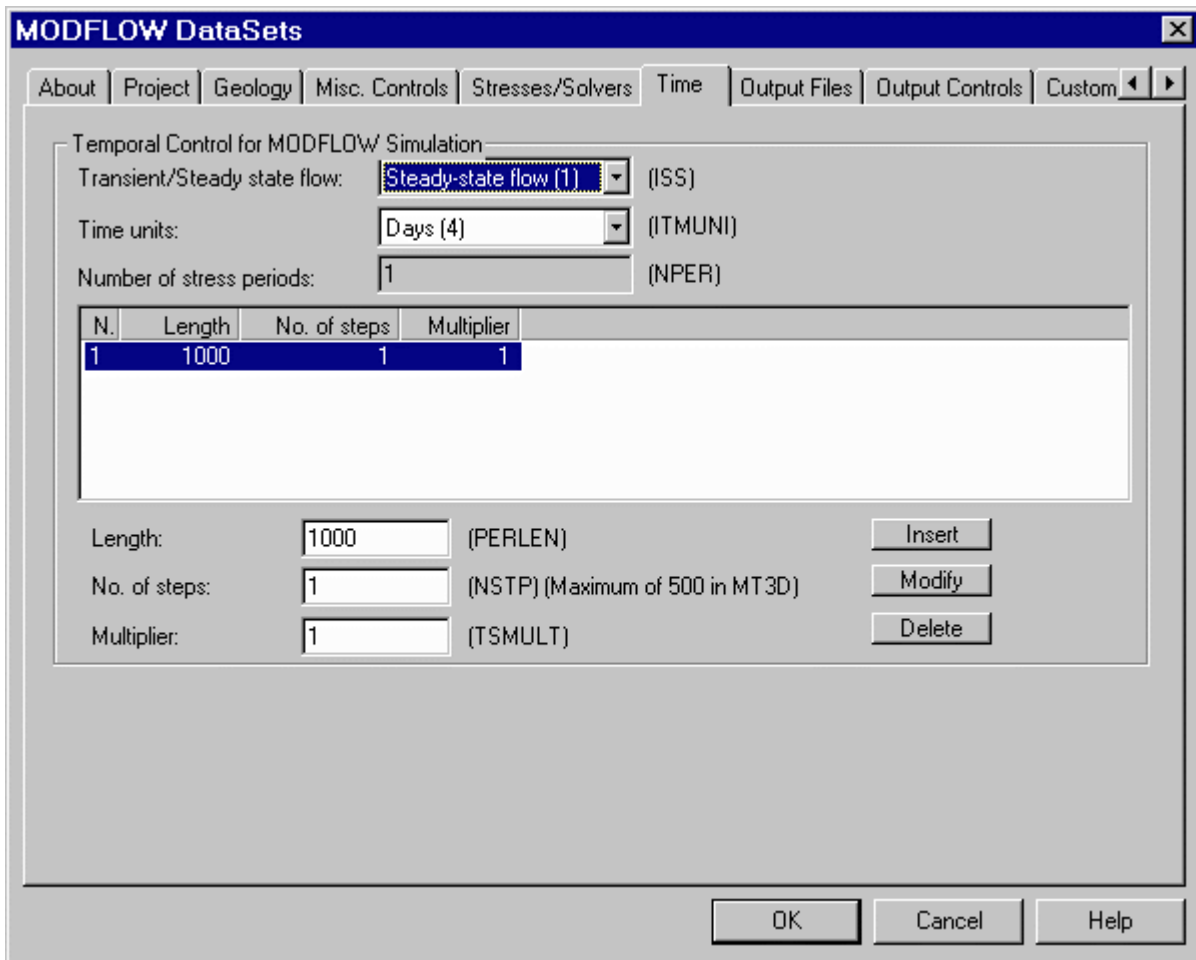


Figure 4. Example, MODFLOW time parameters

On the Output Files tab replace "USERSPEC" with a meaningful name. This will be the *Rootname* for the files created by the MODFLOW/MT3D PIE. Because some versions of MODFLOW and MT3D require that the *Rootname* be eight characters or less, *Rootname* is now limited to a maximum of 8 characters. The versions of MODFLOW and MT3D distributed by the USGS and the University of Alabama respectively are limited to 8 character file names. (The version of MODFLOW from Argus does not have this limitation.) We will change both the "Export Head Data" and "Export Drawdown Data" fields to "Binary file" so we can demonstrate using the MT3D Post Processor with MODFLOW data. We could export the MODFLOW data as a formatted text file and use the MODFLOW post processing PIE instead.

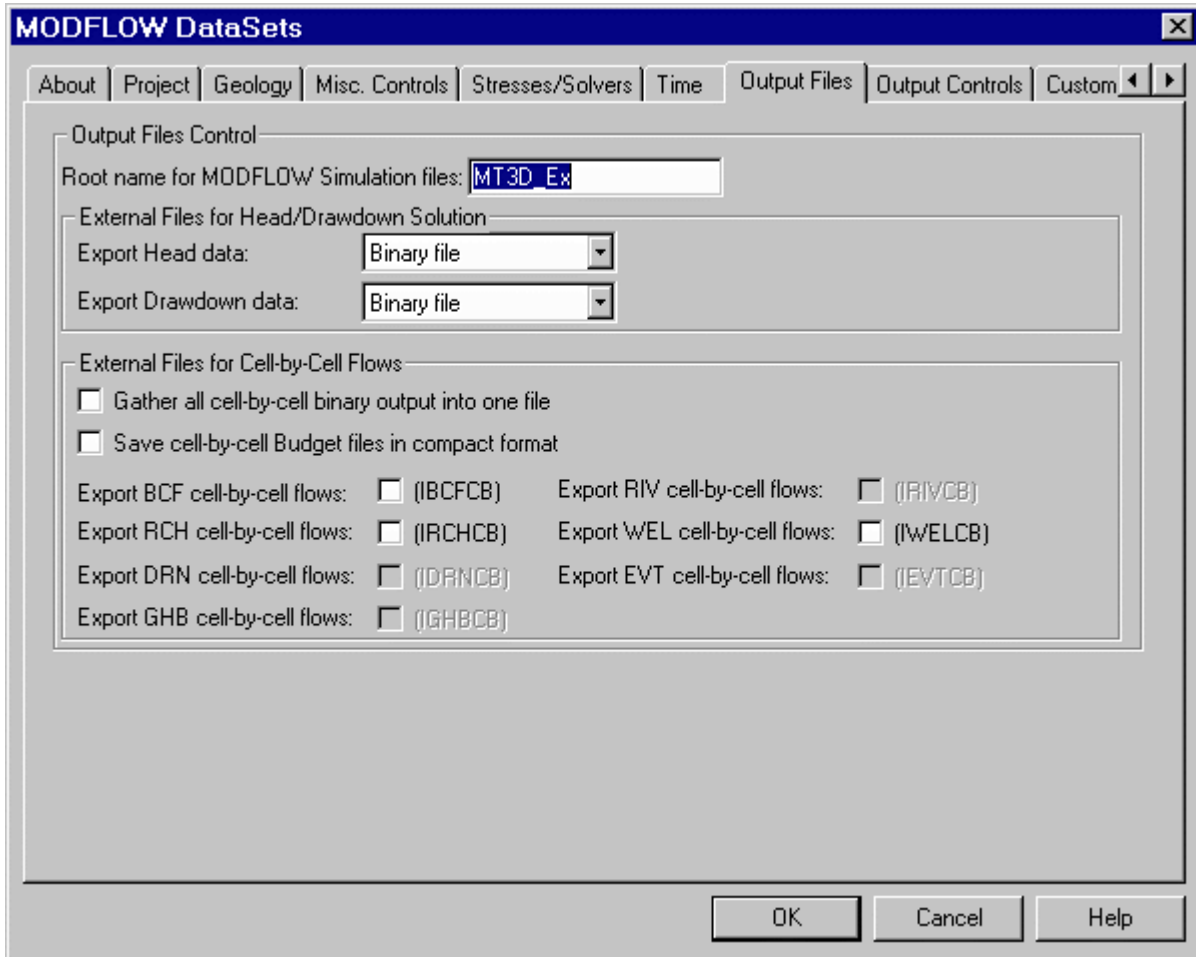


Figure 5. Example, MODFLOW Output file parameters

We don't need to do anything on the Output Controls or PCG tabs so we will go straight to the MT3D BAS tab on which we enter non-spatial data for the MT3D Basic Transport Package. We will enter a title for the MT3D project that will be exported to MT3D and set the length unit to feet. No mass unit was specified in the original model so we will just keep the default unit of kg. The Sink and Source Mixing Package has already be automatically selected but we must manually select the Advection, Dispersion, and Chemical reaction packages.

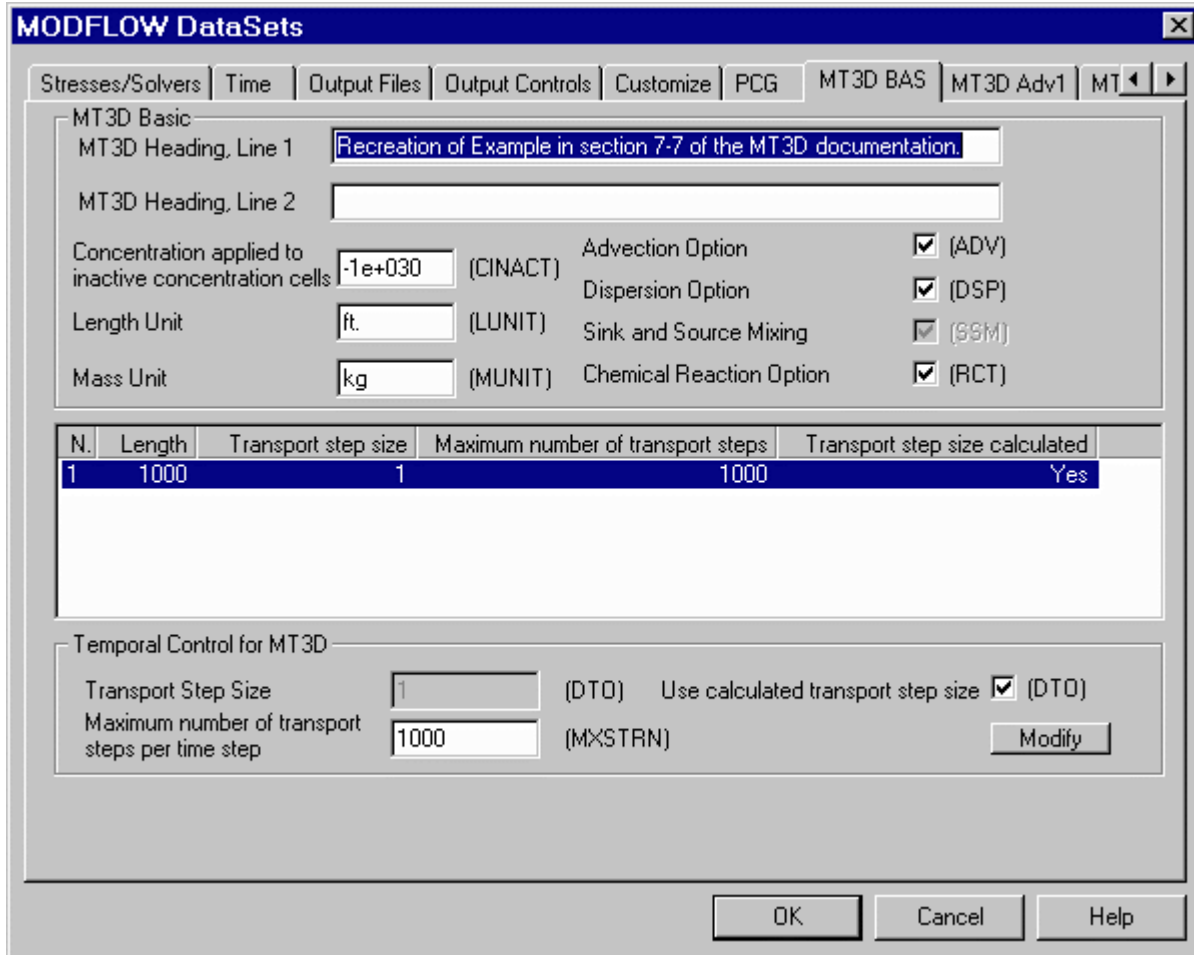


Figure 6. Example, MT3D Basic Package parameters

We don't need to do anything on the MT3D Adv1, MT3D Adv2, or MT3D Disp/Chem tabs so we will skip to the MT3D Out tab. Here we will change the times at which MT3D will print concentrations. From "Each Nth transport timestep within each flow timestep" to "Specified times". We will create out put every 250 days. To do so enter 250 in the Printout Time Dialog box and press the Modify button. Then enter 500 and press the Insert Button. Do the same for 750 and 1000. It doesn't matter if the times are in order or not. They will be automatically sorted when we close the Project Info Dialog box. To see that click the OK button and then select "Edit Project Info..." from the PIE's menu. Go back to the MT3D Out tab and you will see that the times you entered are now sorted in ascending order.

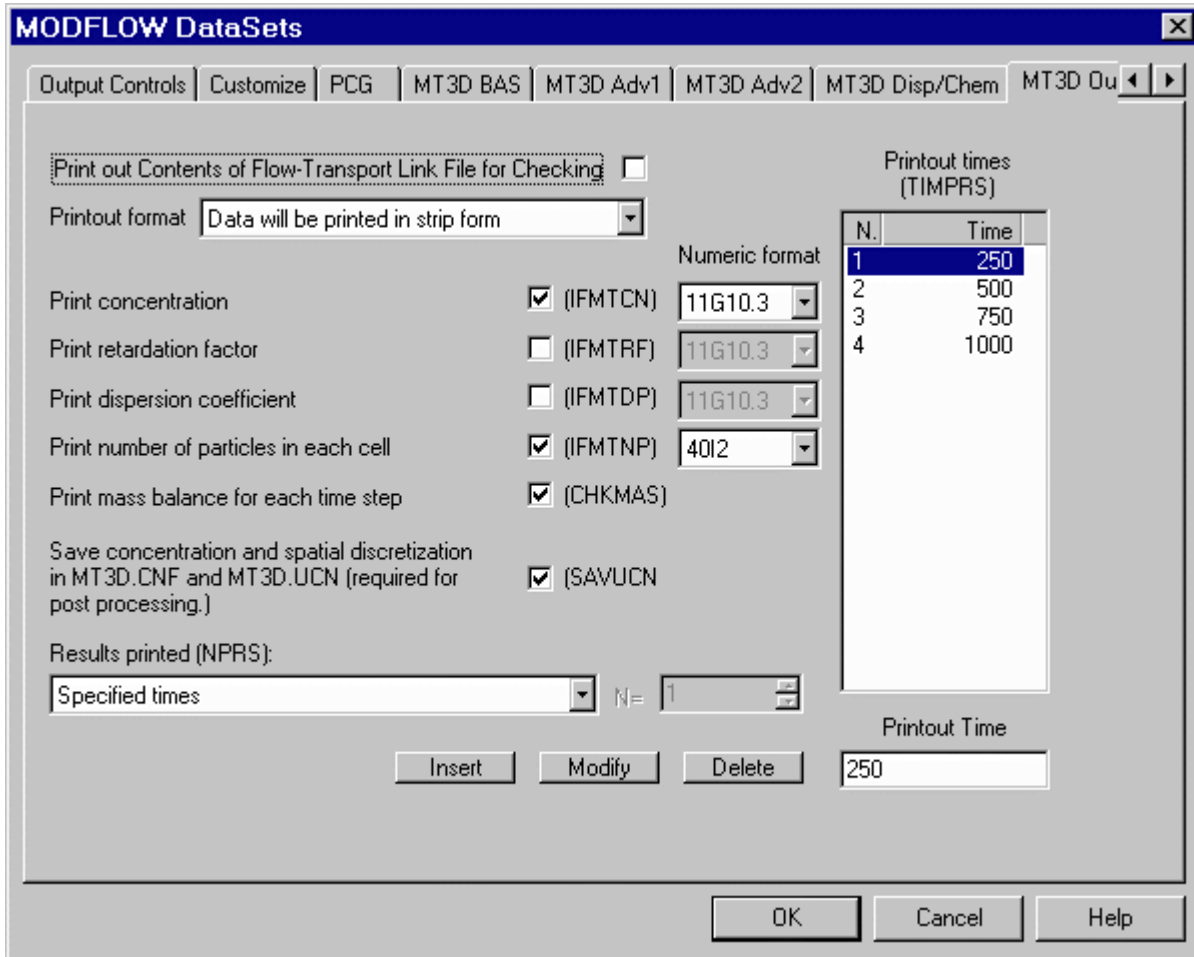


Figure 7. Example, MT3D Output formats

You can get help on any part of the Project Info Dialog box by clicking the Help Button. This will start your web browser with web pages containing the online help. These web pages are all installed on your machine as part of the installation process so you do not need to be connected to the Internet to see them.

Importing Images into Argus ONE

The next step is to import illustrations from Zheng (1990) to use to help setting up the model. You can import a variety of image formats. In this case we will be importing scanned images of Zheng's figures 7.11 and 7.12. First we will change the scale of the model to match the final scale. Zheng's Figure 7.11 shows that total height of the model is 20450 ft. From the Special menu select "Scale and Units" Edit it so that it reads "Every 1 cm on the screen represents 1000 units in the real world" and change "Label units as" to "Feet". Now from the "Special" menu select "Drawing Size" and change the Vertical Extent so that it is somewhat larger than 20450; for example, 25000. Also change the vertical and horizontal origins to -1000. The image has white space beyond the edge of the model. You want the drawing size to be large enough to accommodate that white space.

Next we need to create a layer on which to place the image. Because, we will be placing several overlapping images on the model, we will want one layer for each image. The first layer will be a map layer named "Original Grid". You can download the images from ftp://ftp.argusint.com/pub/ArgusPIEs/MT3D_Files/example7_7_images.zip. Place the image `mt3d_grid.gif` on it and size it so that the scale is correct.

Details for Argus ONE novices:

To create a new layer first select "View | Layers..." to bring up the Layers dialog box. (There are other ways of bringing it up too.) Select the MT3D Domain Outline layer and click the "New" button in the upper half of the dialog box. That will create a new layer beneath the MT3D Domain Outline layer. "Information" and a down arrow are on the right, under "Type". Click on the down arrow and select Maps. This will change the new layer to a Map layer. Enter a name for the new layer such as "Original Grid" by selecting the old name and typing the new one. Click on the far left next to the "eye" icon to make the new layer the active layer. (A check mark will appear next to the active layer.) Click the "Done" button. Zoom out until the area visible on the screen represents approximately 25000 ft. From the "File" menu, select "Place Image". Select the scanned image that represents the grid and click on the "Open" button. The image will appear on the screen. The next step is to resize the image so that its dimensions are correct. First get the lower left-hand corner so that it lies over (0,0) on the screen. You can click on the image and drag it across the screen. However, you can't drag the image off the screen. That includes the white space surrounding the grid on the image. To get the lower left-hand corner of the image over (0,0), you will probably need to change the drawing size again. I ended up with horizontal and vertical origins of -4000 and horizontal and vertical extents of 31,000. You may find it useful to zoom in on the lower left-hand corner of the grid while moving it. That way, you can place the mouse over the corner of the image and drag it to the origin. Now go to the upper left-hand corner of the image. Because the model is 20450 ft long, you want that the upper left hand corner to lie at 20450 on the y-axis. It probably doesn't. See what it does lie at. For example it may lie at 23000. Divide that number by 20450 and convert to a percentage ($23000/20450 = 112.47\%$). From the "Special" menu select "Rotate and Scale". Enter the percent you calculated in the Scale X box and select the radio button for "Position". Accept the default position of X= 0, Y = 0 and click the OK button. The image should have been resized to the correct size. You can also click on one of the corners and drag the image to the correct size. If after you start dragging the image, you hold down the shift key, you can change the size of the image without changing its shape.

The outer rows and columns of the grid are 2000 ft. wide whereas those in the center are only 50 ft. wide. You will also see arrows to 4 points just outside the center of the grid. Those points represent the area that was of interest and they are the corners of the area for which concentration was mapped in figure 7.12. The map that is of most interest is the starting concentration (Zheng's figure 7.12a) We will import this onto a new "Maps" layer. The procedure is much the same as before so I won't cover it in detail here. The file to import is named mt3d_concentration0.gif. When you are finished, the corners of the concentration map should lie nearly over the four, labeled points on the grid. (The match won't be perfect because there is some slight distortion in the original images.) If you want to, you can import the concentrations for other times into the model. In the end, we will compare the final concentration with the concentrations in the original model.

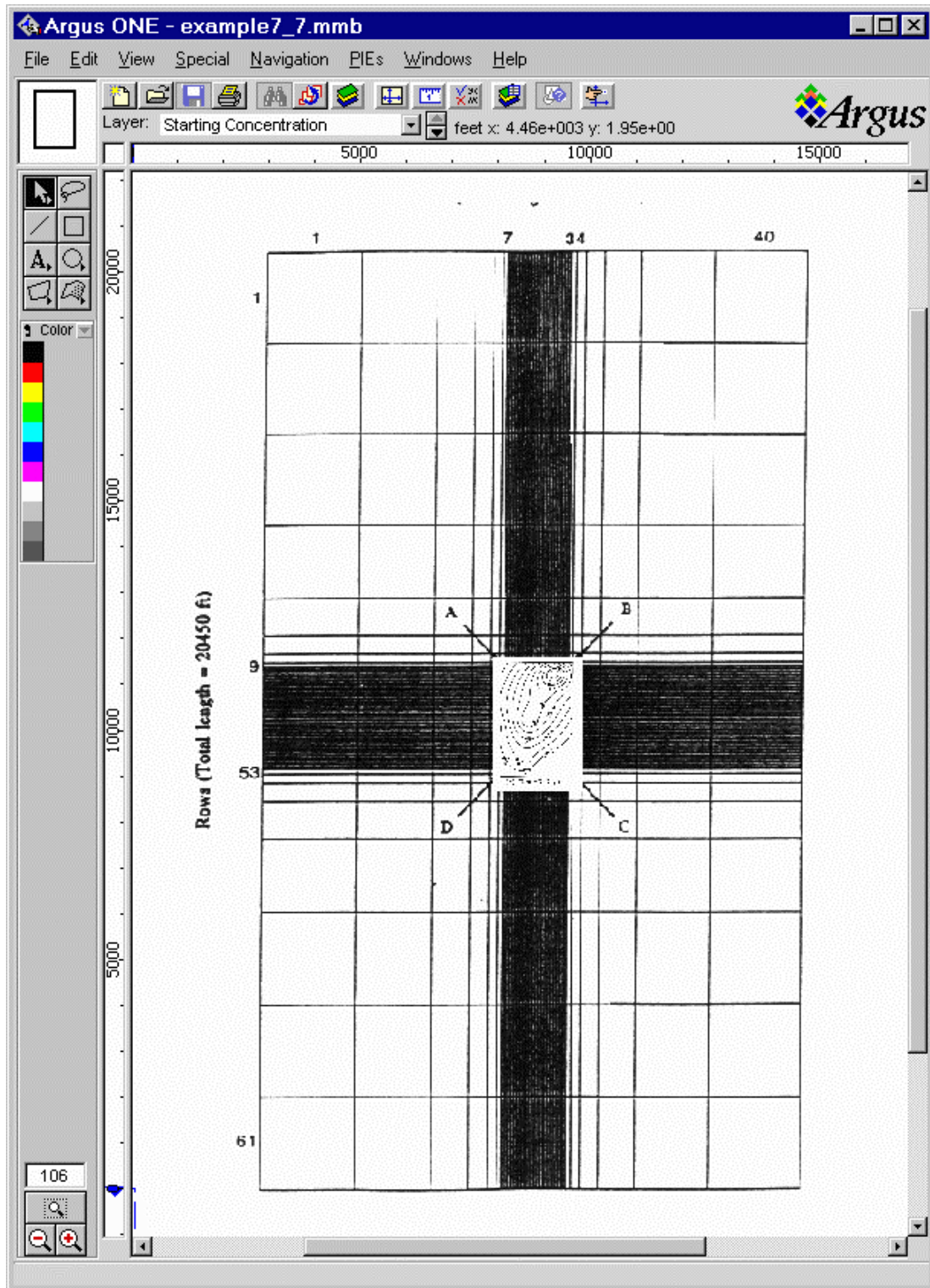


Figure 8. Example, Imported images in Argus ONE

Model Topography

The topography in this example is very simple; the top of the uppermost layer is at 780 ft and each of the 4 layers is 25 ft. thick.

Details for Argus ONE novices:

To enter the elevation of the top layer bring up the "Layers" dialog box by selecting "Layers..." from the "View" menu. (There are other ways of bringing it up too.) Select Elevation Top Unit1 from the list of layers in the upper half of the box. Elevation Top Unit 1 will appear as the only parameter for this layer in the lower half of the dialog box. Click the down arrow under "Type" in the row that has Elevation Top Unit1 in the list of parameters. Select "Expression" from the pop-up menu to bring up the expression editor. Enter 780 in the box at the top of the Expression editor and click on the OK button. This changes the default value for the top of the Unit1 to 780.

Next when you are back in the layers dialog box select Elevation Bottom Unit1 from the list of layers and again bring up the expression editor for it's parameter value. This time, go to this list of layers and functions and click on "Elevation Top Unit1". The parameters for that layer will appear in the box to the right. Double Click on "Elevation Top Unit1" in the list of parameters and it will be transferred to the expression. Edit the expression so that it reads "Elevation Top Unit1 - 25" This will put the elevation for the bottom of the layer 25 ft. below the top.

For Elevation Top Unit2 the expression should just be "Elevation Bottom Unit1". Continue in this way for the rest of the elevations. When you are done, click the "Done" button on the Layers Dialog box.

Recharge

The model uses a uniform recharge rate of 1.14×10^{-3} ft/day to the top layer in every cell. Use the Expression editor to assign default values on the Recharge Layer just as you did for the topography. Make the default elevation the top of Unit1. The Concentration should be 0.

Hydraulic conductivity and longitudinal dispersivity

The upper aquifer (layers 1 and 2) has a horizontal hydraulic conductivity (Kx) of 60, a vertical hydraulic conductivity (Kz) of 6 and a longitudinal dispersivity of 10. The lower aquifer (layers 3 and 4) has a horizontal hydraulic conductivity (Kx) of 520, a vertical hydraulic conductivity (Kz) of 52 and a longitudinal dispersivity of 10. Use the Expression editor to set default values for these parameters. On the Hydraulic Conductivity Unit1 layer and the other Hydraulic Conductivity layers. Longitudinal dispersivity is used by MT3D not MODFLOW but there is no need to wait to assign it. (Note: Cheng quotes a value of "approximately 600 ft per day" for the hydraulic conductivity of the lower aquifer but the value actually used in the model is 520 ft per day.)

Specific Storage and Specific Yield

Because this is a steady state model, Specific Storage and Specific Yield are not used.

Wells

Besides the initial concentration in layers 2 and 3, figure 7.12 (mt3d_concentration0.gif) also shows the location of 8 wells in the third layer. So we don't need to set the top and bottom elevations of these wells manually, we will change the default values for these parameters to link them to the top and bottom elevations of the layer.

Details for Argus ONE novices:

This is similar to entering the default values for the topography. Bring up the Layers dialog box as you did before and select "Wells Unit3" from the list of layers. Select "Top Elevation" from the list of parameters and bring up the Expression editor to change the expression to "Elevation Top Unit3". Change the expression for "Bottom Elevation" to "Elevation Bottom Unit3".

Wells W1 through W6 have pumping rates of $-19230 \text{ ft.}^3/\text{day}$. Well W7 has a pumping rate of $-15384 \text{ ft.}^3/\text{day}$. Well W8 has a pumping rate of $-17307 \text{ ft.}^3/\text{day}$. Enter these on the Wells Unit3 layer. You accept the default value for the concentration (\$N/A) because all of these wells are pumping water out of the aquifer. MT3D does not use concentrations in sinks except for evapotranspiration.

Details for Argus ONE novices:

If the active layer is not Wells Unit3, make it the current layer. The easiest way to do this is to keep the layers floater visible and use it to switch between layers. To bring up the Layers floater, select "Show Layers Window" from the "View" menu. Click to the left of the "eye" icon of the layer you want to be visible. A check mark will appear next to the active layer. Wells Unit3 will appear under a "group layer" named Geological Unit3. Group layers will have an arrow to the right of the "eye" icon. You can use group layers to collapse or expand a group of related layers in the Layers floater. If the group-layer arrow points to the right, the layers making up the group are collapsed and are now shown in the Layers floater. If it points down, they are expanded. You can switch from collapsed to expanded and back by clicking on the arrow. If you don't see Wells Unit 3, it may be a collapsed layer that you can expand by clicking the down arrow next to the group layer. If it still isn't visible check to make sure that you selected the Wells option in the Project Info dialog box. ("PIE's | Edit Project Info... | Stresses and Solvers").

Once you are on the Wells Unit3 layer, you need to add wells. For this purpose, it would be best to have only the Wells Unit3 layer and the Starting Concentrations visible. First press the "None" button at the top of the "Layers" floater. This hides all but the active layer. Now click on the eye icon next to the layer with the starting concentration map. This should make the starting concentration map visible. If it doesn't, you may have placed the image on the wrong layer. Make sure that Wells Unit3 is the active layer.

Locate the Contour button on the left side of the Argus ONE main window. (If you hold your mouse over it for a second or two, a "tool tip" will appear with the word "Contour") Click and hold on the contour button until a pop up menu appears. Select the bottom item from the pop up menu. This is the point contour. You can use it for entering well locations. Zoom in on the area where the wells should appear. Click at one of the well locations. A dialog box will appear. The top and bottom elevations should already be filled in correctly with the values 730 and 705 and the concentrations should be \$N/A (not available). You just need to fill in the pumping rate (Stress1).

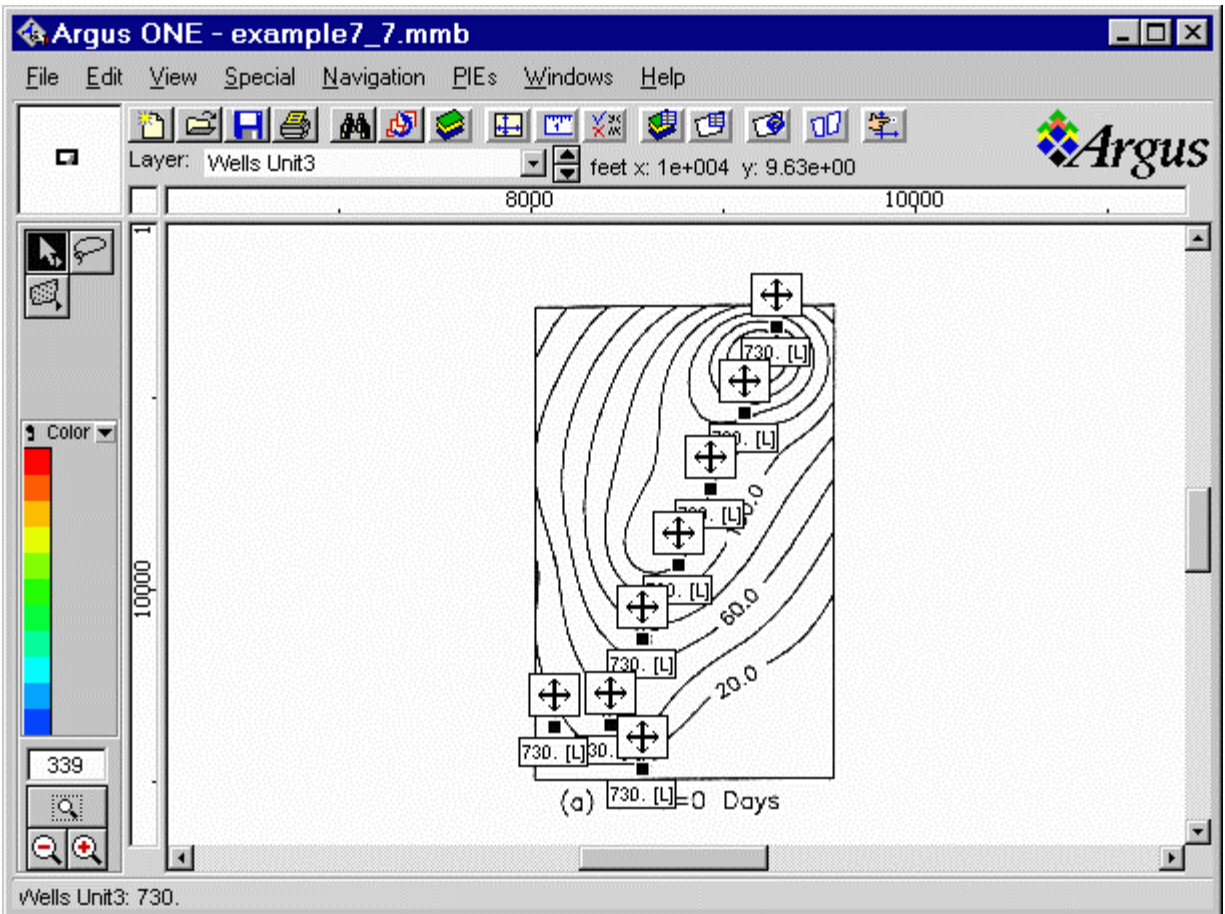


Figure 9. Example, MODFLOW well locations.

Initial Head

The original model had a uniform initial gradient in head from the upper right to the lower left. There are (at least) two ways you could create such an initial gradient. (1) You could import the heads from the original model onto a data layer in Argus ONE using the Array Import Utility that comes with the online MODFLOW Tutorial. (2) You could change the expression for Initial Head Unit1 parameter on the MODFLOW FD Grid layer to base the head on the location of the cell. The following expression will work.

```
(BlockCenterY() - (NthRowPos(0) + NthRowPos(1))/2) /
((NthRowPos(NumRows()) + NthRowPos(NumRows() - 1))/2) -
((NthRowPos(0) + NthRowPos(1)/2))*(787.4-768) + (BlockCenterX()
- (NthColumnPos(0) + NthColumnPos(1))/2) /
((NthColumnPos(NumColumns()) + NthColumnPos(NumColumns() -
1))/2) - ((NthColumnPos(0) + NthColumnPos(1)/2))*(772.58-768) +
768
```

To enter the new expression, you must first unlock the default expression by clicking in the "Lock" column of the Initial Head Unit1 parameter and unselecting "Lock Def Val".

WARNING. You should be cautious about overriding the default expression for any parameter on the MODFLOW FD Grid layer. You need to understand how a parameter on the MODFLOW FD Grid layer is used by the export template before you attempt to modify its expression.

Be sure you put this expression on the parameter named Initial Head Unit1 on the MODFLOW FD Grid and not the Initial Head Unit1 layer.

If you work through this expression, you'll see that it is simply the equation for a plane through three points. Those points are the centers of the cells in the upper left corner of the model, the lower left corner of the model and the lower right corner of the model. At the upper left corner the initial head is 787.399 in the original model. In the lower left corner it is 768.211 and in the lower right corner it is 772.579. All the other layers use the same initial head so for the Initial Head Unit2, Initial Head Unit3, and Initial Head Unit4 parameters, you can either use the same expression or just link them to the Initial Head Unit1 parameter. However, for a link to work, you must make the link in the form "**MODFLOW FD Grid**.Initial Head Unit1" not just "Initial Head Unit1"

Using a formula to set the initial head will work better in this case because doing so makes it simpler to enter the prescribed heads as we will see in the next section.

Prescribed Heads

In the original model, all the cells on the outer edge of the model were prescribed head cells with concentrations of 0.

If you used a formula to enter the initial heads, it will be much easier to specify the prescribed heads than it would otherwise be. To understand why, you have to understand a bit about how MODFLOW works. MODFLOW uses an array called the IBOUND array to specify whether a cell is active, inactive or a constant head cell. Any cell with a positive value in the IBOUND array is an active cell. Any cell with a negative value in the IBOUND array is a constant head cells. Cells with a value of 0 in the IBOUND array are inactive cells. Constant Head cells retain their starting heads throughout the duration of a model.

Normally the MODFLOW/MT3D PIE will take the head assigned on the prescribed head layer and use it to override the head assigned on the initial head layer. (The original expression for the Initial Head Unit1 parameter does exactly that.) Because we have replaced the expression for the initial head, with our own expression, the head assigned to a contour on the Prescribed Head layers will no effect on the actual head assigned to a cell. Instead, contours on the Prescribed Head layers will only affect what cells are prescribed head cells but not the head assigned to those cells. This means that we will be able to use a single long open contour around the outer edge of the model to specify the prescribed heads rather than a series of short open contours each of which would have a different head value.

So, despite the long explanation, you don't need to do much to assign the prescribed heads. Just draw a single open contour just inside the outer edge of the model on the Prescribed Head Unit1 layer. Accept the default value of \$N/A for the MT3D Concentration parameter. It doesn't matter what you assign to the "Prescribed Head" parameter. Copy the contour to the clipboard and paste it on each of the other "Prescribed Head" layers.

Details for Argus ONE novices:

If it is not already visible, show the original grid by clicking on the "eye" icon for the layer on which you placed the image of the original grid. Switch to the Prescribed Head Unit1

layer. Find the Contour button that you used to create the wells. Click and hold it until a pop-up menu appears. Select the middle choice from the pop-up menu. Click in one of the corner cells and then move to each of the other corner cells and click in each of them. Finally go back to the cell you started in and double-click. Move the cursor slightly and a dialog box will appear. Click the OK button.

If the open contour is not already selected (selected contours have black squares at each of their nodes) change to the arrow tool by clicking on the button with an arrow on it and then clicking on the contour. (If you have a button with a hand on it instead of one with an arrow, click and hold on that button until a pop-up menu appears and select the arrow from the pop-up menu.) Copy the selected contour to the clipboard by selecting Copy from the Edit menu or by pressing Ctrl-C on the keyboard. Change to one of the other Prescribed head layers and paste the contour from the clipboard by selecting Paste for the Edit menu or pressing Ctrl-V.

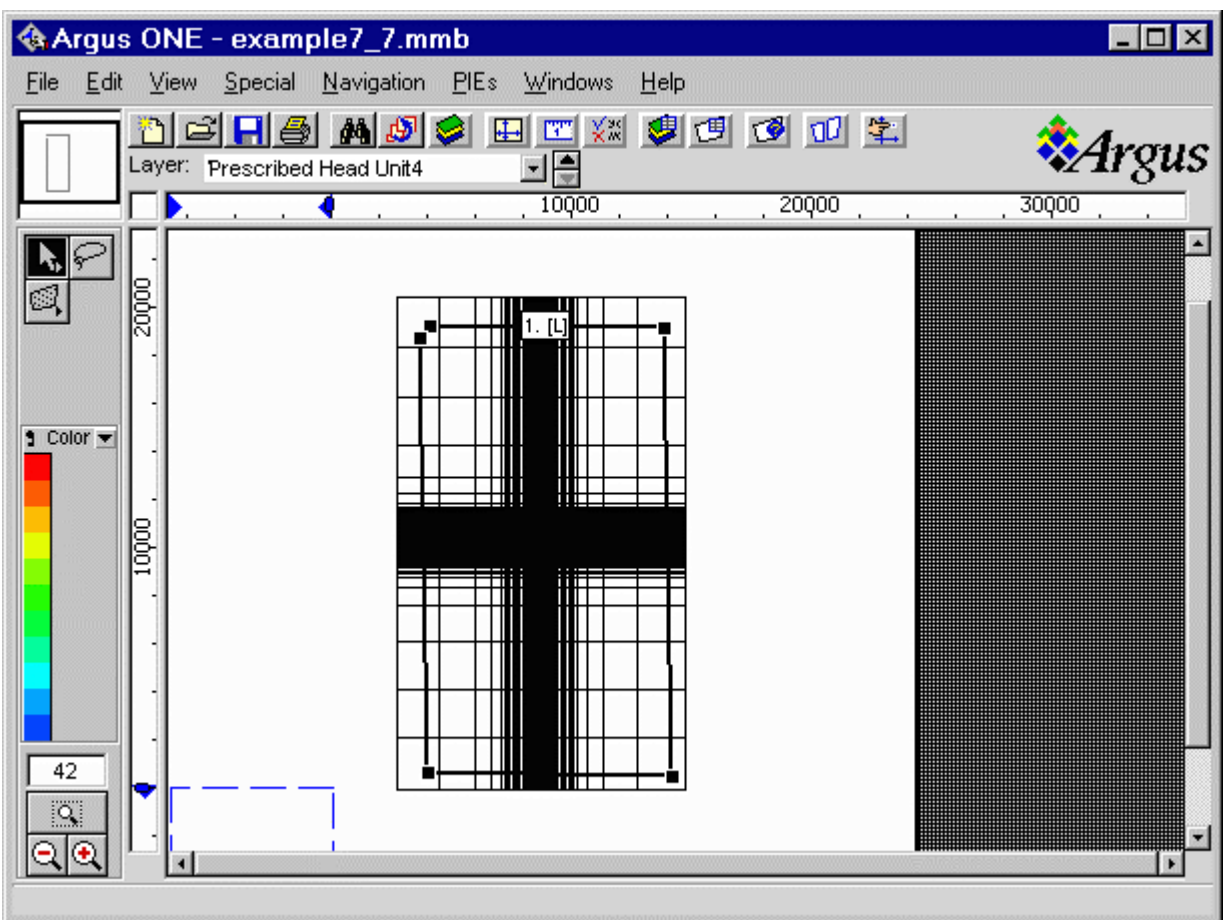


Figure 10. Example, MODFLOW Prescribed head.

The Grid

The largest cells in the original model were 2000 ft. on a side. Those closer to the center were 1600, 800, 400, 200, 100 and finally 50 ft for the smallest cells in the center of the grid.

Details for Argus ONE novices:

Switch to the MODFLOW Domain Outline Layer. Make sure the original grid is visible but you will probably want to hide everything else. Outline the model area with a closed contour and assign it a density of 2000. This is the default grid size for the model.

Switch to the MODFLOW Grid Density layer. Create a series of open contours with progressively smaller values toward the center of the grid. These contours will set the grid size in the area they control.

Move to the MODFLOW FD Grid layer. Select the Magic Wand Tool and click inside the domain outline. A dialog box will appear. Uncheck the "Automatic Angle Calculation Check box and click on the OK button. The grid will be created. Examine the grid to see if it is satisfactory. If not adjust the contours on the MODFLOW Grid Density layer and regrid with the Magic Wand tool. You can also move, add or delete individual grid lines on the MODFLOW FD Grid layer.

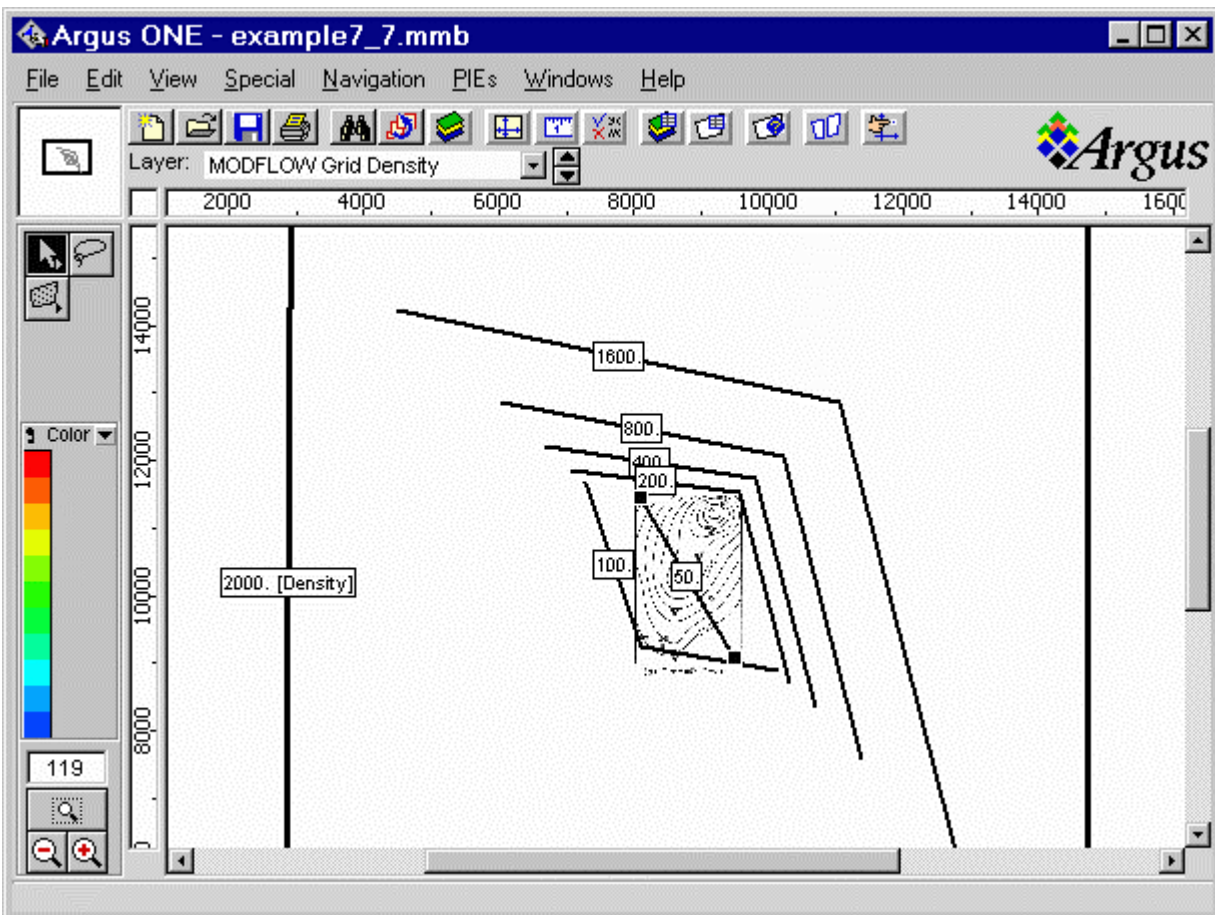


Figure 11. MODFLOW Grid density and domain outline (and initial concentrations).

Run the MODFLOW Model

Be sure that you are using a version of MODFLOW that can create the flow file for MT3D as described in "System Requirements and Installation".

If you are not already on it, Switch to the MODFLOW FD Grid layer. Select "Run MODFLOW/MT3D" from the PIE's menu. Check that the path to MODFLOW is correct. If it isn't, type the correct path or click on the Browse button next to the MODFLOW Path and locate MODFLOW on your computer. See "Changing Default locations of MODFLOW and MT3D" to change the location permanently. Click the Ok button to run MODFLOW. Select the folder in which you want MODFLOW to run and click the Save button. Argus ONE will export the MODFLOW import files and run MODFLOW.

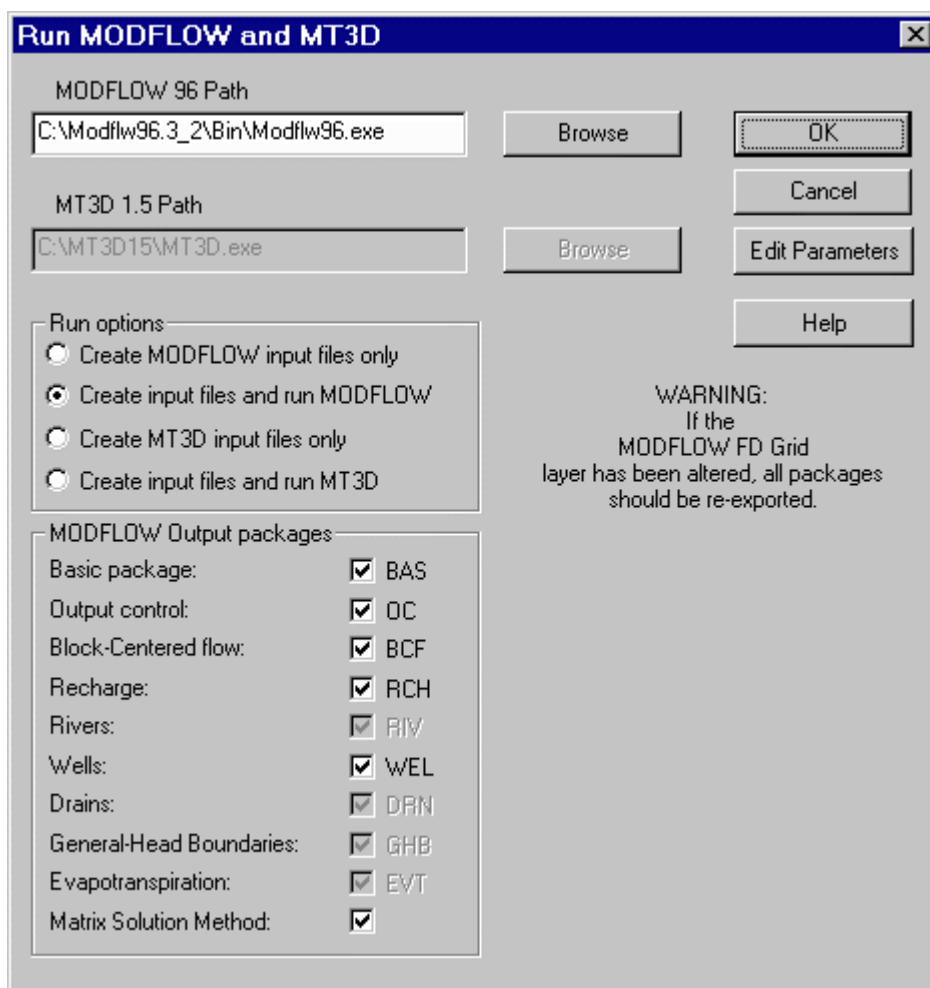


Figure 12. Example, Run MODFLOW.

Post-Processing

You can't do any post-processing yet if you saved the head and drawdown in binary form. The MT3D Post Processing PIE can read the binary head and drawdown file created by MODFLOW but needs the grid configuration file created by MT3D. Thus you must run MT3D before attempting to use the MT3D Post Processing PIE.

MT3D Model

MT3D Domain Outline

All active cells in the MT3D model must be surrounded by the MT3D Domain Outline on the MT3D Domain Outline Layer. In this case, the MT3D Domain Outline is the same as the MODFLOW Domain Outline should be the same as the MT3D Domain Outline so all you need to do is copy the MODFLOW Domain Outline to the MT3D Domain Outline layer. The value of the contour on the MT3D Domain Outline layer can be any non-zero number.

Wells, Recharge and Prescribed Head

In this example, you do not need to change the default values for the wells, recharge and Prescribed heads. If you had needed to change them, you could have set the MT3D Concentration parameters on the appropriate information layers.

Initial Concentration

You have already imported the scanned image of the initial concentrations of layers 2 and 3 into Argus ONE. Now you should trace them on the MT3D Initial Concentration Unit2 or MT3D Initial Concentration Unit3 layer. You should also have a contour with a value of 0 completely around the lowest contour data or everything outside the lowest contour will have a value of the lowest contour.

If you wish to specify a point source, you could place a point contour on the MT3D Point Initial Concentration Unit2 layer. This would override the concentration specified on the MT3D Area Initial Concentration Unit2 layer for the cell containing the point contour. To interpolate between several point values for initial concentration, change method used to probe the MT3D **Area** Initial Concentration Unit2 layer from "Exact Contour method" to "Interpolation method".

Details for Argus ONE novices:

To change the method used to probe the MT3D Area Initial Concentration Unit2 layer from "Nearest Contour method" to "Interpolation method", make MT3D Area Initial Concentration Unit2 the active layer and click on the "Layers..." button on the Layers floater. This will bring up the "Layers Dialog box". At the bottom is a drop down list that says, "When probed for value, use Exact Contour method" Change " Exact Contour method" to "Interpolation method". Then click on the "Done" button.

Hint:

A variety of interpolation PIE's are available from the Argus ONE web site. The 624 interpolation PIE gives especially good results for interpolation. However, it doesn't do a good job of extrapolation so you need to make sure to avoid extrapolation by including extra contours at high and low points on the surface and along ridgelines and valleys.

Because the initial concentration will be the same on layers 2 and 3, the easiest way to specify the concentration on layer 3 is just to link it to the concentration of layer 2. That way any change we make in layer 2 will automatically apply to layer 3 as well.

Details for Argus ONE novices:

Make MT3D Area Initial Concentration Unit3 the active layer and click on the "Layers..." button on the Layers floater. This will bring up the "Layers Dialog box". Click on "Initial Concentration" in the lower half of the dialog box. Then click on the down arrow under "Value" to bring up a pop-up menu. Select "Expression" from the pop-up menu. The Expression Editor will appear. From the list of layers select "MT3D Area Initial Concentration Unit2". "Initial Concentration" will appear in the box to the right. double-click on "Initial Concentration" and "MT3D Area Initial Concentration Unit2.Initial Concentration" will appear at the box on the top. Click on the "OK" button and then the "Done" button.

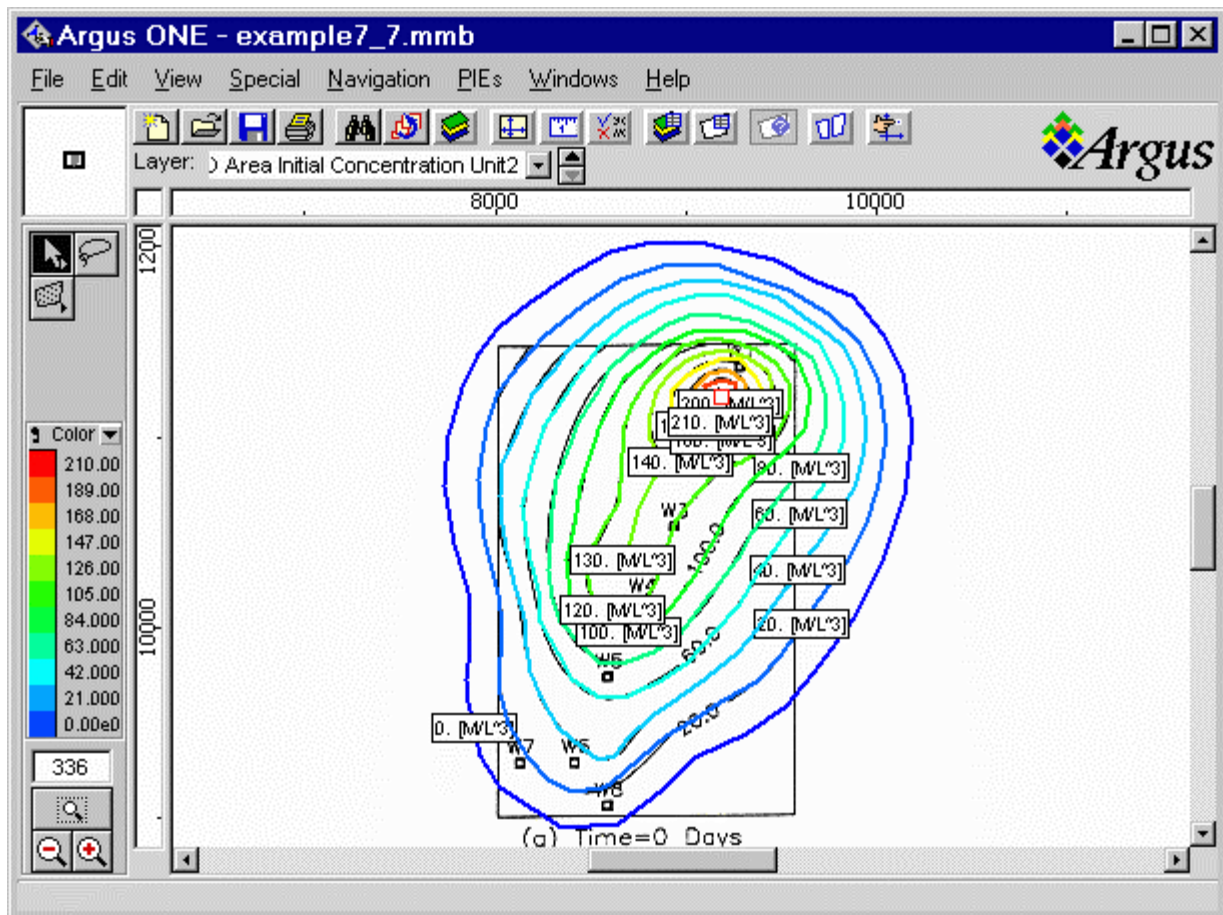


Figure 13. Example, MT3D Initial concentration. (Colormapping used.)

Porosity

We will use a uniform porosity in this model. Set the default value for Porosity in each layer to 0.30. (As it happens, the default value is already 0.3 so you don't need to do anything here.)

Observations

MT3D can print out the concentration at selected observation points for every transport step to the file MT3D.OBS. To specify observation points at the well locations, you can copy the point contours representing the wells from the Well Unit3 layer to the MT3D Observations Unit3 layer. (You can also use open or close contours to designate observation points)

Details for Argus ONE novices:

Make "Wells Unit3" the active layer. If the wells are not already all selected, Select them using the "Edit | Select All" menu item. Copy the contours to the clipboard by selecting Copy from the Edit menu or by pressing Ctrl-C on the keyboard. Change to the MT3D Observations Unit3 layer and paste the contours from the clipboard by selecting Paste for the Edit menu or pressing Ctrl-V.

Run the MT3D Model

You must already have run the MODFLOW model before running MT3D because MT3D uses a flow file generated by MODFLOW. If you change the MODFLOW model, you must rerun the MODFLOW model before running MT3D so that the flows read by MT3D will be correct.

To run the MT3D model, make "MODFLOW FD Grid" the active layer and select "Run MODFLOW/MT3D" from the PIE's menu. Click on the "Create input files and run MT3D" radio button. (You can also just create the input files without running MT3D.) Check that the path for MT3D is correct. If not type in a new path in the "MT3D 1.5 Path" edit box or click on the Browse button and locate MT3D on your computer. If you have already created the input files for MT3D and you haven't done anything to change them, you can reuse the existing file by unchecking the appropriate check boxes. Generally the Sink and Source Mixing package takes the longest time to export so you may speed up the export process significantly by unchecking it.

Click the OK button when you are ready to start exporting data to MT3D. An open file dialog box will appear. You can ignore the name of the file that appears in the dialog box. You will only be choosing a directory. Choose the directory in which you previously ran your MODFLOW model. You must use the same directory because MT3D needs to be able to find the flow file created by MODFLOW. (This need not be the directory where the MODFLOW or MT3D program is located. In fact it is generally better not to clutter those directories with the input and output of models.)

After you click the OK button, the PIE will start exporting the MT3D input files. When it is done, it will start MT3D. You may experience a significant slowdown of other programs while MT3D is running.

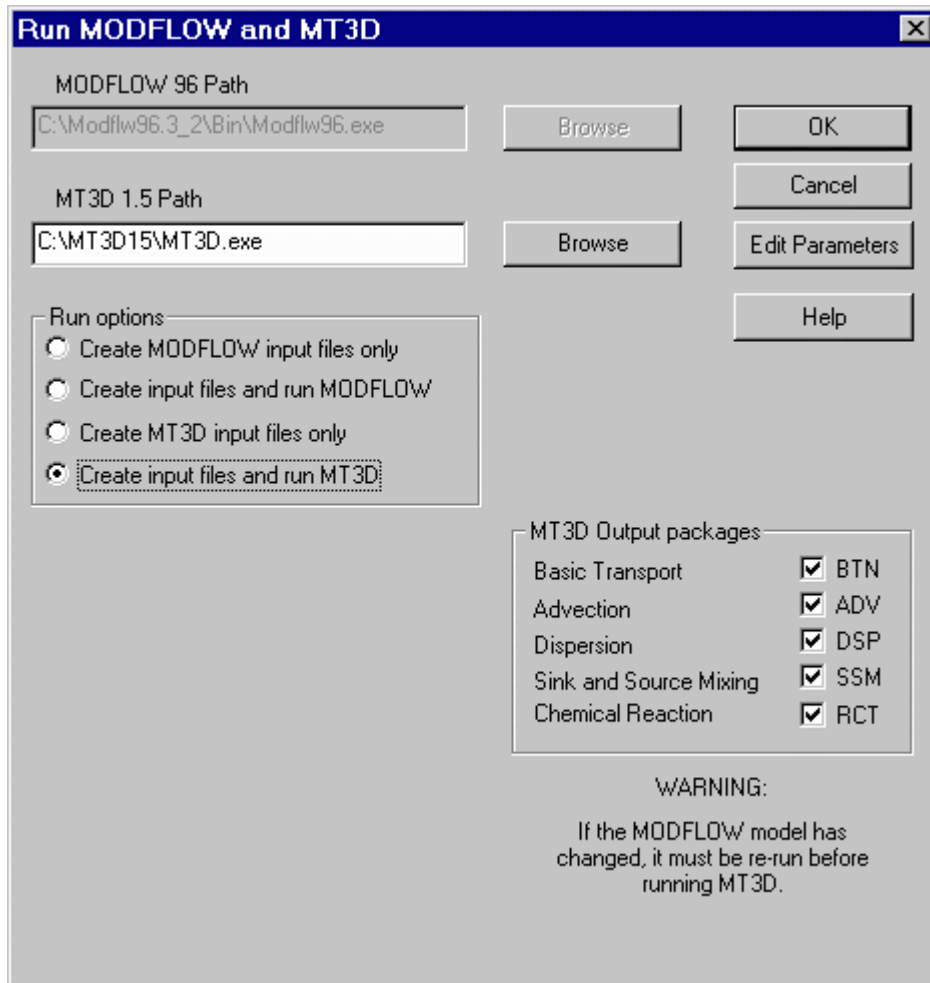


Figure 14. Example, Run MT3D.

Output from the model.

MODFLOW can create several different files when it runs. The main listing file will be *Rootname.mls*. You can examine it with any text editor. MT3D.MAS gives a one-line summary of the mass balance in each transport step. MT3D.OBS gives a one-line mass balance summary for each transport step. MT3D.CNF is the grid-configuration file used in post-processing. MT3D.UCN is binary concentration file that gives the concentration for each transport step for which you specified that concentrations be written. It is used in post processing and can not be read directly with a post processor. (The names MT3D.MAS, MT3D.OBS, MT3D.CNF, and MT3D.UCN are all written into the MT3D code. There isn't any way to direct MT3D to use different names without changing the source code.)

Post-Processing

To plot the concentrations predicted by the model, select "PIEs | MT3D Post Proc..." This will start the MT3D Import Utility. The position of the lower left corner of the model, the grid angle and HNOFLOW and HDRY are passed to the utility automatically. (The configuration of the grid and CINACT are read from the grid configuration file MT3D.CNF.) You can read the

MT3D binary concentration file, or the MODFLOW binary head or drawdown files. Select the type of data you wish to import using the Input Format radio buttons. If you wish, you can apply a log transformation to the data. Use the Log Transformation radio buttons to choose this option. When you have made your choices click on the "Import Data" button. Select the file from which you wish to import. For MT3D concentrations this will be MT3D.UCN. Next select the grid configuration file MT3D.CNF. (The extension "CNF" may not be visible).

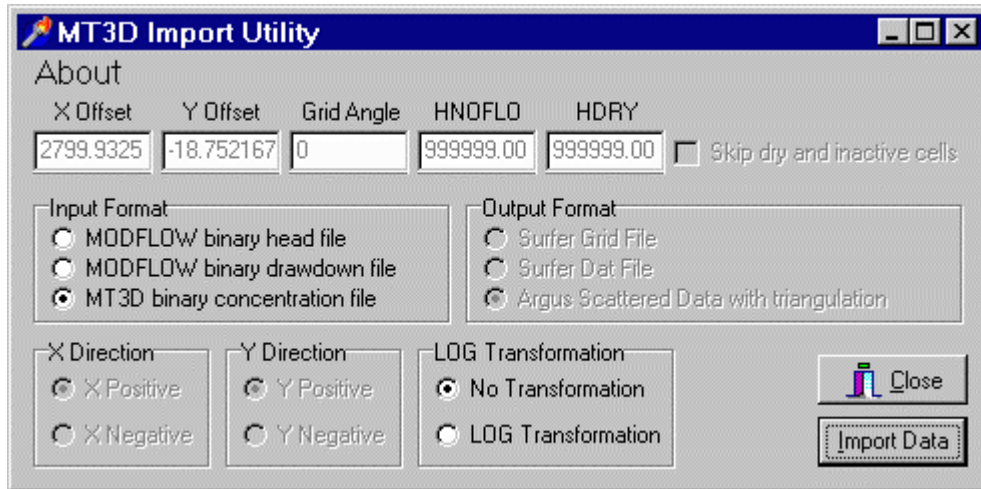


Figure 15. Example, MT3D Import Utility.

When you have selected the files from which you will import data, the Output Format dialog box appears. You can select how you want to import the data. You can select data along any row column or layer or from the water table surface. In this case we will select layer and change the first layer to layer 3. The last layer will change to the same value as the first layer when we leave the "first layer" edit box.

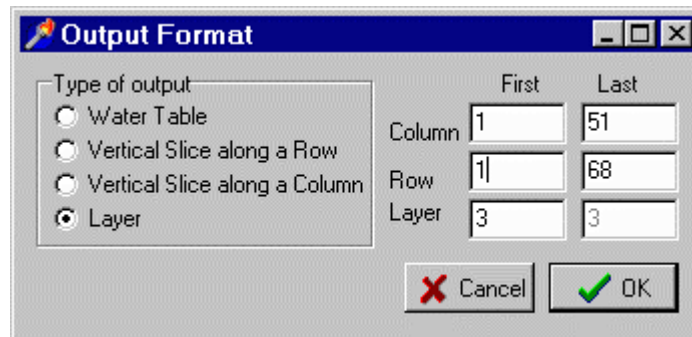


Figure 16. Example, MT3D Import Utility, Output Format.

Next select the transport steps from which to import data. Only those transport steps for which data was written to file will be included in the list. For this example, pick the last choice with an elapsed time of 1000 days.

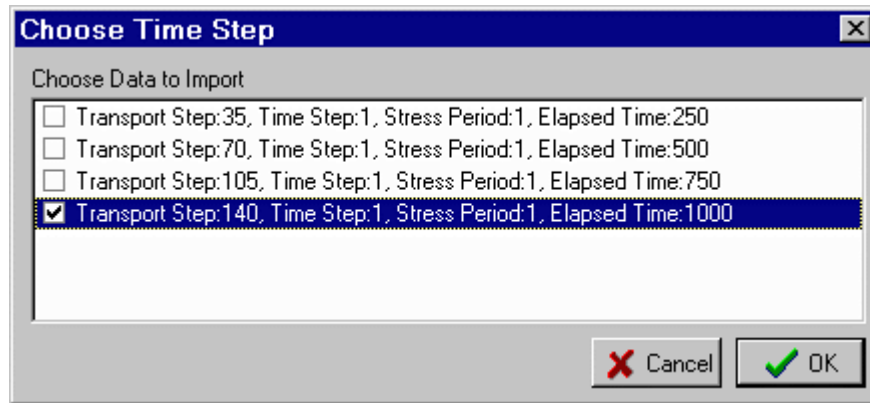


Figure 17. Example, MT3D Import Utility, Time Steps.

Click the OK button and the MT3D Import Utility will close. The MT3D Post processing Pie will read the data from the MT3D Import Utility and import it into Argus ONE. It will create a layer named MT3D Data if that layer does not already exist and import the data to that layer. Any data already on the layer will be overwritten. It will then create a layer named MT3D Post Processing Charts if it does not already exist. If it does already exist, you will be given the choice of clearing that layer or adding the new chart to it. You will then be given a choice of post-processing object to create. As with the MODFLOW Post Processing PIE, your choices are "Contour Map", "Color Map", "3D Surface", and "Cross Section". In this case, we'll chose a contour map and a contour map of the concentration will appear on the MT3D Post Processing Charts layer. (This layer may be hidden so you will have to show it to make it visible. It will be the last layer in the list of layers.)

If you imported the illustration of the final head from the original model you may wish to compare it to the results of the new model. The original diagram had a contour interval of 20 so to make the comparison easier, you should change the contour interval of your contour map to 20 too.

Details for Argus ONE novices:

Make the MT3D Post Processing Charts layer the active layer and double click anywhere on the contour map. The contour diagram dialog box will appear. On the Chart tab, change the Minimum to 0 and Delta to 20. Click on the OK button.

To compare your results, make MT3D Post Processing Charts the active layer and make the layer containing the final concentrations visible. (You must, of course, have imported this diagram before you can make it visible in Argus ONE.) You will see the original diagram (black) together with the new contours (colored). In my model the results were similar but not identical. The peak concentrations were higher and located further to the Northeast in my model.

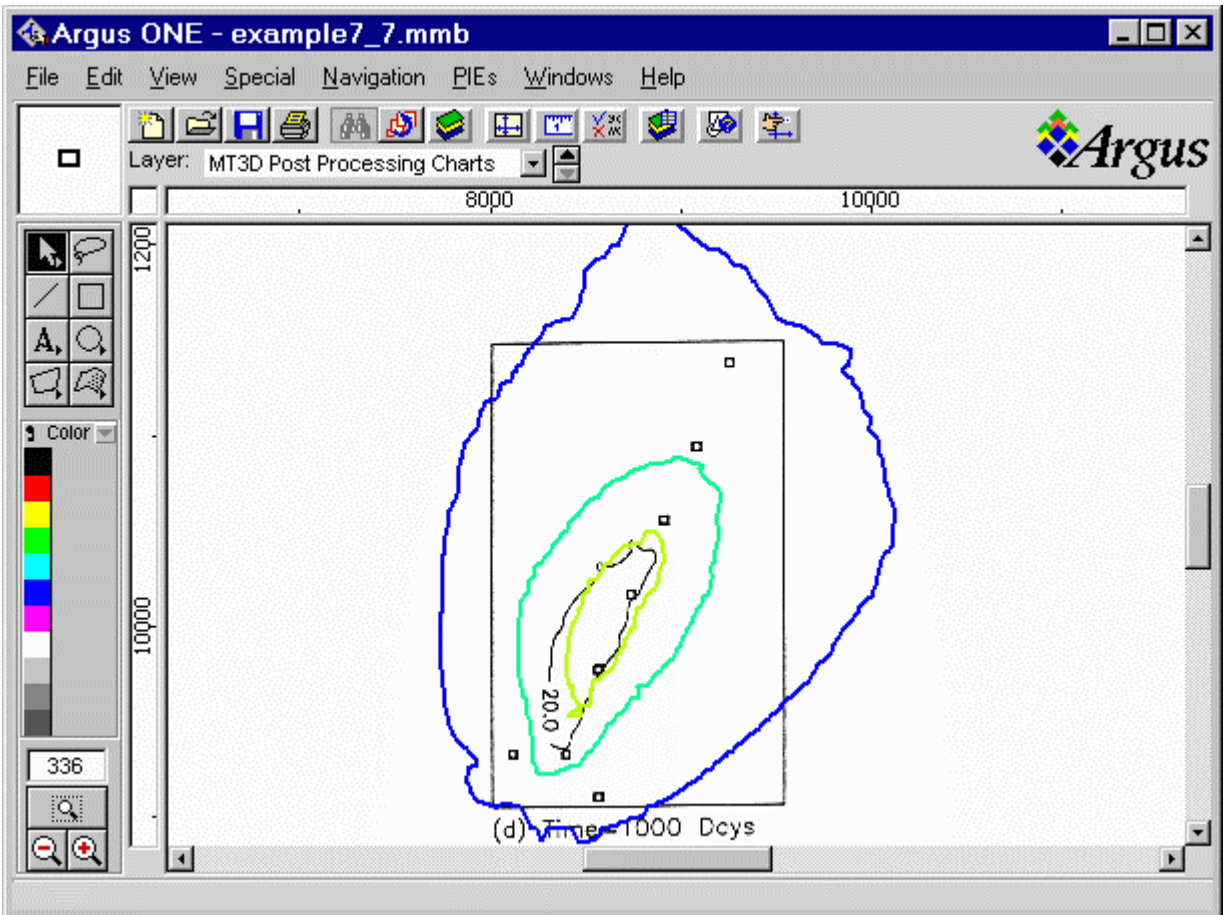


Figure 18. Comparison of results of new and original model.

Acknowledgements

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References

Shapiro, A.M., Margolin, J., Dolev, S., and Ben-Israel, Y. 1997. A Graphical-User Interface for the U.S. Geological Survey Modular Three-Dimensional Finite-Difference Ground-Water Flow Model (MODFLOW-96) Using Argus Numerical Environments. Open-File Report 97-121, U.S. Geological Survey, 53 p.

Zheng, C., 1990. MT3D, a Modular Three-Dimensional Transport Model, S.S. Papadopoulos and Associates, Bethesda, Md,

Appendix 1

Modifying MODFLOW-96 to produce input files for MT3D.

MT3D requires that the flow model produce a specially formatted file that MT3D uses as input. This is accomplished by including a link to MT3D in the source code for MODFLOW and making a few other modifications to the MODFLOW source code to properly incorporate the link to MT3D. The original MT3D documentation (Zheng, 1991) included a modified version of MODFLOW 88 that incorporated a link to MT3D. The way that link is implemented must be modified slightly to incorporate the link to MT3D into MODFLOW 96. The link requires two additional source code files are required for the link: LKMT.FOR and LKMT.INC. These are available with the version of MODFLOW distributed from Zheng's MT3D web site: <http://hydro.geo.ua.edu/mt3d/mt3d150d.htm>. In addition, the following changes must be made in the MODFLOW source code.

Modify CUNIT in the MODFLOW main file.

CUNIT is used to associate file names and abbreviations in the MODFLOW Name file with particular MODFLOW Packages. As shown below, "MT3", the abbreviation used here for MT3D, has been added in position 22 of CUNIT in the MODFLOW main file (usually named MODFLOW.FOR or MODFLW96.FOR).

```
c-RBW begin change: MT3D
DATA CUNIT/'BCF ','WEL ','DRN ','RIV ','EVT ','TLK ','GHB ','
1          'RCH ','SIP ','DE4 ','SOR ','OC ','PCG ','GFD ','
2          ' ','HFB ','RES ','STR ','IBS ','CHD ','FHB ','
3          'MT3 ',' ',' ',' ',' ',' ',' ',' ','
4          ' ',' ',' ',' ',' ',' ',' ',' ','
5          ' ',' ',' ',' ',' ',' ',' ',' '
c-RBW end change
```

Include LKMT2.INC in the MODFLOW main file.

Just before comment C7C5 add a line to include LKMT2.INC.

```
c-RBW begin change: MT3D
C-----SAVE HEADS AND CELL-BY-CELL FLOW TERMS FOR USE IN MT3D
      INCLUDE 'LKMT2.INC'
c-RBW end change
C7C5---PRINT AND OR SAVE HEADS AND DRAWDOWNS. PRINT OVERALL BUDGET.
```

Ensure IUNIT assignments are correct in LKMT.INC

At the beginning of LKMT.INC modify the statements assigning IMT3D and IUSTR to the values used in MODFLOW.FOR for LKMT3D package and the stream package respectively. In this case, IUNIT(22) and IUNIT(18). If, in step 1, you place MT3 in a different position in CUNIT, you must change the IUNIT position for MT3D to correspond to the position that you used for MT3D in step 1.

```

C LKMT3D PACKAGE IMPLEMENTED IN IUNIT (22)
C STR1 PACKAGE IMPLEMENTED IN IUNIT (18)
C MODIFY NEXT TWO STATEMENTS IF NECESSARY
C .....
    IMT3D=IUNIT(22)
    IISTR=IUNIT(18)
C .....

```

Add code that will allow the MT3D flow file to be written correctly.

MODFLOW 96, as distributed by the USGS does not have a method for opening an unformatted file that is also associated with a particular package. The follow modifications to subroutine SBAS50 overcomes that difficulty.

```

C5-----DETERMINE FILE NAME AND THE ACCESS METHOD (DIRECT OR
C5-----SEQUENTIAL). WRITE THE FILE NAME IF THE FILE IS NOT THE
C5-----LISTING FILE. THEN OPEN THE FILE.
    CALL URWORD(LINE,LLOC,INAM1,INAM2,0,N,R,IOUT,INUNIT)
    CALL URWORD(LINE,LLOC,ISTART,ISTOP,1,N,R,IOUT,INUNIT)
    IF(LINE(ISTART:ISTOP).EQ.'DIRECT') THEN
        CALL URWORD(LINE,LLOC,ISTART,ISTOP,2,IRECL,R,IOUT,INUNIT)
        IF(ILIST.NE.0) WRITE(IOUT,35) LINE(INAM1:INAM2),
1          LINE(ITYP1:ITYP2),IU,IRECL
35      FORMAT(1X,/1X,'OPENING ',A,/
1        1X,'FILE TYPE:',A,' UNIT',I4,' DIRECT ACCESS',I10)
        OPEN(UNIT=IU,FILE=LINE(INAM1:INAM2),FORM=FMTARG,
1          ACCESS='DIRECT',RECL=IRECL)
c-RBW begin change: MT3D
        ELSE IF(LINE(ISTART:ISTOP).EQ.'UNFORMATTED') THEN
            IF(ILIST.NE.0) WRITE(IOUT,38) LINE(INAM1:INAM2),
1              LINE(ITYP1:ITYP2),IU,LINE(ISTART:ISTOP)
38      FORMAT(1X,/1X,'OPENING ',A,/
1        1X,'FILE TYPE:',A,' UNIT',I4,' FORMAT:',A)
            OPEN(UNIT=IU,FILE=LINE(INAM1:INAM2),FORM='UNFORMATTED',
1              ACCESS='SEQUENTIAL')
c-RBW end change
        ELSE
            IF(ILIST.NE.0) WRITE(IOUT,36) LINE(INAM1:INAM2),
1              LINE(ITYP1:ITYP2),IU
36      FORMAT(1X,/1X,'OPENING ',A,/
1        1X,'FILE TYPE:',A,' UNIT',I4)
            OPEN(UNIT=IU,FILE=LINE(INAM1:INAM2),FORM=FMTARG,
1              ACCESS='SEQUENTIAL')
        END IF

```