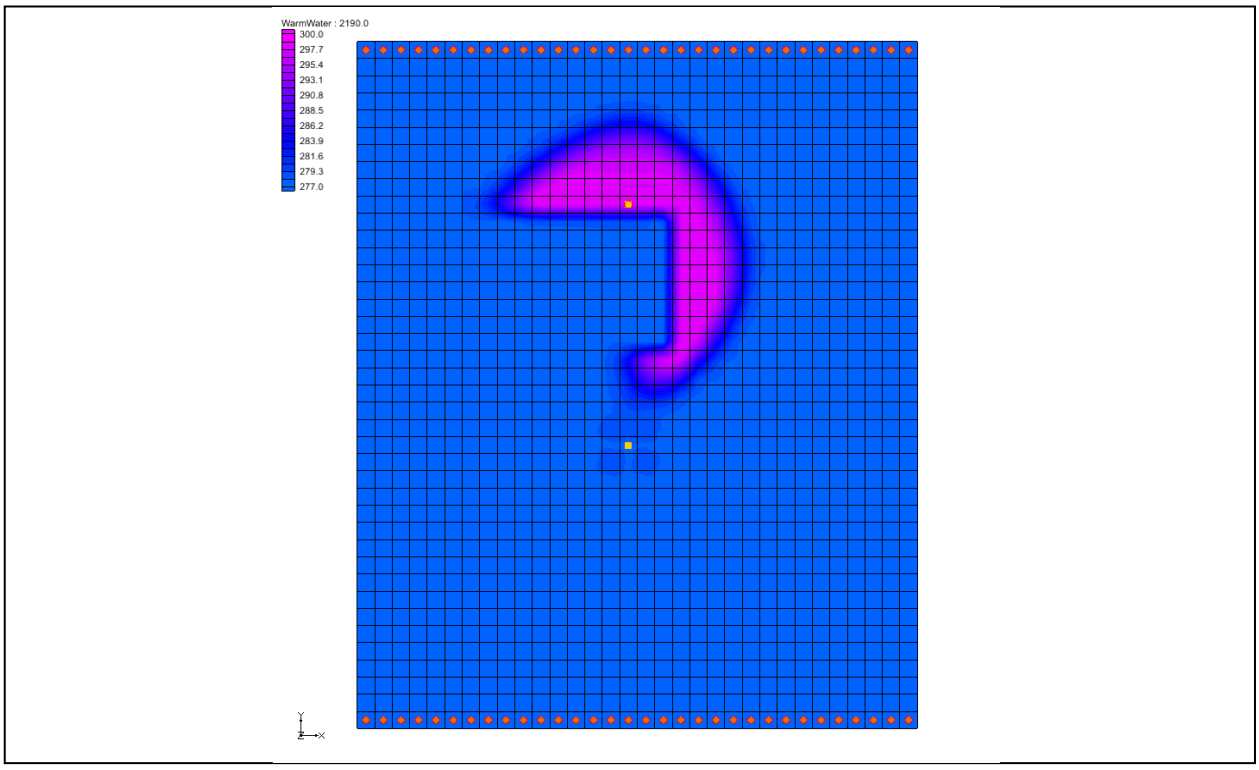
*GMS 10.0 Tutorial*

# *MT3DMS – Heat Transport*

Simulate heat transport using MT3DMS




## Objectives

Construct an MT3DMS model using the grid approach, and learn how to simulate heat transport using MT3DMS.

## Prerequisite Tutorials

- MT3DMS – Grid Approach

## Required Components

- Grid Module
- MODFLOW
- MT3DMS

## Time

- 20-35 minutes

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# 1 Introduction

This tutorial describes how to perform an MT3DMS simulation to simulate heat transport within GMS.

## 1.1 Outline

Here are the steps for this tutorial:

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.

# 2 Description of Problem

The problem to be solved in this tutorial is shown in Figure 1. This problem is similar 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. A well injects warm water into the aquifer with the initial temperature around $5^{o}$C for 3 months and is then turned off for 8 months. This cycle is repeated for 3 years and then the simulation runs for another 3 years. A pumping well serves to withdraw some water migrating from the injection well. A transient flow solution will be provided and a transient transport simulation will be performed over a 6-year period.

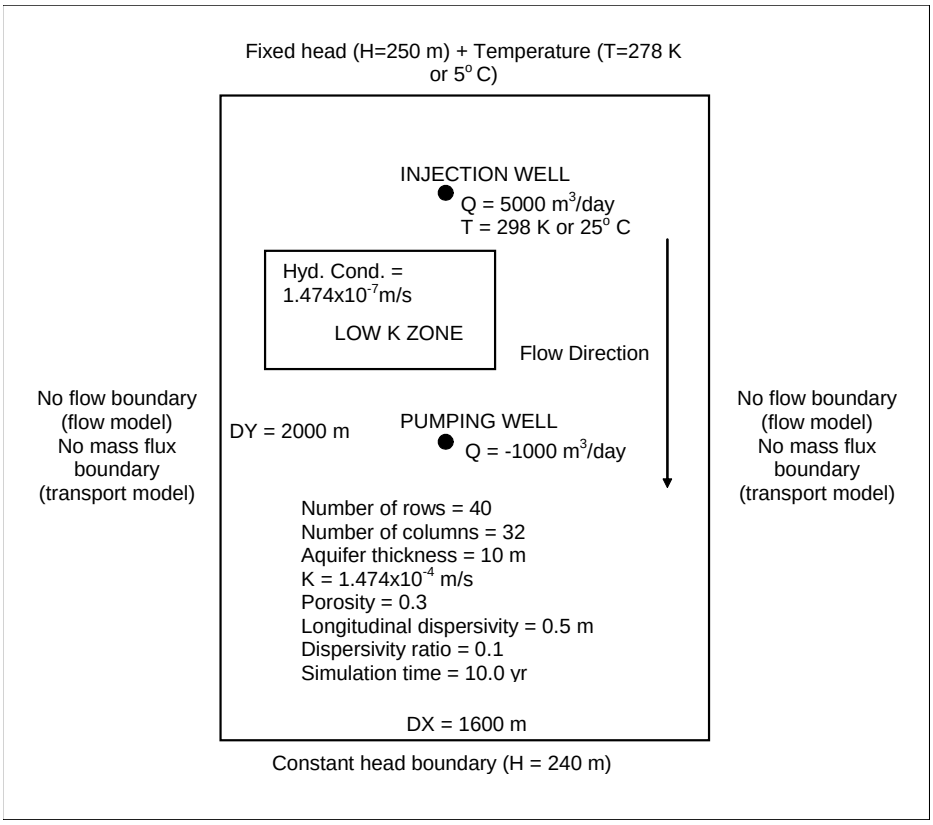


*Figure 1 Sample flow and transport problem*

# 3 Heat Transport Coefficients

Heat transport and solute transport are very similar. The following is a general form of the solute transport equation solved by MT3MDS:

$$(1+\frac{\rho_b K_d^k}{\theta})\frac{\partial(\theta C^k)}{\partial t} = \nabla\cdot[\theta(D_m^k+\alpha\frac{q}{\theta})\cdot\nabla C^k]-\nabla\cdot(qC^k)-q'_s C_s^k \qquad \textbf{(1)}$$

Where $\rho_b$ is the bulk density (mass of the solids divided by the total volume) [$ML^{-3}$], $K_d^k$ is the distribution coefficient of species k [$L^3M^{-1}$], $\theta$ is porosity, $C^k$ is the concentration of species k [$ML^{-3}$], $t$ is time [T], $D_m^k$ is the molecular diffusion coefficient [$L^2T^{-1}$] for species k, $\alpha$ is the dispersivity tensor [L], $q$ is specific discharge [$LT^{-1}$], $q'_s$ is a fluid source or sink [$T^{-1}$], and $C_s^k$ is the source or sink concentration [$ML^{-3}$] of species k.

The similarity between heat transport and solute transport is shown in the following heat transport equation, which was manipulated by Thorne et al. (2006):

$$(1+\frac{1-\theta}{\theta}\frac{\rho_s}{\rho}\frac{c_{Psolid}}{c_{Pfluid}})\frac{\partial(\theta T)}{\partial t} = \nabla\cdot[\theta(\frac{k_{Tbulk}}{\theta\rho c_{Pfluid}}+\alpha\frac{q}{\theta})\cdot\nabla T]-\nabla\cdot(qT)-q'_s T_s \qquad \textbf{(2)}$$

 

Where $\rho_s$ is the density of the solid (mass of the solid divided by the volume of the solid) [$ML^{-3}$], $\rho$ is fluid density [$ML^{-3}$], $c_{Psolid}$ is the specific heat capacity of the solid [$L^2T^{-2}\Theta^{-1}$], $c_{Pfluid}$ is the specific heat capacity of the fluid [$L^2T^{-2}\Theta^{-1}$], $T$ is temperature [$\Theta$], $k_{Tbulk}$ is the bulk thermal conductivity of the aquifer material [$MLT^{-3}\Theta^{-1}$], and *Ts* is source temperature [$\Theta$]. Note that $\rho_b$, $\rho_s$, and $\theta$ are related by

$$\rho_b = \rho_s (1 - \theta) \quad \textbf{(3)}$$

Additionally, there are retardation terms on the left side of both equations 1 and 2. For solute transport, retardation is caused by adsorption of solutes by the aquifer matrix material. With heat transport, retardation is caused by heat transfer between the fluid and solid aquifer matrix. MT3DMS can be used to represent thermal retardation by calculating the distribution coefficient ($K_d$) for the temperature species as a function of thermal properties:

$$K_d^T = \frac{c_{Psolid}}{\rho c_{Pfluid}} \quad \textbf{(4)}$$

Therefore, substituting equations 3 and 4 into the left side of equation 2 will yield the following:

$$(1+\frac{\rho_b K_d^T}{\theta})\frac{\partial(\theta T)}{\partial t} \quad \textbf{(5)}$$

Inspection of Equations 1 and 2 also shows that heat conduction is mathematically equivalent to molecular solute diffusion. To represent heat conduction with MT3DMS, thermal diffusivity for the temperature species is calculated as follows:

$$D_m^T = \frac{k_{Tbulk}}{\theta \rho c_{Pfluid}} \quad \textbf{(6)}$$

In GMS, the user can specify $K_d^T$ and $D_m^T$ in the MT3D interface. $K_d^T$ is the distribution coefficient (slope of the isotherm), which can be specified in the Chemical Reaction Package. $D_m^T$ is the molecular diffusion coefficient (DMCOEF), which can be specified in the Dispersion Package.

# 4 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.

 

# 5 The Flow Model

Before setting up the MT3DMS simulation, the user 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, the user will read in a previously created MODFLOW simulation.

1. Select the **Open** button.
2. Locate and open the directory entitled *Tutorials\MT3D\heat_transport*.
3. Select the file entitled "start.gpr**."**
4. Click **Open.**

# 6 Building the Transport Model

Now that the user has a flow solution, it is possible 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 the user will follow a similar sequence of steps to enter the input data.

## 6.1 Initializing the Simulation

First, the user will initialize the MT3DMS simulation.

1. Expand the "3D Grid Data" item in the Project Explorer.
2. Right-click on the "grid" item in the Project Explorer.
3. Select the **New MT3D** command.

This will create a new MT3D simulation and bring up the *Basic Transport Package* dialog.

## 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, the user needs to define the number of species and name each species. The user will use one species named "WarmWater."

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 "WarmWater."
4. Select the **OK** button.

### Packages

Next, the user will 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*
   - *Chemical Reaction Package*
3. Select the **OK** button.

### Stress Periods

The next step is to set up the stress periods. Since the flow simulation is transient, the transport simulation must match the stress periods defined for the flow simulation. Therefore, it is possible to use the stress periods as defined by the MODFLOW simulation.

### Output Control

Next, the user will 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 provide 100 output time steps):
   - *Initial time step size*: "25.0"
   - *Bias:* "1.0"

 

- *Maximum time step size*: "25.0"
- *Maximum simulation time*: "2200"

6. Select the **OK** button three times to return to the *Basic Transport Package* 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 this 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.

1. Turn on the *Edit Per Cell* toggle in the *Species* spreadsheet.
2. Select the button under the *Starting Conc. Per Cell Column* to open the *Starting Concentrations – WarmWater* dialog.
3. Select **Constant → Grid** button to open the *Grid Value* dialog.
4. Enter a value of "278" ($5^{o}$ C) for the starting value of the warm water species.
5. Select **OK**.
6. Select **OK** to exit the *Starting Concentrations – WarmWater* dialog.

### 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, so no input is necessary.

### Porosity Array

Finally, the user will define the porosity for the cells. The 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* dialog.

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. This tutorial will use the *Third Order TVD scheme (ULTIMATE)* solution scheme. This is the default, so nothing needs to be done.

## 6.4 The Dispersion Package

The molecular diffusion coefficient (DMCOEF) is specified in the Dispersion Package; in a heat transport simulation, DMCOEF represents thermal diffusivity $D_m^T$. Now, the user will enter the data for the Dispersion package.

1. Select the *MT3DMS* | **Dispersion Package** command.
2. Select the **Longitudinal Dispersivity** button to open the *Longitudinal Dispersivity* dialog.
3. Select the **Constant → Grid** option to open the *Grid Value* dialog.
4. Enter a value of "0.5."
5. Click **OK**.
6. Select the **OK** button to exit the *Longitudinal Dispersivity* dialog.
7. Enter a value of "0.1" for the *TRPT* parameter and TRVT parameter.
8. Enter a value of "2.15e-11"[1] for the *DMCOEF* parameter.
9. Select the **OK** button to exit the *Dispersion Package* dialog.

## 6.5 The Chemical Reaction Package

The sorption options are specified in the Chemical Reaction package. In a heat transport simulation, the sorption option represents thermal retardation. To enter the sorption parameters:

1. Select the *MT3DMS* | **Chemical Reaction Package** command to open the *Chemical Reaction Package* dialog.
2. Change the *Sorption* option to "Linear isotherm."

1. This value is based on reference values from the German Engineer Association guidelines for thermal use of the underground (VDI-Richtlinie 4640 2001).

3. Change the *Bulk density* to "1961." Note that these units actually represent [kg/m$^3$]. Once again, this does not agree with the standard units for the model, but these units only need to agree with the Kd (first sorption constant) units.

4. Change the *1st sorption constant* to "0.00021." (Actual units = [m$^3$/kg]).

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

Note that these two values should result in a retardation factor of 1.41. The retardation factor is calculated using the following formula:

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

where

$\rho$ = bulk density

$K_d$ = distribution coefficient (slope of the isotherm)

n = porosity

## 6.6 The Source/Sink Mixing Package

The user must define the data for the *Source/Sink Mixing* package so that the user can specify the temperature of the water at the injection well.

1. Choose the **Select Cells** tool.

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

3. Right-click on the selected cell.

4. Select the **Sources/Sinks** menu command to open the *MODFLOW/MT3DMS Sources/Sinks* dialog.

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

6. Now click the **Add BC** button near the bottom of the dialog.

7. Change the *Type (ITYPE)* to "well (WEL)."

8. Enter "298" (25$^o$ C) for the concentration under the *WarmWater* column.

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

10. Click outside the grid to unselect the cell.

Finally, it is necessary to define the constant temperature at the boundaries of the model.

 

11. Select all cells with the constant head BCs (orange diamond symbols) along the top and bottom boundaries of the grid. Do this by dragging a box around the cells at the top of the model and then holding down the *Shift* key and dragging a second box around the cells at the bottom of the model as shown below.

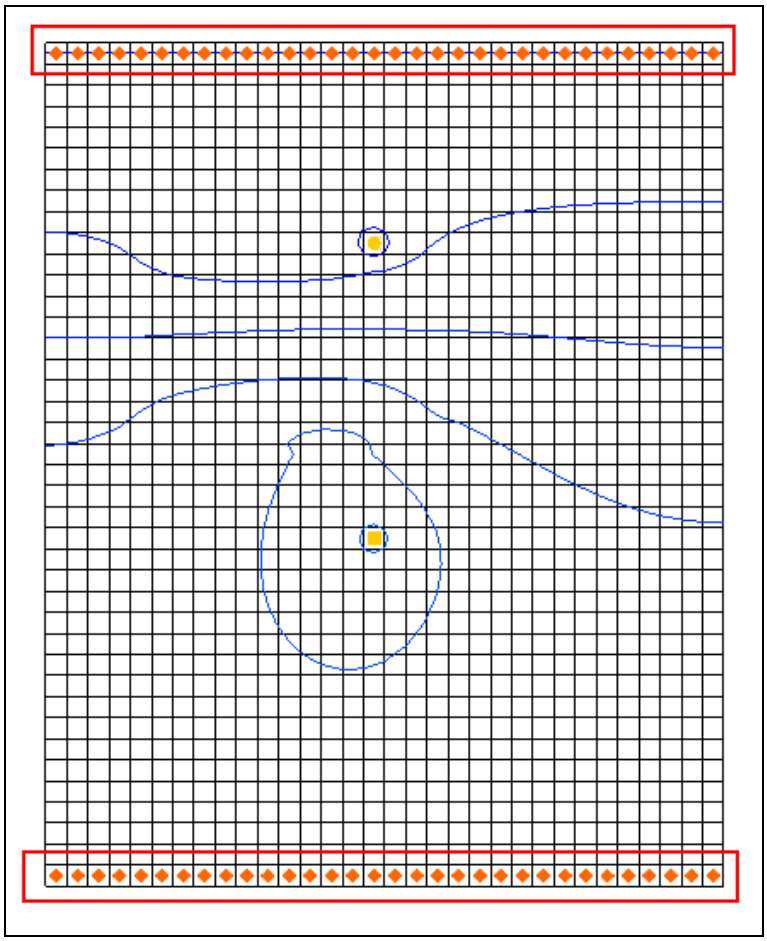

*Figure 2 Selecting cells on the model boundary*

12. Right-click on the selected cells and select the *Sources/Sinks* menu command to open the *MODFLOW/MT3DMS Sources/Sinks* dialog.

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

14. Now click the **Add BC** button near the bottom of the dialog.

15. In the *All* row, enter a concentration of "278" ($5^{o}$ C) in the *WarmWater* column. This will apply this concentration to all of the BCs.

16. Select the **OK** button.

17. Click outside the grid to unselect the cell.

## 6.7 Saving the Simulation and Running MT3DMS

Now save the simulation and run MT3DMS.

1. Select the *File* | **Save As** command.
2. Enter "heat" for the file name.
3. Select the **Save** button.
4. Select the *MODFLOW* | **Run MODFLOW** command.
5. Click **Close**.
6. Select the *MT3DMS* | **Run MT3DMS** command.
7. Select **Yes** at the prompt to save the changes.
8. When the simulation is finished, select the **Close** button.

## 6.8 Changing the Contouring Options

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

1. Click on the **Contour Options** button to open the *Dataset Contour Options – 3D Grid – WarmWater* dialog.
2. Change the *Contour method* to "Color Fill**."**
3. Turn on *Fill Continuous color range* in the *Contour interval* section of the dialog.
4. Select the **OK** button.

The user may wish to select the "WarmWater" dataset in the Project Explorer and select various time steps to see how the temperature changes over time. After looking at the "WarmWater" dataset in the Project Explorer, the user will notice that there is a "WarmWater(Sorbed)" dataset as well. This may be useful to look at after running the simulation.

## 6.9 Setting Up an Animation

Now the user will observe how the solution changes over the one-year simulation by generating an animation. To set up the animation, do the following:

1. Select the *Display* | **Animate** command to open the *Animation Wizard*.
2. Make sure the *Data set* option is on.
3. Click **Next**.

4. Make sure the *Display clock* option is on.

5. Select the **Finish** button.

The user 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. The user may wish to experiment with some of the other playback controls. When finished, close the window and return to GMS.

# 7 Conclusion

This concludes the "MT3DMS – Heat Transport" tutorial. Here are the key concepts in this tutorial:

- It is possible to perform a heat transport analysis using MT3DMS in GMS.
- The important inputs in a heat transport simulation are $K_d^T$ and $D_m^T$.
- $K_d^T$ is the distribution coefficient (slope of the isotherm), which can be specified in the Chemical Reaction Package.
- $D_m^T$ is the molecular diffusion coefficient (DMCOEF), which can be specified in the Dispersion Package.

# 8 Notes

1. Thorne, D., Langevin, C. D., & Sukop, M. C. (2006). Addition of simultaneous heat and solute transport and variable fluid viscosity to SEAWAT. *Computers & geosciences*, *32*(10), 1758-1768.

2. Hecht-Méndez, J., Molina-Giraldo, N., Blum, P. and Bayer, P. (2010), Evaluating MT3DMS for Heat Transport Simulation of Closed Geothermal Systems. *Ground Water*, 48: 741–756. doi: 10.1111/j.1745-6584.2010.00678.x

3. Langevin, C. D., Dausman, A. M. and Sukop, M. C. (2010), Solute and Heat Transport Model of the Henry and Hilleke Laboratory Experiment. *Ground Water*, 48: 757–770. doi: 10.1111/j.1745-6584.2009.00596.x

 