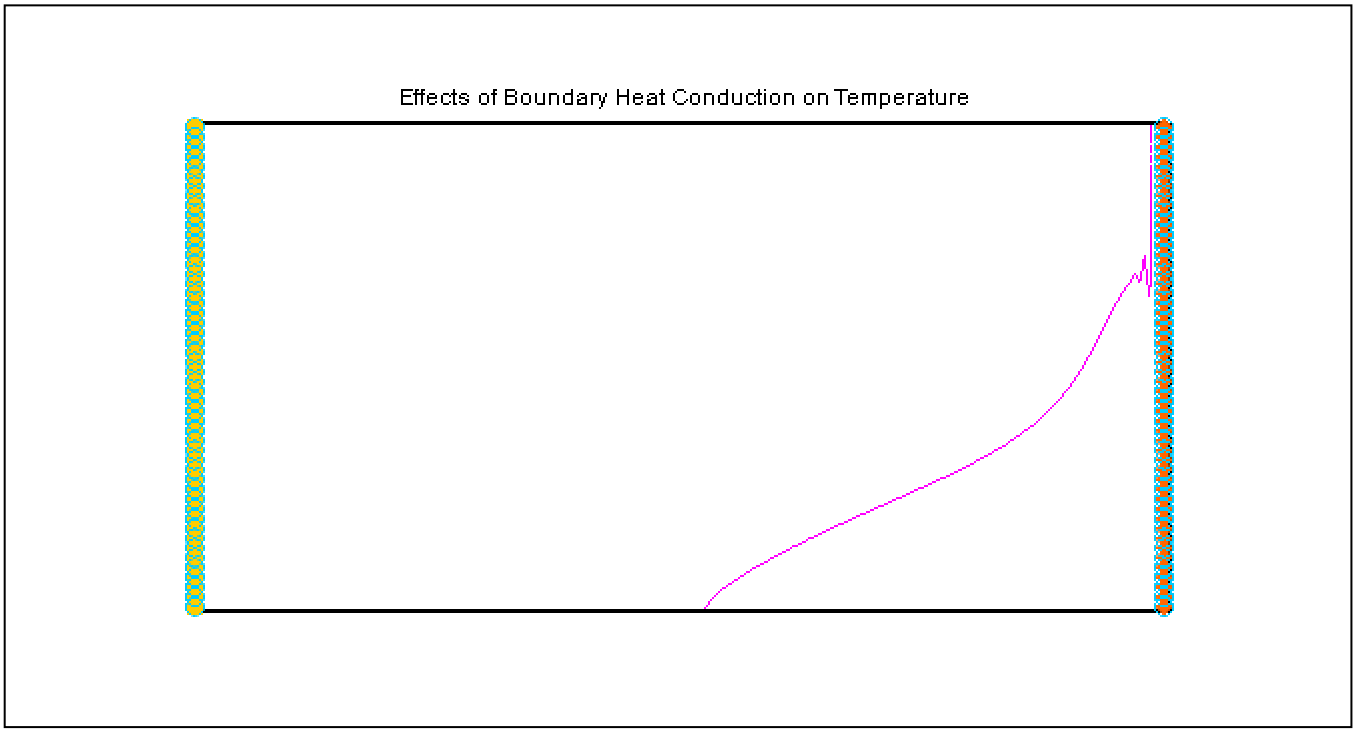
v. 9.2

GMS 9.2 Tutorial

SEAWAT – Thermal Effects

Examine Thermal Effects on a SEAWAT Model



Objectives

Learn how to simulate thermal effects in SEAWAT.

Prerequisite Tutorials

- SEAWAT- Concentration and Temperature Effects

Required Components

- Grid
- MODFLOW
- MT3D
- SEAWAT

Time

- 30-60 minutes

1 Contents

2 Introduction

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

2.1 Outline

This is what you will do:

1. Importing an existing MODFLOW/MT3D simulation
2. Run SEAWAT with different scenarios.
3. Examine the results.

3 Description of Problem

Our 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.

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

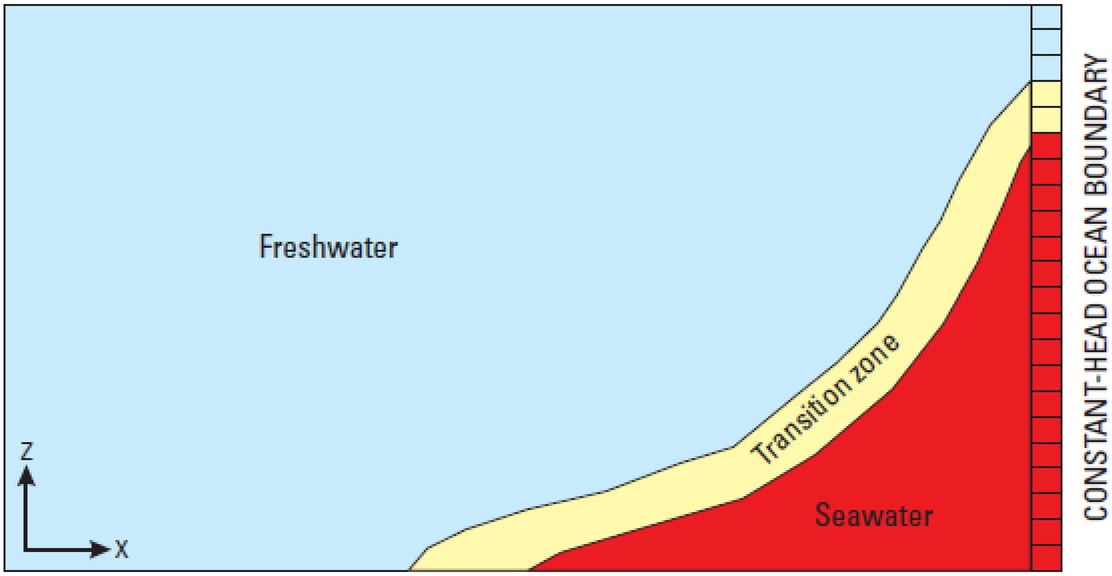


Figure 1. Site to be modeled with SEAWAT.

4 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.

5 Importing the Existing Model

We 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 and click *Open*.

This imports the model.

6 Saving the model with a new name

We're ready to start making changes. Let's 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.

7 Heat Conduction

The existing model simulates the effect of concentration and temperature on fluid density. We 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:

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

Where θ is the porosity. ρ 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:

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

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

The specific heat capacity of freshwater (c_{Pfluid}) is about 4186 (J/kg ^{o}K). Freshwater density is about 1000 (kg/m^3). Using the 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).

7.1 Editing the Dispersion Package

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

1. Select the *MT3D | Dispersion Package* command.
1. Turn on the *Specify DMCOEF for each species* option.
2. Click on the first button in the *DMCOEF - Temperature* column of the spread sheet.
3. Select *Constant -> Grid* command.
4. Enter **0.185**.
5. Click the *OK* button twice to exit the dialog.

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

6. Click on the first button in the *DMCOEF - Salt* column in the spread sheet .
7. Select *Constant -> Grid* command.
8. Enter **1e-10**.
9. Click the *OK* button twice to exit the dialog.
10. Click the *OK* button to exit the *Dispersion Package*.

8 Saving and running SEAWAT

We are ready to save our 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.

9 Viewing the Solution

We will now view the results of the SEAWAT model run.

1. Select the **Salt** data set below the **case3 (MT3DMS)** solution in the *Project Explorer*.
2. Change the time step to **4000.0** in the time step window.
3. Select the **Temperature** data set 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. You will also notice that the contouring options change when you select either **Salt** or **Temperature**. This happens because we are using Display Themes. There is another GMS tutorial that explains Display Themes.

10 Saving the model with a new name

We're ready to start a new scenario. Let's 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.

11 Thermal Equilibrium

In this scenario, we 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.

11.1 Enable the Chemical Reaction Package

We need to enable the Chemical Reaction Package

1. Select the *MT3D | Basic Transport Package* command.
2. Select the *Packages* button.
3. Turn on the *Chemical Reaction Package*.
4. Select the *OK* button twice to exit the *Basic Transport Package* dialog.

11.2 Adding Sorption

This effect is activated only for the **Temperature** species by entering $1.7\text{x}10^{-4}$ [m^3/kg] for K_{d_temp} (Distribution Coefficient – slope of the isotherm).

1. Select the *MT3D | Chemical Reaction Package* command.
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.*
5. Select the *Constant->Grid* button.
6. Enter value of **1760**.
7. Click the *OK* button twice to exit the 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.

8. Select the *Edit* button for *Temperature* with *1st sorption const.*
9. Select the *Constant->Grid* button.
10. Enter value of **.00017**.
11. Click the *OK* button twice to exit the dialog.

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

12. Click the *OK* button to exit the 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

ρ = bulk density

K_d = distribution coefficient (slope of the isotherm)

n = porosity

12 Saving and running SEAWAT

We are ready to run SEAWAT.

1. Select the *SEAWAT | Run SEAWAT* command.
2. Select *Yes* at the prompt to save your changes.
3. When SEAWAT finishes select the *Close* button.

13 Viewing the Solution

We will now view the results of the SEAWAT model run.

1. Select the **Temperature** data set 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.

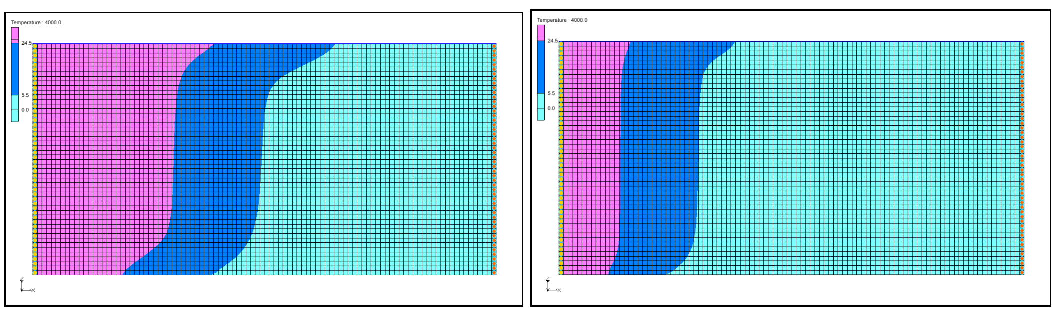


*Figure 2 Comparison of **case3** and **case4** Temperature Fields*

3. Switch back and forth between the **Temperature** data set in **case4 (MT3DMS)** and **case3 (MT3DMS)**.

14 Saving the model with a new name

We're ready to start making changes for another modeling scenario. Let's 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.

15 Boundary Heat Conduction

Now, we 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.

15.1 Modifying the Boundary Conditions

We 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). You can do this by dragging a box around the cells as shown below.

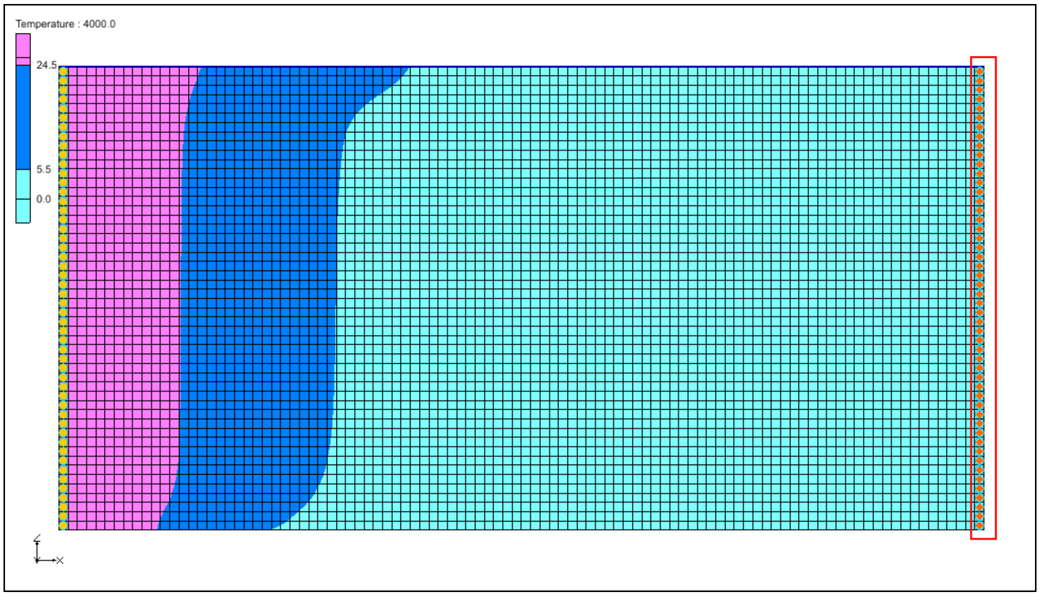


Figure 3 Selecting cells on the east side of the model

3. Select the *MT3D* | *Point Sources/Sinks* command.

First we will adjust the constant head boundary condition.

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

Now we will 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. We need to change the Type (ITYPE) for the new BCs to constant concentration (ITYPE = -1). If you scroll down the spreadsheet you 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, we inactivate 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.

We have successfully set up the heat boundary condition for our model.

16 Saving and running SEAWAT

We are ready to save our 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.

17 Viewing the Solution

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

1. Select the **Temperature** data set below the **case5 (MT3DMS)** solution in the *Project Explorer*.
2. In time step window, select the last time step.
3. 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

18 Conclusion

This concludes the tutorial. Here are the things that you should have learned 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 solid (aquifer) and fluid.
- SEAWAT can simulate boundary heat conduction.

19 Notes

4. Langevin, C.D., Thorne, D.T., Jr., Dausman, A.M., Sukop, M.C., and Guo, Weixing, 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.

