*GMS 10.0 Tutorial*
# SEAWAT – Thermal Effects
Examine Thermal Effects on a SEAWAT Model



Effects of Boundary Heat Conduction on Temperature
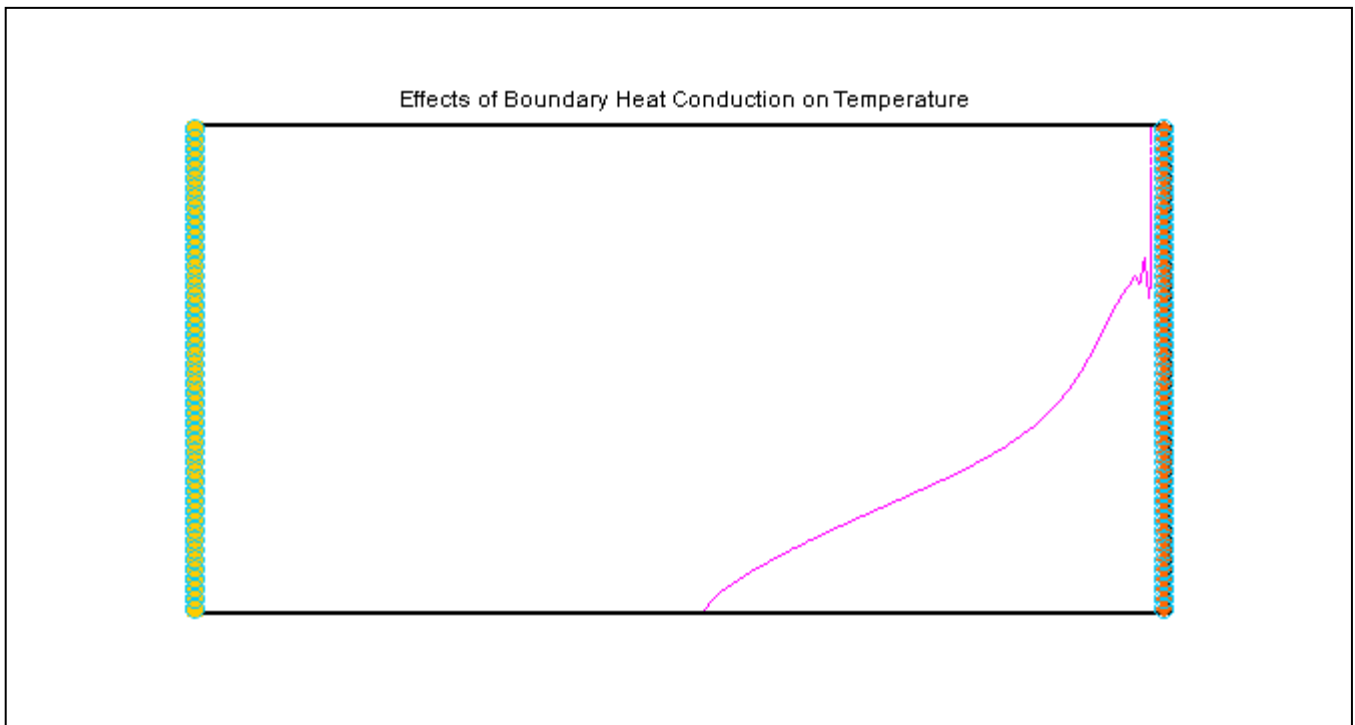
## Objectives
Learn how to simulate thermal effects in SEAWAT.

## Prerequisite Tutorials
- SEAWAT- Concentration and Temperature Effects

## Required Components
- Grid Module
- MODFLOW
- MT3D
- SEAWAT

## Time
- 30-45 minutes

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# 1    Introduction

This tutorial describes how to simulate heat conduction, thermal equilibrium, and boundary heat conduction using SEAWAT.

## 1.1    Outline

Here are the steps to this tutorial:

1. Importing an existing MODFLOW/MT3D simulation

2. Run SEAWAT with different scenarios.

3. Examine the results.

# 2    Description of Problem

The problem is shown in Figure 1; this is a confined aquifer with an initial temperature of $5^{o}$C. Warm freshwater is injected from the west side of the model at a 1 $m^3$/day. The initial concentration of salt in the model is 35 kg/$m^3$.

The user will look at the effect of heat conduction, thermal equilibrium with a solid, and boundary heat conduction in this example. This example problem is very similar to the problem described in the SEAWAT documentation.[1]

1. Langevin, C.D., Thorne, D.T., Jr., Dausman, A.M., Sukop, M.C., and Guo, W. (2007). SEAWAT Version 4: A Computer Program for Simulation of Multi-Species Solute and Heat Transport: U.S. Geological Survey Techniques and Methods Book 6, Chapter A22, 39 p.
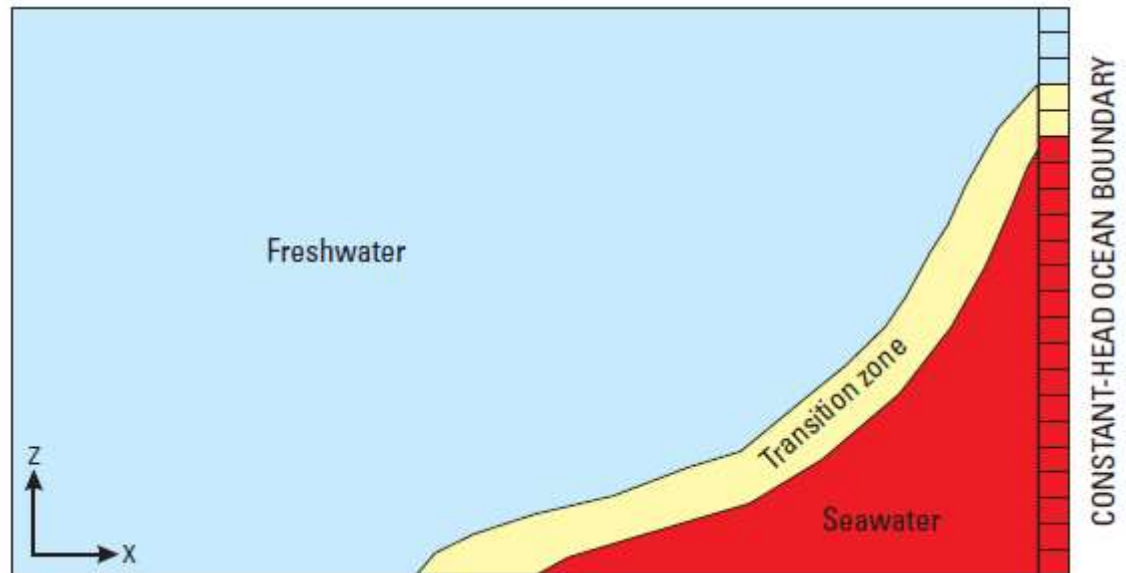
*Figure 1*          Site to be modeled with SEAWAT

# 3      Getting Started

Do the following to get started:

1.  If GMS is not running, launch GMS.

2.  If GMS is already running, select the *File* | **New** command to ensure the program settings are restored to the default state.

# 4      Importing the Existing Model

The user will start with a model that has already been created.

1.  Select the **Open** button (or the *File* / **Open** menu command).

2.  Browse to the *\Tutorials\SEAWAT\Case_Studies\Sample\Case2* folder.

3.  Select the "case2.gpr" file.

4.  Click **Open**.

This imports the model.

# 5      Saving the model with a new name

Now it is possible to start making changes. First, save the model with a new name.

1.  Select the *File* / **Save As** menu command.

2.  Browse to the *\Tutorials\SEAWAT\Case_Studies* folder.

3. Change the project name to "case3."

4. Save the project by clicking the **Save** button.

# 6     Heat Conduction

The existing model simulates the effect of concentration and temperature on fluid density. The user will modify this model to simulate heat conduction.

Heat conduction is included in the simulation by specifying a value for bulk thermal diffusivity ($D_{m\_temp}$). $D_{m\_temp}$ is calculated using the following formula:

$$D_{m\_temp} = \frac{k_{Tbulk}}{\theta \rho c_{Pfluid}} \tag{1}$$

Where $\theta$ is the porosity. $\rho$ is the reference fluid density. $c_{Pfluid}$ is the specific heat capacity of the reference fluid. $k_{Tbulk}$ is the bulk thermal conductivity from solid ($k_{Tsolid}$) and fluid ($k_{Tfluid}$) thermal conductivities. $k_{Tbulk}$ can be estimated using the following equation:

$$k_{Tbulk} = \theta k_{Tfluid} + (1-\theta)k_{Tsolid} \tag{2}$$

The bulk thermal conductivity for a solid (calcite) is $3.59^{[1]}$ (W/[m °K]). The bulk thermal conductivity for a fluid (freshwater) is $0.58^{[1]}$ (W/[m °K]). The porosity in this model is 0.3. Using equation (2), $k_{Tbulk}$ is estimated to be around 2.69 (W/[m °K]).

The specific heat capacity of freshwater ($c_{Pfluid}$) is about 4186 (J/kg °K). Freshwater density is about 1000 (kg/m$^3$). Using equation (1), the bulk thermal diffusivity ($D_{m\_temp}$) is estimated to be around 0.185 m$^2$/day (2.14 x 10$^{-6}$ m$^2$/s).

## 6.1     Editing the Dispersion Package

The bulk thermal diffusivity ($D_{m\_temp}$) can be specified within the Dispersion Package (DSP input file).

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

1. Turn on the *Specify DMCOEF for each species* option.

2. Click on the first button in the *DMCOEF - Temperature* column of the spreadsheet. This will open the *DMCOEF – Effective Molecular Diffusion Coefficient* dialog.

3.  Select **Constant → Grid** command to open the *Grid Value* dialog.

4.  Enter "0.185."

5.  Click **OK**.

6.  Click **OK** to exit the *DMCOEF – Effective Molecular Diffusion Coefficient* dialog.

The bulk thermal diffusivity of 0.185 has been assigned to all the cells in the model. The user will also need to assign the DMCOEF for Salt.

1.  Click on the first button in the *DMCOEF - Salt* column in the spreadsheet. This will open the *DMCOEF – Effective Molecular Diffusion Coefficient* dialog.

2.  Select **Constant → Grid** command to open the *Grid Value* dialog.

3.  Enter "1e-10."

4.  Click **OK**.

5.  Click **OK** to exit the *DMCOEF – Effective Molecular Diffusion Coefficient* dialog.

6.  Click the **OK** button to exit the *Dispersion Package*.

# 7    Saving and running SEAWAT

Now save the changes and run SEAWAT.

1.  Select the **Save** 🖫 button to save the project

2.  Select the *SEAWAT* / **Run SEAWAT** command.

3.  When SEAWAT finishes, select the **Close** button.

# 8    Viewing the Solution

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

1.  Expand the "3D Grid Data" folder and the "grid" item.

2.  Select the "Salt" 📧 dataset below the "case3 (MT3DMS)" 📩 solution in the Project Explorer.

3.  Change the time step to 4000.0 in the time step window.

4.  Select the "Temperature" 📧 dataset below the "case3 (MT3DMS)" 📩 solution in the Project Explorer.

The salinity and temperature fields no longer have the same shape. The temperature field is much more diffuse than the salinity field. The user will also notice that the contouring options change when selecting either the "Salt" or "Temperature" datasets. This happens because Display Themes are being used. Another GMS tutorial explains Display Themes.

# 9    Saving the model with a new name

Now it's time to start a new scenario. First, save the model with a new name.

1.  Select the *File* / **Save As** menu command.

2.  Change the project name to "case4."

3.  Save the project by clicking the **Save** button.

# 10   Thermal Equilibrium

In this scenario, the user will simulate the thermal equilibrium effect between the fluid (freshwater) and the solid (calcite). This effect can be simulated using the MT3DMS Reactions (RCT) Package.

## 10.1   Enabling the Chemical Reaction Package

The user needs to enable the Chemical Reaction 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*.

4.  Select the **OK** button to exit the *MT3D/RT3D Packages* dialog.

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

## 10.2   Editing the Chemical Reaction Package

The thermal equilibrium effect is activated only for the *Temperature* species by entering $1.7 \times 10^{-4}$ [$m^3$/kg] for $K_{d\_temp}$ (Distribution Coefficient – slope of the isotherm).

1.  Select the *MT3DMS* / **Chemical Reaction Package** command to open the *Chemical Reaction Package* dialog.

2.  Change the *Sorption* option to "Linear isotherm."

3.  Change the *Variable Input* to *Cell by cell*.

4.  Select the **Edit** button for *Bulk Density* to open the *Bulk Density Array* dialog.

5.  Select the **Constant → Grid** button to open the *Grid Value* dialog.

6.  Enter value of "1760. "

7.  Click **OK**.

8.  Click **OK** to exit the *Bulk Density Array* dialog.

This set the *Bulk density* to 1760. Note that these units actually represent [kg/$m^3$]. These units do 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.  Select the **Edit** button for *Temperature* for the *$1^{st}$ sorption const* to open the *First Sorption Constant Array* dialog.

10. Select the **Constant → Grid** button to open the *Grid Value* dialog.

11. Enter value of "0.00017."

12. Click **OK**.

13. Click **OK** to exit the *First Sorption Constant Array* dialog.

This set the *1st sorption constant* to 0.00017.  (Actual units = [m$^3$/kg]).

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

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

# 11    Saving and running SEAWAT

Now it is possible to run SEAWAT.

1. Select the *SEAWAT* / **Run SEAWAT** command.

2. Select **Yes** at the prompt to save the changes.

3. When SEAWAT finishes, select the **Close** button.

# 12    Viewing the Solution

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

1. Select the "Temperature" 🖽 dataset below the "case4 (MT3DMS)" 🗂 solution in the Project Explorer.

2. Change the time step to 4000.0 in the time step window.

Notice that the temperature front in "case4" is moving about half as fast as the temperature in "case3." The figure below shows a comparison of the models.
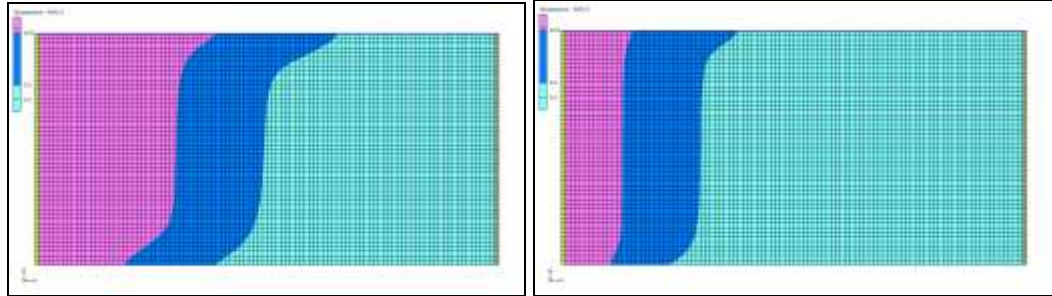
*Figure 2 Comparison of case3 and case4 temperature fields*

3.  Switch back and forth between the "Temperature" 🔲 dataset in "case4 (MT3DMS)" 🔳 and "case3 (MT3DMS)" 🔳.

# 13 Saving the model with a new name

Next, the user will start making changes for another modeling scenario. First, save the model with a new name.

1.  Select the *File* / **Save As** menu command.

2.  Change the project name to "case5."

3.  Save the project by clicking the **Save** button.

# 14 Boundary Heat Conduction

Now, the user will look at the effect of boundary heat conduction in this case. Heat conduction at a seawater boundary is simulated using the MT3DMS constant concentration boundary condition (ITYPE = -1). This boundary condition allows advective and dispersive transport across the boundary. Without a dispersive flux, there is no heat conduction. The constant-head boundary (ITYPE = 1) does not allow dispersive transport to occur.

## 14.1 Modifying the Boundary Conditions

The user will change the boundary condition of all the cells on the east side of the model.

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

2.  Select all the cells on the east side of the model (Figure 2). The user can do this by dragging a box around the cells as shown below.
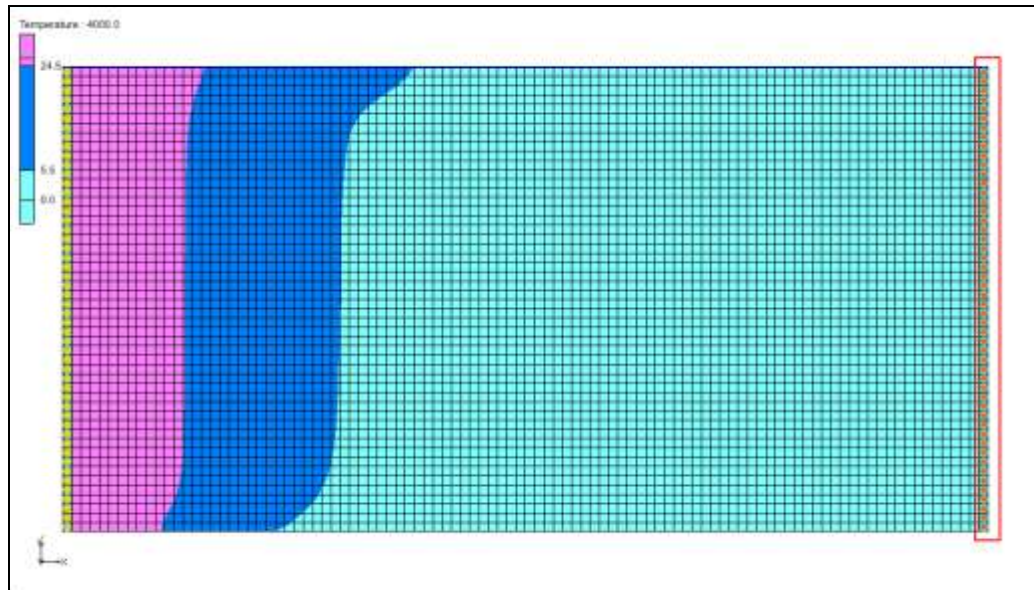
*Figure 3      Selecting cells on the east side of the model*

3.  Select the *MT3DMS* / **Point Sources/Sinks** command to open the *MODFLOW/MT3DMS Sources/Sinks* dialog.

First the user will adjust the constant head boundary condition.

4.  Enter "0.0" for the concentration of *Temperature* in the *All* row.

Now add new boundary conditions.

5.  Select **Add BC** command.

Note that GMS generates 50 more rows corresponding to 50 cells selected on the east side of the model. The user needs to change the Type (ITYPE) for the new BCs to constant concentration (ITYPE = -1). If the user scrolls down the spreadsheet, he or she can see where the new boundary conditions were created because the concentration of *Salt* is 0.0.

6.  Change the *Type (ITYPE)* to "constant concentration" for all the new BCs.

7.  Enter "-1.0" for *Salt* with *constant concentration* Type.

By entering -1, the user inactivates Salt for the *constant concentration* Type.

8.  Enter "5.0" for *Temperature* with *constant concentration* Type.

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

The user has successfully set up the heat boundary condition for the model.


## 15    Saving and running SEAWAT

Now save the changes and run SEAWAT.

1.  Select the **Save** 💾 button to save the project

2.  Select the *SEAWAT* / **Run SEAWAT** command.

3.  When SEAWAT finishes, select the **Close** button.

## 16      Viewing the Solution

The user will now view the results of the SEAWAT model run. The user will compare the differences between two scenarios.

1.  Select the "Temperature" ⊞ dataset below the "case5 (MT3DMS)" 🔒 solution in the Project Explorer.

2.  In time step window, select the last time step.

3.  Expand the "Display Themes" folder.

4.  Select the "Temperature_24" 📝 display theme.

Notice the boundary heat conduction has some effect on the temperature near the vertical ocean boundary (Figure 3). In this example, the boundary heat conduction only affects the simulated salinity slightly.
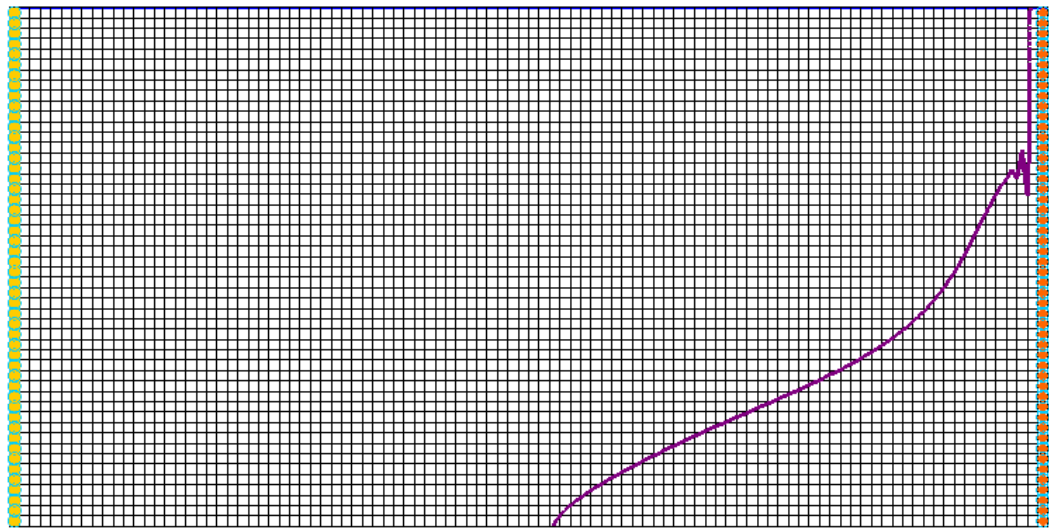


*Figure 4       Boundary heat conduction effect*

## 17      Conclusion

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

- SEAWAT combines MODFLOW and MT3DMS to solve variable density groundwater flow and solute transport problems.

- SEAWAT can simulate heat conduction.

- SEAWAT can simulate thermal equilibrium between a solid (aquifer) and a fluid.

- SEAWAT can simulate boundary heat conduction.