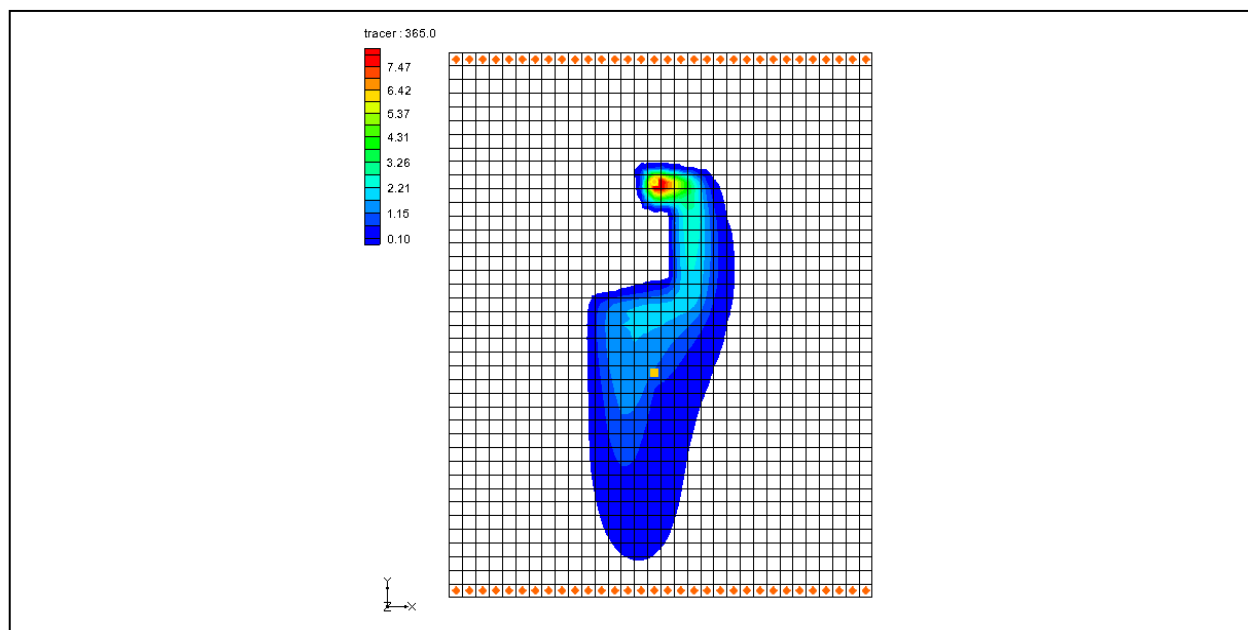*GMS 9.2 Tutorial*
MT3DMS – Grid Approach
Create an MT3DMS model using the grid approach

Objectives

Construct a MT3DMS model using the grid approach. Values are manually assigned to the grid. Simple models can be easily constructed using the grid approach.

Prerequisite Tutorials	Required Components	Time
• None	• Grid • MODFLOW • MT3DMS	• 30-60 minutes

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1   Contents

2   Introduction

This tutorial describes how to perform an MT3DMS simulation within GMS. An MT3DMS model can be constructed in GMS using one of two approaches: the conceptual model approach or the grid approach. With the conceptual model approach, the sources/sinks and zones in the model are defined with GIS objects and automatically assigned to the grid. With the grid approach, values are manually assigned to the grid. While the conceptual model approach is generally preferable for large, complicated models, simple models can be easily constructed using the grid approach. The grid approach is described in this tutorial.

2.1   Outline

This is what you will do:

1. Open a MODFLOW simulation and run MODFLOW.

2. Initialize MT3D and enter the data for several MT3D packages.

3. Run MT3D and read the solution.

4. Set up an animation to visualize the solution.

5. Calculate the mass of the contaminant.

3   Description of Problem

The problem to be solved in this tutorial is shown in Figure 1. This problem corresponds to the sixth sample problem ("Two-Dimensional Transport in a Heterogeneous Aquifer") described in the MT3DMS documentation. The problem consists of a low K zone inside a larger zone. The sides of the region are no flow boundaries. The top and bottom are constant head boundaries that cause the flow to move from the top to the bottom of the region. An injection well with a specified concentration provides the source of the contaminants. A pumping well serves to withdraw contaminated water migrating from the injection well. A steady state flow solution will be computed and a transient transport simulation will be performed over a one year period.
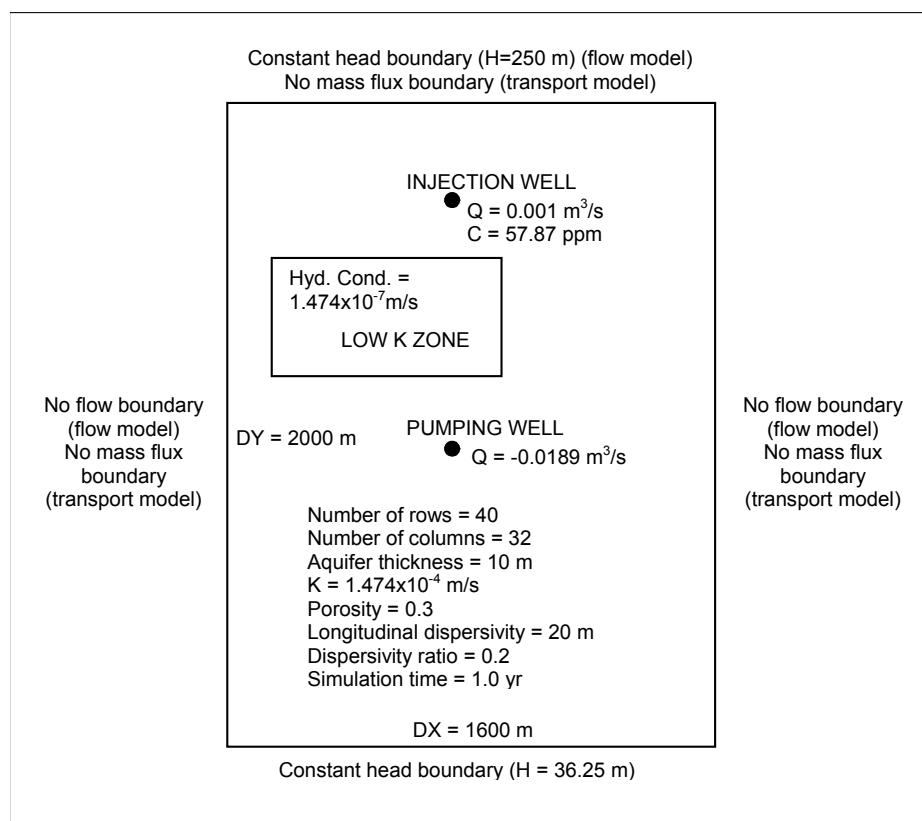

Figure 1.   Sample flow and transport problem.

4   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.

5   The Flow Model

Before setting up the MT3DMS simulation, we must first have a MODFLOW simulation. The MODFLOW solution will be used as the flow field for the transport simulation. In the interest of time, we will read in a previously created MODFLOW simulation.

1. Select the *Open* button .

2. Locate and open the directory entitled **Tutorials\mt3dgrid**.

3. Open the file entitled **flowmod.gpr**.

Now we'll save our project under a new name. Since we're changing the name, we will run MODFLOW to compute solution files with the new name. Otherwise, when MT3D runs it will look for solution files with the new name and not find any.

4. Select the *File | Save As* command.

5. Locate and open the directory entitled **Tutorials\mt3dgrid**

6. Save the project with the name **transport.gpr**.

7. Select the *3D Grid Data* folder from the *Project Explorer*.

8. Click the *Run MODFLOW* button.

9. When it finishes running, select the *Close* button.

6   Building the Transport Model

Now that we have a flow solution, we are ready to set up the MT3DMS transport simulation. Like MODFLOW, MT3DMS is structured in a modular fashion and uses a series of packages as input. Consequently, the GMS interface to MT3DMS is similar to the interface to MODFLOW and we will follow a similar sequence of steps to enter the input data.

6.1   Initializing the Simulation

First, we will initialize the MT3DMS simulation.

1. Right click on the *grid* item in the *Project Explorer* and select the *New MT3D…* command.

6.2   The Basic Transport Package

The MT3DMS Basic Transport package is always required and it defines basic information such as stress periods, active/inactive regions, and starting concentration values.

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 "tracer."

1. Select the *Define Species* button.

2. Select the *New* button.

3. Change the name of the species to **tracer**.

4. Select the *OK* button.

Packages

Next, we will select which packages we wish to use.

1. Select the *Packages* button.

2. Turn on the following packages:

    - *Advection Package*

    - *Dispersion Package*

    - *Source/Sink Mixing Package*

3. Select the *OK* button.

Stress Periods

The next step is to set up the stress periods. The flow simulation was steady state but the transport simulation will be transient. We will run the simulation for a one year time period. To do this we will use a single stress period (since the input values are constant) and allow MT3DMS to determine the appropriate transport step size.

4. Select the *Stress Periods* button.

5. Change the *Length* field to **365**.

6. Make sure the value in the *Trans. step size* is **0.0**. A value of zero signifies that *MT3DMS* will automatically compute the appropriate transport step size.

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

Output Control

Next, we will specify the output options.

1. Select the *Output Control* button.

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

3. Change the specified interval to **10**. This will output a solution at every tenth transport step.

4. Select the *OK* button to exit the *Output Control* dialog.

ICBUND Array

The ICBUND array is similar to the IBOUND array in MODFLOW. The ICBUND array is used to designate active transport cells (ICBUND>0), inactive transport cells (ICBUND=0), and constant concentration cells (ICBUND<0). For our problem, all of the cells are active, therefore, no changes are necessary.

Starting Concentration Array

The starting concentration array defines the initial condition for the contaminant concentration. In our problem, the starting concentrations are all zero and the default is adequate.

HTOP and Thickness Arrays

MT3DMS uses the HTOP array and a thickness array to determine the layer geometry. However, the values for these arrays are determined by GMS automatically from the MODFLOW layer data and no input is necessary.

Porosity Array

Finally, we will define the porosity for the cells. Our problem has a constant porosity of 0.3. This is the default value in GMS so no changes need to be made.

This completes the definition of the Basic Transport package data.

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

6.3   The Advection Package

The next step is to enter the data 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.

6.4   The Dispersion Package

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

1. Select the *MT3DMS | Dispersion Package* command.

2. Select the *Longitudinal Dispersivity* button.

3. Select the *Constant → Grid* option.

4. Enter a value of **20** and click *OK*.

5. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.

6. Enter a value of **0.2** for the *TRPT* parameter.

7. Select the *OK* button to exit the *Dispersion Package* dialog.

6.5   The Source/Sink Mixing Package

Finally, we must define the data for the Source/Sink Mixing package. For our problem, we only have one source/sink: the injection well. To define the source at the injection well, we need to select the well and assign a concentration.

1. Select the cell containing the injection well (the upper well) by clicking anywhere in the interior of the cell.

2. Right-click on the selected cell and select the *Sources/Sinks* menu command.

3. On the left side of the dialog select the **MT3D: Point SS** item.

4. Click the *Add BC* button near the bottom of the dialog.

5. Change the *Type (ITYPE)* to **well (WEL)**.

6. Enter **57.87** for the concentration.

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

8. Click outside the grid to unselect the cell.

6.6   Saving the Simulation and Running MT3DMS

We are now ready to save the simulation and run MT3DMS.

1. Select the *Save* button 💾.

2. Select the *Run MT3D* 🖥 button.

3. When the simulation is finished, select the *Close* button.

6.7   Changing the Contouring Options

When displaying plume data, the color fill option often provides excellent results.

1. Click on the *Contour Options* ▶ button.

2. Change the *Contour method* to **Color Fill.**

3. Select the *OK* button.

6.8   Setting Up an Animation

Now we will observe how the solution changes over the one year simulation by generating an animation. To set up the animation:

1. Select the *Display | Animate* command.

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

3. Turn on the *Display clock* option.

4. Select the *Use constant interval option* and change the *Time interval* to **36.5**. This will result in 11 frames.

5. Select the *Finish* button.

You should see some images appear on the screen. These are the frames of the animation which are being generated.

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.

6.9   Calculating the Mass of the Contaminant

Finally, we will calculate the mass of the contaminant in the aquifer at various times during the simulation.

1. Choose the *Select Cells* tool 🔳.

2. Select the cell containing the well in the lower portion of the model.

3. Select the *MT3DMS | Calculate Mass* command.

This dialog allows the user to calculate the mass of a contaminant in the entire model domain or in the selected cells. The *Definition* section of the dialog explains the formula

that is used to calculate the mass. Basically, the volume of water in each cell is calculated and then multiplied by the concentration computed by MT3D. The user must supply a conversion factor so that the calculated mass will be computed in the correct units. The *Unit conversion factor* section shows an example of a conversion factor. The *Concentration range* section allows the user to specify a range over which the mass will be calculated. This is most useful to ignore negative concentrations that result in MT3D simulations.

4. In the *Concentration range* section, turn on the *Specify range in calculation* toggle.

5. Enter **0.0** for the *Min* and **9.0** for the *Max*.

6. In the *Unit conversion factor* section, enter **0.0283** for the *Factor* so that the resulting mass will be in units of grams.

7. Select the *Use only selected cells in calculation* option near the bottom of the dialog.

8. Select the *Calculate* button.

Notice that the mass values are shown in the spreadsheet on the right side of the dialog.

9. Now select the *Use all cells in calculation* option.

10. Select the *Calculate* button again.

You should now see the total mass in the aquifer for each time step of the solution.

11. When you have finished viewing the results select *Done* to close the dialog

7   Conclusion

This concludes the *MT3DMS – Grid Approach* tutorial. Here are the things that you should have learned in this tutorial:

- MT3D is available only if a MODFLOW model is in memory.

- MT3D relies on the MODFLOW solution files, so if you move or rename your MODFLOW files, you will probably need to regenerate the MODFLOW solution files so MT3D can find them.

- GMS gives MT3D the top and bottom elevation data it requires for each layer from the MODFLOW model.

- You can use the *Animation Wizard* to create an animation in GMS.

- You can calculate the mass of a contaminant in the 3D grid using the *MT3D | Calculate Mass* command.