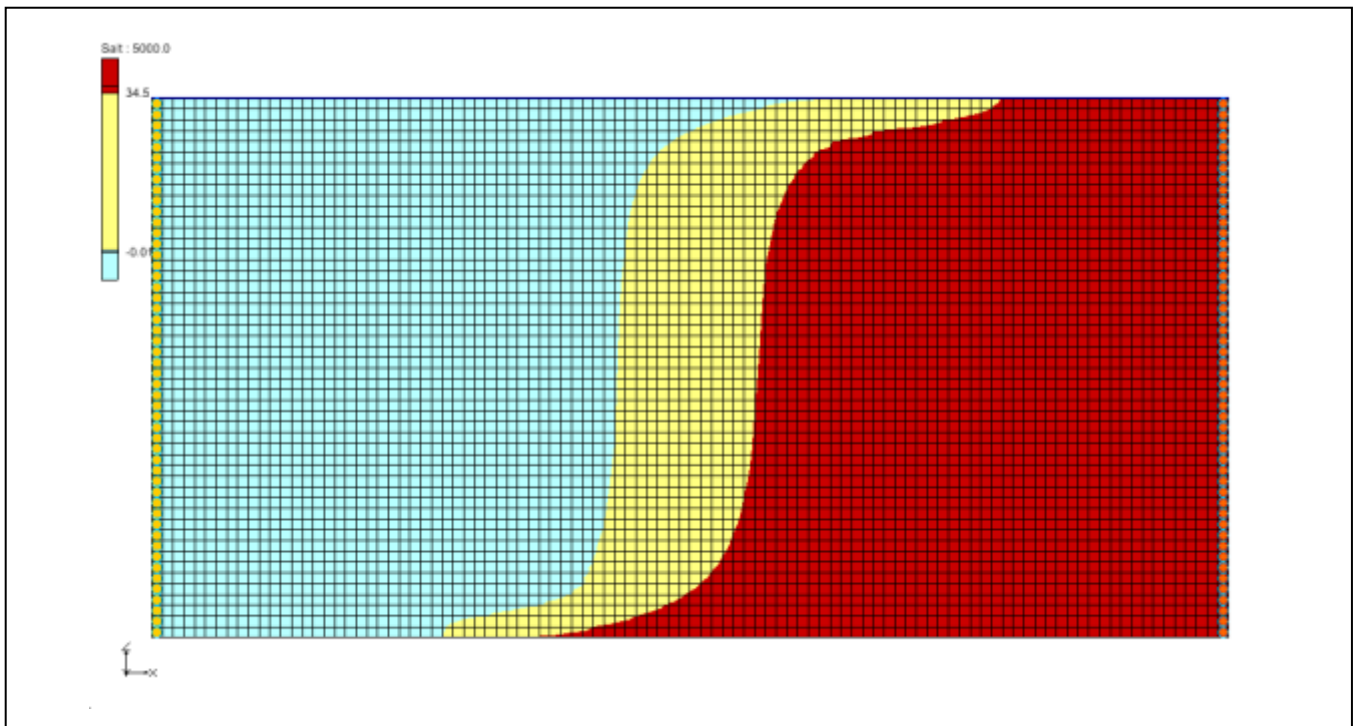


GMS 10.0 Tutorial

SEAWAT – Concentration and Temperature Effects

Examine Concentration and Temperature Impacts on Fluid Density with SEAWAT



Objectives

Learn how to simulate the effects of concentration and temperature on fluid density with SEAWAT.

Prerequisite Tutorials

- MODFLOW – Grid Approach
- MT3DMS – Grid Approach

Required Components

- Grid Module
- MODFLOW
- MT3D
- SEAWAT

Time

- 15-25 minutes



1	Introduction	2
1.1	Outline.....	2
2	Description of Problem	2
3	Getting Started	3
4	Importing the Existing Model	3
5	Initializing the SEAWAT Simulation	4
5.1	Modifying the VDF Package.....	4
6	Saving the Model with a New Name and Running SEAWAT	6
7	Viewing the Solution	6
8	Saving the model with a new name	7
9	Adding Temperature Effects on Fluid Density	7
9.1	Modifying the VDF Package.....	7
10	Saving and running SEAWAT	8
11	Viewing the Solution	8
12	Conclusion	9

1 Introduction

This tutorial describes how to simulate the affects of concentration and/or temperature on fluid density using SEAWAT.

1.1 Outline

Here are the steps for this tutorial:

1. Import an existing MODFLOW/MT3D simulation.
2. Set up a SEAWAT simulation.
3. Run SEAWAT with different scenarios.
4. Compare SEAWAT results for density effects caused by concentration and temperature.

2 Description of Problem

The problem is shown in Figure 1; this is a confined aquifer with an initial temperature of 5°C. Warm freshwater is injected from the west side of the model at a 1 m³/day. The initial concentration of salt in the model is 35 kg/m³.

The user will examine the effects of salinity and temperature on density 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.

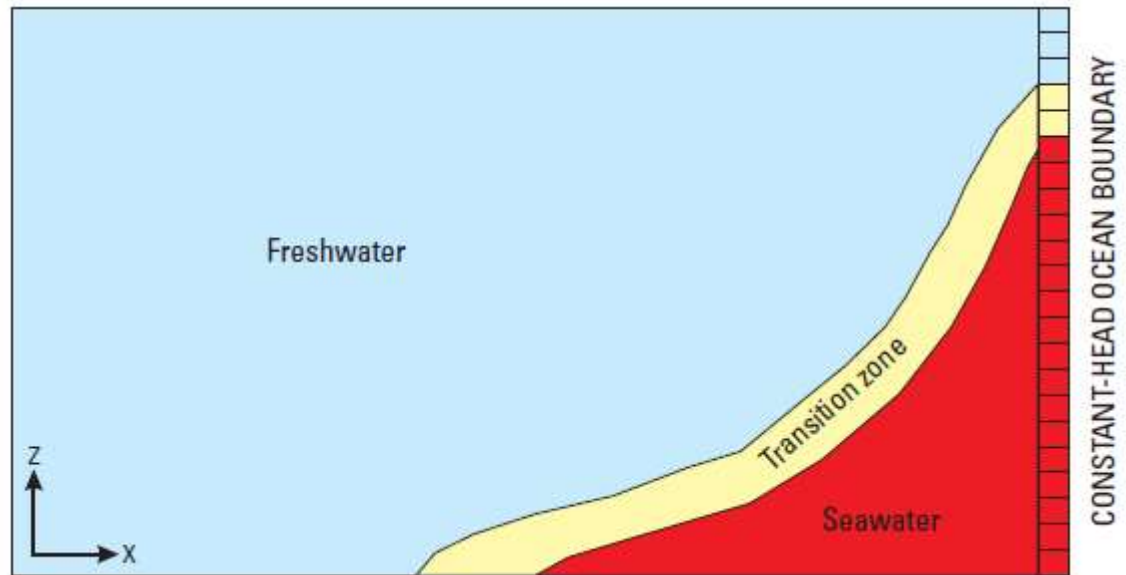


Figure 1 Site to be modeled with SEAWAT


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` folder.
3. Select the “start.gpr” file.
4. Click **Open**.

This imports the model. The user should see a grid with symbols representing well and specified head boundary conditions similar to the figure below.

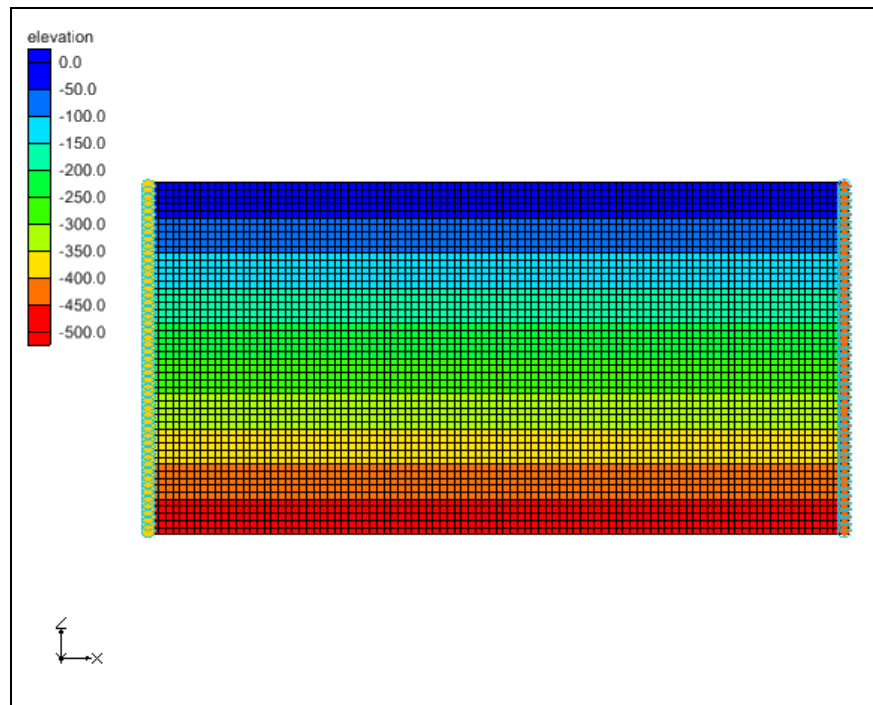




Figure 2 Initial model

5 Initializing the SEAWAT Simulation

SEAWAT uses the combination of MODFLOW and MT3DMS. The user needs to turn on the SEAWAT menu.

1. Expand the “3D Grid Data”  folder.
2. Right-click on the “grid”  item in the Project Explorer.
3. Select the **New SEAWAT** menu command.
4. Turn on *Include transport in simulation* and *Variable-Density Flow (VDF)*.
5. Select the **OK** button to exit the dialog.

5.1 Modifying the VDF Package

For the first scenario, the user will simulate the effect of salinity on the fluid density.

1. Select the *SEAWAT / VDF Package* command to open the *SEAWAT CDF Package* dialog.
2. Enter all the values as given in the following figure:

The screenshot shows the SEAWAT VDF Package dialog box with the following settings:

- Active variable-density water table corrections (IWTABLE)
- Intermodal density calculation (MFNADVFD): Upstream-weighted algorithm (ne. 2)
- Minimum fluid density (DENSEMIN): 0.0 (kg/m³)
- Maximum fluid density (DENSEMAX): 0.0 (kg/m³)
- Length of first transport time step (FIRSTDT): 1.0 (d)
- Flow and transport coupling procedure:
 - Flow/transport coupling (NSWTCP): 0 explicitly coupled
 - Convergence criteria (DNSCRIT): 0.01
- Fluid density calculation:
 - Fluid density calc. (MT3DRHOFLG): 1 Salt
 - Reference fluid density (DENSEREF): 1000.0 (kg/m³)
 - Density/conc. slope (DRHODC): 0.7
 - Density/press. slope (DRHODPRHD): 0.0 (kg/m³)/(m)
 - Reference press. head (PRHOREF): 0.0 (m)

At the bottom, there is a table with columns: Species Name, Species ID, DRHODC, and CRHOREF. The table is currently empty.

Buttons: Help..., OK, Cancel.

Figure 3 VDF inputs for first scenario

MT3DRHOFLG, DENSEREF and DRHODC are three important inputs for this scenario. A value of 1 for MT3DRHOFLG indicates that fluid density calculation will be calculated using the “Salt” species. A DENSEREF value of 1000 indicates that the reference fluid density (freshwater in this case) at 25°C is 1000 kg/m³. A DRHODC value of 0.7 indicates that the density will vary linearly between 1000 kg/m³ for freshwater and 1024.5 kg/m³ for saltwater.

DRHODC can be estimated by dividing the density difference by the concentration difference. In this case, the result is the following:

$$\frac{1024.5(\text{kg/m}^3) - 1000(\text{kg/m}^3)}{35(\text{kg/m}^3) - 0(\text{kg/m}^3)} = 0.7$$

So 35 kg/m³ is the concentration of salt in saltwater; furthermore, 0 kg/m³ is the concentration of salt in freshwater.

3. Select the **OK** button.



6 Saving the Model with a New Name and Running SEAWAT

Now save the changes and run SEAWAT.

1. Select the *File / Save As* menu command.
2. Change the project name to “case1.”
3. Save the project by clicking the **Save** button.
4. Select the *SEAWAT / Run SEAWAT* command.
5. When SEAWAT finishes, select the **Close** button.

7 Viewing the Solution

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

1. Select the “Salt”  dataset below the “case1 (MT3DMS)”  solution in the Project Explorer.

The contour options will change because a display theme has been associated with the “Salt” species. To learn more about display themes see the Display Themes tutorial.

2. Select different time steps in the time step window.

Notice the movement of the freshwater. Select time step 5000.0; the user should see something similar to the figure below.

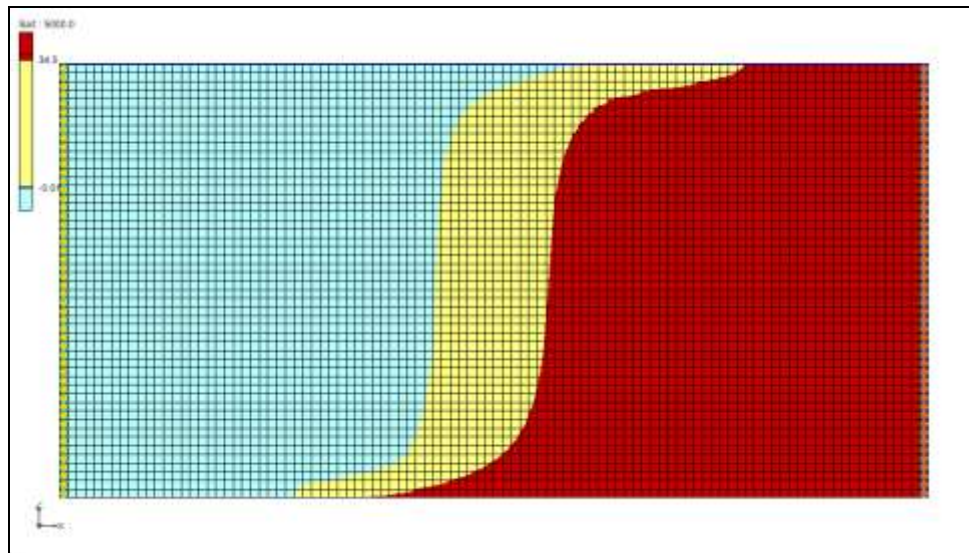



Figure 4 Concentration of salt species at 5000 days

8 Saving the model with a new name

This simulation also included a “temperature” species. The “Temperature”  dataset has no effect on the salinity in this scenario. The effect of temperature on the model is examined in the next scenario.

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

1. Select the *File* / **Save As** menu command.
2. Change the project name to “case2.”
3. Save the project by clicking the **Save** button.

9 Adding Temperature Effects on Fluid Density


The user will look at the effect of temperature on the density in this case.

9.1 Modifying the VDF Package

The temperature effects can be activated in the VDF Package.

1. Select the *SEAWAT* / **VDF Package** command to open the *SEAWAT VDF Package* dialog.
2. Enter a value of -1 for MT3DRHOFLG.

This value means that the fluid density will be calculated using one or more MT3DMS species. In this case, they are the *Salt* and *Temperature*.

3. Click on  twice to generate two species.
4. In *Species ID* column, enter “1” and “2” for each corresponding row.

Notice that the species names have changed to *Salt* and *Temperature*, respectively.

5. For *Salt*, enter “0.7” for *DRHODC*.
6. For *Salt*, enter “0” for *CRHOREF*.
7. For *Temperature*, enter “-0.375” for *DRHODC*.
8. For *Temperature*, enter “25” for *CRHOREF*.

Notice the *DRHODC* value for *Temperature* is negative. The negative value means that the fluid density decreases as the temperature increases.

CRHOREF is the reference (freshwater) concentration/temperature for the species. The reference concentration of *Salt* in freshwater is 0 and the reference *Temperature* of freshwater is 25.

9. The user’s VDF inputs should be the same as the following figure:

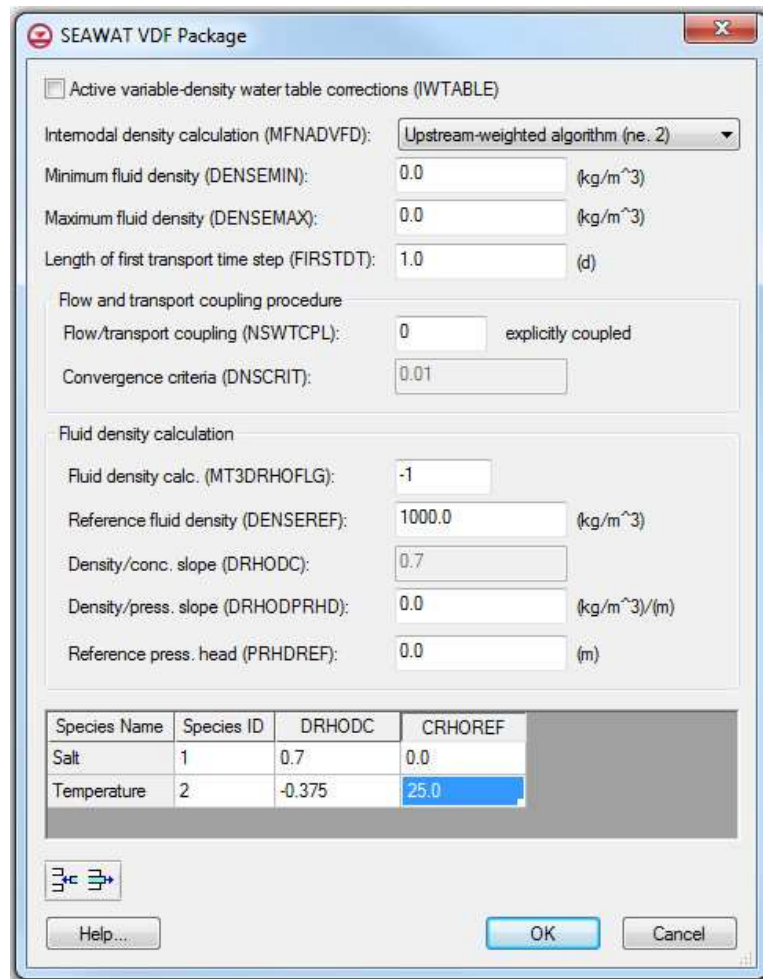



Figure 5 VDF inputs for second scenario.

10. Select **OK** to exit the dialog.




10 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.

11 Viewing the Solution

The user will compare the differences between two scenarios.

1. Switch between the “Salt”  dataset in “case1 (MT3DMS)”  and “case2 (MT3DMS)” . Change the time step to 8000.0 for both datasets and view the differences. The user should see something similar to the figure below.

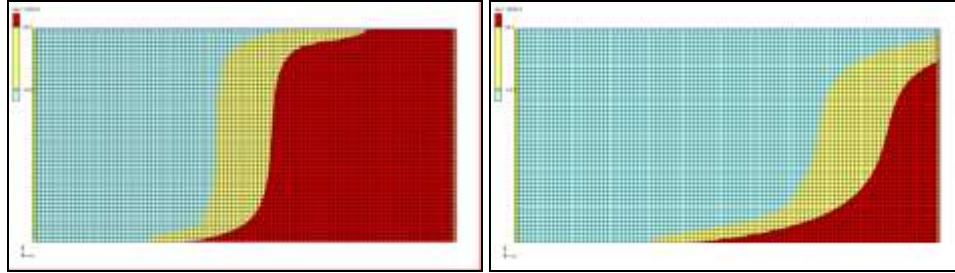


Figure 6 Comparison of salt concentration at time step 8000.0

“Case1” is shown on the left and “case2” is shown on the right. The light blue portion in the figure represents fresh water and the dark red represents salt water. Notice that, in “case2,” the salt water is slightly lower from the top along the left boundary and slightly closer to the right boundary along the bottom of the model. More of the fresh water is “floating” on top of the salt water in “case2” where the fresh water is less dense because SEAWAT is considering temperature in the density calculations.

12 Conclusion

This concludes the “SEAWAT – Concentration and Temperature Effects” 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 simulates the effect of concentration and temperature on fluid density.