

GMS TUTORIALS

MT3DMS – Advanced Transport

This tutorial describes how to include some of the advanced transport options when performing an MT3DMS simulation within GMS. Dispersion, sorption, and dual domain transport are illustrated.

1 Description of Problem

The problem to be solved in this tutorial is a modification of the problem used in the MT3DMS – Grid Approach tutorial. However, the low K zone and the injection and extraction wells have been removed leaving only a simple north-to-south one-dimensional flow field as shown in Figure 11.1. The sides of the region are no-flow boundaries. The top and bottom are constant head boundaries. The initial condition for the plume consists of a small contaminant source zone near the upstream end of the model.

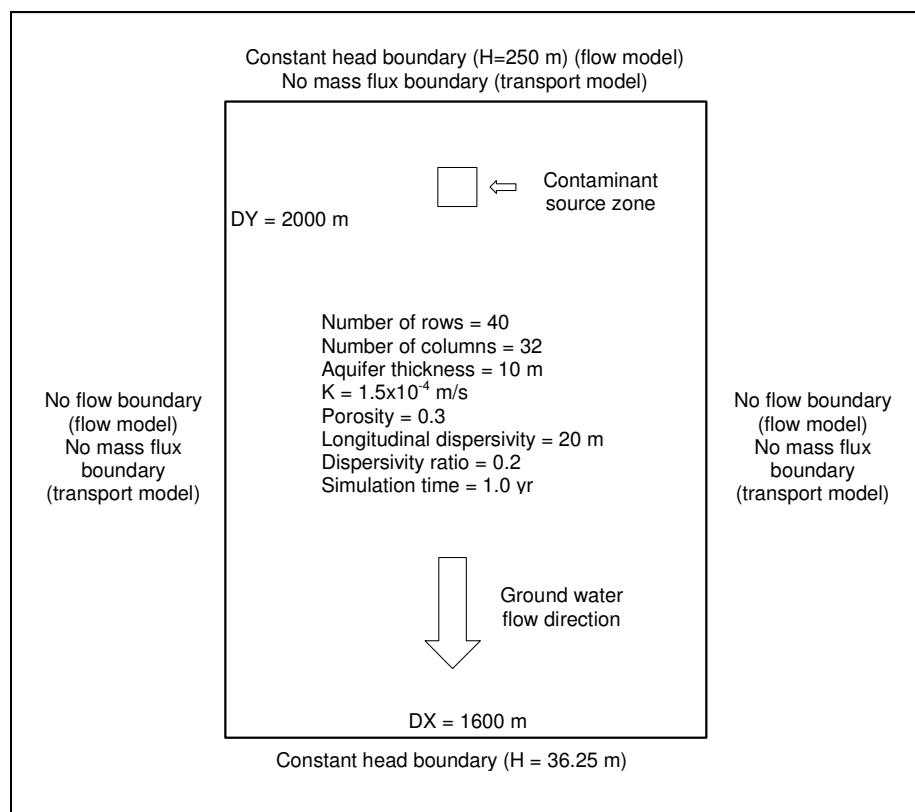


Figure 1.1 Sample Flow and Transport Problem

For this tutorial, we will run four transport simulations representing the following conditions:

1. **Tracer transport.** Simple advective flow.
2. **Dispersion.** We will add dispersion and note the effect on the plume shape.
3. **Sorption.** Same as before but we will turn on sorption.
4. **Dual domain.** In this case we will run a dual domain simulation where we specify a separate set of transport options for the mobile phase and the immobile phase.

2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

3 Required Modules/Interfaces


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

- Grid
- MODFLOW
- MT3DMS

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

4 The Flow Model

Before setting up the MT3DMS simulation, we must first have a MODFLOW solution that 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 **tutfiles\MT3D\mt3dadv**.
3. Select the file entitled **flowmod.gpr**.
4. Select the *Open* button.

Note that the head contours indicate a linear decrease in head from the north to the south.

5 Building the Transport Model

Now that we have a flow solution, we are ready to set up the MT3DMS tracer transport simulation.

5.1 Initializing the Simulation

First, we will initialize the MT3DMS simulation.

1. Select the MT3D | New Simulation command.

5.2 The Basic Transport Package

We first need to define a few things in the MT3DMS Basic Transport package such as stress periods, active/inactive regions, and starting concentration values.

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.

5. Select the *Packages* button.
6. Turn on the following packages:
 - Advection Package
 - Dispersion Package
 - Source/Sink Mixing Package
7. 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.

8. Select the *Stress Periods* button.
9. Change the *Length* field to **365**.
10. 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.
11. Select the *OK* button to exit the *Stress Periods* dialog.

Output Control

Next, we will specify the output options.

12. Select the *Output Control* button.
13. Select the *Print or save at specified times* option.

14. Select the *Times...* button.
15. Select the *Initialize Values...* button.
16. Enter the following values (these values will give us 20 output time steps):
 - Initial time step size: **18.25**
 - Maximum time step size: **18.25**
 - Maximum simulation time: **365**
17. Select the *OK* button twice to exit both dialogs.

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. We can leave the other options at the default values.

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

5.3 Saving the Project

Before continuing, we will save the project under a different name.

1. Select the *File | Save As* command.
2. Change the file name to **tracer.gpr**.
3. Select the *Save* button.

5.4 Defining the Initial Condition

Next, we will edit the initial concentration for four of the cells near the top end of the model to define the initial state of the contaminant plume.

1. Hold the shift key down and select the cells **(5,16)**, **(5,17)**, **(6,16)**, and **(6,17)**. Note that the cell indices (I, J) are displayed at the bottom of the GMS window.
2. Select the *MT3D | Cell Properties* command.
3. Change the *Starting conc.* to **100**.
4. Select the *OK* button.

5.5 Run Options

Next, we will tell MT3DMS to always use the same MODFLOW solution to define the flow field. This will allow us to save the transport simulation under a different name without having to re-run MODFLOW.


1. Select the *MT3D | Run Options* command.
2. Select the *Single run with selected MODFLOW solution* option.
3. Select the *OK* button.

5.6 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.



5.7 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 *MT3D | Run MT3D...* command.
3. When the simulation is finished, click the *Close* button.

5.8 Viewing the Solution

After reading in the solution:

1. Expand the tracer (MT3DMS) Folder  from the Project Explorer.
2. Select the tracer data set .
3. Click on the first time step (**18.25**) in the Time Step Window.
4. Use the up and down arrows on your keyboard to step through the range of time steps associated with the solution.

Note that the plume does not spread out. Rather, it stays together as a concentrated slug of contaminant.

6 Adding Dispersion

Next, we will add dispersion to our simulation and see how it affects the results.

6.1 The Dispersion Package

To enter the data for the Dispersion package:

1. Select the *MT3D | Dispersion Package* command.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant → Grid* button.
4. Enter a value of **20** and select the *OK* button.
5. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.
6. Change the *TRPT* and *TRVT* value to **0.2**.
7. Click the *Close* button to exit the *Dispersion Package* dialog.



6.2 Saving the Simulation and Running MT3DMS

We are now ready to save the simulation under a different name and run MT3DMS.

1. Select the *File | Save As* command.
2. Change the name to **dispersion.gpr**.
3. Select the *Save* button.
4. Select the *MT3D | Run MT3D...* command.
5. When the simulation is finished, click the *Close* button.

6.3 Viewing the Solution

Once again, after reading in the solution:

1. Expand the dispersion (MT3DMS) Folder  from the Project Explorer.
2. Select the tracer data set .
3. Click on the first time step (**18.25**) in the Time Step Window.
4. Use the up and down arrows on your keyboard to step through the range of time steps associated with the solution.

7 Adding Sorption

Next, we will turn on sorption. We will use simple linear sorption. With this option, the sorption and de-sorption of the contaminant is assumed to be a simple function of the contaminant concentration. The relationship between concentration and sorbed mass is defined by a linear isotherm. This theory assumes that the sorption is instantaneous. By contrast, a rate-limited sorption option is also available.

Turning on sorption has the effect of slowing the rate that the plume moves through the system. This effect can be expressed as a retardation factor that represents the ratio of the ground water flow rate to the plume migration rate. The retardation factor is computed as:

$$R = 1 + \frac{\rho K_d}{n}$$

where

ρ = bulk density

K_d = distribution coefficient (slope of the isotherm)

n = porosity

Note that the units used for ρ and K_d do not necessarily need to match the units used for the rest of the model, as long as they are consistent between ρ and K_d . The only place that these values are used is in the calculation of R .

7.1 Editing the Chemical Reaction Package

The sorption options are specified in the Chemical Reaction package. Before we can edit the package data, we must first turn on the package:

1. Select the MT3D | Basic Transport Package command.
2. Select the Packages button.
3. Turn on the Chemical reaction package option.
4. Click the OK button twice to exit both dialogs.

To enter the sorption parameters:

5. Select the MT3D | Chemical Reaction Package command.
6. Change the Sorption option to **Linear isotherm**.

7. Change the Bulk density to **1600**. Note that these units actually represent $[\text{kg}/\text{m}^3]$. Once again, this does not agree with the standard units for the model, but these units only need to agree with the K_d (first sorption constant) units.
8. Change the 1st sorption constant to **0.0001154**. (Actual units = $[\text{m}^3/\text{kg}]$).
9. Click the OK button to exit the dialog.

Note that these two values should result in a retardation factor of 2.0.



7.2 Saving the Simulation and Running MT3DMS

We are now ready to save the simulation under a different name and run MT3DMS.

1. Select the *File* | *Save As* command.
2. Change the name to **sorption.gpr**.
3. Click the *Save* button.
4. Select the *MT3D* | *Run MT3D...* command.
5. When the simulation is finished, click the *Close* button.

7.3 Viewing the Solution

Once again, after reading in the solution:

1. Expand the sorption (MT3DMS) Folder  from the Project Explorer.
2. Select the tracer data set .
3. Click on the first time step (**18.25**) in the Time Step Window.
4. Use the up and down arrows on your keyboard to step through the range of time steps associated with the solution.

8 Simulating Dual Domain Transport

Finally, we will turn on the dual domain transport option. The theory behind dual domain transport is that there are two distinct domains in a transport simulation: the mobile domain (the cracks and fissures where the majority of advective flow occurs) and the immobile domain (the unfractured mass of the aquifer where the primary transport mechanism is dispersion/diffusion). The dual domain option makes it possible to specify separate transport parameters for each of these domains. Numerous case studies have shown that a dual domain simulation may improve calibration and better represent field conditions.

To better illustrate the effect of the dual domain option, we will turn off the sorption option.

8.1 Editing the Chemical Reaction Package

The dual domain option is turned on in the Chemical Reaction package. Before we can edit the package data, we must first turn on the package:

1. Select the MT3D | Chemical Reaction Package command.
2. Change the Sorption option to Dual-domain mass transfer (without sorption).
3. In the Variable input section, select the Cell by cell option. This will allow us to specify a unique value for the immobile phase initial condition in the four cells where the plume is initially defined.

Porosity

Next, we will edit the porosity for the immobile phase. This porosity is generally smaller than the porosity used in the mobile phase.

4. Click the *Edit* button just to the right of the *Immobile porosity* option.
5. Using the *Constant* → *Grid* button, assign a value of **0.1** for the *immobile porosity* to the entire grid.
6. Click the *OK* button to exit the spreadsheet editor dialog.

Initial Concentration

We must also specify the initial concentration of the immobile phase.

7. Turn on the Specify IC of sorbed phase option.
8. Click the Edit button just to the right of the IC immobile phase option.
9. Enter a concentration of **100.0** for the cells (5,16), (5,17), (6,16), and (6,17).
10. Click the OK button to exit the spreadsheet dialog.

Mass Transfer Coefficient

Finally, we must enter a value for the coefficient that defines the mass transfer rate between the mobile and immobile phases.

11. Click the *Edit* button just to the right of the *2nd sorption const.* option.
12. Using the *Constant* → *Grid* button, assign a value of **0.1** for the immobile porosity to the entire grid and select *OK* to exit the dialog.

13. Click the *OK* button to exit the spreadsheet dialog.

This concludes the changes we need to make to the Chemical Reactions Package.

14. Click the *OK* button to exit the *Chemical Reactions Package* dialog.



8.2 Saving the Simulation and Running MT3DMS

We are now ready to save the simulation under a different name and run MT3DMS.

1. Select the *File | Save As* command.
2. Change the name to **dualdomain.gpr**.
3. Select the *Save* button.
4. Select the *MT3D | Run MT3D...* command.
5. When the simulation is finished, click the *Close* button.

8.3 Viewing the Solution

Once again, after reading in the solution:

1. Expand the dualdomain (MT3DMS) Folder  from the Project Explorer.
2. Select the tracer data set .
3. Click on the first time step (**18.25**) in the Time Step Window.
4. Once again, use the up and down arrows to view the different time steps. The result should show a prolonged tail indicating a “bleeding pattern” due to the contaminant migrating from the immobile phase.

At this point, you may wish to change the value of rate constant (second sorption constant) from 0.0005 to 0.0009 and compare the profiles for various mass-transfer constants.

9 Conclusion

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

- How to do a simple tracer simulation with MT3DMS.
- How to add dispersion to a transport simulation

- How to add sorption to a transport simulation and how to compute the retardation factor for a particular set of sorption coefficients.
- How to perform a dual-domain transport simulation.