GMS 7.0 TUTORIALS

MT3DMS - Conceptual Model Approach

1 Introduction

MT3DMS simulations can be constructed using either the grid approach where data are entered on a cell-by-cell basis or using the conceptual model approach where the data are entered via points, arcs, and polygons. This tutorial describes how to use the conceptual model approach.

1.1 Contents

1.2 Outline

This is what you will do:

1. Open a MODFLOW model and solution.
2. Define conditions for a MT3DMS simulation.
3. Convert the conceptual model to MT3DMS.
4. Run MODFLOW and then run MT3DMS.
5. Create an animation.
6. Define additional parameters and rerun MT3DMS.
7. Create a time series plot.

1.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Map
- MODFLOW
- MT3DMS

You can see if these components are enabled by selecting the *File* | *Register* command.

2 Description of Problem

The problem we will be solving for this tutorial is an extension of the problem described in the tutorial entitled *MODFLOW - Conceptual Model Approach*. Thus, if you have not yet completed the MODFLOW tutorial, you may wish to do so now before continuing.

In the MODFLOW tutorial, a site in East Texas was modeled. We will be using the solution from this model as the flow field for the transport simulation. The model included a proposed landfill. For this tutorial, we will be performing two transport simulations to analyze the long term potential for migration of leachate from the landfill. In the first simulation, we will be modeling transport due to advection and dispersion only. In the second simulation, we will include sorption and decay in addition to advection.

3 Getting Started

Let's get started.

1. If necessary, launch GMS. If GMS is already running, select the *File* | *New* command to ensure that the program settings are restored to their default state.

4 Importing the Project

The first step is to import the East Texas project. This will read in the MODFLOW model and solution, and all other files associated with the model.

To import the project:

1. Select the *Open* button .
2. Locate and open the directory entitled **tutfiles\MODFLOW\modfmap\sample**.
3. Open the file entitled **modfmap.gpr**.

5 Defining the Units

First, we will define the units. We will not change the length and time units (these must be consistent with the flow model). However, we need to define units for mass and concentration.

1. Select the *Edit* | *Units* command.
2. Select **kg** for the *Mass* units.

3. Select **ppm** for the *Concentration* units.

4. Select the *OK* button.

6 Initializing the MT3DMS Simulation

Now that the MODFLOW model is in memory, we can initialize the MT3DMS simulation. First, we will initialize the model.

1. Select the *Edit* | *Model Interfaces* command.

2. Turn on the *MT3DMS* | *RT3D* | *SEAM3D* toggle.

3. Select *OK* to exit the dialog.

4. Now, select the *MT3D* | *New Simulation* command.

6.1 Defining the Species

Since MT3DMS is a multi-species model, we need to define the number of species and name each species. We will use one species named "leachate."

1. Select the *Define Species* button.

2. Select the *New* button and change the name of the species to **leachate**.

3. Select the *OK* button to return to the *Basic Transport Package* dialog.

6.2 Defining the Stress Periods

Next, we will define the stress periods.

1. Select the *Stress Periods* button.

Since the flow solution computed by MODFLOW is steady state, we are free to define any sequence of stress periods and time steps we wish. For this model we only need one stress period because the leachate from the landfill will be released at a constant rate. We will enter the length of the stress period (i.e., the length of the simulation) and let MT3DMS compute the appropriate transport time step length by leaving the transport step size at zero.

2. Enter **3000** for the stress period *Length* (days).

3. Enter **4000** for the *Max transport steps*.

4. Select the *OK* button to exit the *Stress Periods* dialog.

6.3 Selecting Output Control

By default, MT3DMS outputs a solution at every transport step. Since this results in a rather large output file, we will change the output so that a solution is written every time step (every 300 days).

1. Select the *Output Control* button.
2. Select the *Print or save at specified times* option.
3. Select the *Times* button.
4. Select the *Initialize Values* button.
5. Enter the following values:
   - *Initial time step size*: **300**
   - *Bias*: **1**
   - *Maximum time step size*: **300**
   - *Maximum simulation time*: **3000**
6. Select the *OK* button three times to return to the *Basic Transport Package* dialog.

6.4 Selecting the Packages

Next, we will specify which of the MT3DMS packages we intend to use.

1. Select the *Packages* button.
2. Turn on the following packages:
   - Advection package
   - Dispersion package
   - Source/Sink Mixing package
   - Transport observation package
3. Select the *OK* button.

Note that the *Basic Transport Package* dialog also includes some layer data. We will address the data for these arrays at a latter point in the tutorial.

4. Select the *OK* button to exit the *Basic Transport Package* dialog.

7 Assigning the Aquifer Properties

MT3DMS requires that a porosity and dispersion coefficient be defined for each of the cells in the grid. While these values can be assigned directly to the cells, it is sometimes convenient to assign the parameters using polygonal zones defined in the conceptual model. The parameters are converted to the grid cells using the *Map → MT3DMS* command.

7.1 Turning on Transport

To assign the porosities and dispersion coefficients to the polygons:

1. In the *Project Explorer*, right-click on the **East Texas** conceptual model and select the *Properties* command from the pop-up menu.
2. Turn on *Transport* and make sure **MT3DMS** is selected as the *Transport model*.
3. Click on the *Define Species* button.
4. Click the *New* button to create a new species. Change the species name to **leachate** and click *OK*.
5. Click *OK* to exit the *Conceptual Model Properties* dialog.
6. Expand the **East Texas** conceptual model if necessary to see the coverages under it.
7. In the *Project Explorer*, right click the **Layer 1** coverage and select the *Coverage Setup* command from the pop-up menu.
8. In the list of *Areal Properties*, turn on the following:
   - *Porosity*
   - *Long. dispersivity*
9. Click *OK*.
10. Repeat steps 7 – 9 for the **Layer 2** coverage .

7.2 Assigning the Parameters to the Polygons

To assign the porosities and dispersion coefficients to the polygons:

1. Make **Layer 1** the active coverage by selecting it in the *Project Explorer*.
2. Choose the *Select Polygons* tool .
3. Double click on the layer polygon.

4. For the *Porosity* enter a value of **0.3**.

5. For *Long. Disp.* enter a value **20**.

6. Select the *OK* button.

To assign the values to layer 2:

7. Make **Layer 2** the active coverage by selecting it in the *Project Explorer*.

8. Double click on the layer polygon.

9. For the *Porosity* enter a value of **0.2**.

10. For *Long. Disp.* enter a value **20**.

11. Select the *OK* button.

12. Click anywhere outside the model to unselect the highlighted polygon.

8 Assigning the Recharge Concentration

The purpose of our model is to simulate the transport of contaminants emitted from the landfill. When the flow model was constructed, a separate, reduced value of recharge was assigned to the landfill site. This recharge represents leachate from the landfill. We will assign a concentration to this recharge. The concentration can be assigned directly to the recharge polygon in the conceptual model.

1. In the *Project Explorer*, right-click on the **Recharge** coverage and select the *Coverage Setup* command from the pop-up menu.

2. From the list of *Areal Properties*, turn on *Recharge conc.* and click *OK*.

3. Make **Recharge** the active coverage by selecting it in the *Project Explorer*.

4. Double click on the landfill polygon.

5. For the *leachate Recharge conc.* enter a constant value of **20000** for the concentration.

6. Select the *OK* button.

7. Click anywhere outside the model to unselect the polygon.

9 Converting the Conceptual Model

At this point, we are ready to assign the aquifer parameters and the recharge concentration to the cells using the conceptual model.

1. Select the *Feature Objects* | *Map* → *MT3DMS* command.
2. Make sure the *All applicable coverages option* is selected and select *OK* at the prompt.

10 Layer Thicknesses

To define the aquifer geometry, MT3DMS requires an HTOP array defining the top elevations of the uppermost aquifer. A thickness array must then be entered for each layer. Since we defined the layer geometry in the MODFLOW model, no further input is necessary.

11 The Advection Package

Before running MT3D, there are a few more options to enter. First, we need to select a solver for the Advection package. We want to use the *Third Order TVD scheme (ULTIMATE)* solution scheme. This is the default, so we don't need to do anything.

12 The Dispersion Package

Next, we will enter the data for the Dispersion package.

1. Select the *MT3D* | *Dispersion Package* command.

The longitudinal dispersivity values were automatically assigned from the conceptual model. All we need to do is specify the remaining three parameters.

2. Enter a value of **0.2** for the *TRPT* parameter for *Layer 1* and *Layer 2*.
3. Enter a value of **0.1** for the *TRVT* parameter for *Layer 1* and *Layer 2*.
4. Ensure that the value of the *DMCOEF* is **0** for both layers.
5. Select the *OK* button to exit the *Dispersion Package* dialog.

13 The Transport Observation Package

Next, we will enter the data for the Transport Observation package.

1. Select the *MT3D* | *Transport Observation Package* command.

We will use this package to determine the mass flux into the river source/sink.

2. Turn off the option to Compute concentrations at observation points and turn on the option to Compute mass flux at source/sinks.

3. Select the *OK* button to exit the *Transport Observation Package* dialog.

14 The Source/Sink Mixing Package Dialog

Finally, we must define the data for the source/sink mixing package. However, the only data required in this package for our simulation are the concentrations assigned to the recharge from the landfill. These values were automatically assigned to the appropriate cells from the conceptual model. Thus, the input data for this package are complete.

15 Saving the Simulation

We are now finished inputting the MT3DMS data and we are ready to save the model and run the simulation. To save the simulation:

1. Select the *File | Save As* command.
2. Locate and open the directory entitled **tutfiles\mt3dmap**.
3. Save the project with the name **run1.gpr**.

16 Running MODFLOW

MT3D requires the .hff file generated by MODFLOW. Since we saved the project in a different folder than the one where we opened the MODFLOW simulation from, the .hff file does not exist in the new location. We need to rerun MODFLOW so that it will recreate the .hff file in the current folder.

To run MODFLOW:

1. Select the *MODFLOW | Run MODFLOW* command.
2. Select *OK* at the prompt if it appears.
3. When the simulation is finished, close the window and return to GMS. The solution is imported automatically.

17 Running MT3DMS

To run MT3DMS:

1. Select the *MT3D | Run MT3D* command.
2. Select *Yes* at the prompt to save your changes.

3. When the simulation is finished, close the window and return to GMS. The solution is imported automatically.

18 Viewing the Solution

We will now view the results of the MT3DMS model run.

1. Expand *run1 (MT3DMS)* in the *Project Explorer* and select the *leachate* data set.
2. In the *Time Step* list below the *Project Explorer*, select the last time step.

It is often helpful to use the color filled contours option. To do this:

3. Select *Contour Options* from the main toolbar.
4. Select the *Contour specified range* option (near the bottom on the left side of the dialog).
5. Enter **1** for the minimum value and **130** for the maximum.
6. Change the *Contour Method* to *Color fill*.
7. Select the *OK* button to exit the *Contour Options* dialog.

You should now see a display of color shaded contours confined to the area adjacent to the landfill. To view the solution for layer two:

8. Select the down arrow ⬇ in the mini-grid display.

To view the solution in cross section view:

9. Select the up arrow ⬆ in the mini-grid display.
10. Select a cell in the vicinity of the landfill.
11. Select the *Side View* button.
12. Use the left and right arrow keys ⬅ ➡ to view the solution along different columns.
13. Select the *Plan View* button when finished.
14. Note that the leachate eventually reaches both the river and the well. We will now view the mass flux of leachate into the river that was computed with the transport observation package.
15. Select the *SourcesSink* coverage in the *Project Explorer* (you may need to expand the *Map Data* folder and the *East Texas* conceptual model).

16. Select the *Select Arcs* tool.

17. Select the specified head arc along the bottom of the model. The computed mass flux is reported along the bottom of the window.

19 Generating a Mass vs. Time Plot

We can also view a plot of Mass vs. Time for a selected feature object. To create the plot:

1. Select the *Plot Wizard* button.

2. Select the *Mass vs. Time* option for the plot type.

3. Select the *Finish* button.

The plot shows the mass flux that leaves the model through the selected river arc.

4. Close the plot window and maximize the GMS graphics window.

5. Select the *Frame* button to resize the view of the model grid.

20 Viewing an Animation

Next, we will observe how the solution changes over the course of the simulation by generating an animation. To set up the animation:

1. Select the *leachate* data set in the *Project Explorer*.

2. Select the *Display | Animate* command.

3. Make sure the *Data set* option is on and click *Next*.

4. Turn on the *Display clock* option.

5. Select the *Finish* button.

6. After viewing the animation, select the *Stop* button to stop the animation.

7. Select the *Step* button to move the animation one frame at a time.

8. You may wish to experiment with some of the other playback controls. When you are finished, close the window and return to GMS.

21 Modeling Sorption and Decay

The solution we have just computed can be thought of as a worst case scenario since we have neglected sorption and decay. Sorption will retard the movement of the plume and decay (due to biodegradation) will reduce the concentration. For the second part of the tutorial we will modify the model so that sorption and decay are simulated. We will then compare this solution with the first solution.

21.1 Turning on the Chemical Reactions Package

Sorption and decay are simulated in the *Chemical Reactions Package*. We need to turn this package on before it can be used.

1. Select the *MT3D* | *Basic Transport Package* command.
2. Select the *Packages* command.
3. Turn **on** the *Chemical reaction package* option.
4. Select the *OK* button to exit the *Packages* dialog.
5. Select the *OK* button to exit the *Basic Transport Package* dialog.

21.2 Entering the Sorption and Biodegradation Data

Next, we will enter the sorption and biodegradation data in the *Chemical Reactions Package* dialog.

1. Select the *MT3D* | *Chemical Reaction Package* command.
2. In the *Sorption* section, select the **Linear isotherm** option.
3. In the *Kinetic rate reaction* section, select the **First-order irreversible kinetic reaction** option.
4. In the lower part of the dialog, enter the following values:

Bulk density	**53500**
1st sorption constant	**0.00000585**
Rate const. (dissolved)	**0.0001**
Rate const. (sorbed)	**0.0001**

5. Switch the layer to layer **2** and enter the following values:

Bulk density	**51500**
1st sorption constant	**0.00000585**
Rate const. (dissolved)	**0.00005**
Rate const. (sorbed)	**0.00005**

6. Select the *OK* button to exit the dialog.

22 Run Options

We are about ready to save the project under a new file name. However, we will face the same problem we did earlier with the .hff file. That is, MT3D will look for a .hff file with the same name as the one we are about to use to save the project. That file doesn't exist. We could rerun MODFLOW to create it, but there's another way.

1. Select the *MT3D | Run Options* command.
2. Select the *Single run with selected MODFLOW solution* option. Make sure that **run1 (MODFLOW)** is the selected solution.
3. Select *OK*.

With this option, GMS tells MT3D to use the .hff file we generated previously.

23 Saving the Simulation

We are now ready to save the new simulation.

1. Select the *File | Save As* command.
2. Save the project with the name **run2.gpr**.

24 Running MT3DMS

To run MT3DMS:

1. Select the *MT3D | Run MT3D* command.
2. When the simulation is finished, close the window and return to GMS. The solution is imported automatically.

25 Viewing the Solution

After the simulation finishes and the solution is read in to GMS:

1. Expand *run2 (MT3DMS)* in the *Project Explorer* and select the *leachate* data set.
2. In the *Time Step* list below the *Project Explorer*, select the last time step.

Notice that at the end of the simulation the plume is smaller and less advanced than in the first simulation.

26 Generating a Time History Plot

A useful way to compare two transient solutions is to generate a time history plot. The fastest way to do this is to create an "Active Data Set Time Series" plot.

26.1 Creating a Time Series Plot

1. Select the *Plot Wizard* button.
2. Select the *Active Data Set Time Series* option for the plot type.
3. Select the *Finish* button.
4. Select a cell in the grid near the landfill. Notice that the plot shows the concentration v. time.
5. Select a different cell and notice that the plot updates. If no cell is selected then the plot will not show any data.

If you want to take the plot data and put it into Excel you can right click on the plot and select the view values option. This brings up a spreadsheet that you can copy and then paste into Excel.

27 Conclusion

This concludes the tutorial. Here are the things that you should have learned in this tutorial:

- If you are starting with a MODFLOW conceptual model and you want to do a transport model, you must turn on transport in the conceptual model properties.
- You can use the *MT3D | Run Options* command to tell MT3D what MODFLOW solution you want to use.

