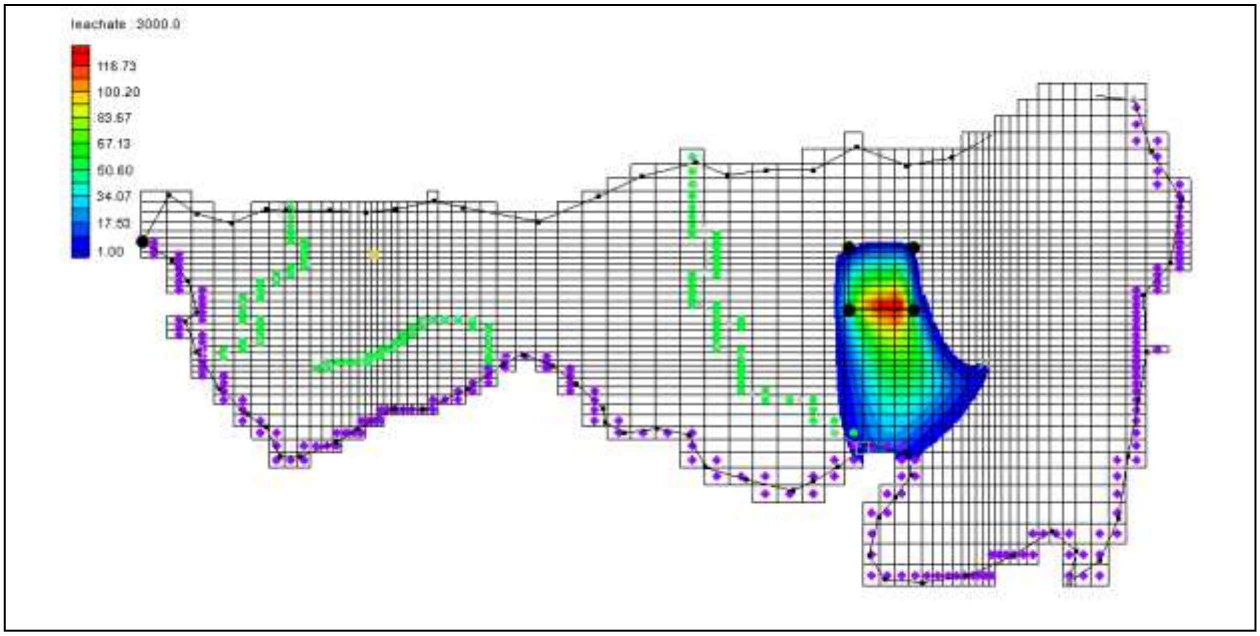
GMS

v. 10.0

GMS 10.0 Tutorial

MT3DMS – Conceptual Model Approach

Using MT3DMS with a conceptual model



Objectives

Learn how to use a conceptual model when using MT3DMS. Perform two transport simulations, analyzing the long-term potential for migration of leachate from a landfill. In the first simulation, model transport is due to advection and dispersion only. In the second simulation, sorption, decay and advection are included.

Prerequisite Tutorials

- MODFLOW – Conceptual Model Approach I
- MT2DMS – Grid Approach

Required Components

- Map Module
- Grid Module
- MODFLOW
- MT3DMS

Time

- 30-50 minutes

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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 Outline

Here are the steps of this tutorial:

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.

2 Description of Problem

The problem for this tutorial is an extension of the problem described in the tutorial entitled “MODFLOW – Conceptual Model Approach I.” Thus, if the user has not yet completed the MODFLOW tutorial, the user may wish to do so now before continuing.

In the MODFLOW tutorial, a site in East Texas was modeled. This tutorial 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, the user will be performing two transport simulations to analyze the long term potential for migration of leachate from the landfill. In the first simulation, the user will be modeling transport due to advection and dispersion only. In the second simulation, the user will include sorption and decay in addition to advection.

3 Getting Started

Do the following to get started:

1. If necessary, launch GMS.
2. 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 *Tutorials\MODFLOW\modfmap\sample2*.
3. Select the file entitled “modfmap2.gpr.”

4. Click **Open.**

5 Defining the Units

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

1. Select the *Edit* | **Units** command to open the *Units* dialog.
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, the user can initialize the MT3DMS simulation. First, the userinitialize the model:

1. Expand the “3D Grid Data” folder.
2. Right-click on the “grid” item in the Project Explorer.
3. Select the **New MT3D**... command to open the *Basic Transport Package* dialog.

6.1 Defining the Species

Since MT3DMS is a multi-species model, the user needs to define the number of species and name each species.The user will use one species named “leachate.”

1. Select the **Define Species** button to open the *Define Species* dialog.
2. Select the **New** button.
3. Change the name of the species to “leachate.”
4. Select the **OK** button to return to the *Basic Transport Package* dialog.

6.2 Defining the Stress Periods

Next, define the stress periods.

1. Select the **Stress Periods** button to open the *Stress Periods* dialog.

Since the flow solution computed by MODFLOW is steady state, the user is free to define any desired sequence of stress periods and time steps. For this model,onlyone stress period is needed because the leachate from the landfill will be released at a constant rate. The user 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 trans. 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, the user will change the output so that a solution is written every time step (every 300 days).

1. Select the **Output Control** button to open the *Output Control* dialog.

2. Select the *Print or save at specified times* option.

3. Select the **Times** button to open the *Variable Time Steps* dialog.

4. Select the **Initialize Values** button to open the *Initialize Time Steps* dialog.

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, specify which of the MT3DMS packages to use.

1. Select the **Packages** button to open the *MT3D/RT3D Packages* dialog.

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. This tutorial will address the data for these arrays at a latter point.

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, expand the “Map Data” folder.
2. In the Project Explorer, right-click on the “East Texas” conceptual model
3. Select the **Properties** command from the pop-up menu to open the *Conceptual Model Properties* dialog.
4. Turn on *Transport.*
5. Make sure **MT3DMS** is selected as the *Transport model*.
6. Click on the **Define Species** button to open the *Define Species* dialog.
7. Click the **New** button to create a new species.
8. Change the species name to “leachate.”
9. Click **OK**.
10. Click **OK** to exit the *Conceptual Model Properties* dialog.
11. Expand the “East Texas” conceptual modelif necessary to see the coverages under it.

12. In the Project Explorer, right-click the "Layer 1" coverage.

13. Select the **Coverage Setup** command from the pop-up menu to open the *Coverage Setup* dialog.

14. In the list of *Areal Properties*, turn on the following:

    - *Porosity*
    - *Long. dispersivity*

Click **OK**.

Repeat steps 12–15 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 to open the *Attribute Table* dialog.
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 to open the *Attribute Table* dialog.
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 this 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. The user 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.
2. Select the **Coverage Setup** command from the pop-up menu to open the *Coverage Setup* dialog.
3. From the list of *Areal Properties*, turn on *Recharge conc.*
4. Click **OK**.
5. Make “Recharge” the active coverage by selecting it in the Project Explorer.
6. Double-click on the landfill polygon to open the *Attribute Table* dialog.
7. For the *leachate Recharge conc.*, enter a constant value of “20000” for the concentration.
8. Select the **OK** button.
9. Click anywhere outside the model to unselect the polygon.

9 Converting the Conceptual Model

At this point, it is possible 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.
3. 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 the user 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, including a solver for the Advection package. This tutorial will use the *Third Order TVD scheme (ULTIMATE)* solution scheme. This is the default, so nothing needs to be done.

12 The Dispersion Package

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

1. Select the *MT3DMS* | **Dispersion Package** command to open the *Dispersion Package* dialog.

The longitudinal dispersivity values were automatically assigned from the conceptual model. All the user must 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,the user will enter the data for the Transport Observation package.

1. Select the *MT3DMS* | **Transport Observation Package** command to open the *Transport Observation Package* dialog.

The user 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*.
3. Turn on the option to *Compute mass flux at source/sinks*.
4. Select the **OK** button to exit the *Transport Observation Package* dialog.

14 The Source/Sink Mixing Package Dialog

Finally, the user must define the data for the source/sink mixing package. However, the only data required in this package for this 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

The user is now finished inputting the MT3DMS data, and it is now possible to save the model and run the simulation. To save the simulation, do as follows:

1. Select the *File* | **Save As** command.
2. Locate and open the directory entitled *Tutorials\MT3D\mt3dmap*.
3. Change the project name to "run1.gpr."
4. Click **Save.**

16 Running MODFLOW

MT3D requires the HFF file generated by MODFLOW. Since the user saved the project in a different folder than the one where the MODFLOW simulation was opened, the HFF file does not exist in the new location. The user needs to rerun MODFLOW so that it will recreate the HFF file in the current folder.

To run MODFLOW, do the following:

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

17 Running MT3DMS

To run MT3DMS:

1. Select the *MT3DMS* | **Run MT3DMS** command.
2. Select **Yes** at the prompt to save the changes.
3. When the simulation is finished, select the **Close** button and return to GMS. The solution is imported automatically.

Here the user may wish to look at the "leachate(sorbed)" item under the "MT3DMS" folder in the Project Explorer to see how it is affected over time.

18 Viewing the Solution

The user will now view the results of the MT3DMS model run.

1. Expand "run1 (MT3DMS)" in the Project Explorer.

2. Select the "leachate" dataset.

3. 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, follow these steps:

4. Select **Contour Options** from the main toolbar to open the *Dataset Contour Options – 3D Grid – leachate* dialog.

5. Select the *Specify a range* option (near the middle on the left side of the dialog).

6. Enter "1" for the minimum value.

7. Enter "130" for the maximum value.

8. Change the *Contour Method* to "Color fill."

9. Select the **OK** button to exit the *Dataset Contour Options – 3D Grid – leachate* dialog.

The user should now see a display of color-shaded contours confined to the area adjacent to the landfill. Do the following to view the solution for layer two:

10. Change the Mini-GridToolbar to layer "2."

Do the following to view the solution in cross section view:

11. Select a cell in the vicinity of the landfill.

12. Select the "Side View" button.

13. Use the up and down arrows to view the solution along different columns.

14. Select the "Plan View" button when finished.

15. Note that the leachate eventually reaches both the river and the well. The user will now view the mass flux of leachate into the river that was computed with the transport observation package.

16. Select the "SourcesSink" coverage in the Project Explorer (the user may need to expand the "Map Data" folder and the "East Texas" conceptual model).

17. Select the **Select Arcs** tool.

18. 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

The user can also view a plot of Mass vs. Time for a selected feature object. To create the plot, do the following:

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** buttonto resize the view of the model grid.

20 Viewing an Animation

Next, the user will observe how the solution changes over the course of the simulation by generating an animation. Do the following to set up the animation:

1. Select the "leachate" datasetin the Project Explorer.
2. Select the *Display* | **Animate** command.
3. Make sure the *Data set* option is on.
4. Click **Next**.
5. Turn on the *Display clock* option.
6. Select the **Finish** button.
7. After viewing the animation, select the **Stop** button to stop the animation.
8. Select the **Step** button to move the animation one frame at a time.
9. The user may wish to experiment with some of the other playback controls. When finished, close the window and return to GMS.

21 Modeling Sorption and Decay

The solution that was just computed can be thought of as a worst-case scenario since the user has 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, the userwill modify the model so that sorption and decay are simulated. The user 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*. The user needs to turn this package on before it can be used.

1. Select the *MT3DMS* | **Basic Transport Package** command to open the *Basic Transport Package* dialog.
2. Select the **Packages** command to open the *MT3D/RT3D Packages* dialog.
3. Turn on the *Chemical reaction package* option.
4. Select the **OK** button to exit the *MT3D/RT3D Packages* dialog.
5. Select the **OK** button to exit the *Basic Transport Package* dialog.

21.2 Entering the Sorption and Biodegradation Data

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

1. Select the *MT3DMS* | **Chemical Reaction Package** command.
2. In the *Sorption* drop-down menu, select the "Linear isotherm" option.
3. In the *Kinetic rate reaction* drop-down menu, 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

It is nearly time to save the project under a new file name. However, the user will face the same problem he or she faced earlier with the HFF file. That is, MT3D will look for a HFF file with the same name as the one the user is about to use to save the project. That file doesn't exist. The user could rerun MODFLOW to create it, but there's another way.

1. Select the *MT3DMS* | **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 that was generated previously.

23 Saving the Simulation

It is now possible to save the new simulation.

1. Select the *File* | **Save As** command.
2. Change the project name to "run2.gpr."
3. Select **Save.**

24 Running MT3DMS

To run MT3DMS:

1. Select the *MT3DMS* | **Run MT3DMS** command.
2. When the simulation is finished, select the **Close** button and return to GMS. The solution is imported automatically.

Again, the userwill notice here that it is possible to view the sorbed dataset.

25 Viewing the Solution

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

1. Expand "run2 (MT3DMS)" in the Project Explorer.
2. Select the "leachate" dataset.

3. 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 the user wants to take the plot data and put it into Excel, the user can right-click on the plot and select the *View Values* option. This brings up a spreadsheet that the user can copy and then paste into Excel.

27 Conclusion

This concludes the tutorial. Here are the key concepts in this tutorial:

- If the user is starting with a MODFLOW conceptual model and he or she wants to do a transport model, the user must turn on transport in the conceptual model properties.

- It is possible to use the *MT3D* | **Run Options** command to tell MT3D what MODFLOW solution to use.

