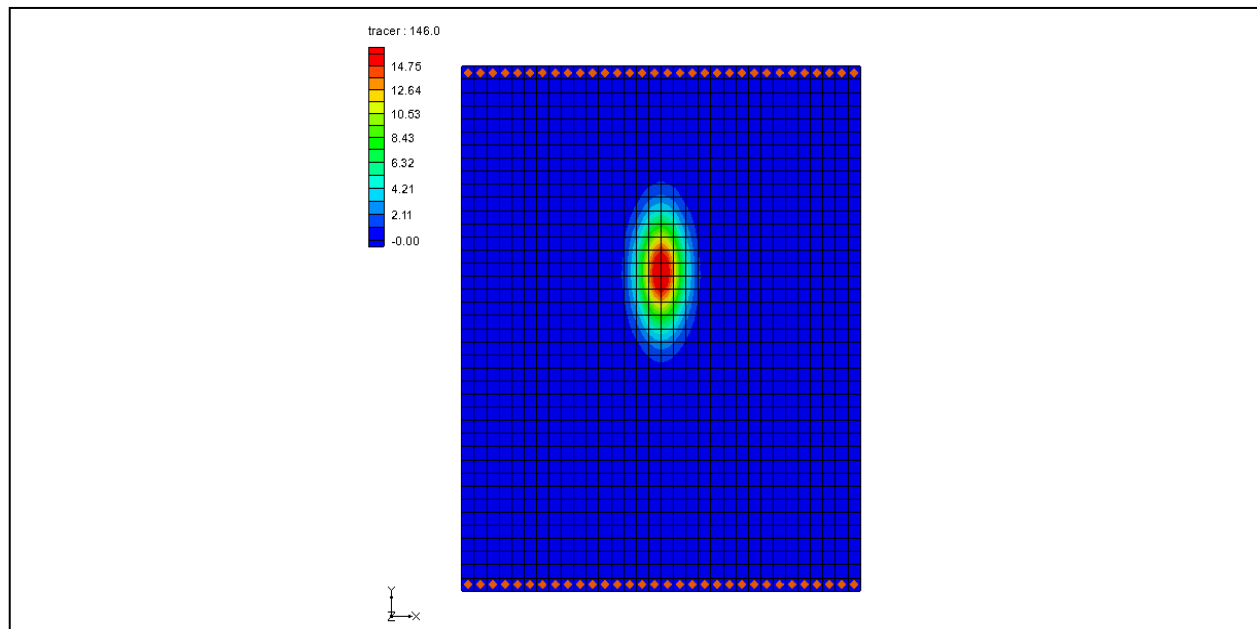


GMS 10.0 Tutorial

MT3DMS – Advanced Transport

MT3DMS dispersion, sorption, and dual domain options



Objectives

Learn about the dispersion, sorption, and dual domain options in MT3DMS

Prerequisite Tutorials

- MT2DMS – Grid Approach

Required Components

- Grid Module
- MODFLOW
- MT3DMS

Time

- 25-40 minutes



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1 Introduction

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.

2 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 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.

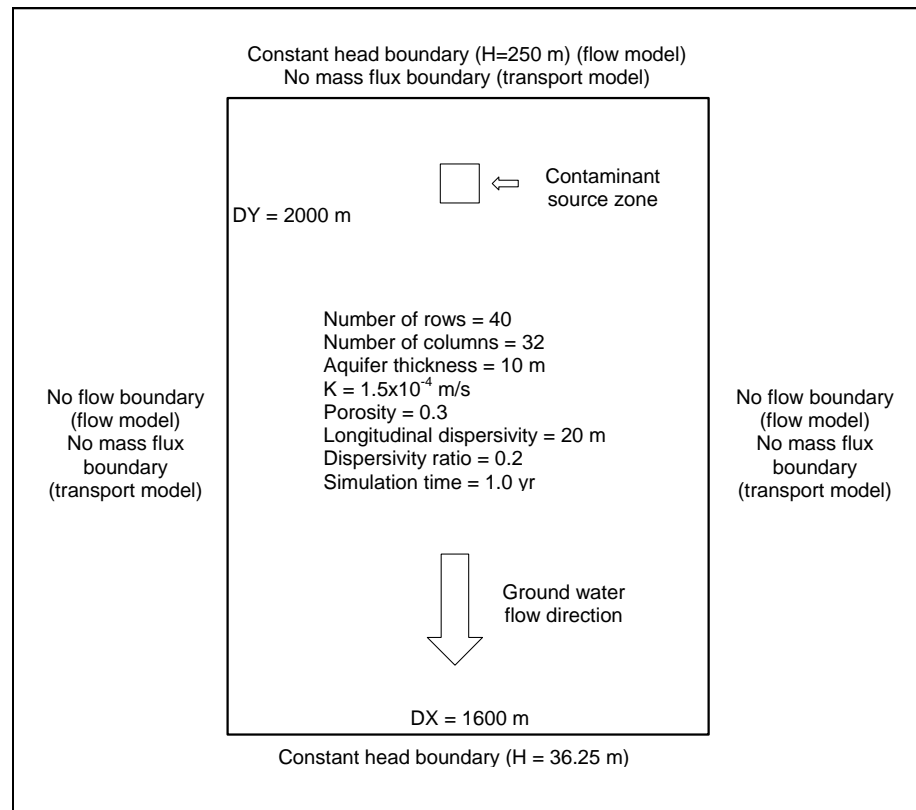


Figure 1 Sample flow and transport problem

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

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


3 Getting Started

Do the following to get started:

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

4 The Flow Model

Before setting up the MT3DMS simulation, it is necessary to have a MODFLOW solution that will be used as the flow field for the transport simulation. In the interest of time, the user will read in a previously created MODFLOW simulation.

1. Select the **Open**  button.
2. Locate and open the directory entitled *Tutorials\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 the user has a flow solution, it is possible to set up the MT3DMS tracer transport simulation.

5.1 Initializing the Simulation

First, initialize the MT3DMS simulation.

1. Select the *MT3DMS / New Simulation* command to open the *Basic Transport Package* dialog.

5.2 The Basic Transport Package

First, it is necessary to define a few things in the MT3DMS Basic Transport Package.

Species

The user will use one species named “tracer.”

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 “tracer.”
4. Select the **OK** button.

Packages

Next, select which 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
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. The user will run the simulation for a one-year time period. To do this, the user will use a single stress period (since the input values are constant) and allow MT3DMS to determine the appropriate transport step size.

1. Select the **Stress Periods** button.
2. Change the *Length* field to “365.”
3. 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.
4. Select the **OK** button to exit the *Stress Periods* dialog.

Output Control

Next, specify the output options.

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 (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”
6. Select the **OK** button three times to return to the *Basic Transport Package* dialog.

Porosity Array

Finally, it is necessary to define the porosity for the cells. This 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. The other options can remain at the default values.

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

5.3 Saving the Project

Before continuing, 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, the user 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 ctrl 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 *MT3DMS* / **Cell Properties** command to open the *3D Grid Cell Properties* dialog.
3. Change the *Starting conc.* to “100.”
4. Select the **OK** button.

5.5 Run Options

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


1. Select the *MT3DMS* / **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. This tutorial will use the *Third Order TVD scheme (ULTIMATE)* solution scheme. This is the default, so nothing needs to be changed.



5.7 Saving the Simulation and Running MT3DMS

It is now possible to save the simulation and run MT3DMS.

1. Select the **Save**  button.
2. Select the *MT3DMS* / **Run MT3DMS** command.
3. When the simulation is finished, click the **Close** button.

5.8 Viewing the Solution

After reading in the solution, do the following:

1. Expand the “3D Grid Data” folder in the Project Explorer.
2. Expand the “tracer (MT3DMS)”  folder from the Project Explorer.
3. Select the “tracer”  dataset.
4. Click on the first time step (18.25) in the *Time Step Window*.
5. Use the up and down arrows on the 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, the user will add dispersion to the simulation and see how it affects the results.

6.1 The Dispersion Package

Do the following to enter the data for the Dispersion package:

1. Select the *MT3DMS* / **Dispersion Package** command to open the *Dispersion Package* dialog.
2. Select the **Longitudinal Dispersivity** button to open the *Longitudinal Dispersivity* dialog.

3. Select the **Constant** → **Grid** button to open the *Grid Value* dialog.
4. Enter a value of “20.”
5. Select the **OK** button.
6. Select the **OK** button to exit the *Longitudinal Dispersivity* dialog.
7. Change the *TRPT* and *TRVT* values to “0.2.”
8. Select the **OK** button to exit the dialog.



6.2 Saving the Simulation and Running MT3DMS

Now 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 *MT3DMS* / **Run MT3DMS** command.
5. When the simulation is finished, click the **Close** button.

6.3 Viewing the Solution

Once again, do the following after reading in the solution:

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

7 Adding Sorption

Next, the user will turn on sorption. The user will use a 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 follows:

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

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 the user can edit the package data, the user must first turn on the package:

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

Do as follows to enter the sorption parameters:

6. Select the *MT3DMS* / **Chemical Reaction Package** command to open the *Chemical Reaction Package* dialog.
7. Change the *Sorption* option to “Linear isotherm.”
8. Change the *Bulk density* to “1600.” Note that these units actually represent [kg/m³]. 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.
9. Change the *1st sorption constant* to “0.0001154.” (Actual units = [m³/kg]).

10. 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

Now 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 *MT3DMS* / **Run MT3DMS** command.
5. When the simulation is finished, click the **Close** button.

7.3 Viewing the Solution

Once again, do the following after reading in the solution:

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

8 Simulating Dual Domain Transport

Finally, the user 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, the user 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. First it is necessary to turn on the package:

1. Select the *MT3DMS* / **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 the user to specify a unique value for the immobile phase initial condition in the four cells where the plume is initially defined.

Porosity

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

1. Click the **Edit** button just to the right of the *Immobile porosity* option.
2. Using the **Constant → Grid** button, open the *Grid Value* dialog.
3. Assign a value of “0.1” for the *immobile porosity* to the entire grid.
4. Click the **OK** button to exit the spreadsheet editor dialogs.

Initial Concentration

The user must also specify the initial concentration of the immobile phase.

1. Turn on the *Specify IC of sorbed phase* option.
2. Click the **Edit** button just to the right of the *IC sorbed phase* option. This will open the *Immobile Porosity Array* dialog.
3. Enter a concentration of “100.0” for the cells (5,16), (5,17), (6,16), and (6,17).
4. Click the **OK** button to exit the spreadsheet dialog.

Mass Transfer Coefficient

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

1. Click the **Edit** button just to the right of the *2nd sorption const.* option.
2. Using the **Constant → Grid** button, open the *Grid Value* dialog.
3. Assign a value of “0.0005” for the second sorption constant to the entire grid.
4. Select **OK** to exit the dialog.

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

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

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

8.2 Saving the Simulation and Running MT3DMS



Now 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 *MT3DMS* / **Run MT3DMS** command.
5. When the simulation is finished, click the **Close** button.

Here the user may wish to view either the “tracer,” or the “tracer(sorbed)” option in the Project Explorer, to see how the simulation is affected over time.

8.3 Viewing the Solution

Once again, do the following after reading in the solution:

1. Expand the “dual domain (MT3DMS)”  folder from the Project Explorer.
2. Select the “tracer”  dataset.
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, the user 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 key concepts 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.