Exercises

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Exercise 1. Introduction to Groundwater Vistas

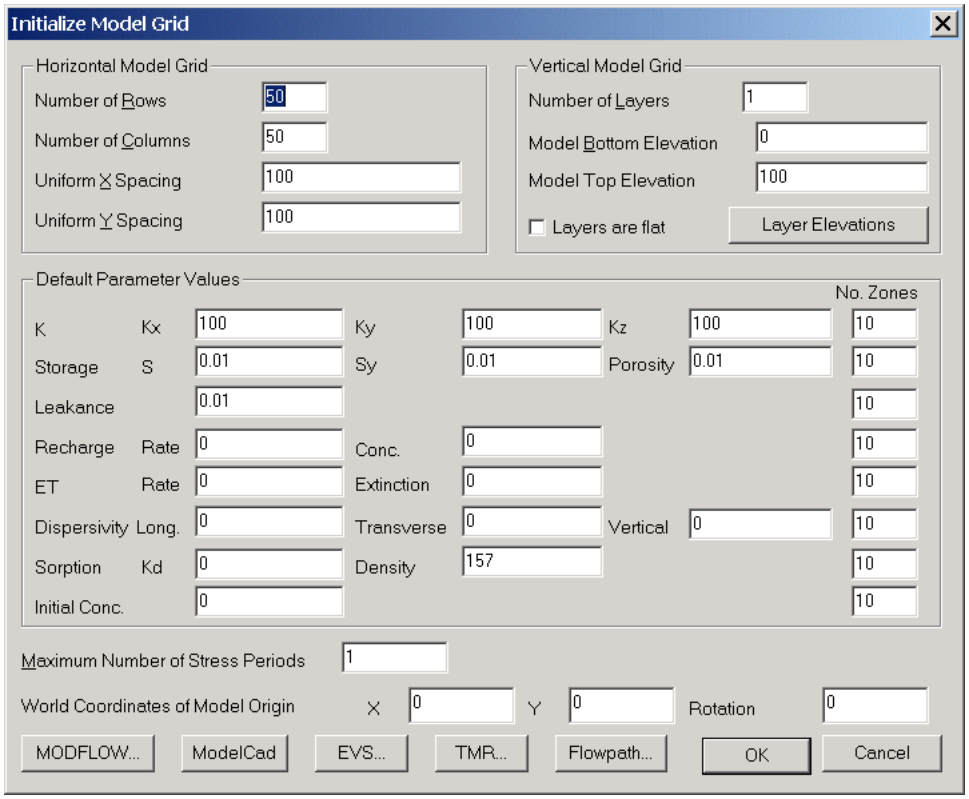
Exercise Description

Groundwater Vistas is a powerful pre- and post-processor for several of the commonly used modeling programs, such as MODFLOW and MT3DMS. The purpose of this exercise is to introduce some of the basics for using the Groundwater Vistas software. Vistas will be used for this course to develop input datasets for MODFLOW, MT3DMS, and SEAWAT, and to post-process model results. Those familiar with Groundwater Vistas may either skip this exercise, or help someone unfamiliar with Vistas learn the basics.

Part I. Getting Started

1. Start Groundwater Vistas

2. Click **File>New** and you should see the following window



Model development will be much easier if you enter correct information for these parameters, particularly the model grid information.

3. For this simple exercise, create a model that has **100 columns** and **100 rows**. Use **uniform x** and **y** spacing of **50** meters.

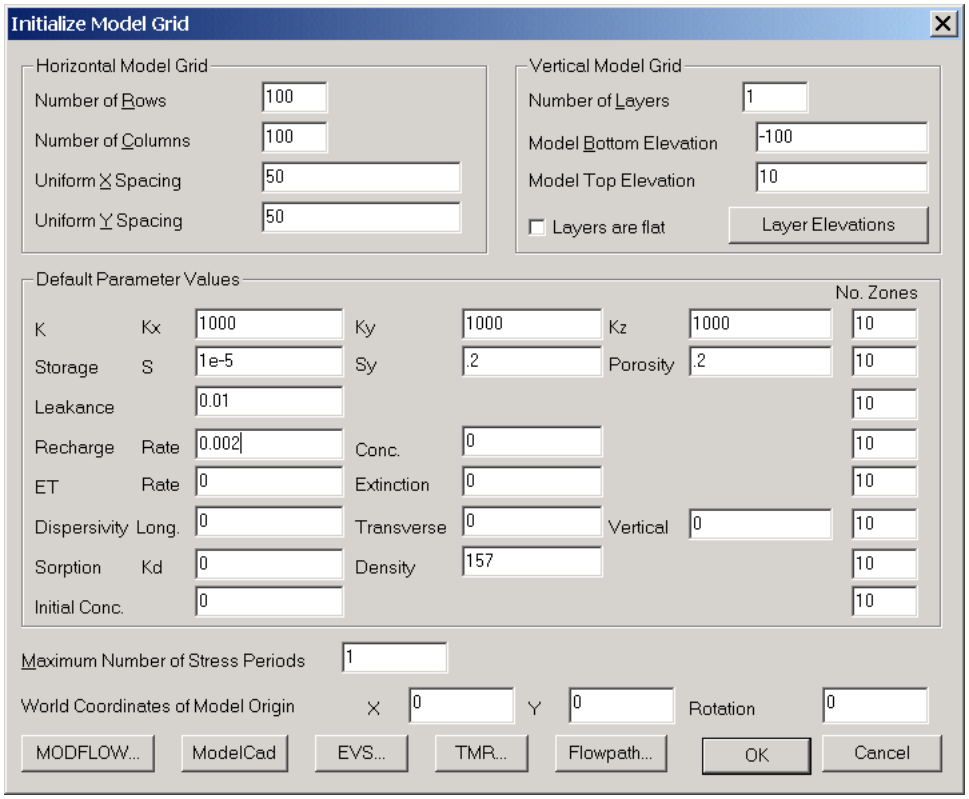
4. For the **vertical grid** information, leave the **number of layers** as **1** and assign a **bottom elevation** of **–100** and a **top elevation** of **10**.

5. Assign a **hydraulic conductivity** value of **1000 m/day** for **Kx, Ky,** and **Kz**.

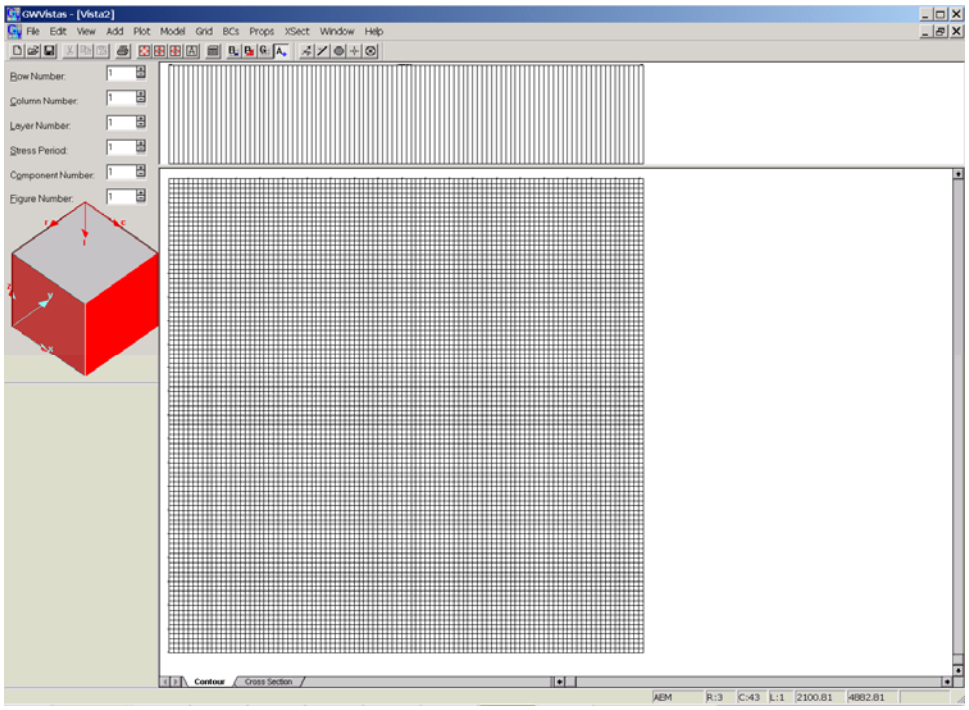
6. Assign values of **1e-5, 0.2,** and **0.2** for **S, Sy**, and **porosity,** respectively.

7. Assign a **recharge rate** of **0.002 m/d.**

8. After you have entered these values, your window should look like the following:



9. Click **Ok** to generate the model template. You should now see the following



10. There are four areas of the Groundwater Vistas main window: **(1) the menus and toolbar across the top, (2) the locator box on the left, (3) the cross section window beneath the toolbar, and (4) the model grid window.**

11. As with any software, it's always a good idea to save the current file. Click **File>Save as**, and save the Groundwater Vista file to the working subdirectory ex01 in your "exercises" folder for this workshop. In this case, you might want to call the file ***Ex01.gwv.***

Part II. Working with Boundaries

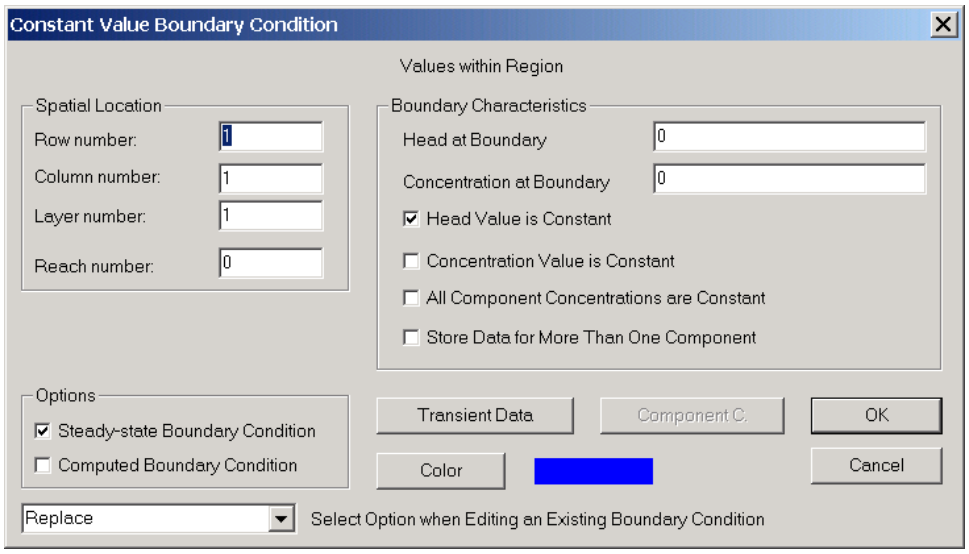
1. Beneath the main menu, there are four buttons labeled **B P G A**. These buttons represent **Boundaries, Properties, Grid**, and **Analytic element.** Whichever one of these buttons is pressed indicates the current editing mode in Vistas. So if we want to work with boundaries, we would press the **B** button.

2. For the sake of this example, lets assume there is an ocean on the east side of this model with an irregularly shaped coastline, and we want to use constant head cells to represent the ocean. Constant head cells can be added by clicking **BCs>Constant head/conc**. Only one boundary type can be edited at a time. The boundary type with the check mark next to it is the current boundary type.

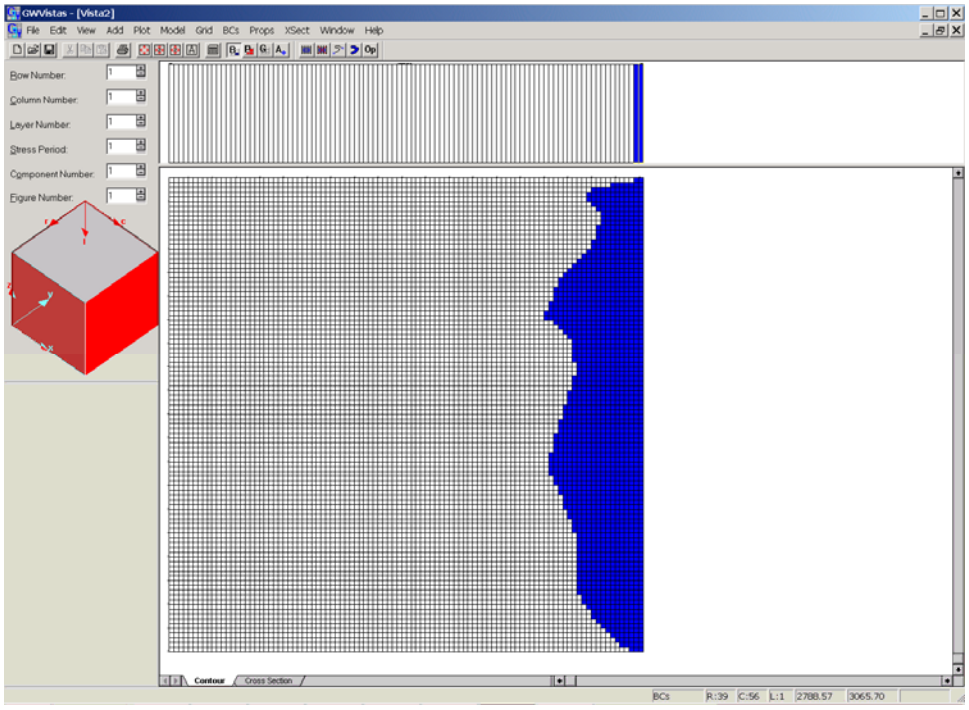
3. To enter a single constant-head boundary, right click on one of the model cells. A window will come up and ask for information about the boundary. To delete this same boundary, right-click again on the same cell.

4. To enter many constant-head boundaries within an irregularly shaped polygon, click on the **polygon tool**, which is located to the left of the **Op** button on the toolbar. With the polygon tool pressed, you can trace a polygon. Double-click when you get to the end of the polygon. Make sure that you do not click outside of the model grid. Once again a window will come up and ask for information about the boundary. In this case, you can accept the default values as shown

below



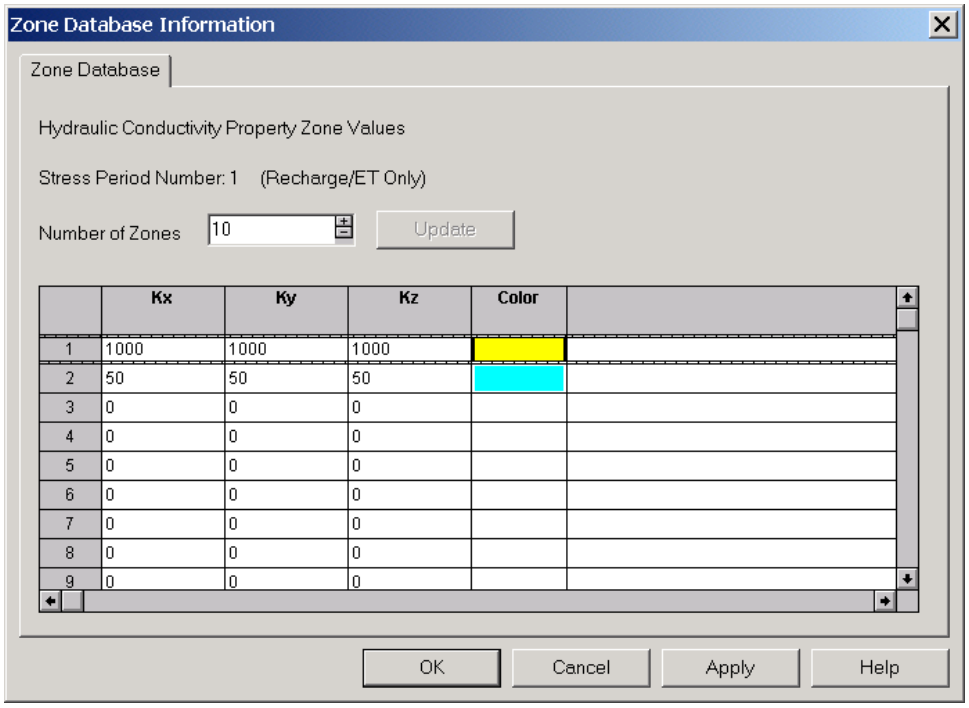
5. Trace out an irregular pattern for the ocean using the polygon tool. Create something that looks like the following:



Part III. Working with Properties

1. Now lets say that we want to add a zone of lower hydraulic conductivity somewhere in the middle of our model grid. Hydraulic conductivity referred to as a **property** in Vista terminology. To work with properties, click the **P** button. Also click on the **Props** menu and make sure there is a check next to **Hydraulic Conductivity.**

2. Groundwater Vistas uses the zone concept for the different property types. To see the zones available for hydraulic conductivity, click on the **Db** button (which means database) on the toolbar. Currently, there are 10 possible zones, but only zone 1 has non-zero hydraulic conductivity values. Enter a value of **50** for **Kx, Ky**, and **Kz** in zone **2**. If you want, you can also change the color of this zone by double-clicking in the color box next to **Kz**. Your database might look like the following



3. When you move the mouse over the model grid, the zone number and zone value are displayed in the lower left corner of the Vista window. To add a new zone to the model grid, use the polygon tool again to trace an irregular shape in the

middle of the model area. When asked for the **zone number**, enter **2**. You now have a heterogeneous distribution for hydraulic conductivity.

Part IV. Running MODFLOW2000

1. At this point, we are ready to run MODFLOW. In this example, we will use the version of MODFLOW that comes with Groundwater Vistas. We will also be using MODFLOW2000, because SEAWAT2000 and SEAWAT Version 4 is based on MODFLOW2000.

2. One of the first things you should always do when using Vistas is verify that the working directory is set properly. To set the working directory, click on **Model>Paths to Models** and at the bottom of the box where it says "Working Directory", browse for the correct working directory (***ex01***). Groundwater Vistas will create model datasets in the working directory and will also read model output from files in the working directory. Some of the errors that you will encounter while using Vistas are the result of an inaccurate working directory.

3. Information regarding a MODFLOW2000 simulation can be found in two places—under the **Model>MODFLOW** menu and under the **Model>MODFLOW2000** menu. Normally, you should browse through each one of the options under these menus to make sure the parameters are set properly.

4. Go to the **Model>MODFLOW>Packages** menu. Set the MODFLOW Version to **MODFLOW2000**. Also, change the solver to **PCG2**, which works better than SIP in most cases, and click **OK**.

5. After you have looked through each of the menus and are satisfied that the parameters are set properly, you need to create the MODFLOW2000 datasets. Go to **Model>MODFLOW2000>Create Datasets**. If you look in your working subdirectory, you will see that the MODFLOW2000 datasets have been created.

6. Use a text editor to inspect each of the files created in the working subdirectory. If you are new to MODFLOW2000 you will notice changes in the input files. For

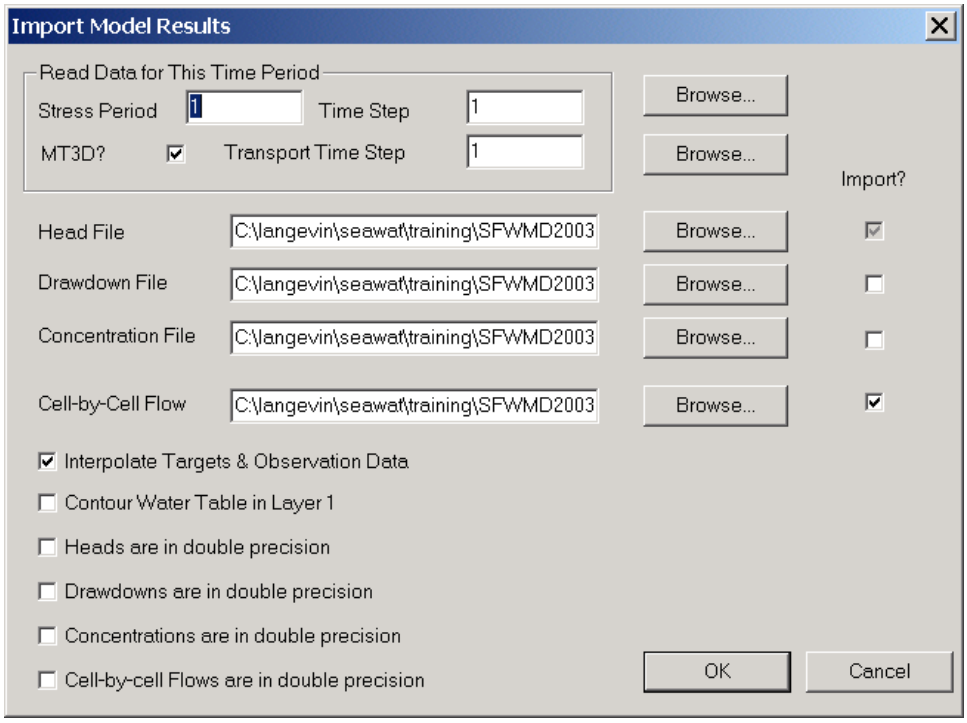
example, all information regarding the model grid is now stored in the ***discretization file*** (with suffix .dis). Also look at the name file. The name file controls the overall simulation options.

7. Next, run MODFLOW2000 by going to **Model>MODFLOW2000>Run MODFLOW2000.**

8. When MODFLOW2000 finishes, you will be asked if you want to import results. Click **yes**.

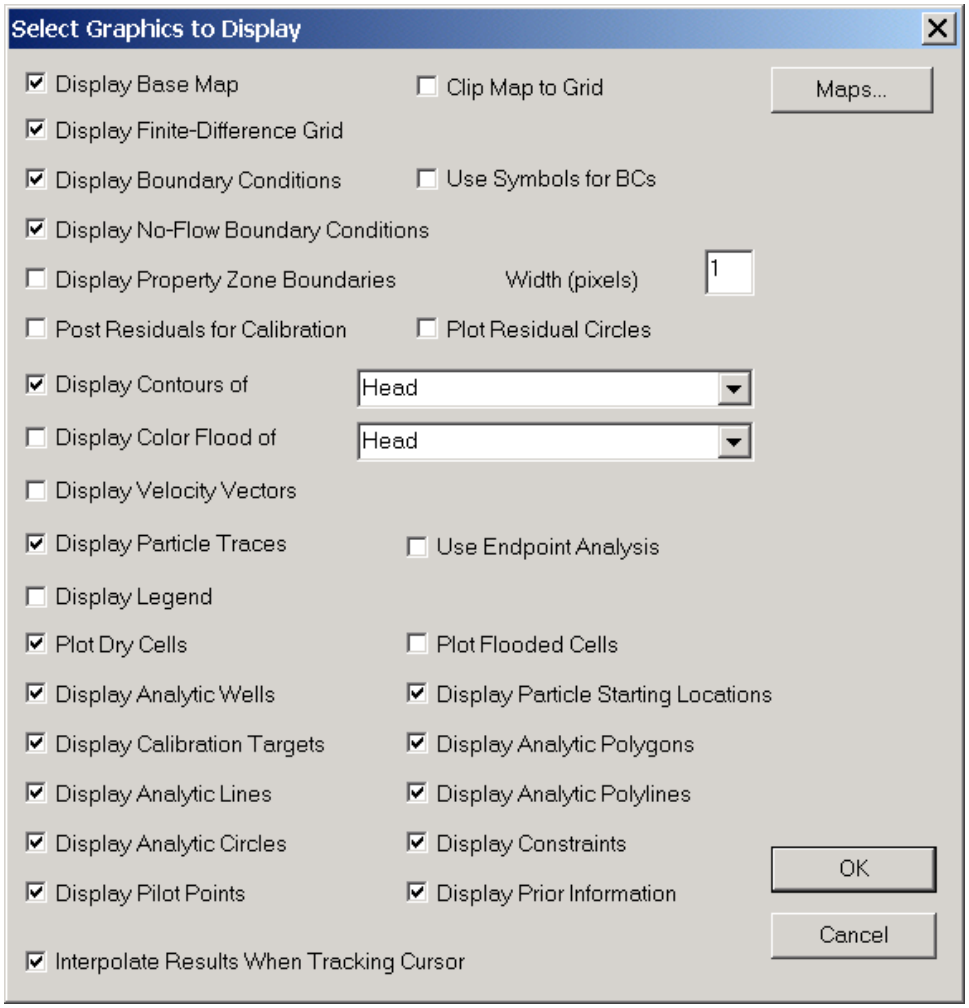
Part V. Importing and Plotting Results

1. When you import model results you should see the following window



2. Normally you want to import the head file and also the cell-by-cell flow file. If you import the cell-by-cell flow file you will able to view the water budget and draw velocity vectors. Later, when we use MT3D and SEAWAT, we will also import concentrations.

3. After you have imported results, there are several ways to make useful plots. Most of the plotting options are listed under the Plot menu. Look at the **Plot>What to Display** window. This is the main window for turning on or off display options.



Toward the bottom right corner of the main Vista window, there is a number that changes as you move the cursor over the model grid. This number reflects the value of whatever option is selected next to the **Display Contours** of box. So for in this case, Head has been selected. So when you move the cursor over the model grid, you will see the head value for each location.

4. If you are unhappy with the way your contours look, you can change the contour interval, label font, etc. under **Plot>Contour>Parameters (Plan)**…

5. Vistas has several options for showing water budget information. If the **B** button is pushed, then as you move the mouse over the different boundaries, in the bottom left-hand corner of the main Vista window, you can see discharge

information for each boundary cell (F=xxx.xxE-xx). This discharge value has units of **L^3/T**, which for this case is **m^3/day**.

6. You can also view detailed water budget information for the entire model or a subset of the model by going to **Plot>Mass Balance**, and then selecting an option. <u>According to the constant-density model, how much groundwater is discharging into the ocean?</u>

Exercise 2. PARTICLEFLOW—Understanding Advection and Dispersion

Exercise Description

The purpose of this exercise is to demonstrate the concepts of advection and dispersion, and to demonstrate the role of aquifer heterogeneity on solute transport. The PARTICLEFLOW software used for this exercise was developed by Paul Hsieh of the USGS. Documentation for the software is included in the ***Ex02*** subdirectory (***ofr01-286.pdf***).

Part I. Advection in a Uniform Flow Field

1. Go to the subdirectory ***Ex02\pflow*** and click on the file ***pflow.html***. To run this program, you will need a web browser, such as Internet Explorer or Netscape.

2. Briefly look over the description of the equations and then click on the button under the title Running the Model that says "click here to run the model". After you do this, a new window should come up with the title Particle Transport and Dispersion.

3. First click Start and then enter the following data

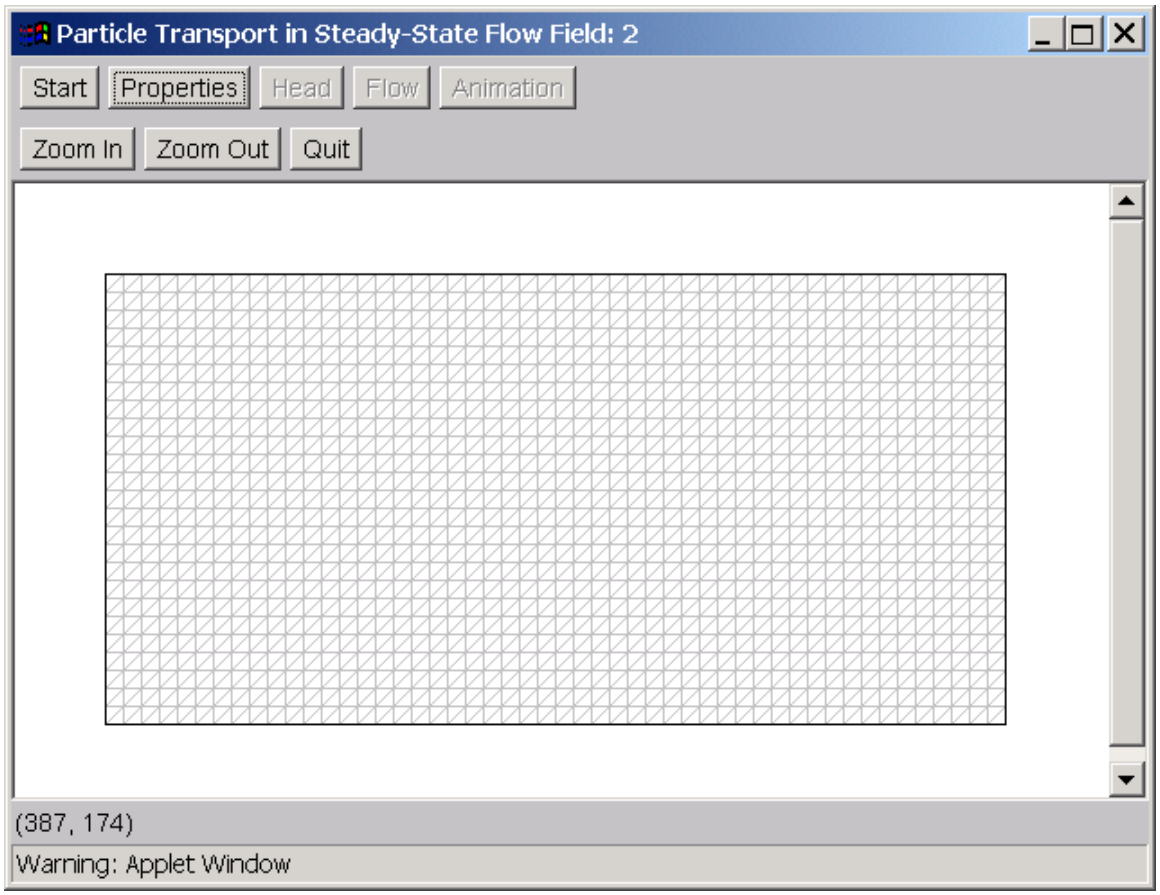
    i. Grid spacing (meters): 10

    ii. Number of columns: 50

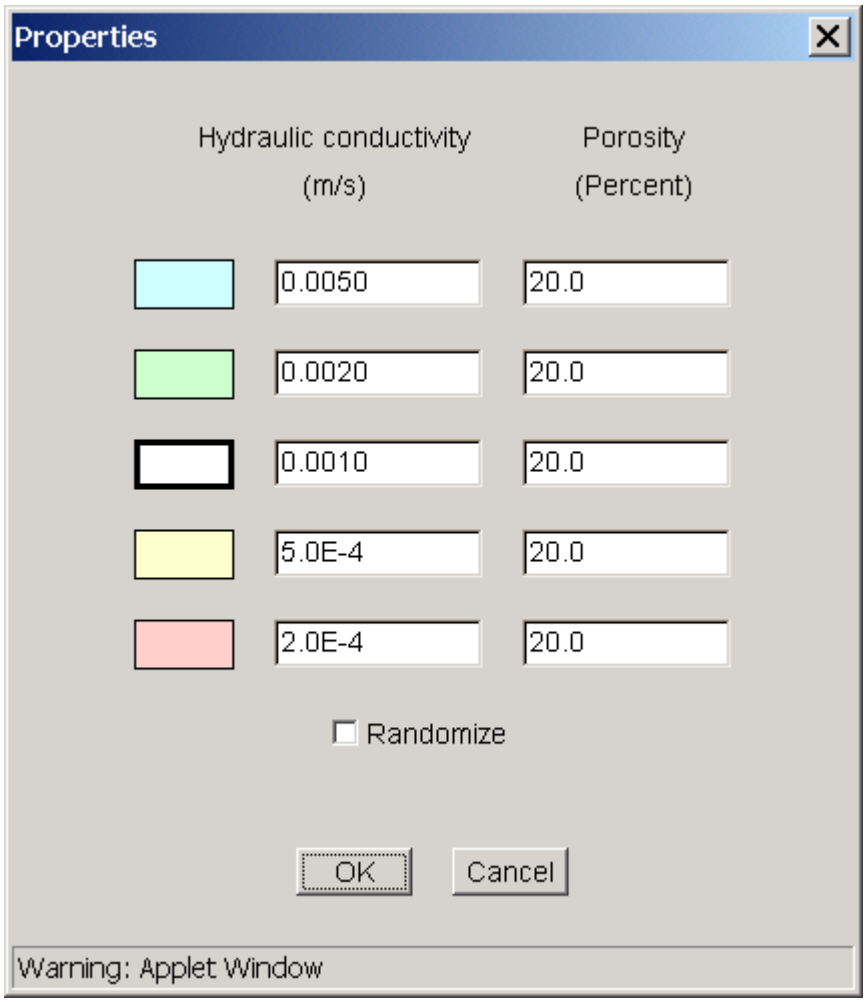
    iii. Number of rows: 25

    iv. Average hydraulic gradient: 0.001

4. Then click ok, and you should see a model grid as shown below.

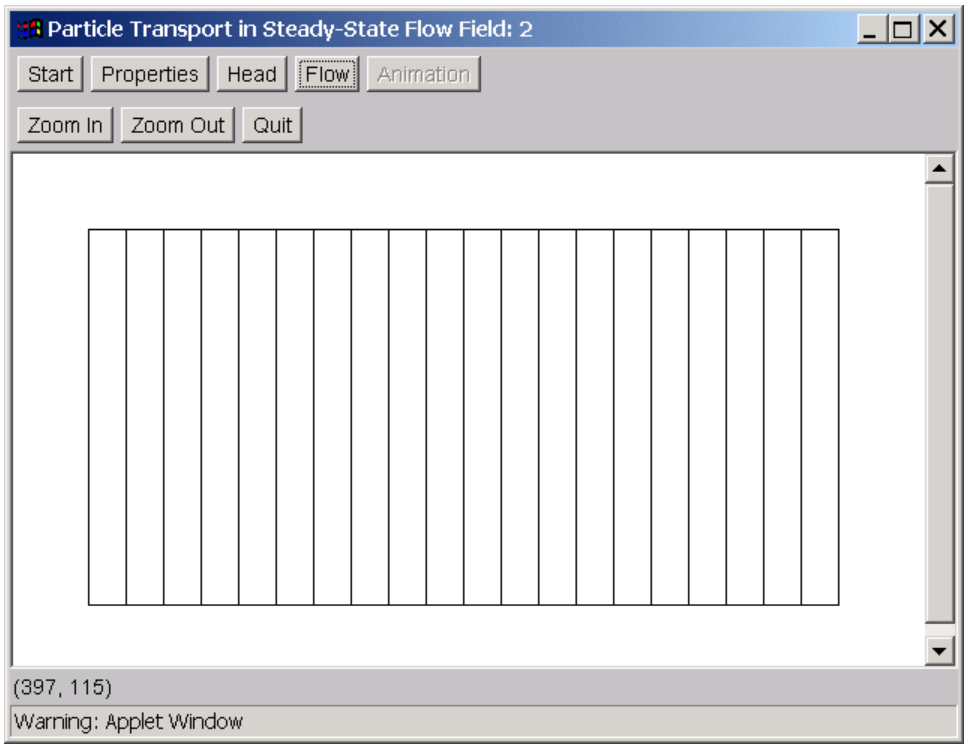


5. Next click on the Properties button to assign hydraulic properties (hydraulic conductivity and porosity). You should see the following window



6. Do not change the default setting, which assigns a uniform hydraulic conductivity of 0.001 m/s and porosity of 0.2 [zone 3] to the entire model domain. Click OK to proceed.

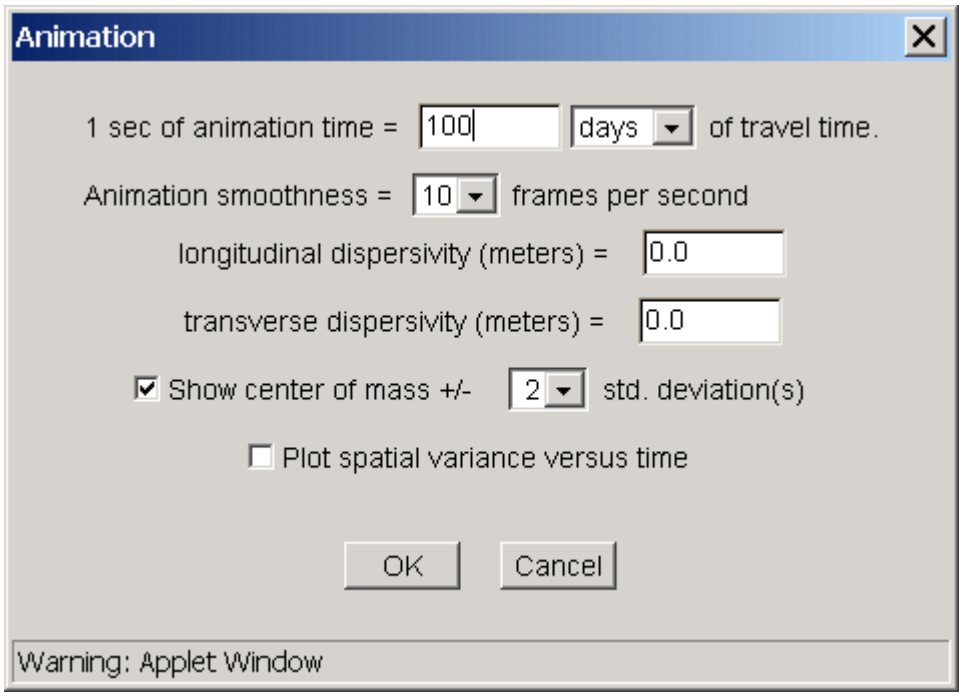
7. In the main window, click the Head button. When inside the Head window, click Compute and you will see a uniform head distribution as shown below



8. Next, click on the Flow button. Under the Options, select Particle Movement. Also, set Initial particle (placement) spacing to 1 meter, and activate the option Keep previous particles. Click OK to proceed.

9. In the main window, move the mouse to an area near the left boundary where you would like to define a source area. Double-click the left mouse button when you want to enclose the source area.

10. Click the Animation button and assign the input as shown



11. Finally, click OK and you will return to the main window. Click the mouse anywhere within the main window and you should see the particles move downgradient. Click the mouse again to stop particle movement. Note the two arrow bars on the side, which mark the center of the particle plume as it travels downgradient. The shape of the plume remains the same in this uniform flow field as there is nothing to cause the plume to spread.

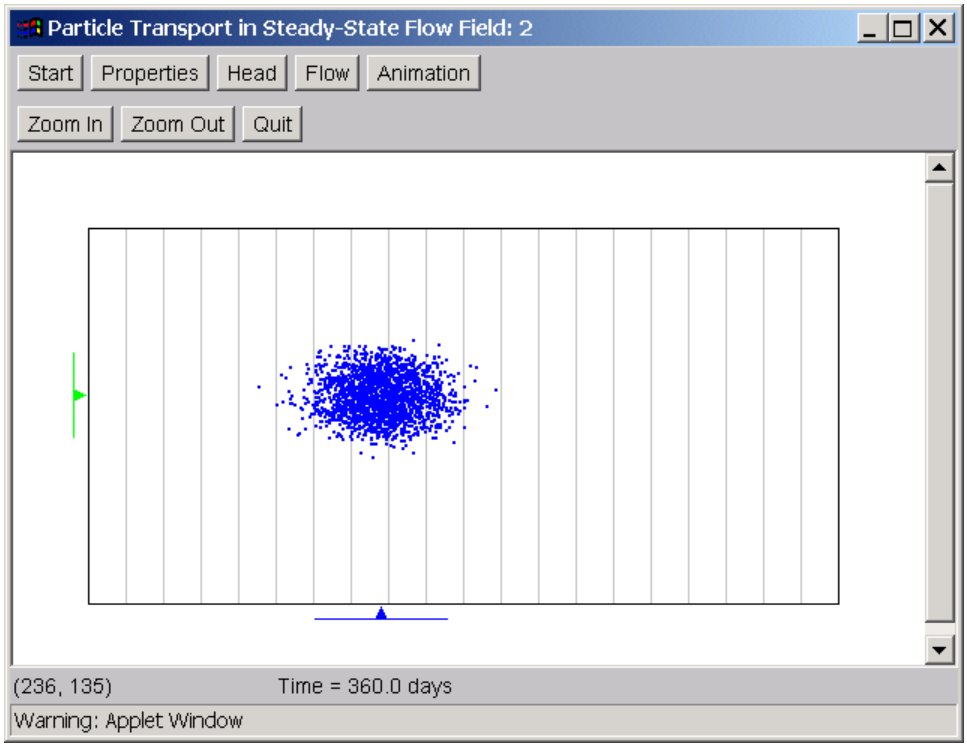
Part II. Advection and Dispersion in a Uniform Flow Field

1. In the main window, click on the Animation button. Assign the following dispersivity values

   Longitudinal dispersivity (meters): 1.0

   Transverse dispersivity (meters): 0.1

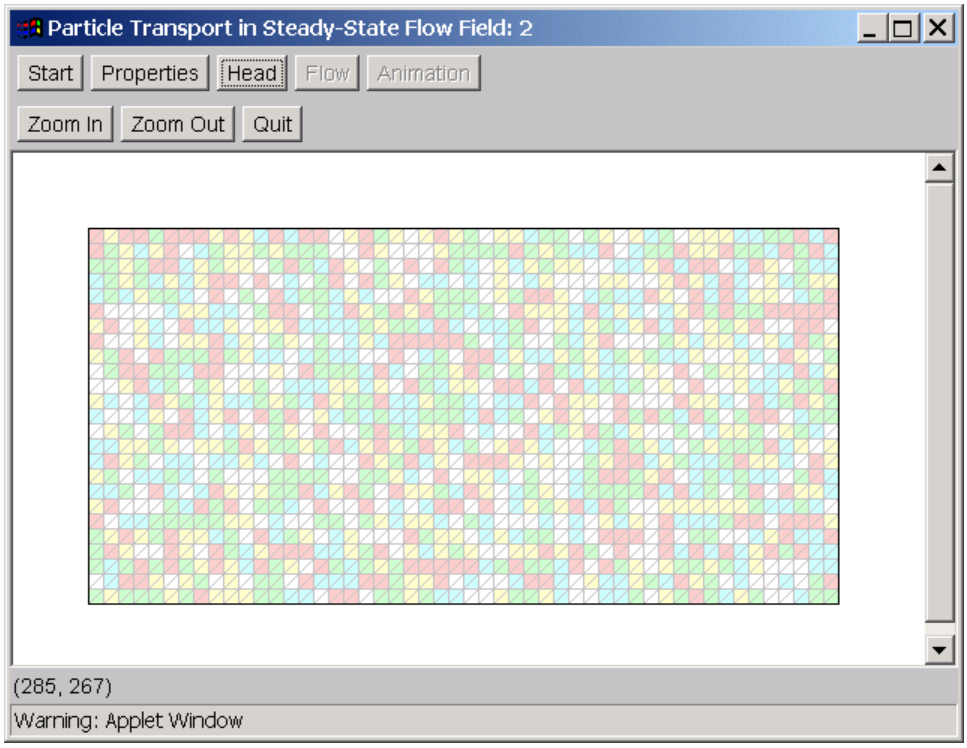
2. Click anywhere in the main window and watch how the particles move downgradient. Note how the addition of dispersion has led to the spreading of the particle plume in both the longitudinal and transverse directions. Much more spreading occurs in the longitudinal direction because we have specified the longitudinal dispersivity to be 10 times greater than the transverse dispersivity. Also note that the center of the plume remains the same as in the previous case with advection only, when the two cases are compared at the same observation time.



3. Go back to the Animation window and assign different values of longitudinal and transverse dispersivity to see how they affect solute transport. A key point to pay attention to is how some particles travel a lot faster than the average while some other particles lag significantly behind, due to the dispersion imposed. This phenomenon becomes more profound when the dispersivities are increased.

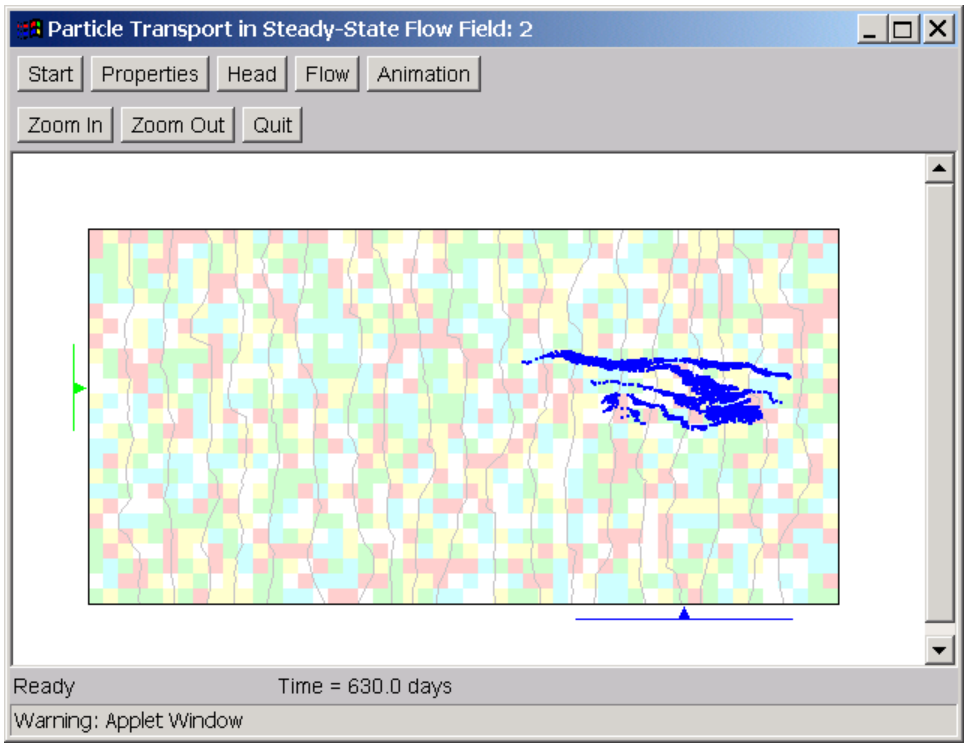
Part III. Advection in a Heterogeneous Flow Field

1. In the main window, click on the properties button. Do not change the default values of hydraulic conductivity and porosity. However, click on the checkbox next to the Randomize option, which generates a random K distribution



2. Next, repeat the steps as described previously to compute the head distribution and start the particle animation. **Make sure to change the longitudinal and transverse dispersivities back to zero.** Then watch the advection of particles in

the heterogeneous flow field, like the snapshot shown below



3. Note how the aquifer heterogeneity has led to the spreading of particles even though the dispersivities are set to zero.

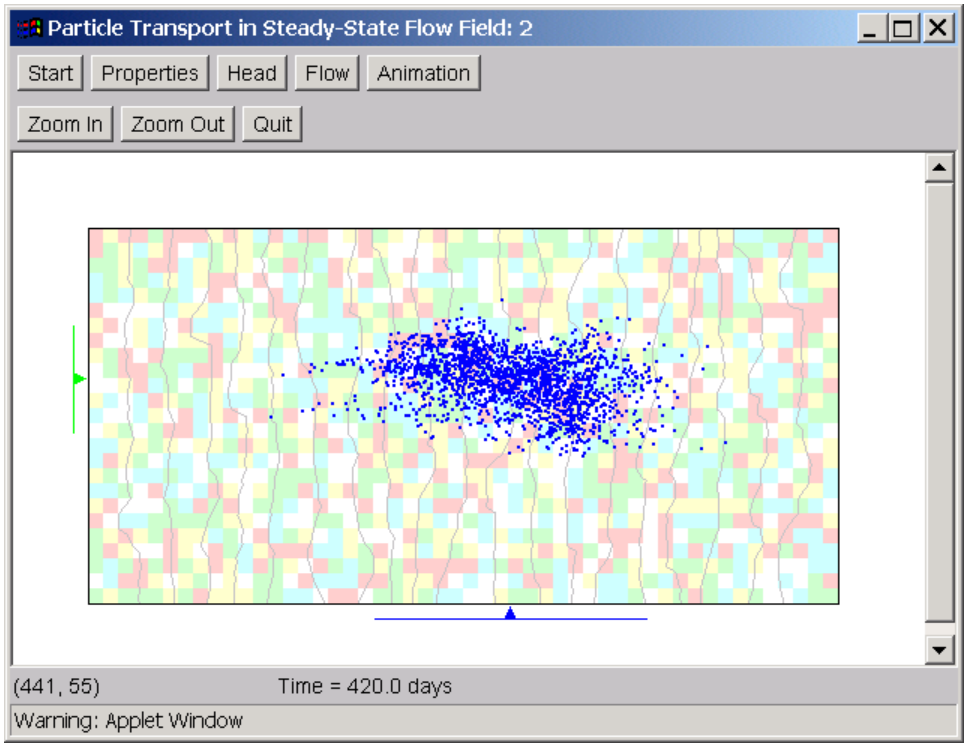
Part IV. Advection and Dispersion in a Heterogeneous Flow Field

1. In the main window, again click on the Animation button. Assign

   Longitudinal dispersivity (meters): 1.0

   Transverse dispersivity (meters): 0.1

2. Watch how the particles move in the heterogeneous flow field with both advection and dispersion. Compared with the previous case, the addition of dispersion enhances the spreading of the particle plume.

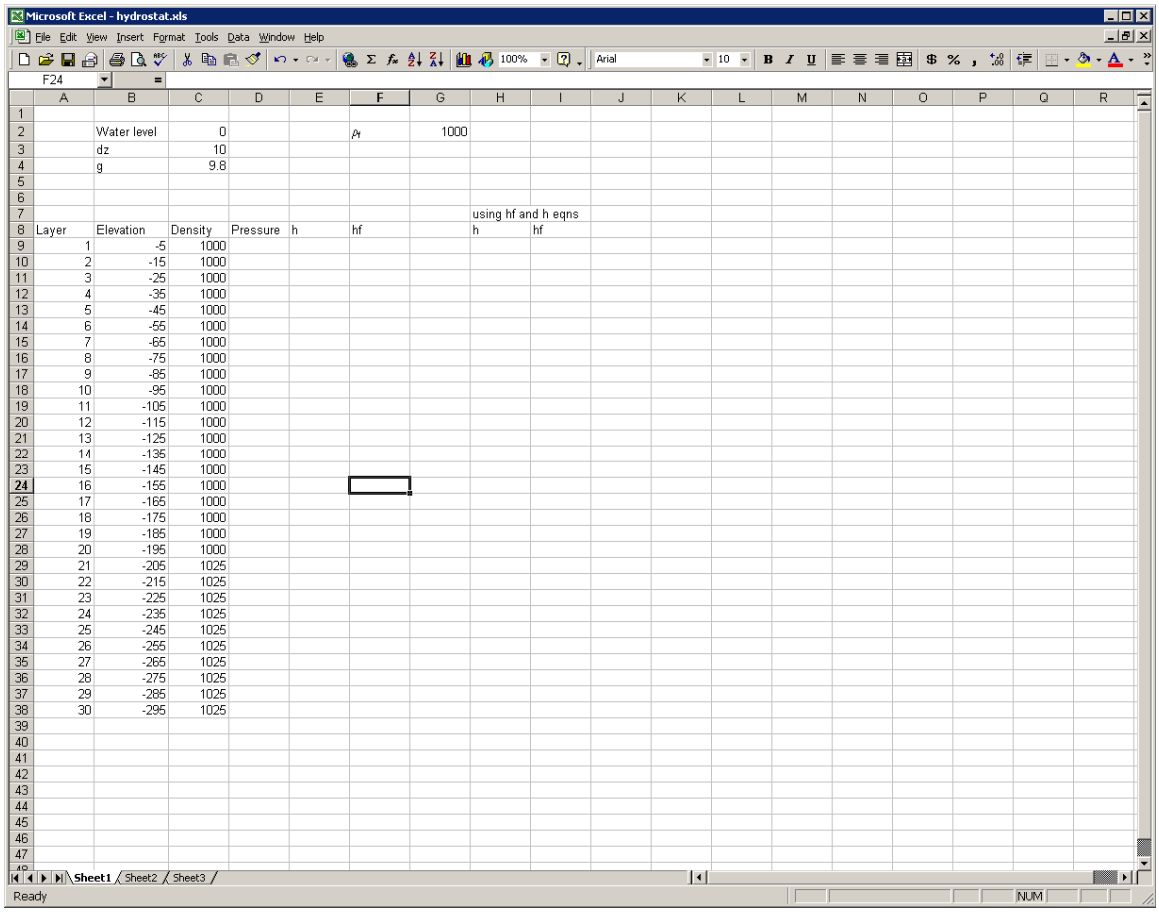


Exercise 3. Calculation of Head and Equivalent Freshwater Head

Exercise Description

The purpose of this exercise is to familiarize course participants with the equations for calculating head and equivalent freshwater head. These calculations will be made for a one-dimensional hydrostatic water column that contains freshwater overlying saline water.

Using Excel, calculate the vertical profile of pressure, head, and equivalent freshwater head. Begin by setting up your spreadsheet as follows:



Microsoft Excel - hydrostat.xls

	A	B	C	D	E	F	G	H	I
2		Water level	0			ρ_f	1000		
3		dz	10						
4		g	9.8						
7								using hf and h eqns	
8	Layer	Elevation	Density	Pressure	h	hf		h	hf
9	1	-5	1000						
10	2	-15	1000						
11	3	-25	1000						
12	4	-35	1000						
13	5	-45	1000						
14	6	-55	1000						
15	7	-65	1000						
16	8	-75	1000						
17	9	-85	1000						
18	10	-95	1000						
19	11	-105	1000						
20	12	-115	1000						
21	13	-125	1000						
22	14	-135	1000						
23	15	-145	1000						
24	16	-155	1000						
25	17	-165	1000						
26	18	-175	1000						
27	19	-185	1000						
28	20	-195	1000						
29	21	-205	1025						
30	22	-215	1025						
31	23	-225	1025						
32	24	-235	1025						
33	25	-245	1025						
34	26	-255	1025						
35	27	-265	1025						
36	28	-275	1025						
37	29	-285	1025						
38	30	-295	1025						

These are the type of calculations that would be required to specify a hydrostatic boundary condition in SEAWAT. In this example, the model has 30 layers, and each layer is 10-m thick. The water level is 0 m. In column C, under density, the values represent 200-m of freshwater overlying 100 m of seawater. Try to design your spreadsheet to refer to the values of water level, dz, and g above so you can change them and note their effects on the profiles.

Part I. Calculate Vertical Profile for Pressure

Using the standard equations for pressure, calculate the pressure in each cell (in column D under Pressure). Remember to account for the cell thickness in your pressure calculation.

Part II Calculate Vertical Profile for Head

In column E, under h, calculate the vertical profile for head using the value of pressure in the adjacent column. How does head vary in a variable-density setting under hydrostatic conditions?

Part III. Calculate Vertical Profile for Equivalent Freshwater Head

In column f, under hf, calculate the vertical profile for head using the value of pressure in each cell. How does equivalent freshwater head vary in a variable-density setting under hydrostatic conditions?

Part IV. Convert Between Head and Equivalent Freshwater Head

Using equations 3 and 4 in the original SEAWAT manual (Guo and Langevin, 2002), calculate head and equivalent freshwater head in columns H and I using the values of equivalent freshwater head and head in columns E and F. Do you get the same answer?

If your spreadsheet was designed properly, you should be able to change the different values, such as the density profile, and see how it affects pressure, head, and equivalent freshwater head.

Save this spreadsheet. You may use it one day to help calculate values for our boundary conditions.

Exercise 4: Hand Calculations of Density, Density Slopes, Heads, and Pressures

Exercise Description

The purpose of this exercise is to familiarize course participants with the equations for calculating density, density slopes, heads and pressures. These are important calculations when setting up a variable-density numerical model.

1. Calculations of Density Slopes

Fill the tables using Equation 40 shown on Page18 (Guo and Langevin 2002)

(a) Assuming ρf =1000 kg/m3, ρs=1025 kg/m3

	C0	Cs	Δρmax	ΔCmax	Density Slope
TDS in kg/m3	0	35	25	35	0.7143
TDS in lbs/ft3					
TDS in g/l					
TDS in mg/l					
Normalized TDS concentration					
Chloride in kg/m3					
Chloride in lbs/ft3					
Chloride in g/l					
Chloride in mg/l					
Normalized Chloride concentration					

(b) Assuming pf = 62.44 lbs/ft3, ps= 64.001 lbs/ft3

	C0	Cs	Δρmax	ΔCmax	Density Slope
TDS in kg/m3					
TDS in lbs/ft3					
TDS in g/l					
TDS in mg/l					
Normalized TDS concentration					
Chloride in kg/m3					
Chloride in lbs/ft3					
Chloride in g/l					
Chloride in mg/l					
Normalized Chloride concentration					

2. Calculation of Fluid Density

Calculate the fluid density of the samples shown below using Equation 40 on Page 18 (Guo and Langevin 2002, or the values in Question 1):

(1). Sample 1: TDS=10000 mg/l

(2) Sample 2: TDS =35000 mg/l

(3) Sample 3: Chloride concentration = 5000 mg/l

(4) Sample 4: Relative Chloride concentration = 0.5

(5) Sample 5: Chloride concentration = 19000 mg/l

(6) Sample 6: Chloride concentration =200 mg/l and TDS =2000 mg/l

Discussion: what assumption(s) you have to make in order to make these calculations? In (6) which concentration would provide a better estimate of density?

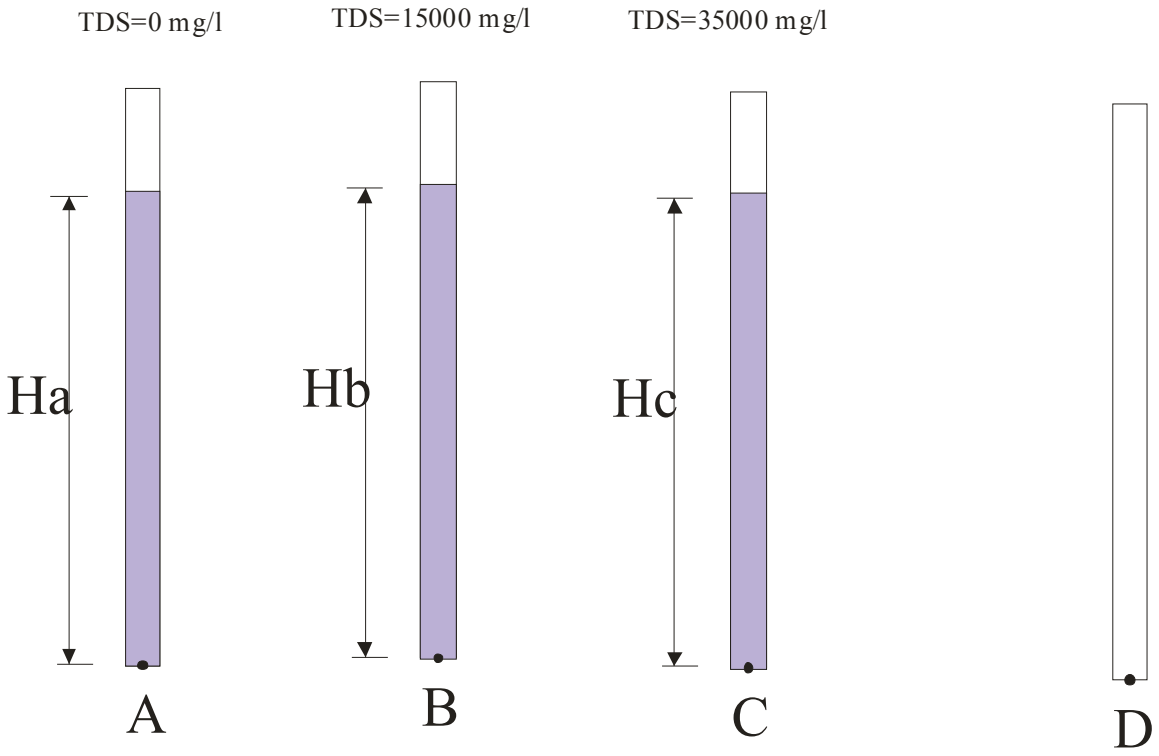
3. Calculation of Heads and Pressure

The figure below shows four tubes, three of them, A, B, C, are filled with water with different quality.

(1) What are heads at A, B and C?

(2) Calculate the hydraulic static pressures at Points A, B and C: Pa, Pb and Pc?

(3) If you fill Tube D with freshwater to the levels so that the hydraulic pressure at point D satisfies the condition: Pd=Pa, Pd=Pb and Pd=Pc, respectively, what are these levels? What are these heads called?



Exercise 5: Henry Problem

Exercise Description

The purpose of this exercise is to use SEAWAT to simulate the classic Henry problem. As described in class, some people consider there to be two cases of the Henry problem—each with different values for molecular diffusion. Code developers often use the Henry problem to test variable-density programs because an analytical solution exists for the problem (Simpson, 2004, is probably the best solution). In addition to Henry's original paper, information for the Henry problem can be found in Langevin et al. (2003, page 34) and Guo and Langevin (2002, page 70).

Part I. Getting Started

1. Start Groundwater Vistas
2. Click **File>New**. Model development will be much easier if you enter correct information for these parameters, particularly the model grid information.
3. For the Henry problem, create a model that has **21 columns** and **1 row**. Use **uniform x spacing** of **0.1** and **uniform y spacing** of **1** meter. The 1-meter y spacing has no influence on the solution; however, it does allow flows to be read in units of m^3/day/m.
4. For the **vertical grid information**, use **10 layers** and assign a **bottom elevation** of **0** and a **top elevation** of **1**.
5. Assign a **hydraulic conductivity** value **of 864 m/day** for **Kx, Ky**, and **Kz**.
6. Enter in a **porosity** of **0.35**
7. Enter in a **Storage** value of **0.0001**
8. Click **OK** to generate the model template.
9. Save your work into the ***Ex05*** folder.

Part II. Boundary Conditions and Properties

1. Beneath the main menu, there are four buttons labeled **B P G A**. These buttons represent **Boundaries, Properties, Grid,** and **Analytic element**. Whichever one of these buttons is pressed indicates the current editing mode in Vistas. So if we want to work with boundaries, we would press the **B** button.
2. In the Henry problem the ocean is along the east side. We want to use constant head cells to represent the ocean. Constant head cells can be added by clicking **BCs>Constant head/conc**. Only one boundary type can be edited at a time. The boundary type with the check mark next to it is the current boundary type.
3. Click on the small box  in the top left hand corner to add a window of **constant head/conc** cells. Then create a window in the cell at the bottom of the model (the map view of the model NOT the cross section view), this will be the cell in **column 21 of layer 1**. (An alternative is to right-click on the cell to add a boundary.) After you finish, a screen should pop up allowing you to enter in the information for the **constant head/conc cells** (or cell in this case). The **head** at the **Boundary** should be set to **1 m**. The **concentration** is set to **35 kg/m^3**, and the **constant head box** should be checked. You may or may not check the constant concentration box depending on how you want to represent the solute transport boundary. For this problem, we are going to use the CHD package to set the constant-head cells. GWV will use the CHD package if data are entered in the **Transient Data** box. Go down and un-check the **Steady-State Boundary Condition** option. Click the **Transient Data** box and another screen will open.

Enter in **1** for **Starting Stress Period**, **1** for **Ending Stress Period**, **1** for **Head value**, and **35** for the **Concentration value**. Click "**OK**", and then click "**OK**" again. The cell in **column 21** of **layer 1** should turn blue.

4. Now, we want to copy that down to every consecutive layer. This is done by going to **layer 2** (you can do this on the left side of the screen). Once in layer 2, go to **BCs>Copy**. Another window will pop up asking layer to copy from, the layer will be **1**, and to **copy all reaches**. Click "**OK**", and the cell in **column 21 layer 2** should turn blue. **Do this for all 10 layers**. (An alternative here is to right-click in column 21 of each layer and add the boundary.)
5. The cells in column 21 in all 10 layers should turn blue. According to the Henry problem, the length of the box is 2 meters. In our current configuration, however, the center of column 21 is at 2.05 m. One way to more precisely locate this boundary is to decrease the width of column 21. To change the width of this column go to **Grid>Edit>Column Spacings**. Go down to **21** and change the width to **0.01**. Click "**OK**" and the width should narrow on the screen.
6. For this simulation, we will start with seawater throughout the entire model domain by setting the initial concentrations to **35 kg/m^3**. Go to **Props>Initial Concentrations**. Click the **Db** button, and in **Row 1, Column 1** (labeled **Initial C**) enter in a value of **35** and change the color to red if you want (we typically have seawater as red and freshwater as blue). Click "**OK**".
7. A constant flux of fresh ground water is applied to the left boundary at a rate of **5.702 m^3/day**. The well package is used to create this boundary. A simulated "**well**" is put into each layer along the left hand column. Go to **BCs>Well**. Then

go to the window box  and create a small window in **Layer 1, Column 1**. Since there are **10 layers**, the total influx **5.702 is divided by 10**. Enter in **0.5702** for the **Flow Rate in Well** box. Click "**OK**" and the cell should turn red. You now want to copy this flux into every layer. Go to the next layer, **BCs>Copy**, and copy the well boundary condition (same as step 4 above for the constant head cells). Do it for every layer.

8. Click "**OK**". The entire column along the left hand side should be red representing the wells.
9. Henry represented mixing with a velocity independent coefficient, which can be represented here by specifying a value for the molecular diffusion coefficient. Go to **Props** and check **Diffusion – Decay on Soil**. Then click the **Db** button and set the value of **Diffusion** to 1.629. This is the value originally used by Henry. To run the other case, you would enter a value of 0.57.

Part III. SEAWAT Settings

1. For this simulation, we will use a simulation length of 2 days. This is done by going to **Model>Modflow>Stress Period Setup**. Change the **Period Length** to **2**, **No. of time steps** to **1**, and the **Time Step Multiplier** to **1**. Note that the Time Step Multiplier will not matter for this particular simulation because the number of MODFLOW time steps is set to 1. If we wanted to save flow data at different time intervals, we could adjust these parameters accordingly.
2. The stress periods will be set to transient. This is done by going to **Model>Modflow-2000>Stress Period Types> Set all to transient.**
3. For this simulation, the variable-density flow equation is solved using the PCG2 solver. To correctly set the solver, go to **Model>Modflow>Packages**.
    a. Here, next to Solver, make sure the **PCG2** solver is selected.
    b. Also, change the **MODFLOW Version** to **SEAWAT-2000**.
    c. Change the **Root File Name** to: ***henry***.
    d. Underneath the **Package option** we want to create the **CHD** package. Click the box to create that package, and change the **Unit No**. to **20**.
4. We are also going to set output options so the heads are printed to a file. Go to **Model>Modflow>Package Options**
    a. Click the "**Output Control**" tab.
    b. Make sure to click the box next to **Always save data at the last time step of the run**.

c. Go to the "**Block-Centered Flow**" tab, and change all 10 layers to **0-Confined**. The Henry problem is specified as confined conditions. In actuality, it may be ok to leave the LAYCON type as 3 for layers 2 through 10, however, in many practical applications, the program will be more stable for confined conditions.

d. Go to the "**Density**" tab and look at the values. This tab is only useful if you want GVW to correct boundary heads for equivalent freshwater values. With SEAWAT-2000 and SEAWAT Version 4, this is done automatically (i.e. heads are entered, not equivalent freshwater values). So for this simulation, do not check the box for **Correct Boundaries for Density**. If you were using the previous version of SEAWAT, you would want to check this box, and you would also want to specify a concentration of 35 for the maximum brine concentration.

e. Go to the "**CHDs**" tab and check the box next to **Use Same Head Value for Beginning and End of Stress Period**.

f. Click "**OK**"

5. For this simulation, we will solve the transport equation with the implicit finite-difference method. This is done by going to **Model>Mt3D/Rt3D>General Options**.

   a. Click the "**Advection**" tab. Set the solution scheme to **Finite Difference**, and the **Weighting** to **Upstream**.

   b. Click the "**Basic Transport**" tab. Set the **Time Units** to **DAY**, the **Length Units** to **M** and the **Weight Units** to **KG**.

c. Click the "**Time Stepping**" tab. Set the **Transport Time Step Size** to **0.0001 day**, change the **Maximum transport steps per flow step** to **99999**, and put in a **timestep multiplier** of **1.5**. Change the **Maximum Time Step Size** to **0** (which means the time step lengths will not be limited).

d. Click the "**Printing**" tab, and next to the **Frequency of output**, set it to **Every N Time Steps**, and print every **2** time steps.

e. Click the "**GCG Solver**" tab. Change the **Solver Option** to **SSOR**. Click the box to **Include Full Dispersion Tensor**. You may want to experiment later with different solvers.

f. After all this is done, click "**OK**".

6. Now go to **Model>Mt3D/Rt3D>Packages**. Set the root file name to ***henry.*** Also, uncheck the Include and Create boxes for the Reactions package, which is not required for this simulation.

7. We need to set the SEAWAT options so that a variable-density simulation will be performed.

   a. This is done by going to **Model>SEAWAT>SEAWAT2000 VDF Options**. At the top, check the box next to **Use SEAWAT2000 Version 4.**

   b. Change the option next to **Fluid Density Calculation (MTDNCONC or MT3DRHOFLG in v4)** to **1 – Species 1 couples flow and transport**.

   c. The **Coupling Procedure (NSWTCPL)** is for the implicit coupling between flow and transport in SEAWAT. For most cases, this can be

inactivated by specifying a value less than or equal to 1 for. Set the value to 0 or 1.

d. Set **DENSEMIN** and **DENSEMAX** to **0**. These are the density limiters, which are generally not used. Set the **Reference Fluid Density (DENSEREF)** to **1000** (this is the density of fresh water). Set the **Density-Concentration Slope (DENSESLP)** to **0.714** (this is the change in density between fresh and seawater divided by the change in concentration of fresh and seawater. i.e. 25/35=0.714). Set **FIRSTDT** to **0.01**.

8. ***IMPORTANT! Don't forget to set your path to models to the correct directory.*** This is done by going to **Model>Path to Models**, go to the directory for Exercise 5 so your datasets are written to the correct place.
9. Next we will create the SEAWAT datasets into that file. Go to **Model>SEAWAT>Create SEAWAT datasets**.

Part IV. Running SEAWAT

1. At this point, we are ready to run SEAWAT. In this example, we will use the executable provided to you in the exe folder.
2. We are going to create a ****.bat*** (batch) file to run the program and to pause at the end so the window does not close.
3. Open the program ***UltraEdit*** (or a text editor of your choice) which should be in the ***Start*** menu of your computer. Then type the following into a blank sheet:

```
..\..\exe\swt_v4.exe henry.nam
pause
```

4. Then go to **File>Save as>** and save the file into the directory that you are working in (***EX05***) as the name ***swt_v4.bat.***
5. You will now go into the working directory of ***EX05*** and double click on ***swt_v4.bat.***
6. SEAWAT should run the henry problem.

Part V. Importing and Plotting Results

1. Next go to **Plot>Import Results**. A window should pop up.
2. You want to import the head file and the concentration file. Next to the head file browse for ***henry.hds***. Next to the concentration file, browse for ***MT3D001.ucn***. Click the boxes to import both of those files.
3. At the top of the window, next to **Stress Period** and **Time Step** you will browse to make sure you are reading in the head file.
4. Next to the **Transport Time Step** you will browse and go down to the bottom of the file. It should have gone to **transport step 23**. Click on that and click "**OK**".
5. Then click "**OK**" again and the datasets should import into Vistas.
6. After you have imported results, there are several ways to make useful plots. Most of the plotting options are listed under the **Plot** menu. Look at the **Plot>What to Display** window. This is the main window for turning on or off display options. Go to **Display Contours of** and set it to **Head**. Go to **Display Color Flood of** and set it to **Concentrations**.
7. Click "**OK**".
8. If all has been set correctly, you should see a saltwater interface with the "ocean" on the right hand side and fresh water above it and on the left hand side of the grid.
9. Vistas has several options for showing water budget information. If the **B** button is pushed, then as you move the mouse over the different boundaries, in the bottom left-hand corner of the main Vista window, you can see discharge

information for each boundary cell (F=xxx.xxE-xx). This discharge value has units of L^3/T, which for this case is m^3/day.

10. You can also view detailed water budget information for the entire model or a subset of the model by going to **Plot>Mass Balance**, and then selecting an option. <u>According to this model, how much groundwater is discharging into the ocean? Why is the flow into the constant head cells greater than the inflow from the wells?</u>
11. If time permits, use Modelviewer to animate the results of this simulation. Make sure to use the MT3DMS option in Modelviewer when opening the files. Open Modelviewer and go to **File>new**. You can look at a MODFLOW or MT3DMS results. To view the salinity distribution select MT3DMS. For "cnf" scroll to the directory you are running your model in and select the MT3D.cnf file. Then specify the concentration file (MT3D001.UCN), and select "OK". We will leave the other two boxes blank. .You can leave the time to visualize as it is, or go to another time. The data type "concentration" will be used in this visualization. Click "OK". A blank box will appear. Go to **Show>solid** and you will see some colors appear; however, this view still looks odd. Why do you think that is? You can move the view around with the left-click on the mouse. There is also a place in the menu to animate the concentrations and change the min/max color scheme for concentrations.

Part VI. Testing different solution schemes

1. Try running the Henry problem with a different solver.
2. Go to **Model>MT3D/RT3D>General Options**, and click on the "**Advection**" tab. Change the Solver to **TVD**. Click "**OK**".
3. Create your SEAWAT datasets **Model>SEAWAT>Create SEAWAT datasets**.
4. Run SEAWAT (***swt_v4.bat***) again. This will take a few minutes so get up and stretch your legs.
5. What are the transport time step lengths? What would you change, if you wanted them to be calculated based on a Courant number?
6. When it's done, import the results and plot them again.
7. Does it look different from the first run? What looks different? Why? Which result do you think is more accurate?

Exercise 6: Modified Henry Problem

Exercise Description

Simpson and Clement (2003, 2004) showed that the Henry problem isn't a good test of variable-density codes because you can get similar answers with a constant density code and equivalent freshwater heads assigned to the seawater boundary. Simpson and Clement (2004) suggest a modified version of the Henry problem in which the inflow rate is cut in half. This causes the seawater to intrude farther. The resulting concentrations cannot be obtained with a constant density model.

Part I. Getting Started

1. Copy the ***GWV*** file you created in Ex05 into the working directory of Ex06.

2. Change the **Model>Path to Models** to this working directory.

3. The modified henry problem decreases the amount of flow in from the left hand side "wells" by 50%.

4. Go to **BCs>Well**.

5. Go to **BCs>Modify>Reach**. The reach number for all the wells created along the left hand side is zero.

6. A box pops up with **Reach Number**, leave **0** in the box and click **"OK".**

7. It will ask **"Continue with Boundary Cell modification?"** Click **"yes".**

8. Next it will ask **"Modify all layers?"** Click **"yes"**. Any changes made to the box that pops up will modify every simulated **"well"** in the system with a reach number of **0**. These are all the wells on the left hand side.

9. The current influx is: 0.5702 m^3/day, and this needs to be reduced by 50% to 0.2581 m^3/day. Replace **0.5702** with **0.2581**. Click **"OK**".

10. Create your SEAWAT datasets **Model>SEAWAT>Create SEAWAT datasets**.

Part II. Running the Model and Viewing results

1. At this point, we are ready to run SEAWAT. In this example, you can use the batch file, ***swt_v4.bat,*** that you created in Ex05 (copy the batch file into Ex06).

2. After the model finishes running import the results as in Ex05 by going to **Plot>Import Results** (make sure you are importing results from Ex06).

3. Do these results in Ex06 look different from Ex05?

4. What is the main difference? What would be the general procedure for running a constant-density model of the same problem?

Exercises 7-10. Saltwater Intrusion (SWI) Exercise

Exercise Description

A growing coastal city is interested in developing a wellfield in order to provide potable drinking water to its residents. You have been contracted by the city to perform a numerical analysis to determine the effects of groundwater withdrawals on the position of the saltwater interface. The city is particularly interested in knowing if the planned withdrawal rate will result in pumped water that exceeds the drinking water standard for chloride, which is 250 mg/L. In addition, you have been asked by the city to delineate a wellfield protection zone by determining the approximate recharge area for the wellfield. The city is also interested in knowing what would happen if a spill was to occur at the airport. At what concentrations would a conservative contaminant plume reach the proposed wellfield?

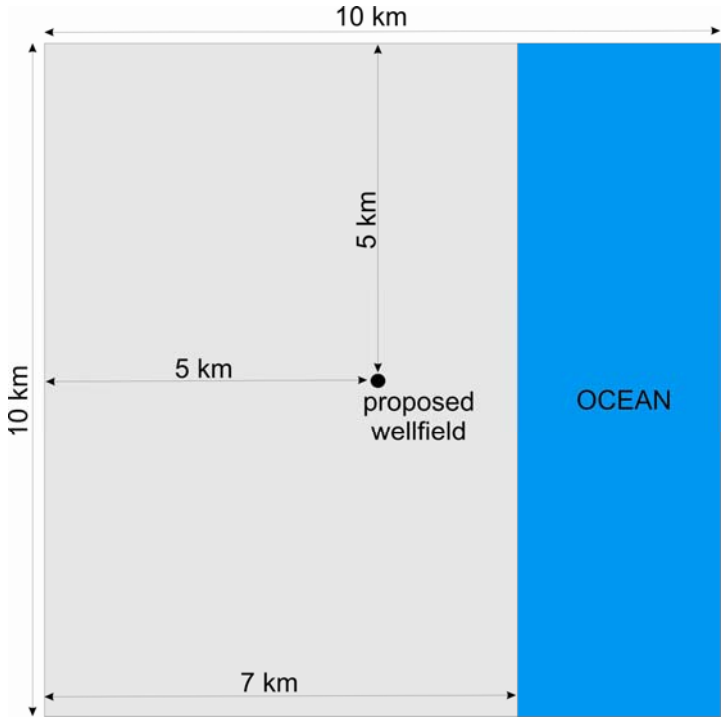


Figure 1. Map of the study area.

The study area consists of a 10 by 10 km area of a coastal plain aquifer system centered on the proposed wellfield (Figure 1). The hydrogeology of the area consists of a shallow and deep aquifer, and both aquifers intersect the sea floor (Figure 2). The two aquifers are separated by a discontinuous confining layer that thickens to the east. The confining layer is present in the eastern part of the study area, but is absent in the western part. A low permeability unit, which slopes downward to the east, underlies the deep aquifer and can be considered a no flow boundary. Extensive field investigations have been performed, and the aquifer properties for the different units are summarized in Table 1. Annual average recharge was determined to be 25.4 cm/yr (10 in/yr).

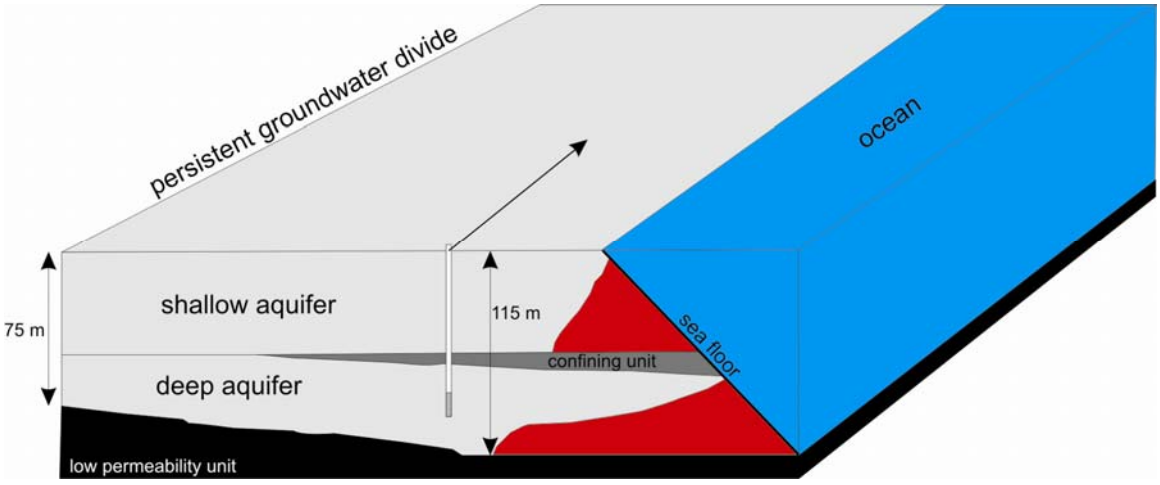


Figure 2. Block diagram showing the hydrogeology of the area.

Unfortunately, due to limitations in available property, the city has only one option for wellfield location, which is shown on the map in Figure 1. The city is hoping to capture at least 25% of the recharge for the area, but there is an obvious concern that excessive pumping from the deep aquifer could cause the saltwater interface to move inland and contaminate the wellfield.

Table 1. Aquifer hydraulic parameters.

Unit	K_H (m/d)	K_V (m/d)	S (-)	S_y (-)	n (-)	α_L (m)	α_T (m)
Shallow Aquifer	100	1	1×10^{-5}	0.2	0.2	10	1
Confining Unit	0.001	0.001	1×10^{-5}	0.2	0.2	10	1
Deep Aquifer	2000	200	1×10^{-5}	0.2	0.2	10	1

Exercise 7. SWI Part I. Design, run, and calibrate a 2D cross-section model to obtain the steady-state pre-withdrawal distribution of head and salinity

Based on the geometry of the system, the pre-withdrawal conditions can be obtained by running a 2D cross-section model. The resulting heads and salinities can then be used as initial conditions for the 3D model to evaluate interface movement in response to pumping. Because 3D saltwater intrusion models can take a long time, across-sectional model is developed first using one row, 100 columns, and 25 model layers. The model has already been constructed for you.

This exercise was designed such that a 2D model could be used to represent pre-withdrawal conditions. If the hydrogeology were to vary in the north-south direction, or if an irregular boundary were to exist, the problem of obtaining equilibrium conditions would be more difficult.

IA. Determine length of simulation period required to reach equilibrium

1. Using Groundwater Vistas, go into the folder ***SWI_IA*** and open the GWV file called ***SWI_IA.gwv***.

2. As always, check the **Model>Paths to Models** option, and make sure the correct working directory has been set.

3. Create the SEAWAT datasets by going to **Model>SEAWAT>Create Datasets**.

4. Run SEAWAT by double-clicking on the ***swt_v4.bat*** file in the ***SWI_IA*** folder.

5. When SEAWAT finishes, record the amount of time it took to run the simulation, then check to see if equilibrium has been achieved. An easy way to do this is to open the file ***MT3D001.mas*** with Excel and graph the "Total Mass in Aquifer" as a function of time. Based on this graph, can you tell if equilibrium was achieved?

6. The answer to number 5 is no—equilibrium has not been achieved, because the total mass in the aquifer continues to change with time. Thus, aquifer salinities have not reached steady state. In order to reach equilibrium conditions, the simulation period needs to be extended. In Vistas, go to **Model>MODFLOW>Stress Period Setup**. Note that the simulation period is currently set for 2000 days. Clearly this is not enough time. Change this value to 100,000 days.

7. Recreate the SEAWAT datasets (**Model>SEAWAT>Create Datasets**).

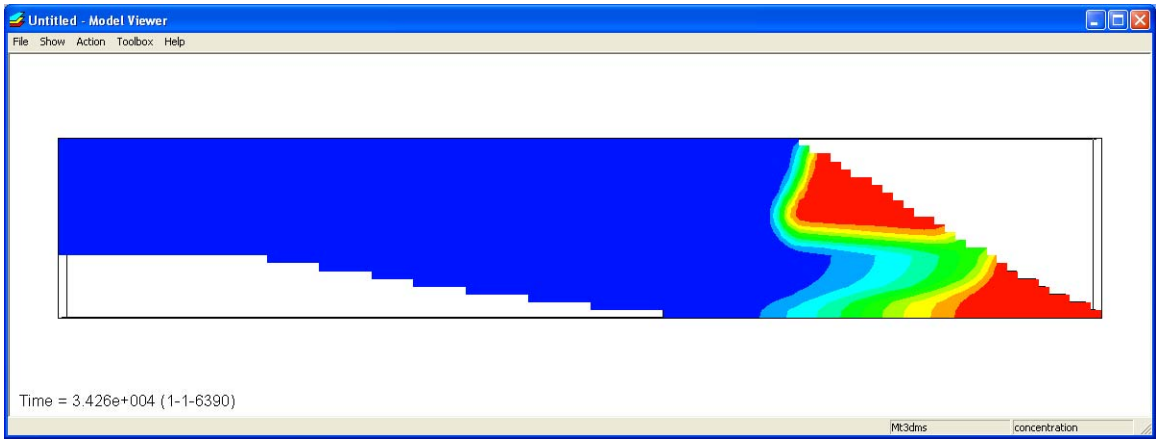
8. Rerun the model (double-click on the ***swt_v4.bat*** file in the ***SWI_IA*** folder). This simulation may take a little while to finish. You should record how long it took to run the simulation on your computer. (If the run is taking too long, you can proceed to step 9, and use the MT3D001.mas file from the **results** folder)

9. Once the simulation is finished, check again to see if equilibrium has been achieved (open the file ***MT3D001.mas*** with Excel and graph the "Total Mass in Aquifer" as a function of time).

10. Use the Modelviewer program to animate salinity as a function of time. Make sure to use the MT3DMS option in Modelviewer when opening the files. Open Modelviewer and go to **File>new**. You can look at a MODFLOW or MT3DMS results. To view the salinity distribution select MT3DMS. For "cnf" scroll to the directory you are running your model in and select the MT3D.cnf file. Then specify the concentration file (MT3D001.UCN), and select "OK". We will leave the other two boxes blank. .You can leave the time to visualize as it is, or go to another time. The data type "concentration" will be used in this visualization. Click "OK". A blank box will appear. Go to **Show>solid** and you will see some colors appear; however, this view still looks odd. Why do you think that is? Could it have something to do with the dimensions of the model? How do you think this can be fixed? (Hint: go to **Toolbox>Geometry** and increase the vertical

discretization in "z") You can move the view around with the left-click on the mouse. There is also a place in the menu to animate the concentrations.

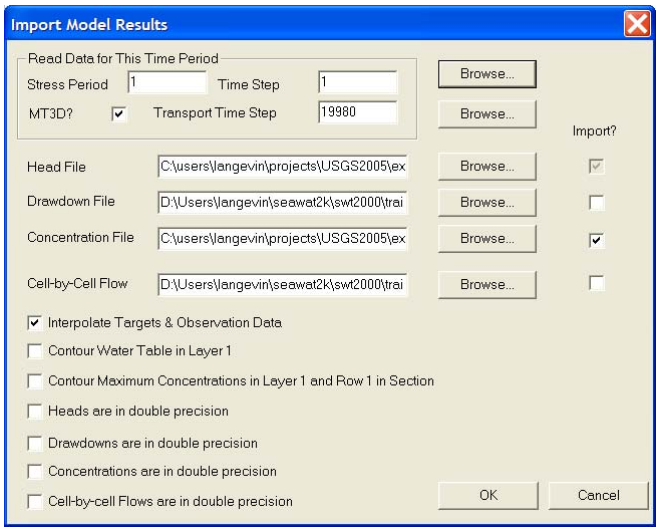
11. Play around with Modelviewer and get comfortable with how to view and animate results.

12. 

13. Based on the mass balance graph and the Modelviewer animation, about how many years does it take to reach equilibrium?

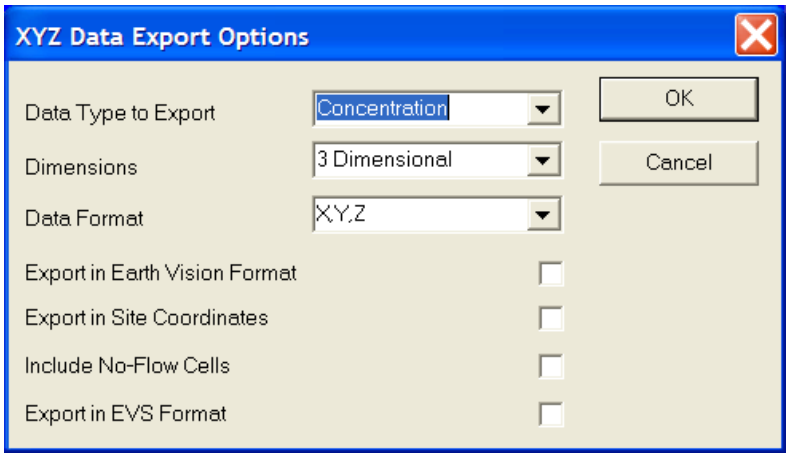
14. A final step here is to import the SEAWAT results into GWV so that we can use them in a subsequent analysis. Go to Plot>Import Results. When the dialog box comes up, click on both of the browse buttons next to Time Step and Transport Time Step and select the last value. Also check the import box next to the

Concentration file if it is not checked, and then click ok.



15. After the results have been imported, go to **File>Export** and then select the save type as **ASCII XYZ (*.dat)**. You may use the default file name if you like.

16. When the next dialog box comes up, select concentration as the **Data Type to Export**, and then click Ok.



17. The file that you created (possibly called ***SWI_IA.dat***) will be used later to compare with other simulation results.

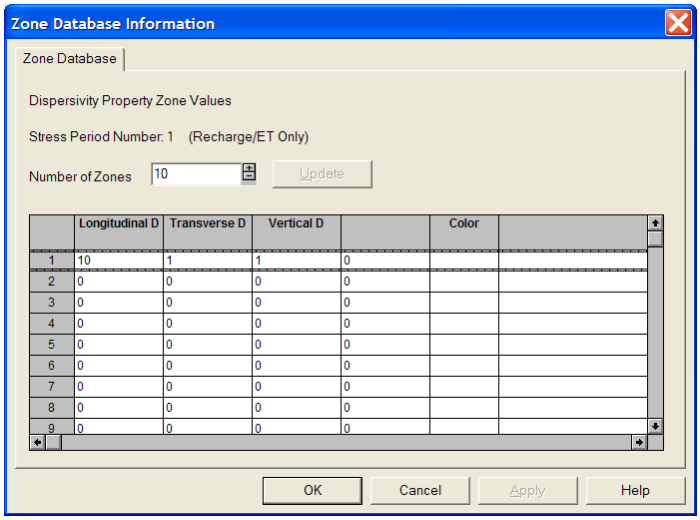
IB. Evaluate the level of numerical dispersion

In IA, the TVD solver was used with a specified Courant number of 0.5, and because the longitudinal and transverse dispersivities (α_L and α_T) were specified as 10 and 1 m, respectively, the simulation included dispersion. In addition to the intended dispersion, the simulation also had some numerical dispersion. The purpose of this analysis is to determine the approximate level of numerical dispersion by rerunning the previous simulation with the dispersivity values set to zero.

1. Go into the folder ***SWI_IB*** and open the GWV file called ***SWI_IB.gwv***. This file should be the same as the file that you ended up with in IA.

2. As always, check the **Model>Paths to Models** option, and make sure the working directory has been set to ***SWI_IB***.

3. Go to **Props>Dispersivity** and then go to **Props>Property Values>Database**. You should see the following window:

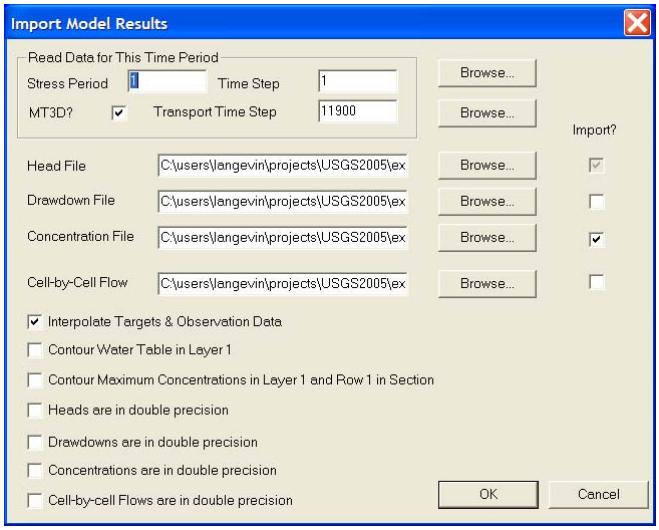


4. Change all three of the dispersivity values to zero.

5. Create the SEAWAT datasets by going to **Model>SEAWAT>Create Datasets.**

6. Run SEAWAT by double-clicking on the ***swt_v4.bat*** file in the ***SWI_IB*** folder.

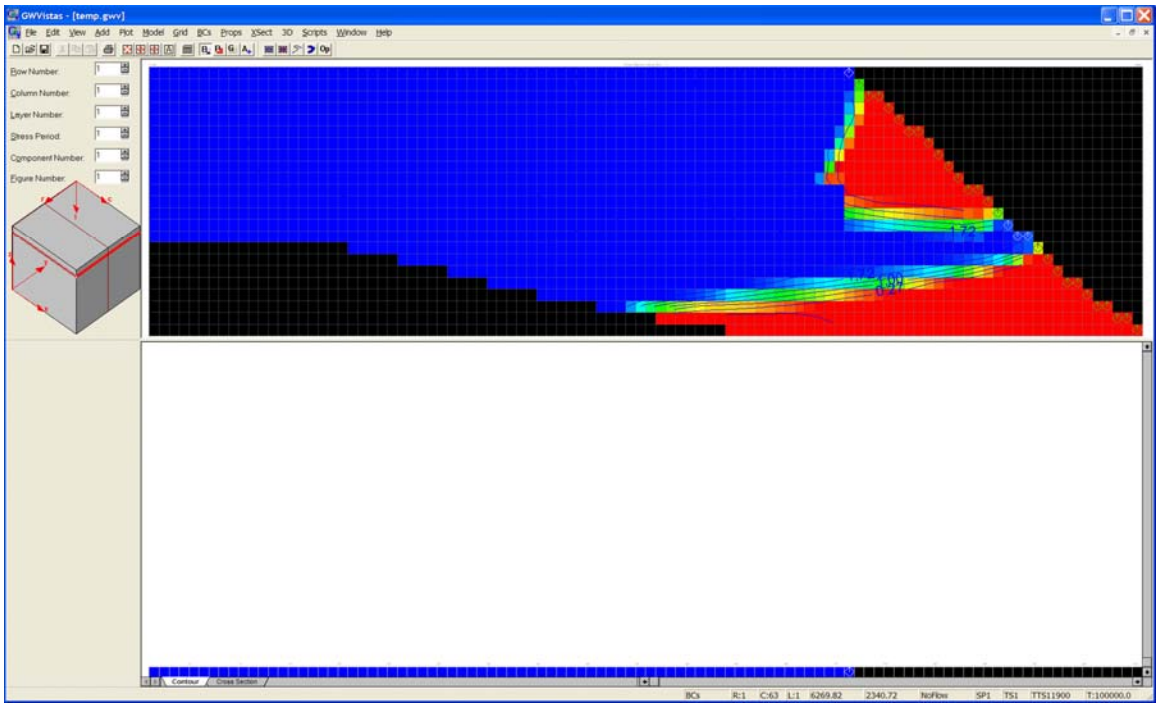
7. Import the model results into GWV by select **Plot>Import Results**.



8. Check both of the browse buttons next to Time Step and Transport Time Step and make sure to select the last value in the list. For the Time Step, there should be only one possibility because you have only one MODFLOW timestep.

9. Next, check the import box next to the Concentration File and then click ok. GWV should read the last transport timestep and then plot a color flood of

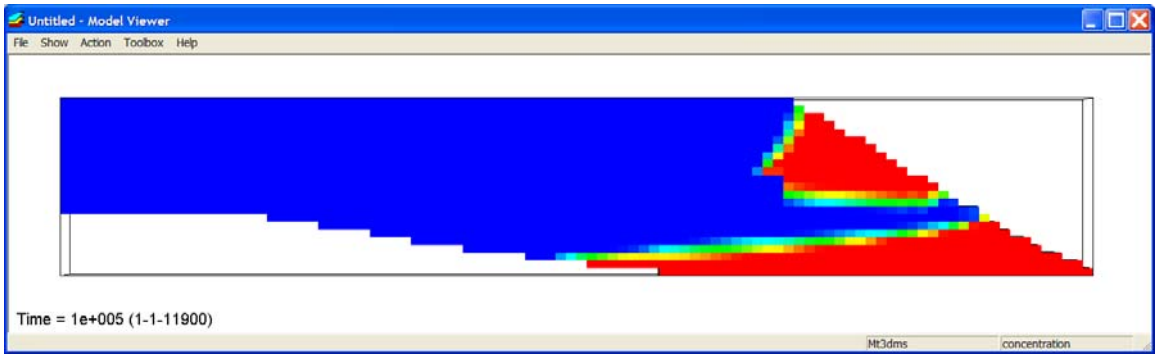
concentrations on your screen.



10. Based on this color flood plot of concentration, what can be said about the level of numerical dispersion? How well does the TVD scheme minimize numerical dispersion for this particular problem?

11. Has this simulation reached equilibrium?

12. Use Modelviewer to watch an animation of groundwater salinity for this simulation.



IC. Evaluate transport solution schemes and parameters to determine compromise between accuracy and efficiency

The simulation in IA was performed using TVD with a specified Courant number of 0.5. Although the IA simulation took a while to run, the results can be considered highly accurate. The purpose of this analysis is to change some of the simulation parameters, and then compare the results with simulation IA.

1. Go into the folder ***SWI_IC*** and open the GWV file called ***SWI_IC.gwv***. This file should be the same as the file that you ended up with in IA.

2. Check the **Model>Paths to Models** option, and make sure the working directory has been set to ***SWI_IC***.

3. Go to **Model>MT3D/RT3D>General Options** and click on the **Advection** tab. As a user of SEAWAT, you will spend a lot of time modifying the parameters under this **Advection** tab and the parameters under the **Time Stepping** tab.

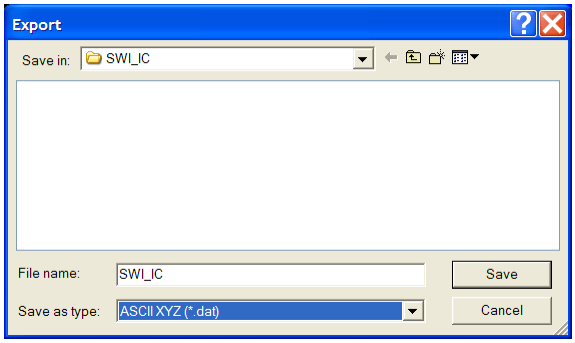
4. Change the specified Courant number from 0.5 to 1.0 and click ok. Now, create the data sets (**Model>SEAWAT>Create Datasets**) and run the simulation (double-click on the ***swt_v4.bat*** file in the ***SWI_IC***). Can you tell what happened?

5. Next, go back to that same **Advection** tab, and try changing the Courant number to 0.75. Recreate the SEAWAT data sets and run the model. Record the length of time to run the simulation. Did it run faster or slower than the simulation in IA?

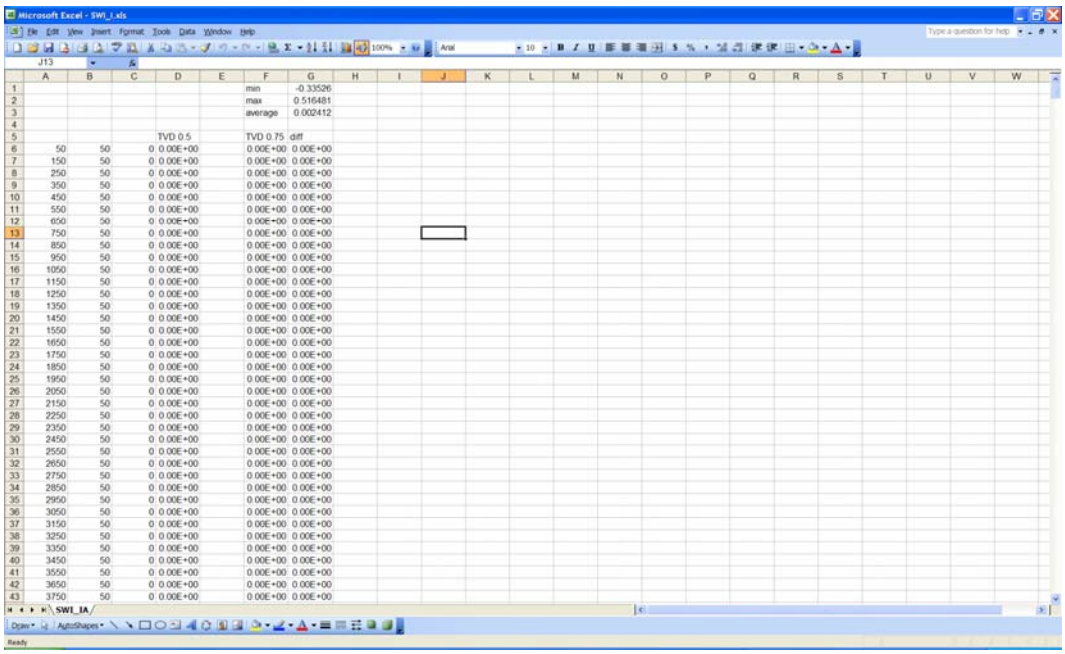
6. How different are the results from this simulation compared to the results from the simulation in IA? The first thing to do is to import the results from this simulation into GWV by selecting **Plot>Import Results**. Make sure to browse to

the last time step and transport timestep and also to check the import box next to the concentration file.

7. Next go to **File>Export** and create the same type of ASCII file that you made in IA, which means that you need to select concentration as the Data Type to Export in the following dialog box.



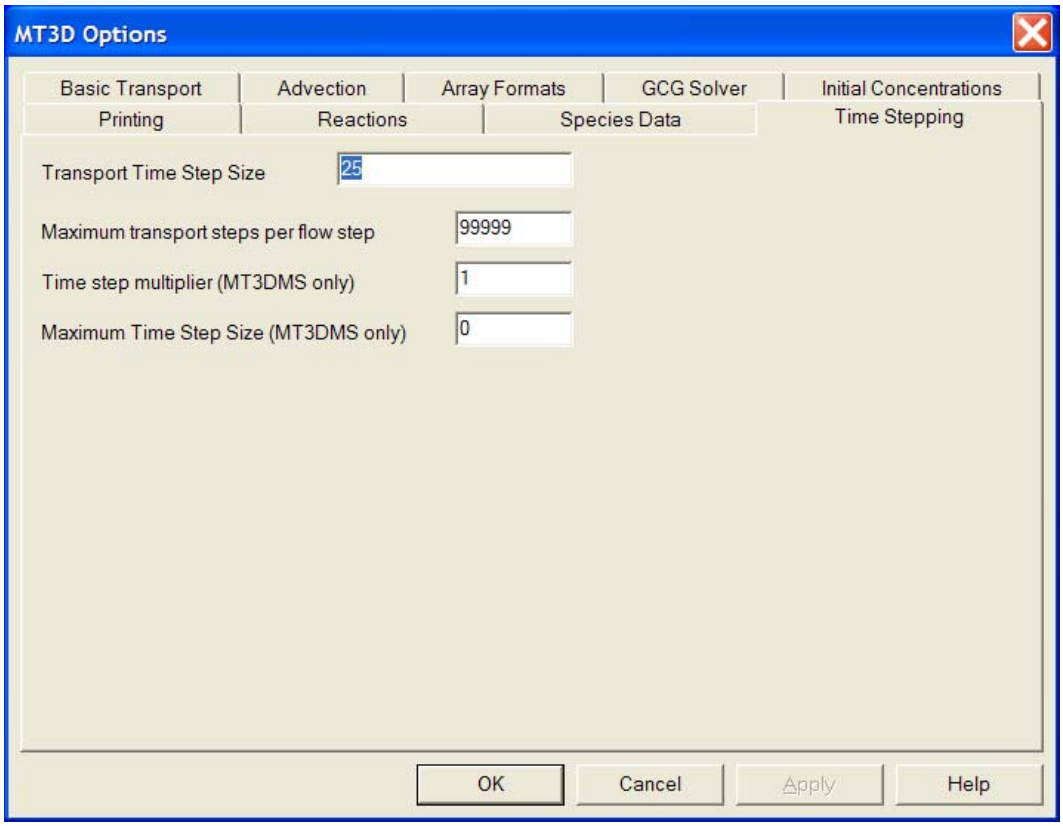
8. In folder ***SWI_IA***, you should have a file called ***SWI_IA.dat***, and in folder ***SWI_IC***, you should now have a file called ***SWI_IC.dat***. Now import both of these files into Excel and calculate the minimum, maximum, and average concentration difference for the active model cells. Your spreadsheet should look something like the following:



9. Save this spreadsheet as ***SWI.xls*** in the ***SWI_IC*** folder.

10. For the next simulation, try using the finite-difference solver (with upstream weighting) for transport, but specify a constant transport time step length of 25 days. This is done by going to the **Advection** tab again and changing the solution scheme to finite difference. Because we'll be specifying the transport time step length, the specified Courant number will not matter.

11. Now click on the Time Stepping tab and set the parameters according to the following:



12. Now recreate the datasets and rerun the simulation. Was it faster than previous simulations? How many transport time steps did it take?

13. Import the results into GWV and then export the ASCII file again and import the concentrations into the ***SWI.xls*** spreadsheet. How different are the concentrations

when using the finite-difference solver? Is this an acceptable compromise between accuracy and efficiency?

14. If time permits, try experimenting with the different solver parameters. How fast can you get the simulation to run?

ID. Simulate age as a second species

SEAWAT is also capable of simulating age another species in the model. This can aid when having groundwater observations which include age data. The purpose of the following problem is to show how age can be simulated.

1. Go into the folder SWI_ID and open the GWV file called SWI_ID.gwv. This file should be the same as the file that you ended up with in IC.

2. Check the **Model>Paths to Models** option, and make sure the working directory has been set to ***SWI_ID***.

3. Go to **Model>MT3D/RT3D>Packages,** and click the 2 boxes to **Include** and **Create** the Reactions (RCT) package.

4. Next we need to tell MT3D that we want to simulate two species. Go to **Model>MT3D/RT3D>MT3DMS Options,** change the "Number of Components" to 2, change the "Number of Mobile Components" to 2. Then click the boxes next to "Store Recharge Concentrations for All Components" and "Store Initial Concentrations for All Components".

5. Go to **Model>MT3D/RT3D>General Options** and click on the **Reactions** tab. For "Type of Sorption Simulated" enter in "No sorption". For Type of Rate Reaction we want a “Zero-Order Decay” reaction. This will set up the reactions package very close to what you will need, but manual changes have to be made to simulate age.

6. Create the SEAWAT datasets.

7. I have already created a modified version of the reaction package called "SWI_ID_mod.rct". Open this package and compare it to "SWI_ID.rct" that was created by GWVistas.

8. Note at the top, that there is a 100 on the first line of both files. This 100 can be found in the **MT3DMS Supplimental User's Guide** and is the flag that tells SEAWAT it is a zeroth-order reaction (as opposed to first order or no reaction at all). (Find the MT3DMS Supplimental User's Guide and find the information listed on a zeroth-order reaction)

9. Scroll down and note that there is **a -1.000e+00** before the "1st Order Constant for Component 2" in the modified reactions package (as opposed to a zero in the package created by Vistas). This negative one is the rate coefficient and signifies that 'production' will be occurring at a zeroth order.

10. What we have done is created a reactions package that will track the movement of water with time. All the water in the simulation begins with an age of zero days. As the water moves in the simulation, its age is simulated daily (which is the time measurement of our model).

11. Before we can run SEAWAT, we need to make sure we are using the new reactions package created. This is done by modifying the name file and the batch file (I have done this already). Open SWI_ID.nam and SWI_ID_mod.nam and compare the two. Note the name for the reactions package has been altered in the modified version of the name file. Why is it important to change the name of the Name file to something other than what is created by GWVistas?

12. Open the batch file and make sure the executable is running SWI_ID_mod.nam.

13. Run the model.

14. How long did it take to run? Was the run time longer than the model run in SWI_IC? What made the difference?

15. Import the results into Vistas, however this time import MT3D002.ucn. This is the second species representing age. You will likely have to change the color flood options to view the data. Go to **Plot>Color Flood Options** and change the maximum range to 100,000 which is the length of our model. Click "OK".

16. Go to **Plot>What to Display,** and Display Contours of Concentration instead of Contours of Head.

17. Now, when you look at the results, the oldest water is in red, and the youngest water in blue. If you put your cursor in the model, the age where the cursor is can be seen at the bottom. This number changes as you move the cursor. If you put your cursor over the red areas you will see the age is close to 100,000.

18. Where is the oldest water in the model? What is happening in the confining unit? Why do you think this occurs?

19. Can you think of other times when you might have to manually change a package and create a new name file? This is an important step to learn in modeling as GUI's cannot do everything for us. We always need to be able to alter things and refer to a manual to aid us. Even though Vistas could have been used to create the reactions package, this example provides us guidance on how to modify things ourselves.

IE. Using PEST to calibrate the model

After the cross-sectional model was developed, data was "discovered" from 1998 in boxes from a warehouse that belonged to the city. Data exist from 7 monitoring wells in the area. The data included water-levels, salinities, and age data from isotopes (tritium-helium) from 1998. Regression is used to determine what information is provided by the data about the system.

There are a number of automated calibration programs that can aid in model calibration. PEST (by John Doherty) is a powerful calibration tool. It uses observations from the field and compares them with simulated results (the different between the field observations and simulated observations is considered the residual). PEST will run the model over and over changing parameters in an attempt to minimize the residuals (find the best fit between the simulated results and observed field data). To simplify things (and because this is not a PEST course), I have prepared everything for you to do the parameter estimation. However, I will take you through some of the files and steps to help better comprehension.

1. Go into the folder ***SWI_IE*** and open the GWV file called ***SWI_IE.gwv***.

2. Check the **Model>Paths to Models** option, and make sure the working directory has been set to ***SWI_IE***.

3. This file should be approximately the same as the file that you ended up with in ***SWI_ID***, however the length of the model has been decreased to 45,000 days from 200,000 days and the transport time step size has been increased to 50 from 25. I have also altered the file to include the heads and concentrations from the previous run in SWI_IE.

4. Go to **Model>MODFLOW>Package Options,** then click on the tab "Initial Heads". Note where the Initial Head Location says "Read Heads Directly from binary head-save file". The file name below is browsed to the location

where the SWI_IE_orig.hds, the Stress Period and Time Step are both set to 1. That is because we only have 1 stress period and time step in the Modflow portion of our SEAWAT model.

5. Go to **Model>MT3D/RT3D>General Options** and click on the "Initial Concentrations" tab. Note the box is checked "Set Initial Concentrations from Binary File", then the Concentration file name is browsed to SWI_IE_orig.UCN. Note that the Transport Time Step size is 4000. That means we want to import concentrations for that time step. Where did the 4000 come from? Why use that number as opposed to a different number?

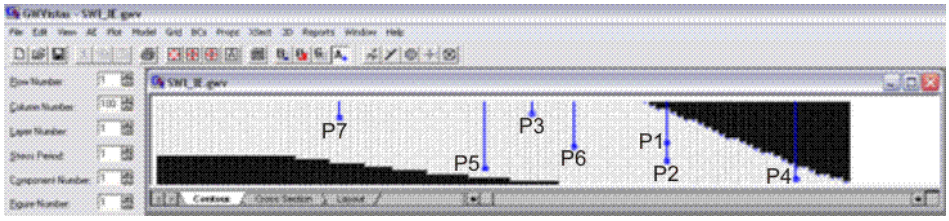
6. The names of the *.hds and *.UCN files were manually changed, therefore when subsequent runs are done, these two imported files will not be written over by the output of those subsequent runs.

7. What is the purpose of changing the initial heads and concentrations? What is the purpose of changing the run time from 200,000 days to 45,000 days?

8. This version of the model has all the new monitoring wells put in as target or well observations. If you view a cross section in the Vistas file, you can observe the different target observations as blue lines running vertically representing the wells.

Table 2. Data for each well

Well	Date	Water Level (ft)	Age (years)	Concentrations (mg/l)
P1	2/24/1998	0.77	88.98	19.00
P2	2/24/1998	2.17	100.61	1.74
P3	2/24/1998	2.12	38.52	0
P4	2/24/1998	0.00	8.03	35.00
P5	2/24/1998	2.43	78.45	0
P6	2/24/1998	1.98	109.1	0
P7	2/24/1998	3.17	32.43	0



9. Our model is run for 45,000 days, or just a little over 123 years. We have a start date of our model for: 1/1/1875 and ending in March of 1998. Therefore, our observations fall near the end of our model run.

10. All the files to run PEST are set up in the SWI_IE folder. The "Pest Control File" is SWI_IE.pst. This file is the overall control for the parameter estimation run process. It contains information on which parameters we want to estimate, what our observations are, the weights of those observations, etc...

11. Open SWI_IE.pst in the text editor. Upon first look, it is overwhelming, but we will "skip" to what's important for our process. (as a side note, John Doherty has developed a number of utilities, one of those utilities creates a *.pst file for you, as well as other files needed in the optimization process)

12. Go down to the line that says "* parameter data". There are 7 parameters listed under parameter data. We can estimate these parameters, tie the parameters to one another, or fix them so they don't change.

-*shall_hk*, is the horizontal hydraulic conductivity of the shallow aquifer

-*shall_vk* is the vertical hydraulic conductivity of the shallow aquifer.

-*deep_hk* is the horzontal hydraulic conductivity of the deep aquifer

-*deep_vk* is the vertical hydraulic conductivity of the deep aquifer

-*confine* is the vertical and horizontal hydraulic conductivity of the confining unit

-*dsp* is dispersivity of all the layers in the model

-*porosity* is porosity of all the layers in the model

13. For our simulation we have decided to estimate the horizontal hydraulic conductivity of the shallow and deep aquifers. These two parameters have "log" next to them. They are log transformed in this model.

14. The vertical hydraulic conductivities are tied to the horizontal hydraulic conductivities. The tied parameter means that the ratio from horizontal to vertical hydraulic conductivity will remain the same when PEST changes the horizontal hydraulic conductivity.

15. We have fixed the confining unit, the dispersivity, and the porosity. However, if we have problems calibrating the model, we might decide to add these parameters to the estimation process later, that's why they are included now. It's easier to put them in and fix them now, than to create a new *.pst file later on if we decide we want to add them to the estimation process.

16. Column 4 next to the parameters listed, contains the starting value for each parameter, these are the starting values you have been using in your model up to this point.

17. The following two columns (5 & 6) contain the range of values from low to high, respectively. We think we have a decent idea of the hydraulic conductivities for these two aquifers so we put in a reasonable range.

18. Go down to the line that says "* observation data". This is where our observations are placed in the model. You can see the heads, concentrations, and age here. The third column contains the weights for each observation. Why do you think the weights are different for the heads, concentrations, and age? What is the purpose of this?

19. Beneath the observation data is the "* model command line" which runs SEAWAT. When doing an automated parameter estimation process, the model is run within PEST. Why do you think this is?

20. Open the modified name file (SWI_IE_mod.nam) that SEAWAT uses and note that some of the file names have changed even though we have all of the same packages. Why do you think that is?

21. Next in the PEST control file comes the "* model input/output". These are template files that mirror some of the input files in our model. Note that the files modified in the name file are the ones seen here. Open SWI_IE_modlpf.tpl. Open SWI_IE_mod.lpf. Compare the two files. What is the difference between the two? What do you think PEST is doing with these different files.

22. After the template file are the instruction files (*.ins). These are the files created that read simulated observations from the model and compare them to the measured observations listed above in the PEST control file. Open head.ins and modeled_hd.smp. Can you see where the instruction file directs PEST to read numbers from the output file, modeled_hd.smp?

23. We will now run PEST. In the SWI_IE folder you should see an icon for a command promp (a dos window) that looks like this: 

. Double-click on this prompt and a black dos window will show up. In that window type**: ..\..\exe\pest swi_ie.pst.**

24. PEST will begin running. Take a little break because this will take a few minutes.

25. When you sit back down go ahead and open the swi_ie.rec file. Even if the model is still running, you should still be able to open this file. This is one of the main PEST output files that sums everything up for you.

26. If you start reading this file from the beginning, you can note the "Number of parameters : 7" and the "Number of adjustable parameters : 2".

27. It will print out much of model input information. Scroll down to "OPTIMIZATION RECORD". This gives you information on optimization of the model.

28. Note beneath the optimization record:

INITIAL CONDITIONS:

Sum of squared weighted residuals (ie phi) = 3000.0

Contribution to phi from observation group "heads" = 1000.0

Contribution to phi from observation group "conc" = 1000.0

Contribution to phi from observation group "age" = 1000.0

Current parameter values

shall_hk 100.000

shall_vk 1.00000

deep_hk 2000.00

deep_vk 200.000

confine 1.000000E-03

dsp 10.0000

porosity 0.200000

29. This information is very important in the optimization process. The Sum of squared weighted residuals (i.e. phi) is also referred to as the objective function. Right now it is 3000. This number is a measure of how close the measured observations from the field are to the modeled observations. The values listed below that are how much is contributed from each observation group. Is it an accident that each contribute 1000 to phi? Could this be related to the weights in the control file? As PEST continues to optimize, the objective function (or phi) should get smaller. Which means, as the regression changes the parameter values, the difference between the measured observations from the field and the simulated observations should get smaller. If you are ever optimizing a model, and the objective function is not falling, there is a problem with the optimization process or your model.

30. Scroll down to "OPTIMISATION ITERATION NO. : 2". What is the objective function now?

31. Scroll down to the "Current parameter values" and the "Previous parameter values". What are the values of the horizontal and vertical hydraulic conductivities of the shallow and deep aquifer? Are they rising or falling from your original values?

32. The optimization should cease after 5 regression iterations. What is the final objective function from "OPTIMIZATION ITERATION NO. : 5"? What are your final parameter values? They should be close to what is seen in Table 3. These are the parameters we will use in the "new" calibrated model in the following exercises.

Table 3: Parameters used in the calibrated model. For the two estimated KH parameters and associated tied KV parameters, the starting values are shown in parentheses.

Unit	K_H (m/d)	K_V (m/d)	S (-)	S_y (-)	n (-)	α_L (m)	α_T (m)
Shallow Aquifer	50 (100)	0.5 (1.0)	1×10^{-5}	0.2	0.2	10	1
Confining Unit	0.001	0.001	1×10^{-5}	0.2	0.2	10	1
Deep Aquifer	1000 (2000)	100 (200)	1×10^{-5}	0.2	0.2	10	1

Exercise 8. SWI Part II. Design and run a 3D model to determine the effects of groundwater pumping on saltwater interface movement

In this part of the exercise, you will determine if the recommended pumping rate can be sustained without exceeding the chloride drinking water standard of 250 mg/L. The general procedure for this exercise will be to convert the calibrated model from SWI_IE into a 3D model, and then perform simulations with and without pumping.

IIA. Convert the calibrated model into a 3D model of the study area

The first step here is to set the initial heads and concentrations for the 3D model using the results from a previous 2D simulation. Then, convert the 2D model into a 3D model. Lastly, perform a simulation without pumping to verify that the initial concentrations and heads are at equilibrium for the 3D situation. The last step is optional, however, it is good practice to ensure that the conversion from 2D to 3D occurred without error.

1. We want to use a model similar to what you created in SWI_IA for the 3-D model. However, we need to re-run SWI_IA with the new hydraulic conductivities from Table 3 to get heads and concentrations for this run (We are not going to simulate age as a 2nd species since model calibration has been done and the 2nd species increases model run time. Age can always be added back in at a later time.)

2. Go back to your SWI_IA directory and open the GWVistas file. Go to **Props** and select **Hydraulic Conductivity**. Then go into the database, Db, and change the Kx and Ky for zone 1 (shallow aquifer), to 50 (from 100). Change the Kz for zone 1 to 0.5 (from 1).

3. Now change the Kx and Ky for zone 3 (deep aquifer) to 1000 (from 2000), and change the Kz to 100 (from 200).

4. Now, create your datasets and run SEAWAT (make sure the model reaches equilibrium).

5. The GWV file you have now created in exercise IA has been copied into the subdirectory ***SWI_IIA*** and has been renamed as ***SWI_IIA.gwv***. The root name for the files has also been changed from ***SWI_IA*** to ***SWI_IIA*** to maintain consistency.

6. Open the file ***SWI_IIA.gwv*** and set the **Model>Paths to Models**.

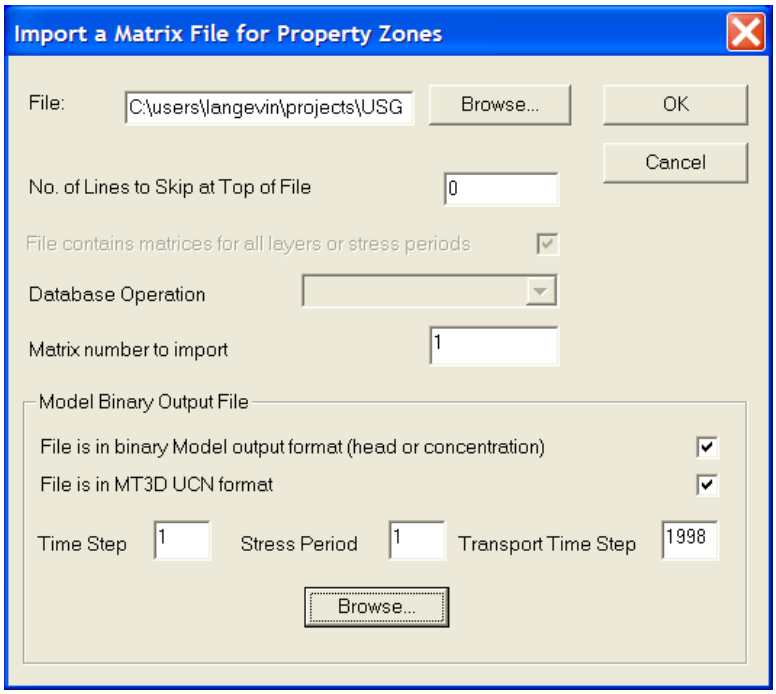
7. The first thing we want to do is set the initial concentrations of the 3D model to the concentrations from the last transport time step of the simulation performed in SWI_IA.

8. First, go to **Props>Initial Concentrations**.

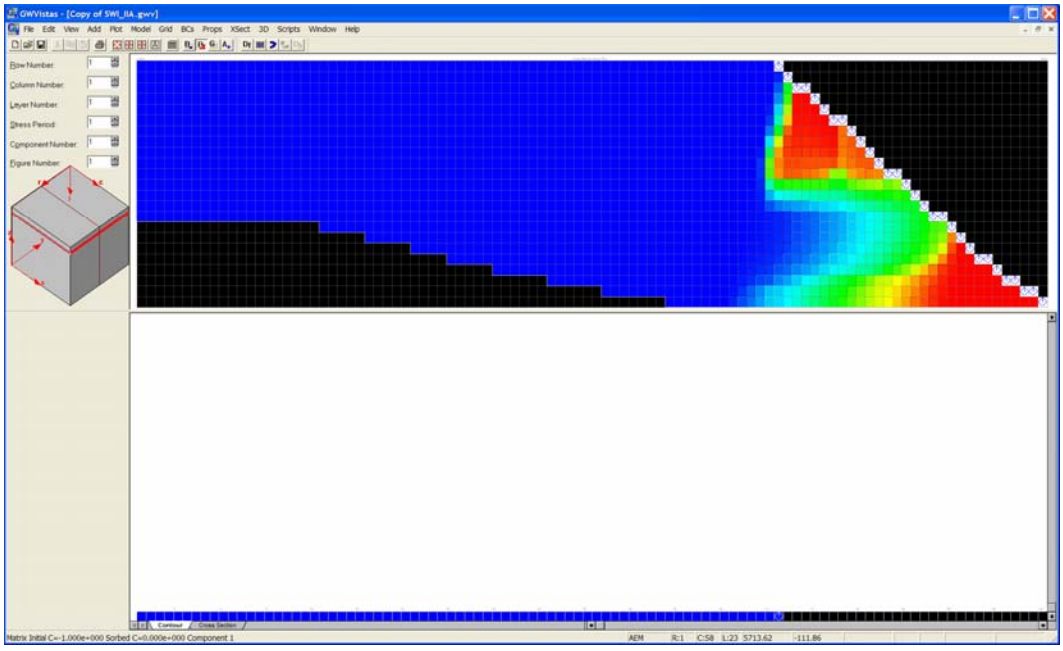
9. Next, go to **Props>Options** and check the Use Matrices option for Initial Concentrations. Note that this option is already set for Initial Heads. This allows us to work with the initial concentrations in a spreadsheet-like editor as opposed to using zone numbers and a zone data base.

10. Now we will use the matrix import utility to read in the concentrations from the ***mt3d001.ucn*** file that was created during the simulation in SWI_IA. The way to do this is to go to **Props>Import>Matrix**. The first thing you do in this window is browse to the ***mt3d001.ucn*** file that you created in IA. Note that you will have set the file type on the bottom of the browse window to "Concentration File (*.ucn)". Next, check the box that says "File is in binary Model output format (head or concentration)". Now check the box that says "File is in MT3D UCN format." Lastly, click the browse button and select the last transport timestep in the ucn file (it should probably be transport timestep 20208). When your window

looks like the following, then click OK.



11. After you click OK, GWV should set the initial concentrations to the last transport time step of simulation IA. If the procedure worked correctly, your GWV window will look like the following:



12. Follow the same procedure for Initial Heads, except import the file SWI_IA.hds and do not check the box next to "File is in MT3D UCN format."

13. Now what we want to do is convert the 2D model into a 3D model with 100 rows. Unfortunately, there is not an easy way to do this task. Perhaps the easiest way is to zoom in on one of the rows and manually divide the row into 100 rows. This is done by going to **Grid>Insert Row**, and clicking the "G" button on the GWV toolbar if it is not already depressed. Then, each time you right-click on the cell, the row will be split in half. As you add more rows, it becomes more difficult to divide them. After a while, you will need to **select Grid>Uniform>Row Spacing** and set the value to 100. This will spread the rows out and allow you to continue adding rows. When you have reached 100 rows (you can check by putting the mouse on the bottom row and noting the row number), set the uniform row spacing one last time to 100. Understandably, this is a frustrating process, but by doing so, the boundary conditions, aquifer properties, and all the model parameters will retain their appropriate values.

14. For the 3D simulation, use a simulation period of 20 years (7300 days). This value is set under **Model>MODFLOW>Stress Period Setup**. Change the value from 2000 to 7300 days.

15. In order to speed up the simulation, and based on our analysis of the different transport solvers for the 2D problem, use the finite-difference transport solver with a specified transport time step length of 25 days.

16. If time permits, try running this simulation without the pumping well to ensure that the initial concentrations and heads do not change with time. Note, however, that the heads and concentrations may change slightly due to the fact that we are using a different solver. If the simulation takes too long, you may copy the model results from the **results** folder into the **SWI_IIA** folder.

17. Does a graph of the total mass in the aquifer versus time indicate that the initial concentrations and heads are at equilibrium?

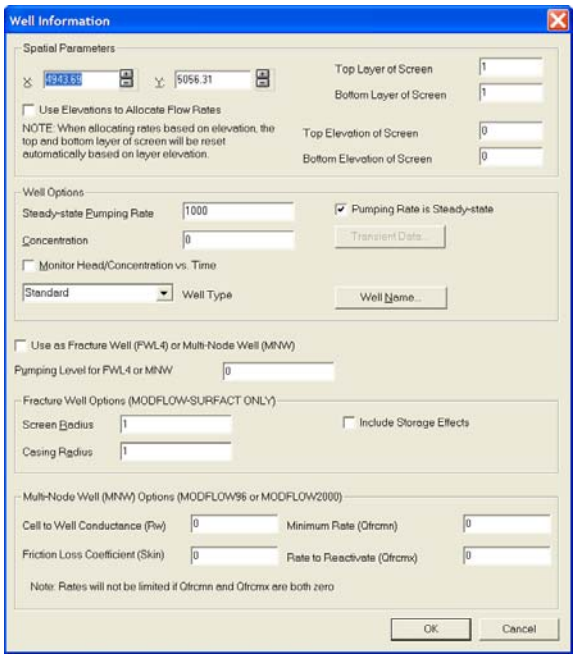
IIB. Evaluate the effects of saltwater intrusion in response to groundwater withdrawal

The city has determined that they would like to capture about 25% of the groundwater recharge. In this part of the exercise, you will perform a simulation to determine if the drinking water standard for chloride would be violated with this withdrawal rate. Your simulation period will remain at 20 years, as the city's water supply plan only focuses on the next 20 years.

1. The file you created in exercise IIA has been copied into the subdirectory ***SWI_IIB*** and has been renamed as ***SWI_IIB.gwv***. The root name for the files has also been changed from ***SWI_IIA*** to ***SWI_IIB*** to maintain consistency.

2. Open the file ***SWI_IIB.gwv*** and set the **Model>Paths to Models**.

3. Add a pumping well to row 50, column 50 and layer 20. There are several ways to do this, but here we will use the GWV-created ability to add the well as an analytic element. Go to **AE>Well** and click on cell (50, 50). You should see the following window:



4. Set the top layer and bottom layer of screen to 20.

5. The recharge rate for our area is about 25 cm/yr, and the total land area is 10 km by 7 km. If we want to try and intercept 25% of the recharge, then what pumping rate should we assign? (Hint: go into the GWV file **Model> MT3D/RT3D >General Options** and look under the **Basic Transport** tab to see the model units. Pumping rates should be calculated in the same units in a volume over time). What should the sign of the pumping rate be? Assign this value to the "Steady-State Pumping Rate" box.

6. In order to record the concentration in cell (20, 50, 50), check the box next to "Monitor Head/Concentration Versus Time" and then click OK. This will save the concentration in that cell using the observation feature in MT3DMS.

7. If you ever want to edit this pumping rate, you can scroll down to layer 20, click the "A" button on the GWV toolbar, and double-click on the analytical well. Another option is to click **Edit>Analytic Element List** and double click on the desired feature to edit.

8. Create the SEAWAT data sets and run the model with the pumping rate set at 25% of the recharge. The simulation may take a while.

9. Concentrations at the well are stored in the file ***mt3d001.obs***. This file contains the concentration in cell (20, 50, 50) for each transport time step. Note that this concentration is in total dissolved solids (TDS). Import this file into Excel and prepare a graph of chloride concentration versus time. You will be able to make the conversion by assuming the chloride concentration in seawater is about 19,000 mg/L. Note that the TDS of seawater is about 35 g/L (the concentration value assigned to the ocean boundary). After 20 years of pumping, has the drinking water limit for chloride been violated?

10. What was the approximate inland migration rate of the 250 mg/L isochlor at the base of the deep aquifer during the 20 years of pumping?

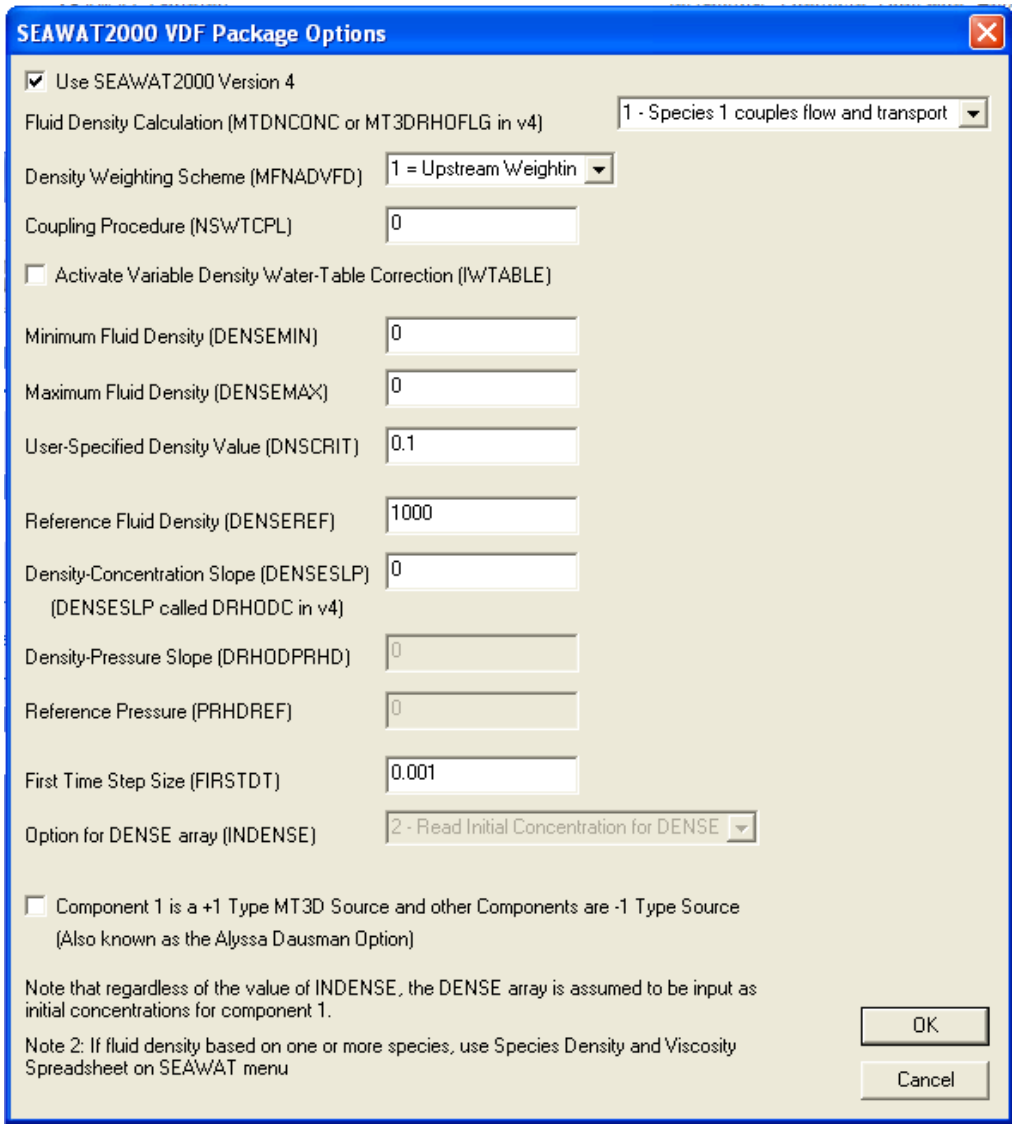
IIC. Evaluate the sensitivity of model results to density dependence

It is difficult to determine *a priori* whether or not density variations are necessary to incorporate in a simulation of coastal groundwater flow. The purpose of this analysis is to shut off the variable density component in SEAWAT and quantify the effects on the simulated concentration in cell (20, 50, 50) and on the water budget. There are three ways to perform a simulation where the density effects are neglected: (1) make the DENSESLP equal to zero, (2) remove the vdf package from the simulation, and (3) use MODFLOW and MT3DMS. We will try the first two here. Prior to performing the simulations, think about what you might expect to happen in a constant-density simulation of our saltwater intrusion problem.

1. The file you created in exercise IIB has been copied into the subdirectory ***SWI_IIC*** and has been renamed as ***SWI_IIC.gwv***. The root name for the files has also been changed from ***SWI_IIB*** to ***SWI_IIC*** to maintain consistency.

2. Open the file ***SWI_IIC.gwv*** and set the **Model>Paths to Models**.

3. There are three ways to perform the constant-density simulation with solute transport. The first way is to set the DENSESLP parameter to zero. Why would setting this parameter to zero be equivalent to running a constant density simulation? Set the parameter to zero by going to **Model>SEAWAT>SEAWAT 2000 VDF Options** and set the Density-Concentration Slope to zero.

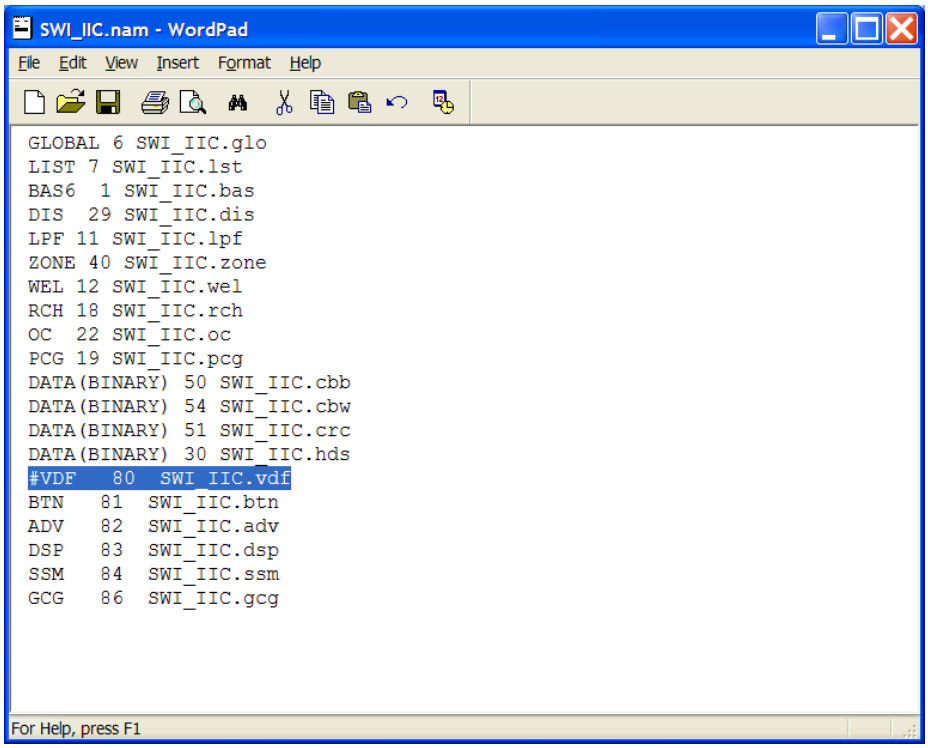


4. Next, create the SEAWAT data sets and run the simulation. When the simulation finishes, compare the simulated concentration at cell (20, 50, 50) with the simulated concentration from IIB. Are the results different? In general, what happens to the solute when density effects are neglected?

5. Rename the output file called ***SWI_IIC.lst*** that you just created so that when you run the next simulation, you won't overwrite this file.

6. Another way to perform a constant-density simulation, just like the previous simulation, is to use the Ground Water Flow (GWF) Process instead of the

Variable-Density Flow (VDF) Process. A simple way to do this is to open the ***SWI_IIC.nam*** file and put a "#" symbol in front of the VDF line. By commenting out this line, the VDF Process is not used, and the simulation defaults to the GWF Process. Make sure you save your changes to the Name file.



7. After you manually modify the Name file, run the simulation again by double-clicking on ***swt_v4.bat*** . Do not recreate the SEAWAT data sets or GWV will overwrite the Name file that you just modified.

8. When the simulation is complete, compare the simulated water budget at the end of the listing file (***SWI_IIC.lst***) with the simulated water budget from the DENSESLP=0 simulation. Why are the values different? And if you make an adjustment for density, why are the numbers not identical, particularly the storage values? Those interested in the answer will find a hint by comparing the flow convergence output for the first transport time step.

Exercise 9. SWI Part III. Determine wellfield protection area

Numerical models, such as the SEAWAT model developed for this exercise, can be used to delineate the recharge areas for groundwater pumping wells. In this exercise, you will use MODPATH to perform forward and backward particle tracking analysis to delineate the recharge area for the city's proposed wellfield. The cell-by-cell flow file that was created during the 20 year pumping simulation from SWI_IIB contains the intercell flows for the entire simulation. Flows from the last transport time step will be used to determine the well-field protection area. By performing this particle tracking analysis, we are assuming that these intercell flows remained constant throughout the simulation. If we wanted to see the effects of transient intercell flows on the particle movement, we would need to rerun the SEAWAT simulation with additional MODFLOW time steps so that the intercell flows could be saved more frequently.

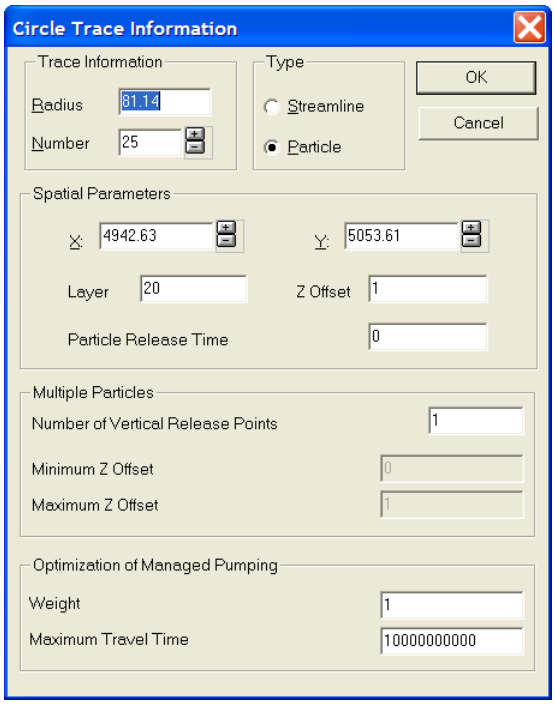
IIIA. Run backward particle-tracking MODPATH simulation

1. The GWV file you should have created in exercise IIB has been copied into the subdirectory ***SWI_IIIA*** and has been renamed as ***SWI_IIIA.gwv***. The root name for the files has also been changed from ***SWI_IIB*** to ***SWI_IIIA*** to maintain consistency. The output files from the SEAWAT simulation in IIB, which are required for particle tracking, have also been copied into the ***SWI_IIIA*** folder.

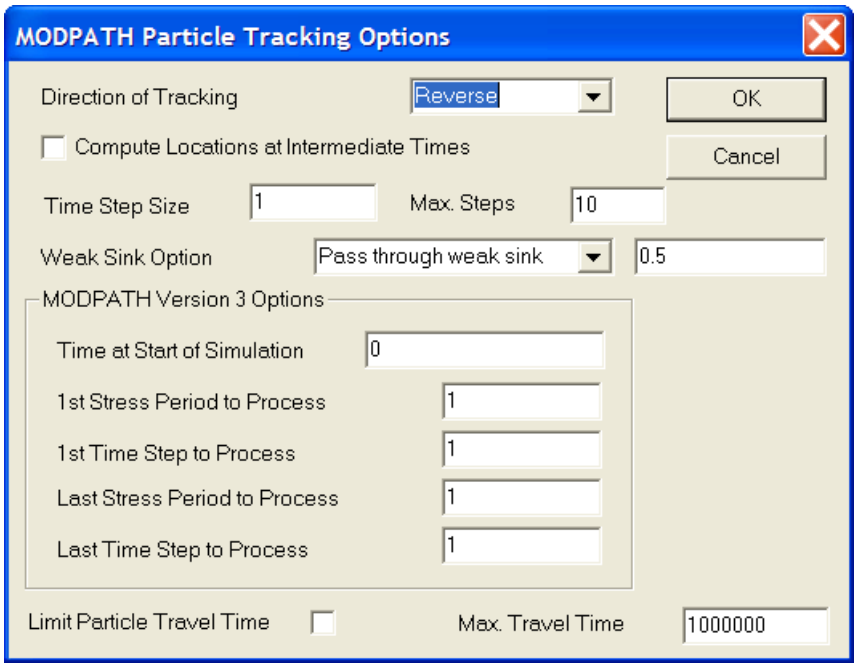
2. Open the file ***SWI_IIIA.gwv*** and set the **Model>Paths to Models**..

3. Scroll down to layer 20 and zoom in on the pumping well. Then, select **AE>Particle>Circle** and drag the circle outward from the center of the cell. Also,

increase the number of particles to 25 or more.

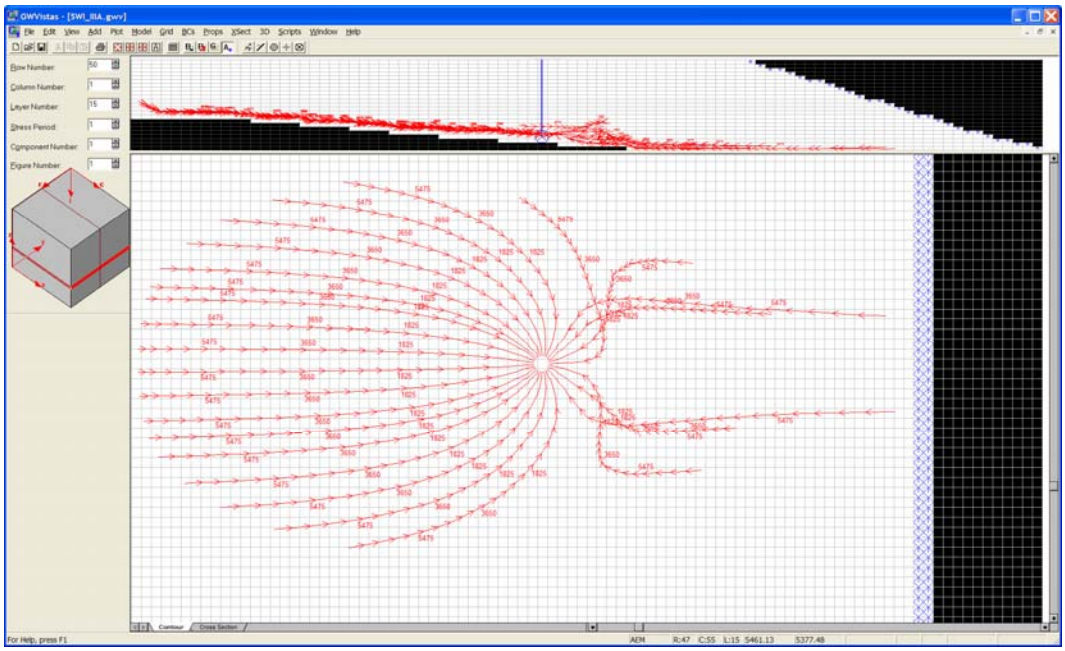


4. Go to **Model>MODPATH>Particle Options** and set the tracking direction to reverse.



5. To run MODPATH, go to **Model>MODPATH>Create Data Sets** and then **Model>MODPATH>Run MODPATH**. If for some reason, MODPATH does not run, check the **Model>Paths to Models** and make sure the path for the MODPATH *.dll is set correcly. (Note the MODPATH dll will be located in the C:\gwv5 subdirectory, or the subdirectory in which you installed GWVistas).

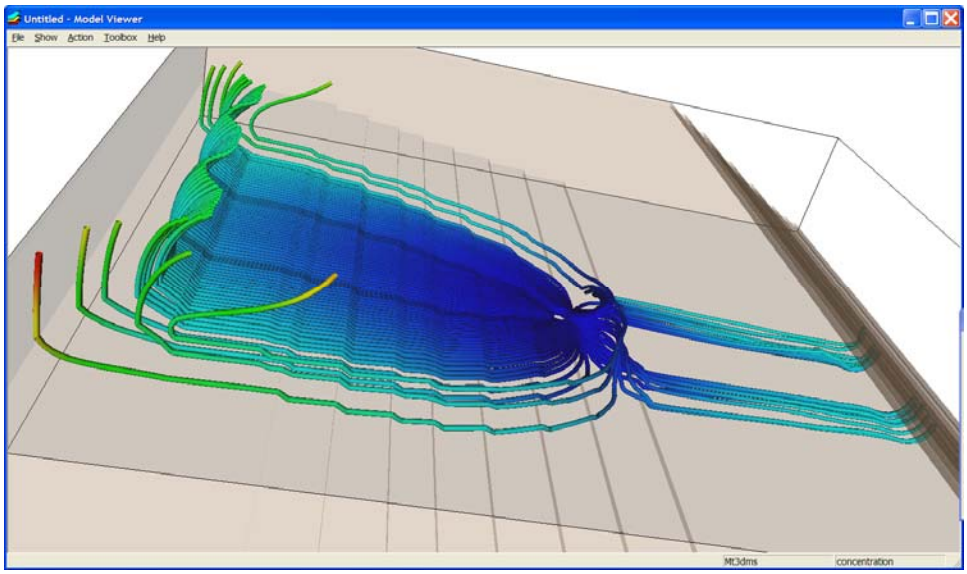
6. When MODPATH finishes, GWV will automatically import the results, if you click yes to the next dialog box. GWV has options for displaying arrows and particle times. These options can be set under **Plot>Particles>Options**. Try experimenting with the different options. You should be able get a view that looks something like the following:



7. You'll notice that MODPATH did not track the particles all the way back to their original recharge locations. This is because the simulation time is set to 20 years. If you increase the simulation time under **Model>MODFLOW>Stress Period Setup**, MODPATH will track the particles back to their original starting locations (if you create the data sets and run MODPATH).

8. Use Modelviewer to prepare a 3D plot of the particle paths (you will need to create the SEAWAT data sets to do this, you need the *.nam file for

Modelviewer, as well as the *.ptl). The following plot was created after MODPATH was run using 100 particles.



9. Is the capture zone clearly delineated?

IIIB. Run forward particle-tracking MODPATH simulation

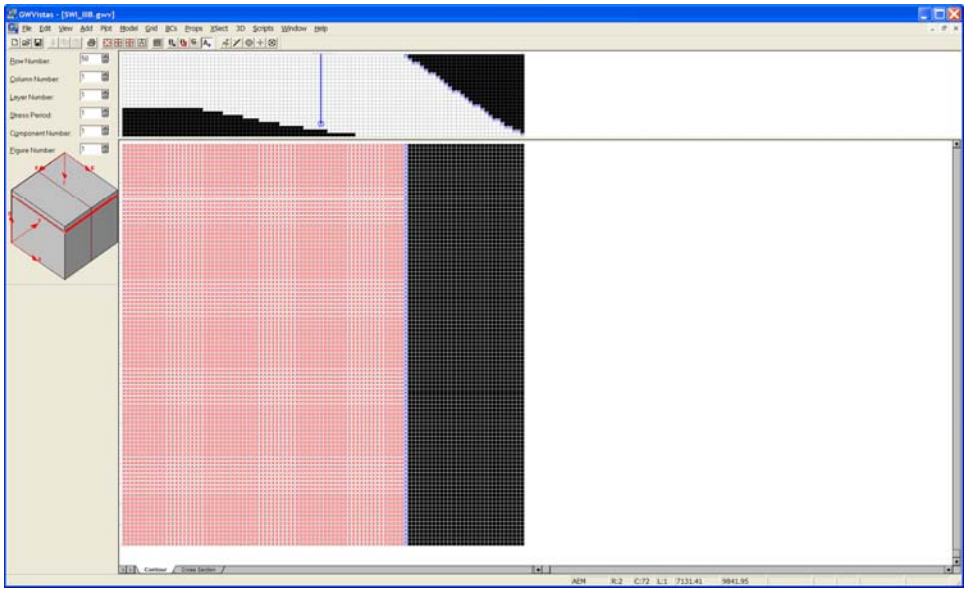
In this MODPATH simulation, place a single particle at the center of each active cell in layer 1. Then run a forward tracking MODPATH simulation to determine the recharge area for the proposed wellfield.

1. The GWV file you should have created in exercise IIB has been copied into the subdirectory ***SWI_IIIB*** and has been renamed as ***SWI_IIIB.gwv***. The root name for the files has also been changed from ***SWI_IIB*** to ***SWI_IIIB*** to maintain consistency. The output files from the SEAWAT simulation in IIB, which are required for particle tracking, have also been copied into the ***SWI_IIIB*** folder.

2. Open the file ***SWI_IIIB.gwv*** and set the **Model>Paths to Models**..

3. Begin by increasing the stress period length to 73000 (200 years)so that all particles will reach their final destination.

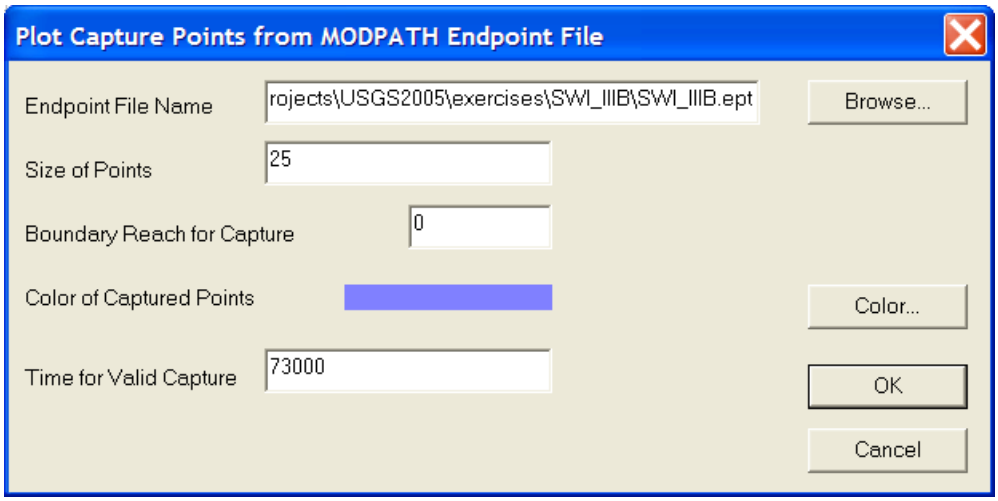
4. To add a particle to every active cell in layer 1, go to **AE>Particle>Window** and draw a box around the entire active area. Trace the box carefully so you do not go outside of the model domain. Then click OK two times. If the procedure was successful, you should see a red particle in every cell.



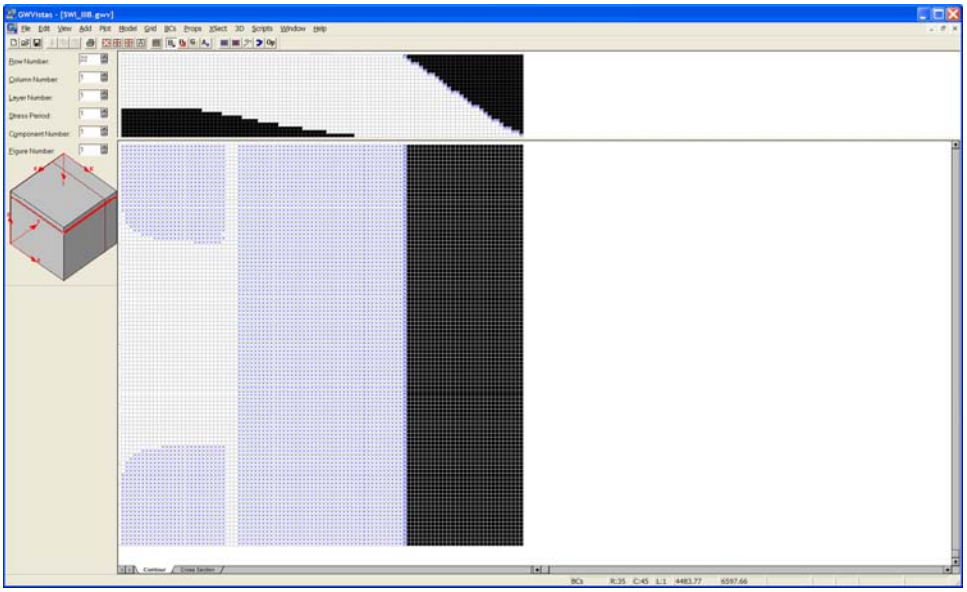
5. Next, go to **Model>MODPATH>Create Datasets** and then **Model>MODPATH>Run MODPATH** and click Open to the pathline file when MODPATH is finished.

6. Now go to **Plot>What to Display** and uncheck the Display Particle Traces box and the Display Particle Starting Locations box and check the Use Endpoint Analysis box.

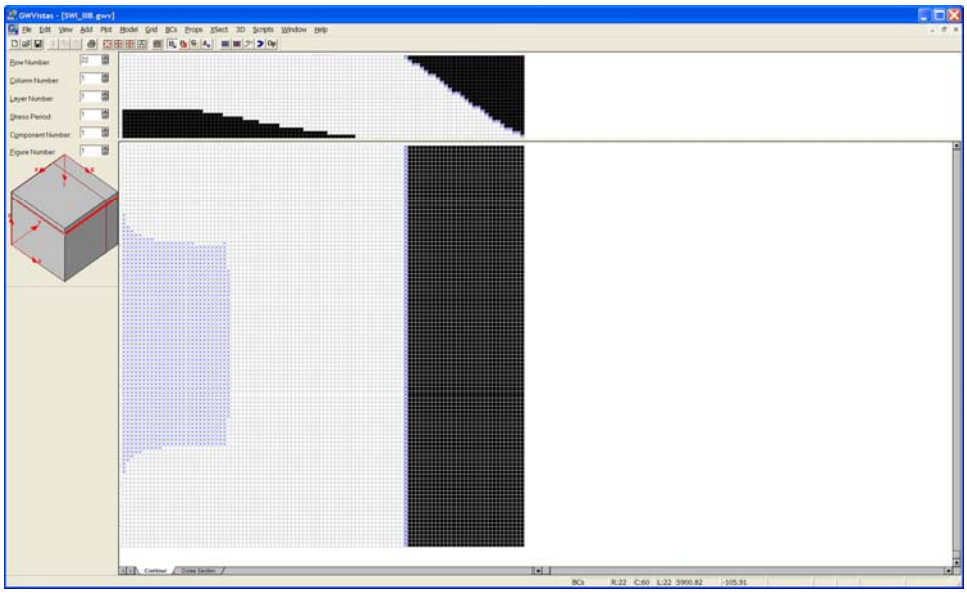
7. Now go to **Plot>Particles>Endpoint Analysis** and fill out the box as follows:



8. If everything worked correctly, you should see the following plot, which shows blue for all the particles that discharged into the ocean and white for all particles captured by the pumping well or perhaps trapped in the confining layer.



9. The wellfield recharge area cannot be shown directly, because the pumping well is represented in GWV using the analytic element feature as opposed to a BC such as the MODFLOW Well Package. By adding a well BC to cell (20, 50, 50) and assigning it a reach other than zero, which is the reach used for the constant head cells, then the endpoint analysis can be performed again to show the true wellfield capture area.



10. Comparison of the last two figures shows that some of the particles remain trapped in the confining unit. Why is there no contribution from the ocean?

Exercise 10. SWI Part IV. Simulation of multi-species solute transport

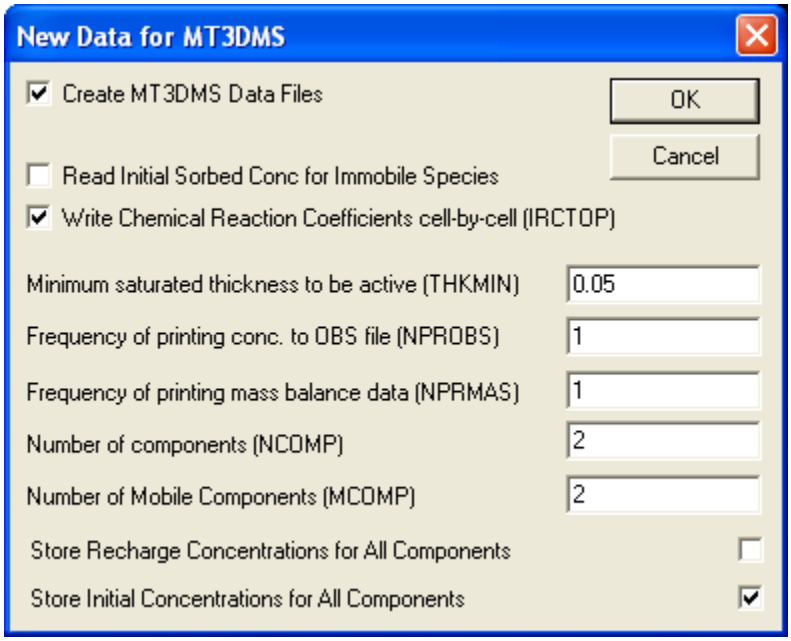
A plume of naturally occurring poor-quality groundwater was detected by monitoring wells in the northwestern part of the study area. The plume is roughly located at the interface between the shallow and deep aquifers. The city is concerned that this poor-quality groundwater could migrate to the wellfield. The results from the particle-tracking simulation suggest that the plume is just outside of the wellfield capture zone, however, particle-tracking analysis is based solely on advection. A multi-species simulation will be performed as part of this exercise to determine if the plume will reach the wellfield within the 20-year period of interest.

IVA. Perform multi-species solute transport simulation using SEAWAT

1. The GWV file created in exercise IIB has been copied into the subdirectory ***SWI_IVA*** and has been renamed as ***SWI_IVA.gwv***. The root name for the files has also been changed from ***SWI_IIB*** to ***SWI_IVA*** to maintain consistency.

2. Open the file ***SWI_IVA.gwv*** and set the **Model>Paths to Models**.

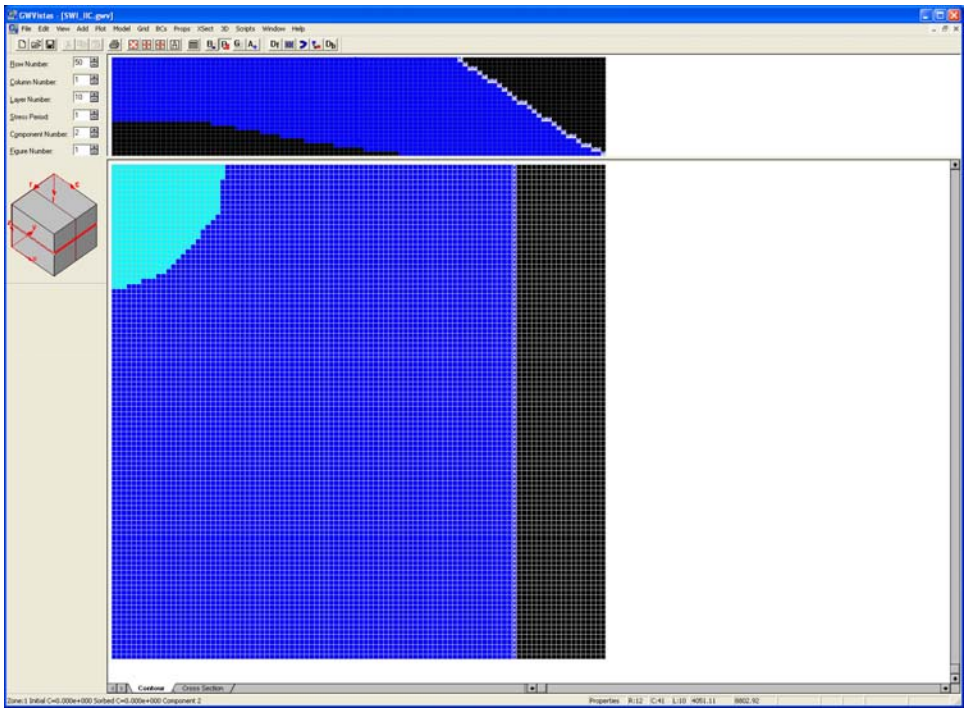
3. The plume of poor-quality water will be tracked as component species number 2. Another species can be added to the simulation by selecting **Model>MT3D/RT3D>MT3DMS Options**. Increase the number of components (NCOMP) and the number of mobile components (MCOMP) to 2. Also, check the box next to "Store Initial Concentrations for All Components." The plume of poor-quality water will be included in the model in the initial concentrations as a discontinuous source. Click "OK".



4. To modify the properties of component number 2 (such as the initial concentrations), change the component number to 2 on the left-hand-side of the GWV window.

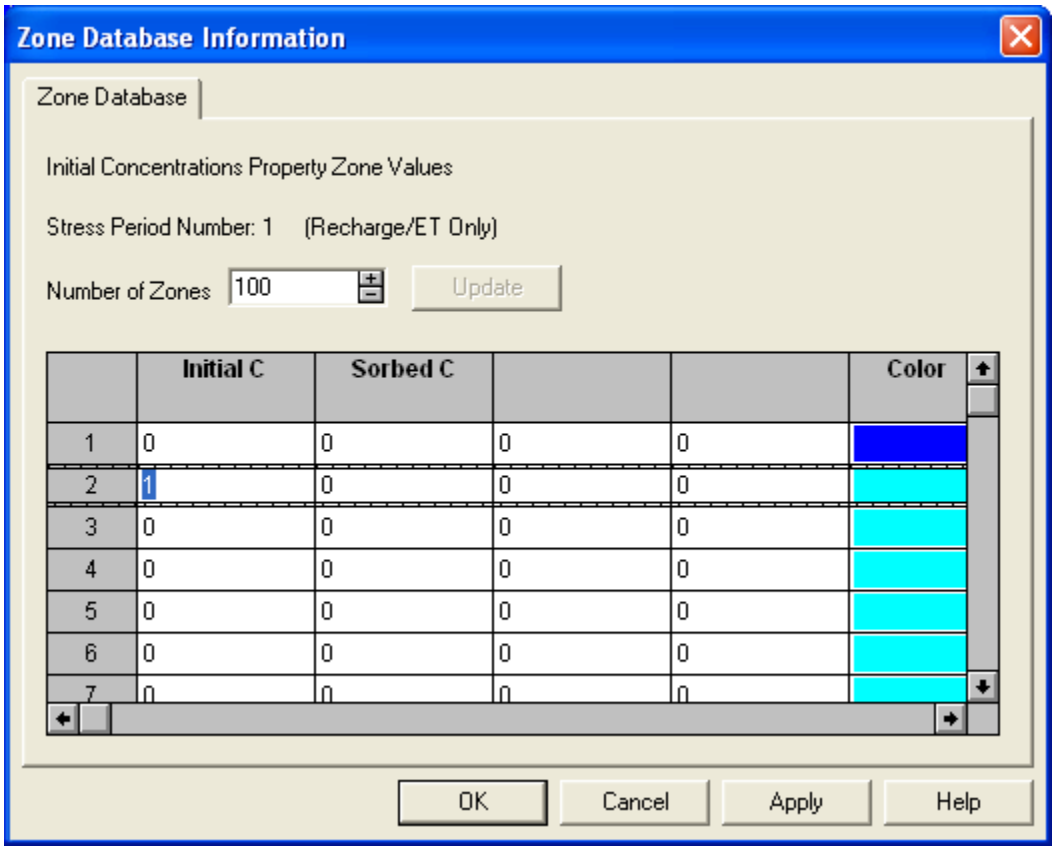
5. Next, go to **Props>Initial Concentrations**. Because you are working with component number 2, you no longer see the initial concentrations of salinity. Instead, you should see that all initial concentrations are zero (by default). To see the initial salinity concentrations, you can simply change the component number.

6. Change the initial concentrations in the northwestern part of the model to represent the plume of poor-quality water. Because the plume is located at the interface between the shallow and deep aquifer, put the plume in layer 10. Make sure you change the layer number to 10. Once you have selected layer number 10 and component 2, and the initial concentrations are checked under the Props menu, use the polygon digitize tool to change the zone number of the northwestern part of the model to 2. The area for the poor-quality water should be roughly traced according to the following figure.



7. Assign a concentration value of 1.0 for zone 2. The value of 1.0 means that the simulated concentrations of component 2 will be the fraction of poor-quality water. To assign the value, go to **Props>Property Values>Database** and change

the initial concentration of zone 2 to 1.0

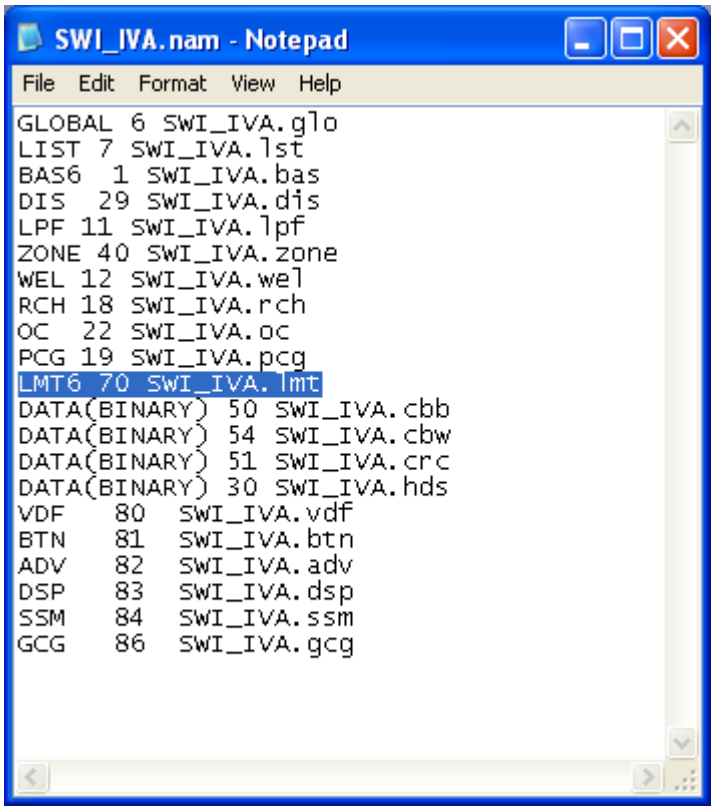


8. Before creating the datasets and running SEAWAT, we are going to set up SEAWAT to save the intercell advective fluxes for a subsequent simulation with MT3D. This file, called a flow and transport link file (with the .ftl extension), is created by selecting **Model>MODFLOW>Packages** and checking the box next to the MT3D flow output.

9. Create SEAWAT datasets.

10. Before running SEAWAT, you'll need to edit the name file, ***SWI_IVA.nam***. Due to a bug in GWV, the line that causes the MT3D flow output file to be written to a file needs to be added manually. Open the name file with a text editor and add the following line. Note that the LMT6 line can be added anywhere in the file. Do not recreate the SEAWAT datasets after you have made this change or it will

overwrite the ***SWI_IVA.nam*** file.



11. Run SEAWAT. As SEAWAT is running, you will notice that there are more iterations for each transport timestep compared with previous simulations. This is because of the second component. When SEAWAT is finished, record the simulation time before you close the window. If the simulation takes too long, you can grab the results from the ***SWI_IVA\results*** folder.

12. In a file manager, take a look at the output files from this simulation. You will see a couple of new files: ***MT3D002.OBS***, ***MT3D002.UCN***, and ***MT3D002.MAS*** (disguised by the file manager as a "Microsoft Access Stored Procedure Shortcut"). These files contain information about species number 2—the poor quality water. These results can be processed and evaluated using Modelviewer, GWV, and an ASCII text editor.

13. How far does the plume of poor-quality groundwater migrate over the 20 years?

IVB. Perform multi-species solute transport simulation using MT3DMS

In this simulation, the MT3D flow output file created in IVA will be used with the standard version of MT3D to simulate salinity as component 1 and the poor-quality groundwater as component 2. To speed up the simulation, we could simulate transport for only the poor-quality groundwater, but we will simulate both components here to compare with IVA.

1. The GWV file created in exercise IVA has been copied into the subdirectory ***SWI_IVB*** and has been renamed as ***SWI_IVB.gwv***. The root name for the files has also been changed from ***SWI_IVA*** to ***SWI_IVB*** to maintain consistency. The MODFLOW version under **Model>MODFLOW>Packages** was also changed from SEAWAT2000 to MODFLOW2000 so that all of the SEAWAT data files would not be created.

2. Open the file ***SWI_IVB.gwv*** and set the **Model>Paths to Models**.

3. In the previous simulation, the flow and transport equations were solved for each and every transport timestep, resulting in a fairly long simulation. One way to shorten computer runtimes, is to store the intercell fluxes from a SEAWAT simulation, which includes the density effects, and then simulate transport using those intercell fluxes. In the previous simulation, you told SEAWAT to save an MT3D flow output file (***SWI_IVA.ftl***). This file has been copied into the ***SWI_IVB*** folder and renamed as ***SWI_IVB.ftl***. We can now use that flow output file to run the standard version of MT3DMS contained with GWV. One limitation with this approach is that the intercell fluxes are only saved at the end of MODFLOW timesteps and stress periods. Thus, for a simulation where the intercell fluxes are changing rapidly with time, it may be necessary to add many MODFLOW timesteps, or to simply stick with a SEAWAT simulation.

4. To create the MT3DMS data files, go to **Model>MT3D/RT3D>Create Datasets**. Because the MODFLOW version was changed to MODFLOW2000, only the

MT3DMS data files are created as part of this step. If the MODFLOW version remained SEAWAT2000, then all of the MODFLOW2000 files would be created as well.

5. Run MT3DMS by going to **Model>MT3D/RT3D>Run MT3D**. This command runs the windows version of MT3D that is distributed with GWV. This simulation should run faster than the simulation in SWI_IVA because only transport is simulated, and thus, the variable-density flow equation is not solved every transport time step (NOTE: if it doesn't run, make sure the **Model>Path to Models** for MT3D is set to the correct folder. It will likely be c:\gwv5\MT3DWIN32.dll).

6. Are the results from this simulation different from the previous simulation with SEAWAT? If so, why might they be different?