# HST3D Example Problem 2

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# HST3D Example Problem 2

## *Introduction*

Before beginning this example, it would be a good idea to read Chapter 2 of the Argus One user's guide as well as "Overview" through "Expressions" in Chapter 3.

This describes a simplified real-life example of how to use HST3D based on data provided by John Passehl of the USGS (United State Geological Survey). It is a simplified model of the Biscayne aquifer, which is part of the "Surficial Aquifer".

You will need the following to reproduce this example

Argus ONE 4.2.0p or later.
HST3D GUI and related PIE's installed
Shape file import PIE (installed automatically with Argus ONE)
JoinContours PIE (installed automatically with HST3D GUI)
MoreConversions PIE (installed automatically with HST3D GUI)

Maps.exp (a base map)
Specified_State_NL1.exp (This file contains the location of a canal that will be placed on a Specified State layer.)

The following Shape files
fig. 13 - Surficial aquifer bottom
Fig. 17 - Biscayne aquifer transmissivity map
fig. 17pt - Biscayne aquifer transmissivity points
fig. 18 - initial water table
fig. 16 - Biscayne aquifer bottom

The following Excel files:
start_pressure.xls (pressures at the upstream end of the canal)
end_pressure.xls (pressures at the downstream end of the canal)

## Starting a New Project

To begin, create a new HST3D project. Select PIEs|New HST3D Project. If " New HST3D Project" does not appear on the PIEs menu, the HST3D PIE is not properly installed. The "coordinate system" dialog box will appear. At present, the PIE only supports Cartesian coordinates so select Cartesian and click OK
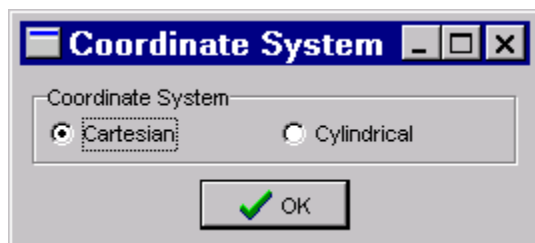


## Specifying Non-spatial data.

Next, the "Edit Project Info" dialog box will appear. It is used to edit all the non-spatial data in the model. On the Project tab, enter the title lines of the model. For this model select U.S customary Units, days and scaled mass fraction.
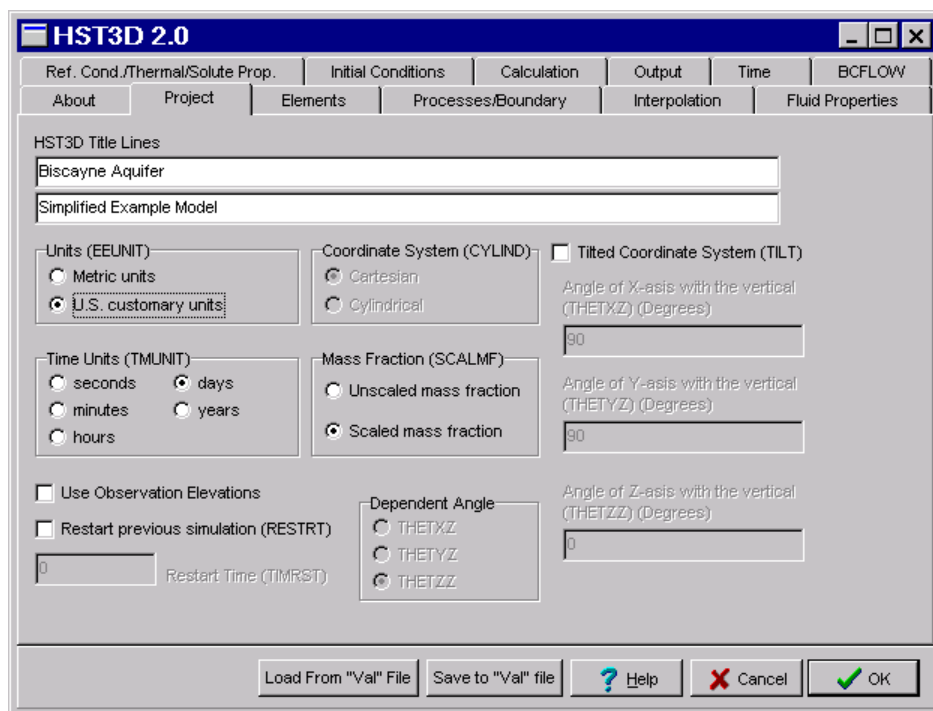
Next switch to the Elements tab and create 10 element layers. The elevations should range from 9 at the top to -270 at the bottom. 9 feet is the highest surface elevation in the study area and -270 is the elevation of the base Surficial Aquifer at its lowest point in the study area. The intervening elevations are divided equally between these two values. (Note: HST3D does not require that the element layers all have the same thickness.)

| Element Layer Number | Element Layer Name | Top Elevation | Bottom Elevation |
|---|---|---|---|
| 1 | Element Layer1 | 9 | -19 |
| 2 | Element Layer2 | -19 | -47 |
| 3 | Element Layer3 | -47 | -75 |
| 4 | Element Layer4 | -75 | -103 |
| 5 | Element Layer5 | -103 | -131 |
| 6 | Element Layer6 | -131 | -159 |
| 7 | Element Layer7 | -159 | -187 |
| 8 | Element Layer8 | -187 | -215 |
| 9 | Element Layer9 | -215 | -243 |
| 10 | Element Layer10 | -243 | -270 |

Number of Element Layers: 10

Next on the Processes/Boundary tab, we choose the type of processes to be simulated and the types of boundary conditions in the model. In this example, we will simulate solute transport with a free surface. The boundary conditions will include specified pressure, specified mass fraction, specified fluid flux, and wells. We will also select "Allow interpolation along open contours for specified pressure parameters".
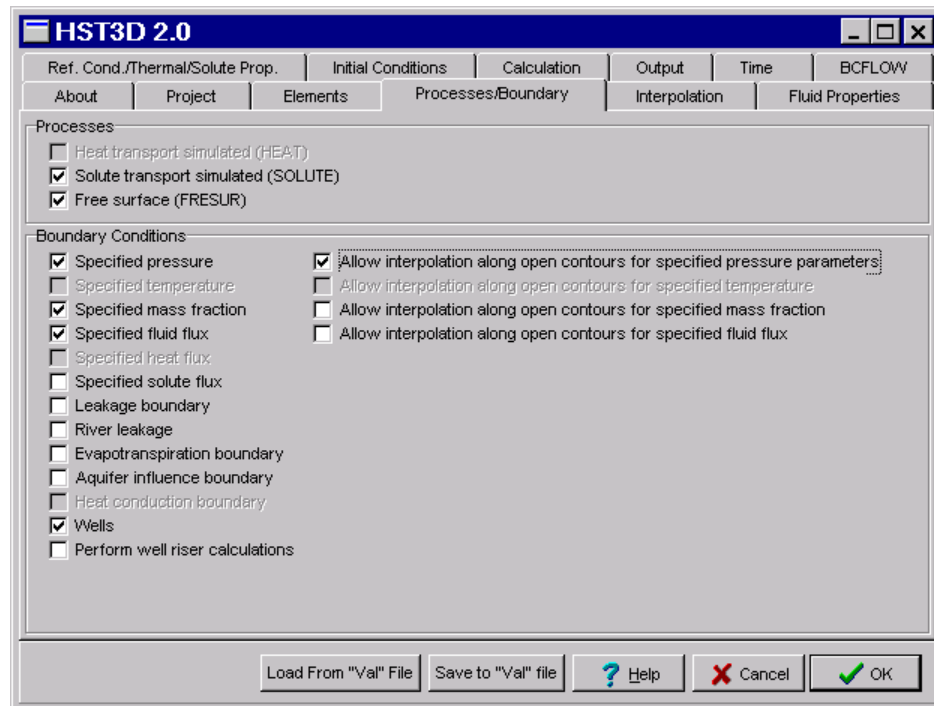


On the Interpolation tab, select specified pressure.
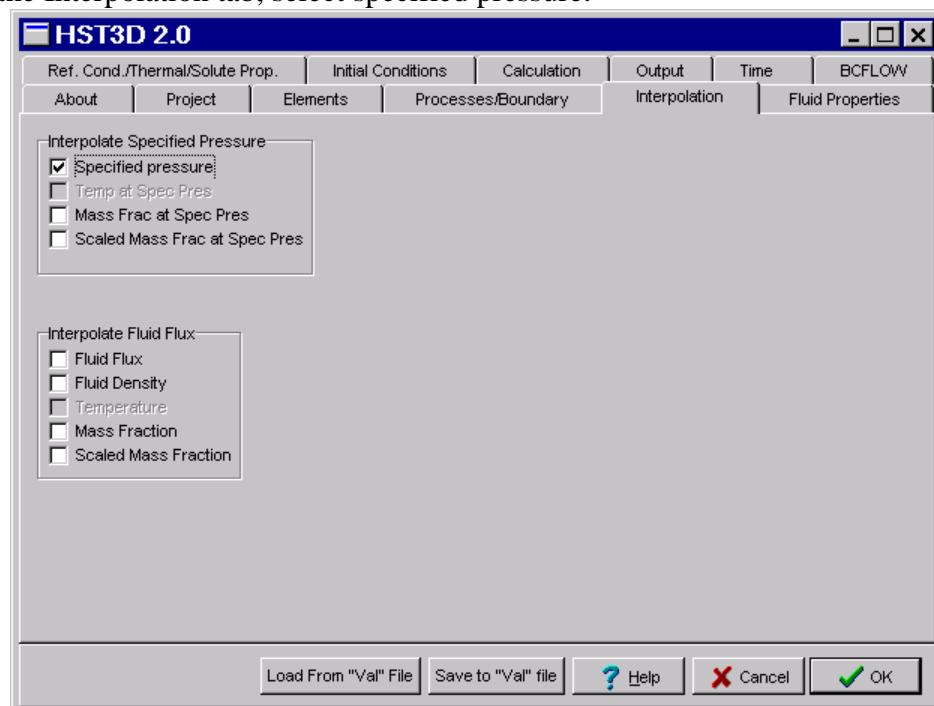
On the Fluid Properties tab, we will select the following properties.

| | |
|---|---|
| Compressibility of the Fluid: | 2.3e-8 |
| Reference Pressure for Density: | 0 |
| Reference Temperature for Density: | 68 |
| Reference Mass Fraction for Density: | 0 |
| Fluid Density at Reference Condition: | 62.42 |
| Maximum Mass Fraction: | 3.57e-2 |
| Fluid Density At Maximum Solute Mass Fraction: | 63.98 |
| Viscosity Multiplication Factor: | 1 |

On the Ref. Cond./Thermal/Solute Prop tabs, we will select the following properties.

| | |
|---|---|
| Atmosphere press | 0 |
| Reference pressure | 0 |
| Reference temperature | 68 |
| Effective molecular diffusivity | 0 |
| Solute decay constant | 0 |

On the Initial Conditions tab, we will select a specified initial water table.

On the Calculation tab, we will set the factor spatial-discretization to 0 and the factor temporal-discretization to 1. This is a good way to start because it is free of oscillations in the solution. However, it may have excessive numerical dispersion. Later, we might want to change to centered in space (FDSMTH = 0.5) and centered in time (FDTMTH = 0.5). It is normal for field-scale examples to use upstream in space differencing because you will probably have insufficient memory to allow you to use a sufficiently fine grid to avoid oscillation. We will use the generalized conjugate gradient iterative solver with red-black renumbering. We will use the standard incomplete LU factorization. The other options may be left at their default values

On the output tab, you can choose which data to print. You also need to specify the data input file name and extension for output. You can specify the path for HST3D now or when you are ready to run HST3D.

On the Time tab, we will set the following options:

| | |
|---|---|
| Duration | 1826 |
| AUTOTS | Yes |
| Max change in pres | 1 |
| Max change in mass frac. | 0.1 |
| Min time step | 0.00003 |
| Max time step | 30 |
| Solution method printout interval | 1 |
| Pres/temp/mass fraction printout interval | -30 |
| Flow-balance printout interval | -30 |
| Boundary flow printout interval | -30 |
| Well printout interval | -30 |
| Print pressure: | pressure |
| Print mass fraction : | yes |
| Print contour map data : | yes |
| Print velocity vector map data | yes |
| Map printout interval | -30 |
| Maximum number of time periods to be used for any object: | 1 |

(We will change the last parameter later.)

You can resize the dialog box or use the scroll bar to see all the options.

We will not use the BCFLOW tab at this time.

You don't need to worry about what these mean right now. If you want to know about them, check the online help for HST3D.

## HST3D 2.0

| About | Project | Elements | Processes/Boundary | Interpolation | Fluid Properties |
|---|---|---|---|---|---|

| Ref. Cond./Thermal/Solute Prop. | Initial Conditions | Calculation | Output | Time | BCFLOW |
|---|---|---|---|---|---|

| | |
|---|---|
| Start Time (TIMCHG) (t) | 0 |
| Duration (t) | 1826 |
| End of Period (TIMCHG) (t) | 1826 |
| Automatic time step (AUTOTS) | Yes |
| Not used | 1 |
| Max change in pres. (DPTAS) (F/L^2) | 1 |
| Max change in temp. (DTTAS) (T) | 9 |
| Max change in mass frac. (DCTAS) | .1 |
| Min time step (DTIMMN) (t) | 0.00003 |
| Max time step (DTIMMX) (t) | 30 |
| Solution Method Printout Interval (PRISLM) | 1 |
| Conductance/Dispersion Printout Interval (PRIKD) | 0 |
| Pres/Temp/Mass Frac Printout Interval (PRIPTC) | -30 |
| Density/Viscosity Printout Interval (PRIDV) | 0 |
| Velocity Printout Interval (PRIVEL) | 0 |
| Flow-,Heat, and Solute-Balance Printout Interval (PRIGFB) | -30 |
| Boundary Flow Printout Interval (PRIBCF) | -30 |
| Well Printout Interval (PRIWEL) | -30 |
| Print Pressure (IPRPTC n1) | Pressure |
| Print Temperature (IPRPTC n2) | No |
| Print Mass Fraction (IPRPTC n3) | Yes |
| Print Checkpoint Dumps (CHKPTD) | No |
| Checkpoint Dump Printout Interval (PRICPD) | 0 |
| Save Only Last Checkpoint Dump (SAVLDO) | No |
| Print Contour Map Data (CNTMAP) | Yes |
| Print Velocity Vector Map Data (VECMAP) | Yes |
| Map Printout Interval (PRIMAP) | -30 |

| 1 | Maximum number of time periods for any object | Add Time | Delete Time | Insert Time |
|---|---|---|---|---|

| Load From "Val" File | Save to "Val" file | ? Help | ✗ Cancel | ✓ OK |
|---|---|---|---|---|

We have now entered the non-spatial data for the model. Click OK and the HST3D layer structure will be created.

## *Importing a Map*

We will start by importing a base map for the project. Move to the "Maps" layer and File|Import Maps|Text File. Select the file Maps.exp. It is in the Argus Interware\Examples\Hst3d Examples directory. The map is larger than the current drawing area so you will get a dialog box asking if you wish to expand the drawing area. Click the OK button.
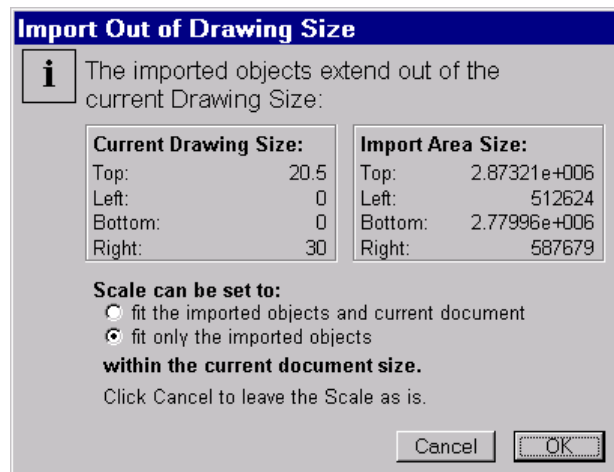


The base map will be imported into the model.
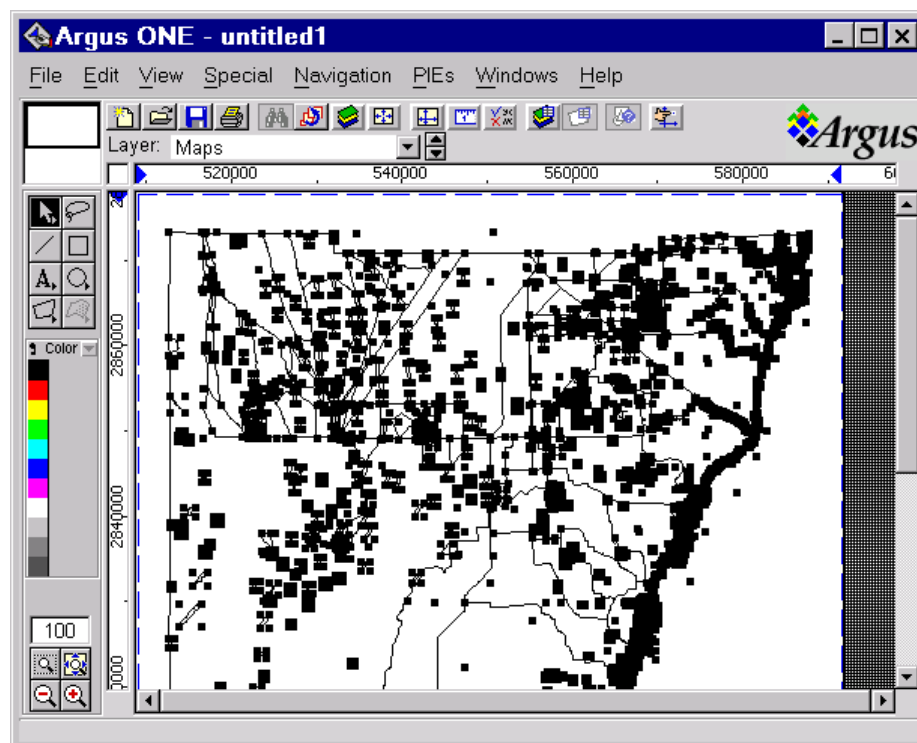
## *Creating New Layers*

For this exercise, we will pretend that the units for this map are feet so we can demonstrate proper unit conversions to U.S customary units. U.S customary units are generally more difficult to work with because of the numerous unit conversions you must perform. Thus, you may prefer to use metric units for your models. If you wish, you can change the units to feet in the "Special|Scale and Units" dialog box.

Next, we will create a number of additional layers that are not automatically created by the PIE. These layers will be used to hold a variety of data that we will use in our model. To begin with, we will create a group layer called "Non_Standard Layers" under which the new layers will be created.

We will start by creating a layer to hold the transmissivity values of the Biscayne Aquifer. Actually, we will have two such layers. In one, we will have point values of transmissivity and in the other, we will have transmissivity contours from a map. We will use both of these to calculate the permeability and compare the two to assess the strengths and weaknesses of each source of data.

Click the "Layers…" button on the Layers floater or the "Layers Dialog" button on the main Argus ONE window or select "View|Layers…" Click the "New" button under "Layer:" to create a new layer. Change the name of the layer to Nonstandard Layers. Change the Type of the Layer to "Group". Click the "New" button under "Layer:" again. This time change the name to "Biscayne aquifer transmissivity map" and change the units to 1000's of ft^2/s. Click the Done button.



15
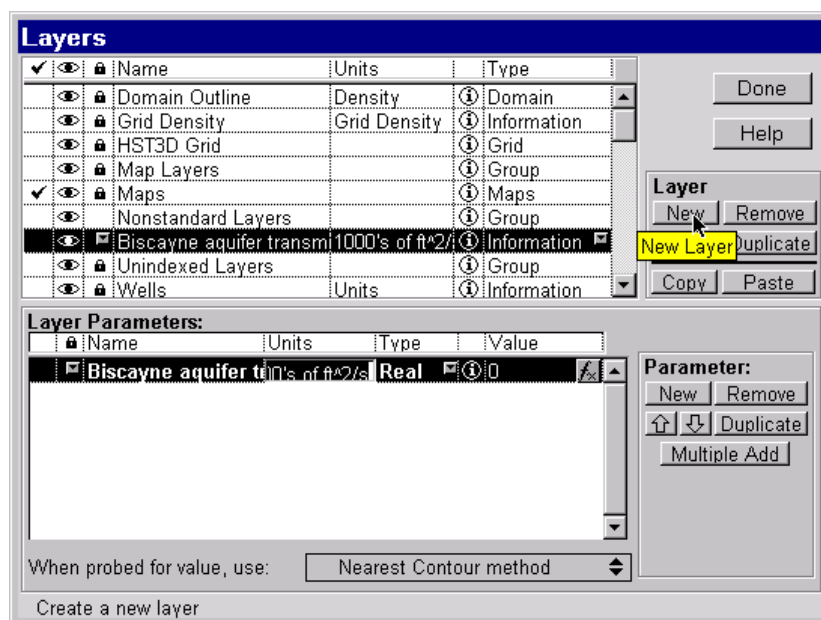
### *Importing a Transmissivity Map*

Next, we will import the transmissivity map into this layer. The transmissivity map is an ArcInfo shape file so we will use the shape file import PIE to import the data. Make "Biscayne aquifer transmissivity map" the active layer and select "File|Import Biscayne aquifer transmissivity map|Import Shp file…". The shape file is "fig17.shp". Select it. Select "Import to the current layer" and then select "ZVALUE[Number - Integer]". You will get an error message. "Some objects intersected themselves or other. Those objects cannot be imported. Do you want to import the rest of the objects?" The reason we get this message is that we forgot a very important step. We have to turn on "Allow Intersection" before importing this map. Cancel the import and select "Special|Allow Intersection" or click the "Allow Intersection" button. Now, let's try it again. This time there is no problem importing the contours.
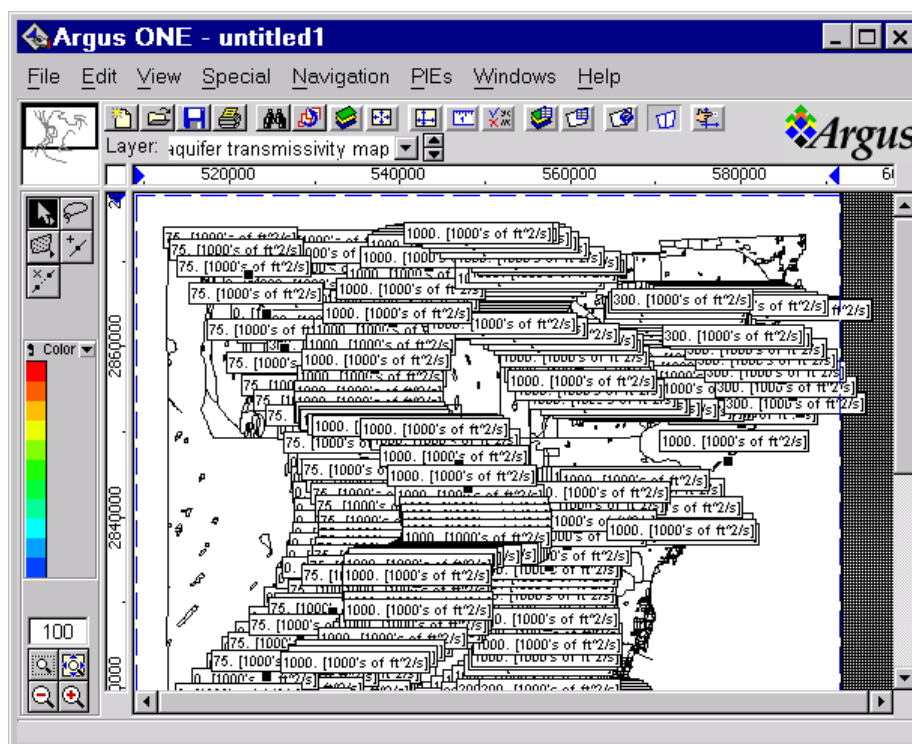
## Joining Contours

The map is made of many, small, short contours that meet at their endpoints. Each contour has it's own label which is why the map looks so strange. We will join those contours that have the same value.

Select File|Import Biscayne aquifer transmissivity map|Join Contours". Then select " Biscayne aquifer transmissivity map". The contours will disappear briefly and then reappear but now the multiple contours will have been joined into a much smaller number of long continuous contours. (I have also hidden the base map by clicking on the "eye" icon on the Layers floater so that only the transmissivity map is visible.)
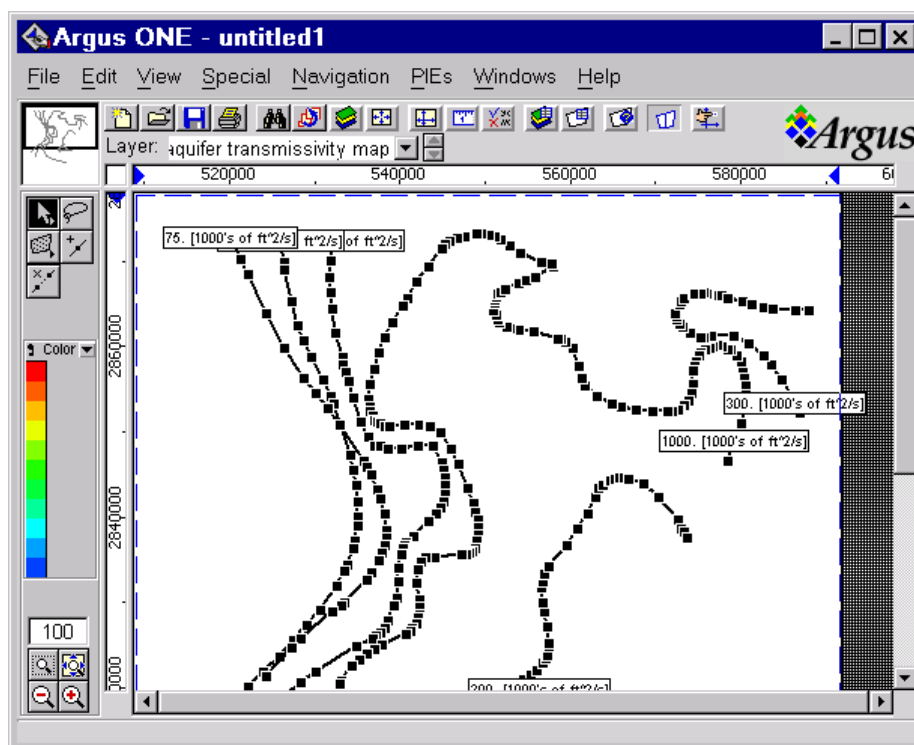


## Importing More Data

We also have the point values of transmissivity on which this map is based. We will import that into another layer named "Biscayne aquifer transmissivity points". The shape file is named fig17pts.shp. Because this is point data, we don't need to turn "Allow Intersection" on and we have no need to use the Join Contours PIE. The procedure for creating the layer and importing the points is the same as it was before.

Next, we will create a new layer named "Biscayne Aquifer bottom" and import fig16.shp into it. You must turn "Allow Intersection" on first. You may wish to run the "Join Contours" pie after importing the shape file. The units for this layer are "feet".

Next, we will create a new layer named "Surficial Aquifer bottom" and import fig13.shp into it. Again you must turn "Allow Intersection" on and you may wish to run the "Join Contours" pie after importing the shape file. However, before running the "Join Contours" pie you may wish to delete some of the contours. In the illustration below, I have hidden the labels so that you can see the contours more clearly. You will see that depressions are indicated by hatch marks. You may wish to delete those hatch marks. As you delete them, you will find that in one or two cases, there are a few identical hatch marks directly on top of one another. Such hatch marks would have been joined into a single contour that doubles back on itself by the "Join Contours" PIE. Argus will not accept such contours so those contours will be lost when the "Join Contours" PIE is used. The error message will be "Several contours are not simple, that is, cross themselves. These contours were skipped. (Try importing into Maps layer)". You can ignore the error message in this case.

There is also a gap in one of the contours that you may wish to close. To close the contour, select one of the open ends and move it over the other open end. When the end is close enough to the other end, the cursor will change to a hollow cross. If you release it at this point, the points will line up exactly.
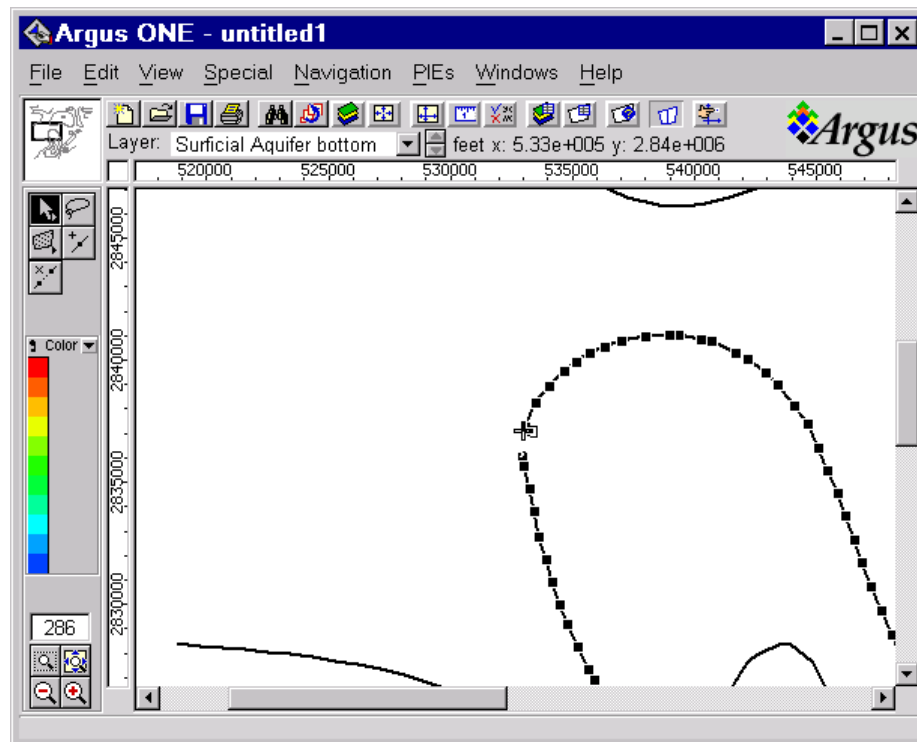
### *Importing the Initial Water Table*

Finally, we will import the initial water table. This is going to give the most trouble of any of the files we import. We will use a Maps layer to diagnose the problem and solve it. Create two layers. One should be named "Initial Water Table Map" and it should be a "Maps" layer. The other should be named "Imported Initial Water Table" and it should be an Information layer. Move to the "Imported Initial Water Table" layer, Make sure "Allow intersection" is on and import fig18.shp into it. You will get a warning message "Some objects intersected themselves or other. Those objects cannot be imported. Do you want to import the rest of the objects?" Select OK. Now go to the "Initial Water Table Map" layer and import fig18.shp there too. Go back to "Imported Initial Water table" and locate the "Color" drop down menu. Select "Imported Initial Water table" from the menu. In the figure below, only the "Initial Water Table Map" and "Imported Initial Water table" layers are visible. We imported the same data into both you can see where there is a gap in the colored lines where the black line on the "Initial Water Table Map" shows through. That contour could not be imported into the information layer but it could be imported into the map layer. To make it easier to see, I have hidden the contour labels by selecting "View|Show Contour Value". (There is another, similarly named command named "View|Show Contour Value**s**". That is not the one we want.)
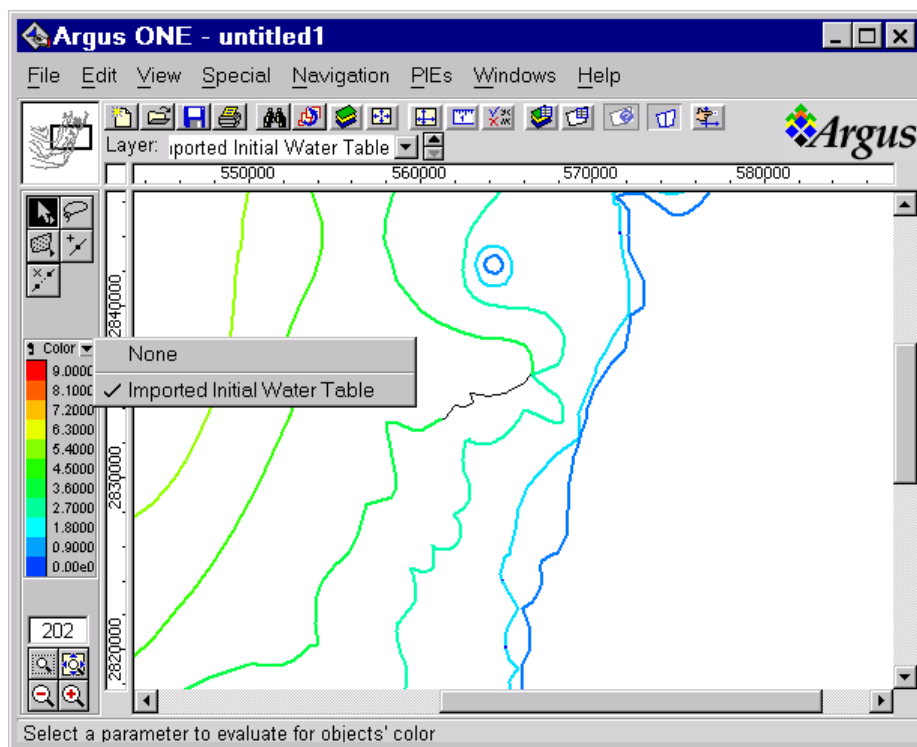
Zoom in on that contour and you will see the problem. The contour doubles back on itself.
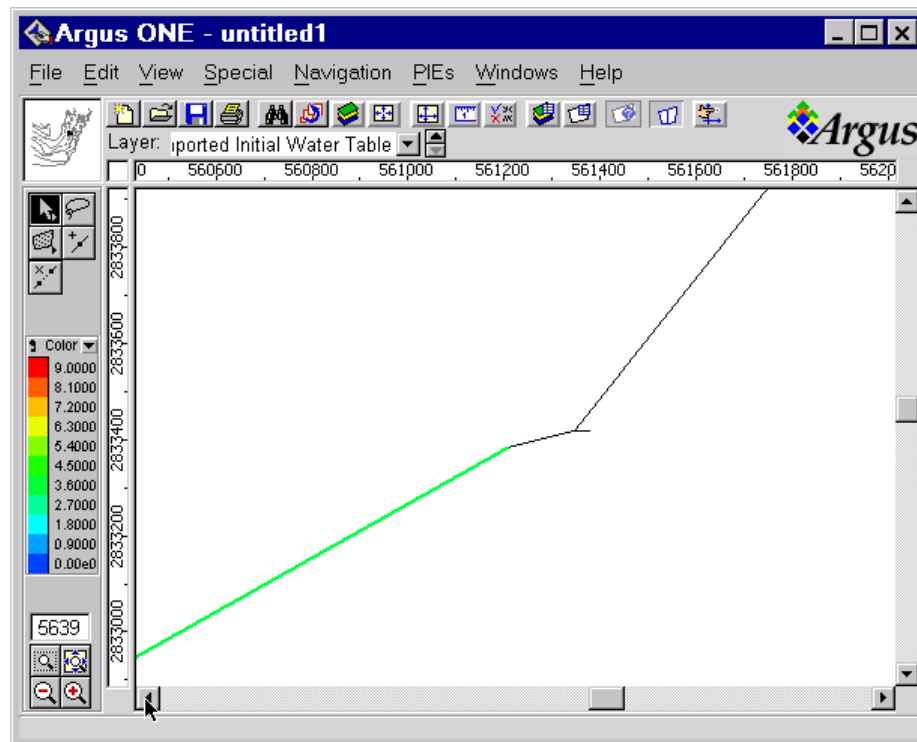
To fix the problem, select the contour on the "Initial Water Table Map", copy it to the clipboard, and paste it in a text editor. The second and fourth vertices are identical as shown below. Delete the second and third vertices and change the number of vertices (on line 1) from 14 to 12.
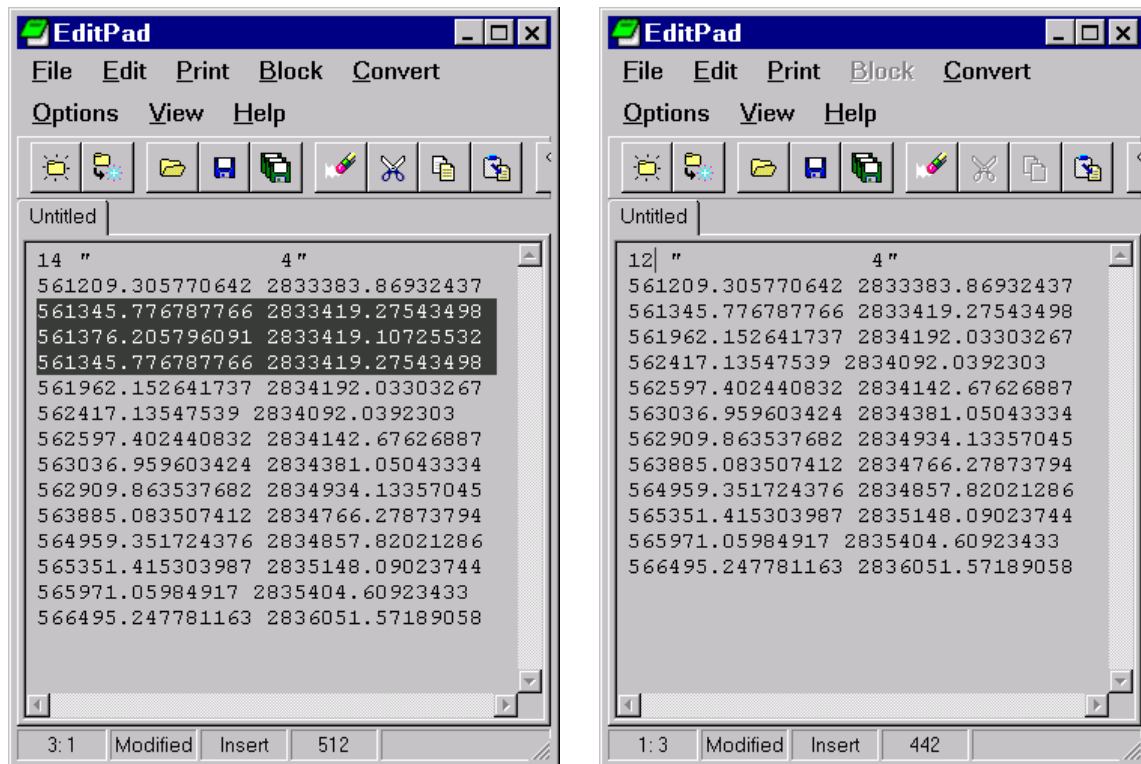


Copy the text from the text editor back to the clipboard and paste it in the Imported Initial Water Table layer.

This solves one problem but we have two more. First, some of the contours do not have the correct value. We can see this because they have a different color from other contours to which they are connected. You will need to correct this problem. Double click on the contours with the incorrect values and assign them the same values as their neighbors.
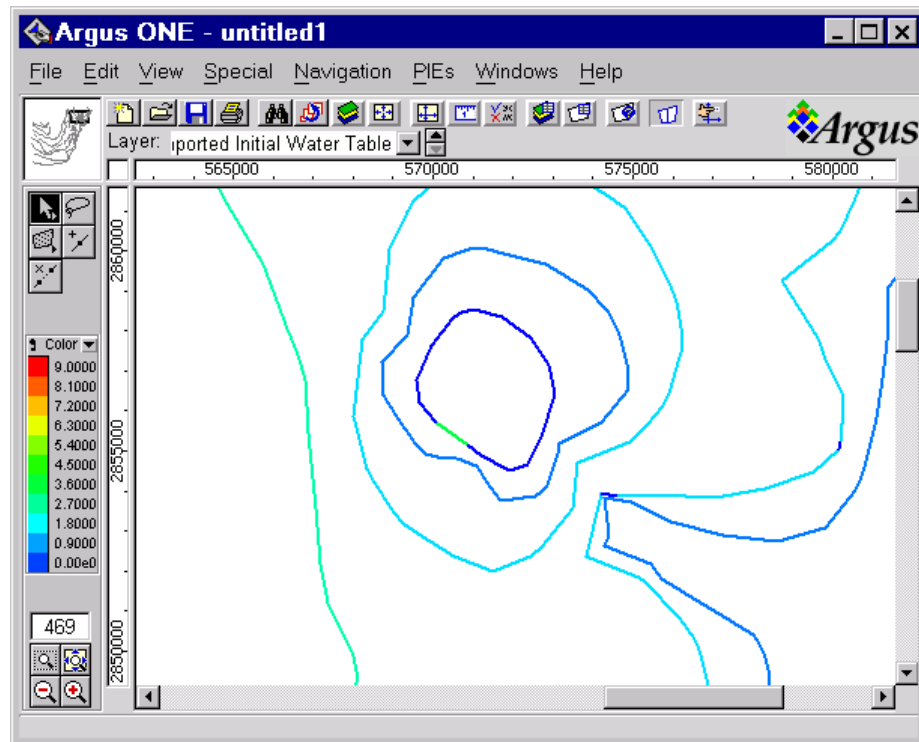
The other problem is that the contours are discontinuous. You can see this if you zoom in. You will need to align the ends before you can join the contours with the Join Contours PIE. You will find that some of the contours have several vertices that are very close together near the ends of the contours. You may wish to delete some of these extra vertices to make it easier to align the ends of the contours.
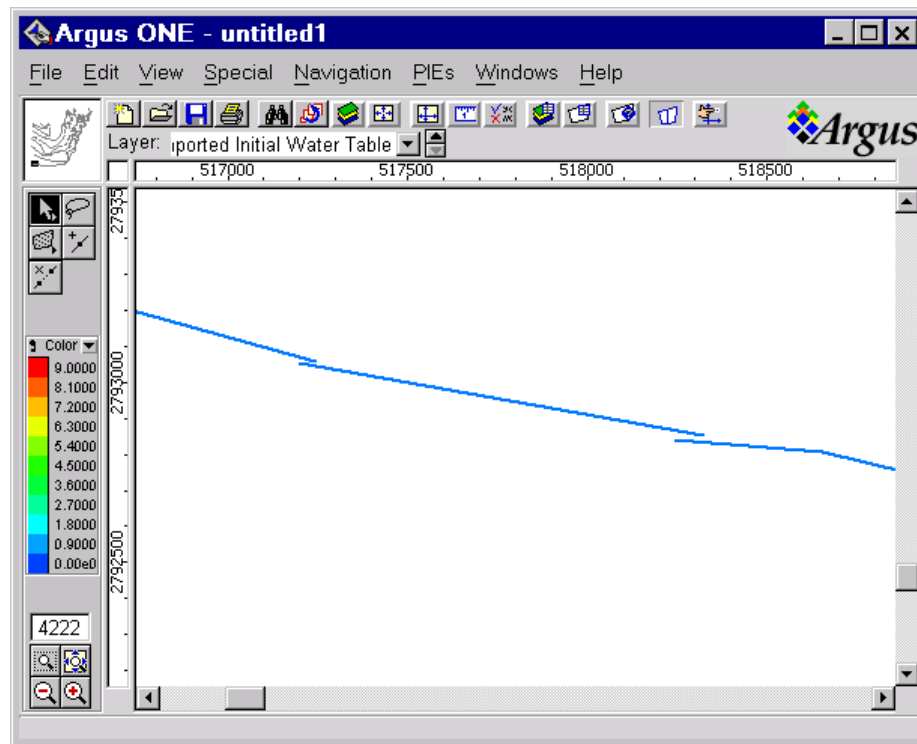


## Calculating the permeability of the Surficial Aquifer

For the Surficial aquifer, we will use a constant hydraulic conductivity of 500 ft/day. We will need to convert this to permeability. To show how the conversion is performed, we will use the expression editor. First, create a new layer named "Surficial Aquifer Permeability" and create parameters as shown in the table below.

| Parameter name | Units | Expression |
|---|---|---|
| hydraulic conductivity | ft/day | 500 |
| fluid density | kg/m^3 | 998.23 |
| Viscosity | Pa-s | 0.001002 |
| Surficial Aquifer Permeability | ft^2 | Hydraulic Conductivity * Pa2psi(Viscosity) /24/3600 / kg_per_cu_m2lb_per_cu_ft(Fluid Density) * 144 |

The expression for Surficial Aquifer Permeability deserves a bit of explanation. The relationship between intrinsic permeability and hydraulic conductivity is

$$K = \frac{k\rho g}{\mu}$$

where
$K$ = hydraulic conductivity,
$k$ = intrinsic permeability,
$\rho$ = fluid density,
$g$ = gravitational acceleration, and
$\mu$ = fluid viscosity.

The More Conversions PIE has a function to convert density in kg/m³ to specific weight in lb/ft³. The conversion incorporates the gravitational acceleration so we don't need to include that explicitly in the function for calculating permeability. The More Conversions PIE also has a function for converting pressure in Pascals to pressure in pounds per square inch (psi). Because the units for viscosity are Pa-s, we can use this to convert the viscosity from Pa-s to psi-s. The constants in the expression are for unit conversions. Hydraulic conductivity is in ft/day whereas the viscosity (after conversion) is in psi-s. We need to divide by 24 hr/day and 3600 s/hr to get the time units to cancel out. Similarly, we need to multiply by 144 in²/ft² to convert the pressure units from psi to lb/ft². We end up with permeability in ft². Of course, if we had used metric units throughout the model, we would have had fewer difficulties with unit conversions. I used English units in this model to illustrate how to deal with unit conversions in case you must use English units.

### *Calculating the permeability of the Biscayne Aquifer*
We need to make a similar conversion for the Biscayne transmissivity values. Transmissivity is related to hydraulic conductivity by the formula

T = Kb

Where
T = Transmissivity,
K = hydraulic conductivity, and
b = aquifer thickness.
Create the following parameters on the "Biscayne aquifer transmissivity map" and "Biscayne aquifer transmissivity points" layers respectively

| Parameter name | Units | Expression |
|---|---|---|
| hydraulic conductivity | ft/day | Biscayne aquifer transmissivity map/ (HST3D Grid.Elevation NL1 - Biscayne Aquifer bottom) * 1000 |
| fluid density | kg/m^3 | 998.23 |
| Viscosity | Pa-s | 0.001002 |
| permeability | ft^2 | Hydraulic Conductivity * Pa2psi(Viscosity) /24/3600 / kg_per_cu_m2lb_per_cu_ft(Fluid Density) * 144 |

| Parameter name | Units | Expression |
| --- | --- | --- |
| hydraulic conductivity | ft/day | Biscayne aquifer transmissivity points / (HST3D Grid.Elevation NL1 - Biscayne Aquifer bottom) * 1000 |
| fluid density | kg/m^3 | 998.23 |
| Viscosity | Pa-s | 0.001002 |
| permeability | ft^2 | Hydraulic Conductivity * Pa2psi(Viscosity) /24/3600 / kg_per_cu_m2lb_per_cu_ft(Fluid Density) * 144 |

The only difference between these expressions and the previous ones are that in this case we calculate the hydraulic conductivity by dividing the transmissivity by the aquifer thickness (HST3D Grid.Elevation NL1 - Biscayne Aquifer bottom). HST3D Grid.Elevation NL1 is the elevation of the top of the model and thus also the top of the Biscayne aquifer.

### *Correcting Errors in the Transmissivity Data*

We need to examine at the data on both the Biscayne transmissivity layers. We will see problems with the data. On the transmissivity map, we have a transmissivity contour that extends past the edge of the aquifer. In the illustration below, this contour is the blue contour that has been selected. The base of the Biscayne aquifer is shown with black contours. It turns out that in the area past the edge of the Biscayne aquifer, the transmissivity values on the map actually come from a different aquifer. We need to delete the portion of the contour that represents the incorrect aquifer. That portion is shown with hollow squares. I selected just those vertices by using the lasso tool, which is the button shown in black on the left side of the illustration.
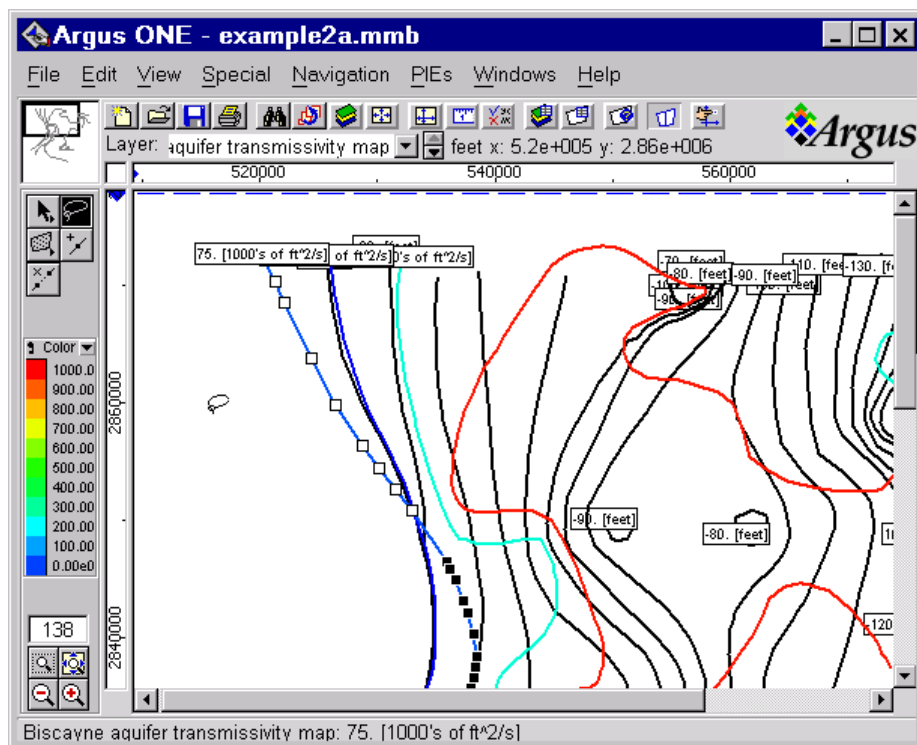
If you look at the point values of transmissivity, you will find that some of them are also beyond the edge of the aquifer. Those represent a different aquifer and should be deleted. You should always look for inconsistencies such as this in your data and resolve them. In this case, it turns out that the problem was that some transmissivity values didn't come from the right aquifer but the problem might have been that the base of the aquifer was mapped incorrectly.

### Creating the Grid

Now might be a good time to decide how we will interpolate the bottom elevations of the layers and which source of data we will use for the permeability of the Biscayne aquifer. Because the bottom elevations of the layers are used in determining the permeabilities, we will address the elevations first. We need to see how the bottom elevations will look on the grid. Thus, we must first create the grid. Hide all layers except the Maps layer in which you have the base map and the Domain Outline layer. Make the Domain Outline layer the active layer and draw the domain outline (shown in green below) around the study area. In this case, I assigned the domain outline a grid density of 3000 ft. I have not attempted to pick the natural boundaries of the model area in this example. Later, we may come back and modify the domain outline to reflect the natural boundaries of the system better.
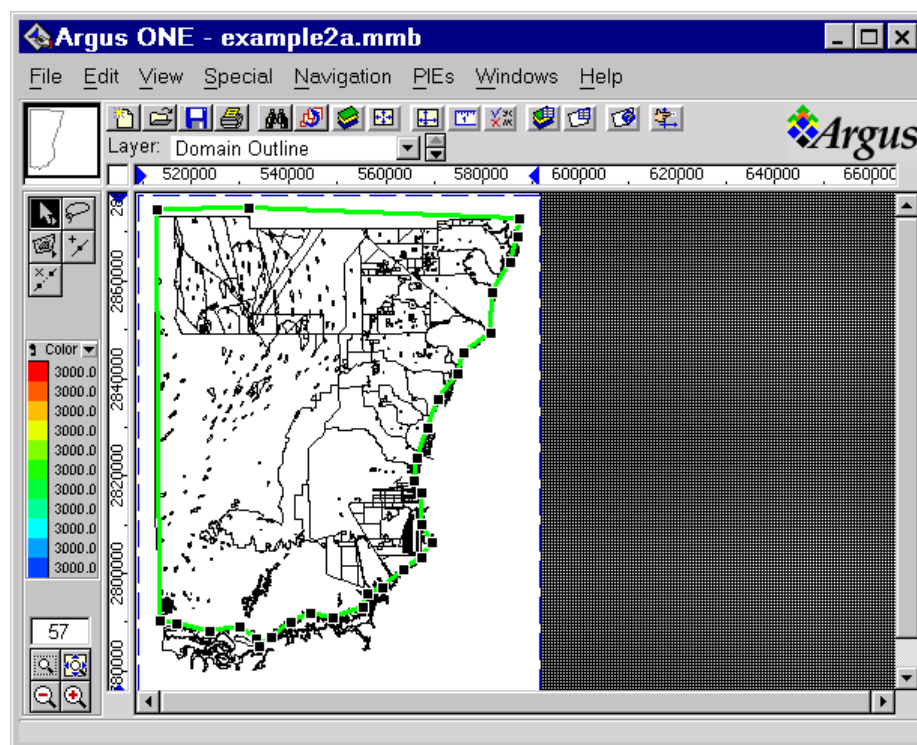
Next go the HST3D Grid layer and click inside the Domain Outline with the Magic Wand Tool to create the grid. You will be prompted to either allow Argus ONE to find a grid at the best angle or to create a grid at some specific angle that you designate.
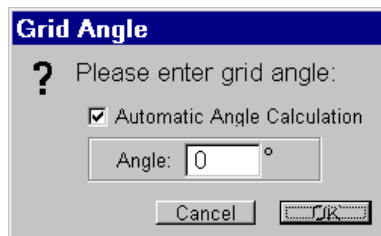


The grid will be created. This is a grid of HST3D Elements. You should read the HST3D documentation to see the difference between the grid of elements and grid of cells (Kipp 87 p77.) or "The HST3D Grid" in the introduction of the online help.
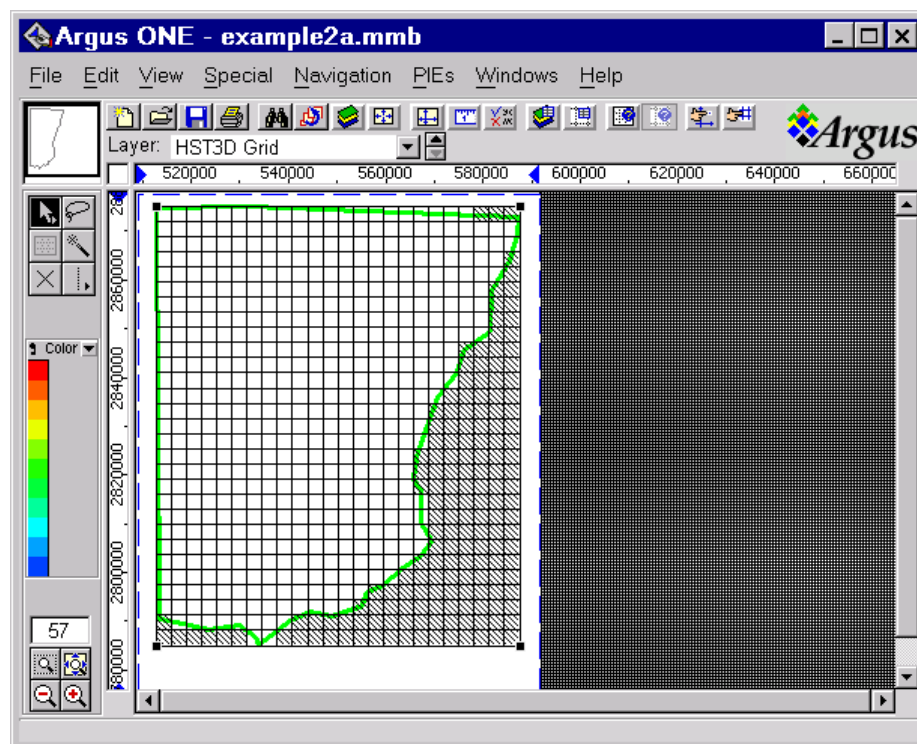
### *Viewing the Bottom Elevation of the Surficial Aquifer*

Next we will map the bottom elevation of the Surficial aquifer on the grid using several different interpolation schemes to see which is most suitable for our data. Open the Layers dialog box and create a new parameter on the HST3D Grid layer named "Surficial Bottom". Make the default expression for this layer "Surficial Aquifer bottom". Make sure the parameter is a block parameter and not a layer parameter.
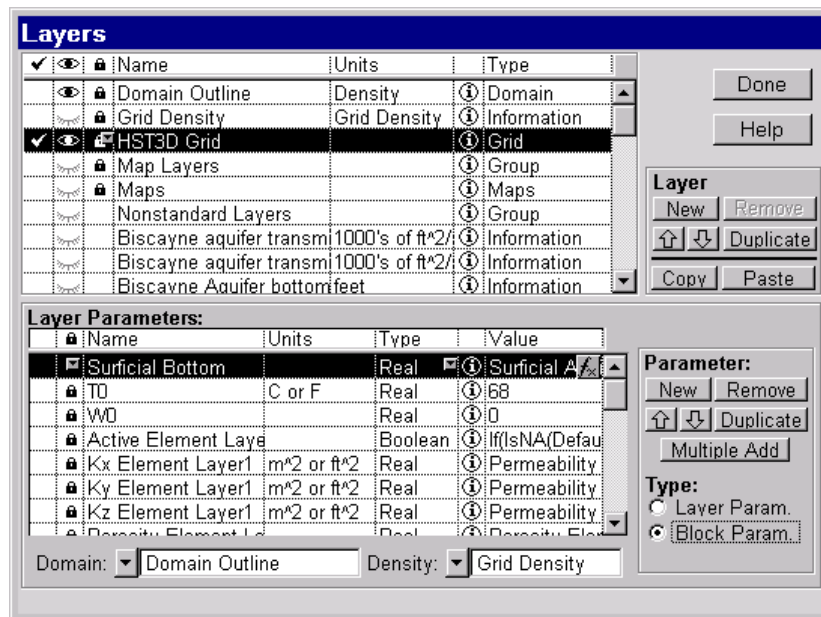
Next, color the block cells using the "Surficial Bottom" parameter of the HST3D Grid layer.
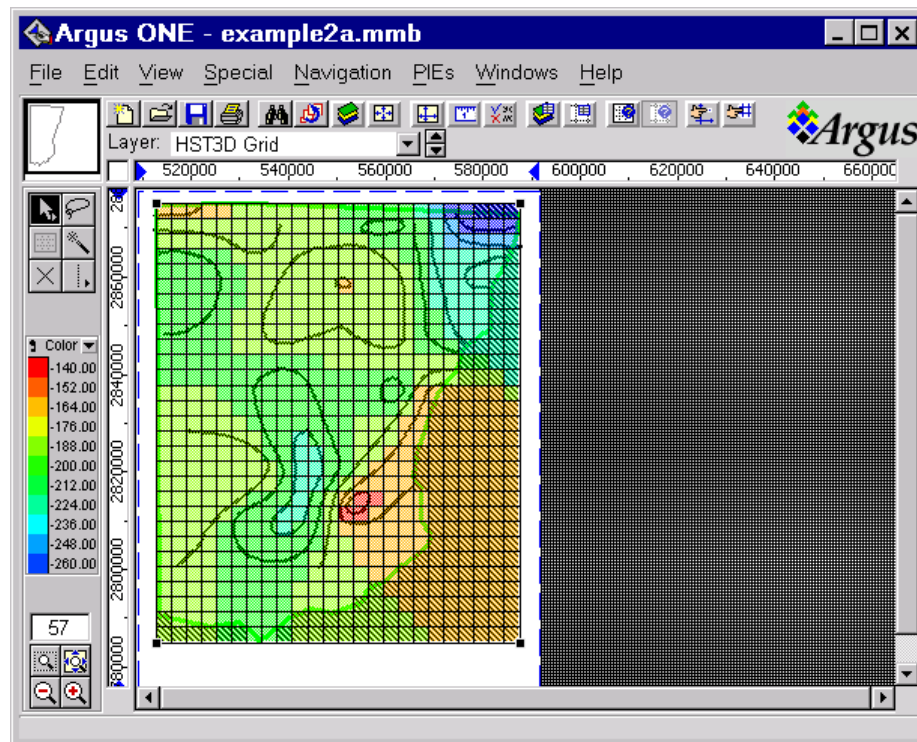
By default, the "Nearest" interpolation scheme is used so each block is assigned the value of the contour that is nearest to the center of the block. Try changing the interpolation to one of the other choices. (Don't use the "Exact" method; it is only for cases where all the contours are closed.) You might want to try the 624 Interpolation option, for example. You should also try the interpolation method. The 624 Interpolation option is fast but tends to do poorly at extrapolation. The Interpolation method tends to be slower but does better at extrapolation. If you find that you wish to use the interpolation method but that it is very slow, you may be able to speed things up by increasing the spacing of vertices on your contours. In some cases, the vertices are very close together as shown below.
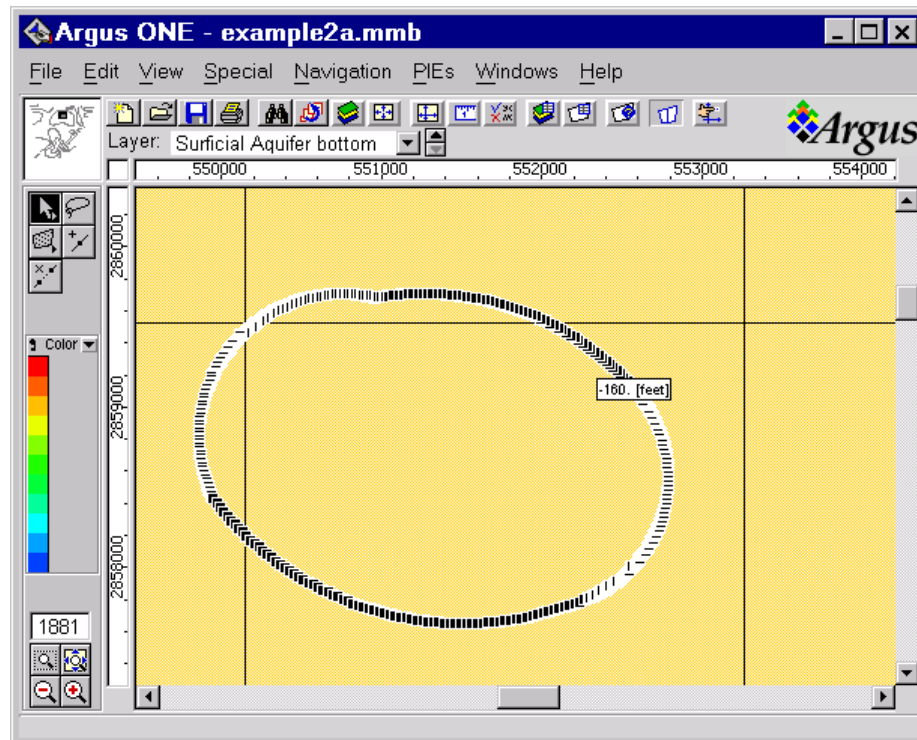
You can use the "Declutter Contours" PIE to eliminate vertices that are close together. In this case, the desired vertex spacing was set at 1000. This is still smaller than the grid size of 3000 so it should not affect the values assigned to grid cells much but it will make the interpolation process a good bit faster.
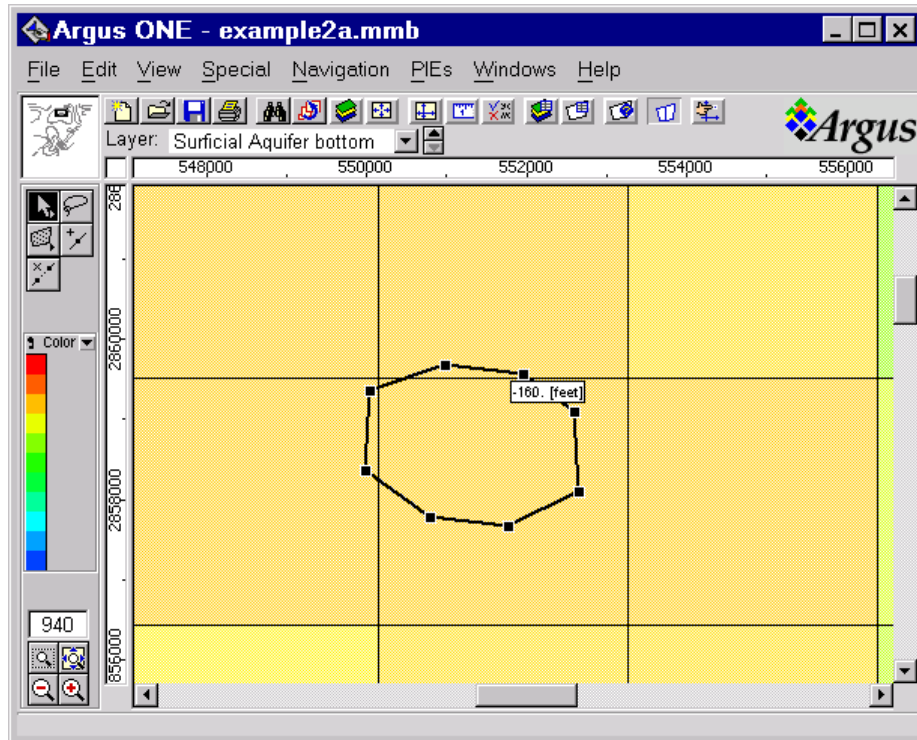
## *Visualizing Other Parameters*

We can use similar procedures to visualize the other parameters. Here is what I find. You may wish to visualize these parameters yourself to see if you agree.

For the initial water table, the interpolation method works well but the 624 interpolation does not. With this grid density, Nearest, Interpolation and the TriInterpolation PIE (624 Interpolation) all give acceptable results for the bottom elevations of the Biscayne and Surficial aquifers in the active parts of the model. I personally prefer the 624 interpolation but you may have a different opinion. For the Surficial aquifer, the permeability is a constant so it doesn't matter what interpolation scheme is used. When using the interpolation method, the mapped values of permeability for the Biscayne aquifer don't look good. As shown below, there appears to be a band of high transmissivity near the eastern edge of the aquifer. This is probably not real but rather is an artifact of the way transmissivity was mapped. It looks like the mapped transmissivity values were drawn without consideration of the aquifer thickness. The transmissivity should probably have been lower where the aquifer pinches out. This effect is just as bad with 624 interpolation and in addition, 624 Interpolation extrapolates very high values of permeability in some locations where such permeabilities are not justified.
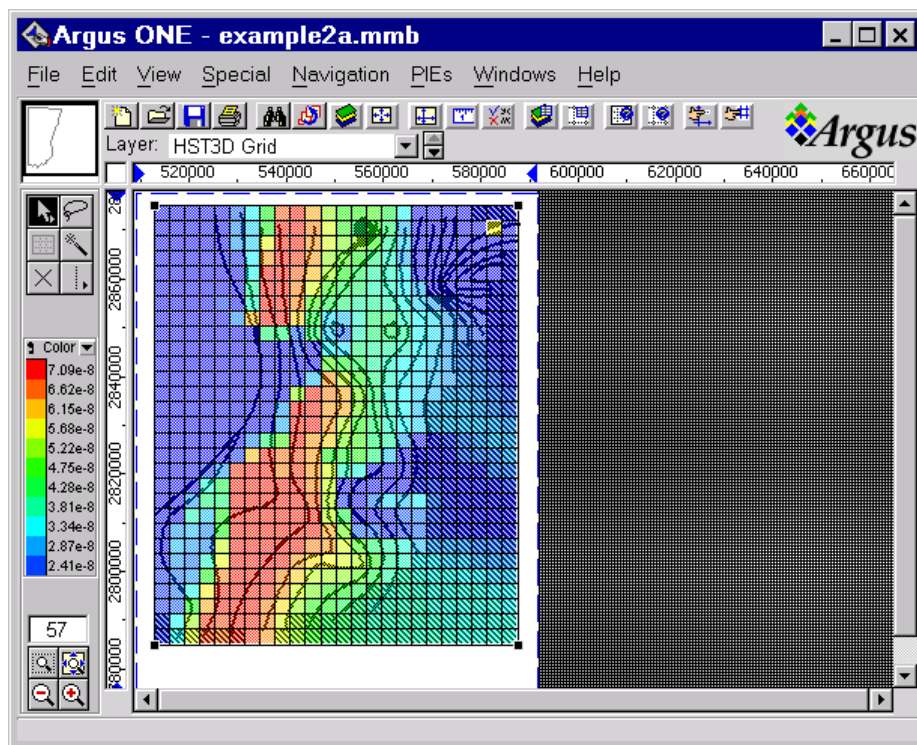
The point values of permeability are better in than those calculated from the permeability map in that they show less of a tendency to extrapolate a band of high permeability near the outcrop area. However, in the northwest corner of the model, there is an area of high permeability that does not appear to be justified by any data. It might be worthwhile to place a few estimated data points in this area with reasonable permeability values to prevent the interpolation process from introducing unreasonable permeability values.
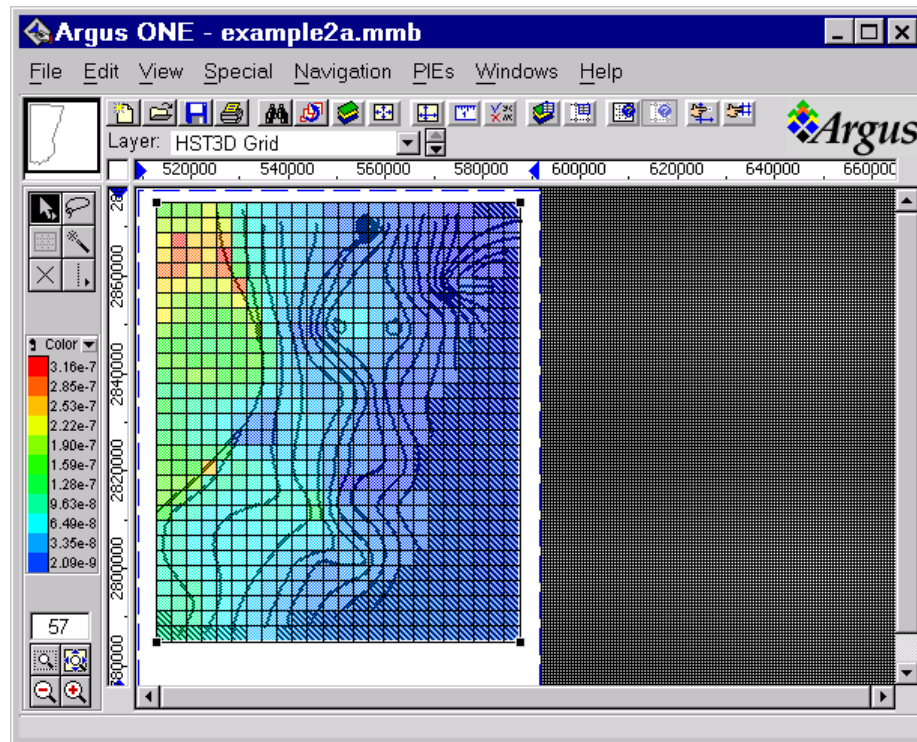


## Converting Point Contours to a Data Layer

If you are satisfied with one of the interpolation methods for the point contours and want to speed up the interpolation a bit, you can convert the point contours to data points on a data layer. To do this, bring up the Layers dialog box and select the "Biscayne aquifer transmissivity points" layer. Click on the "Duplicate" button in the upper half of the dialog box to make a new layer with all the same properties as the old one.

Next, convert the new layer to a data layer. To do this, locate the "Type" column and click on the down arrow next to where it says "Information". A pop-up menu will appear. Select "Data" from the list of choices.

Next, go to the HST3D Grid layer and select "File|Export|Edit Template". Click on the "Load" button. Locate the file "contour2data.met" in the Argus Interware|ArgusPIE|HST3D_GUI directory and select it. After the file is loaded, read the instructions at the beginning of the file. At the time this was written, the instructions said that line 30 would need to be changed. You have to change "New Layer" in line 30 to "Biscayne aquifer transmissivity points". When you have done so, click the "Done" button and then select "File|Export|By Template". Choose a file name and the export template will save the contours to that file in the format for a data layer.

Finally, go to the new data layer (named "Biscayne aquifer transmissivity points1") and select "File|Import|Text File". Accept the default choice of "Scattered Data" and click on the OK button. Next, choose the file you just saved to import the data into a data layer.

### *Using Elevations to Assign Active Cells and Permeabilities*

Our next task is to assign permeabilities to the correct cells based on the elevations of the bottoms of the aquifers. We will assume that if the middle of a cell is above the base of the Biscayne aquifer, it should be assigned the permeability of the Biscayne Aquifer. If the middle of the cell is above the base of the Surficial aquifer but below the base of the Biscayne Aquifer, it should be assigned the permeability of the Surficial aquifer. Otherwise, it should be assigned a permeability of 0.

To do this, we will create a new information layer for each element layer. The Information layers will be named Aquifer Index[i] where i designates which element layer the information layer refers to. Thus for Element Layer1, we will create an information layer named Aquifer Index1. The expression for the Aquifer Index1 layer will be

If((HST3D Grid.Elevation NL1 + HST3D Grid.Elevation NL2)/2>=Biscayne Aquifer Bottom, 1, If((HST3D Grid.Elevation NL1 + HST3D Grid.Elevation NL2)/2>=Surficial Aquifer Bottom, 2, 0))

This expression will return a 1 if the middle of the cell
(HST3D Grid.Elevation NL1 + HST3D Grid.Elevation NL2)/2
is above the base of Biscayne aquifer. It will return a 2 if the middle of the cell is above the base of the Surficial aquifer but below the base of the Biscayne aquifer. It will return 0 if the middle of the cell is below the base of the Surficial aquifer. We would use similar expressions for the other Aquifer Index1 layers except instead of HST3D Grid.Elevation NL1 and HST3D Grid.Elevation NL2 we would use HST3D Grid.Elevation NL[i] and HST3D Grid.Elevation NL[i+1] where i designates the element layer.

We will use the result of Aquifer Index[i] in two different expressions for each Element Layer. The first will be for Active Area Element Layer[i]. If Active Area Element Layer[i] is true at a location, that location will be part of the active area of the model. In Argus ONE, any non-zero value is true and 0 is false. Any cell that whose middle is below the base of the Surficial aquifer should be inactive and all other cells should be active. Thus the expression for Active Area Element Layer[i] is very simple, it is simply Aquifer Index[i].

The other place where we will use Aquifer Index[i] is in the expression for permeability. The expression for Permeability Element Layer[i].kx should be
"Index(Aquifer Index[i]+1, 0, Biscayne aquifer transmissivity points.permeability,Surficial Aquifer Permeability.Surficial Aquifer Permeability)"
This says that if Aquifer Index[i]+1 is 1, the permeability should be 0 (i.e. inactive). If Aquifer Index[i]+1 is 2, the permeability should be the permeability of the Biscayne aquifer. If Aquifer Index[i]+1 is 3, the permeability should be the permeability of the Surficial aquifer.

We will assume, for no particularly good reason, that the permeability in the y direction is the same as the permeability in the x direction and that the permeability in the z direction is 1/10'th the permeability in the x direction. Thus, the expressions for Permeability Element Layer[i].ky and Permeability Element Layer[i].kz should be kx and kx/10 respectively.

### Assigning Other  Aquifer Properties

Similarly, we will assume the following values throughout the model

| | |
|---|---|
| Porosity | 0.15 |
| Vertical compressibility | 1e-7 |
| Longitudinal dispersivity | 3000 |
| Transverse dispersivity | 600 |
| Distribution coefficient | 0 |

### Assigning the Initial Water Table

Our next task is to assign the initial water table. This is a little harder than it looks. For the element layers, we could assign default values to the related information layers and those values would be used in the model. We have a layer created by the PIE called Initial Water Table. Couldn't we just make the default value for that layer be the layer into which we imported the initial water level contours? Better yet, couldn't we just import those contours into the Initial Water Table layer to begin with and skip creating a layer to hold the contours. Unfortunately, the answer is no. That works for layers related to elements because the HST3D Grid is a grid of elements and each element is linked to the information layers related to elements. There is no similar grid for cells. Instead, the HST3D GUI expects every active cell on a node layer to be either intersected or enclosed by a contour. Because the water table will be different at every cell, we will need to have a separate contour for every cell. That sounds difficult but the HST3D GUI provides an easy way to do this.

Go the HST3D Grid Layer and select "File|Export|Edit Template". Click the load button and load "grid.met" from the Argus Interware|ArgusPIE|HST3D_GUI directory. Click the "Done" button and select "File|Export|By Template". Next go to the Initial Water Table layer and import the file you just exported as a text file. It will be named "HST3D Grid.exp" unless you choose a different name. You will end up with a point contour at every cell. Now make the default value for the layer "Imported Initial Water table". If you color the points, you will see that each point has been assigned an appropriate value.
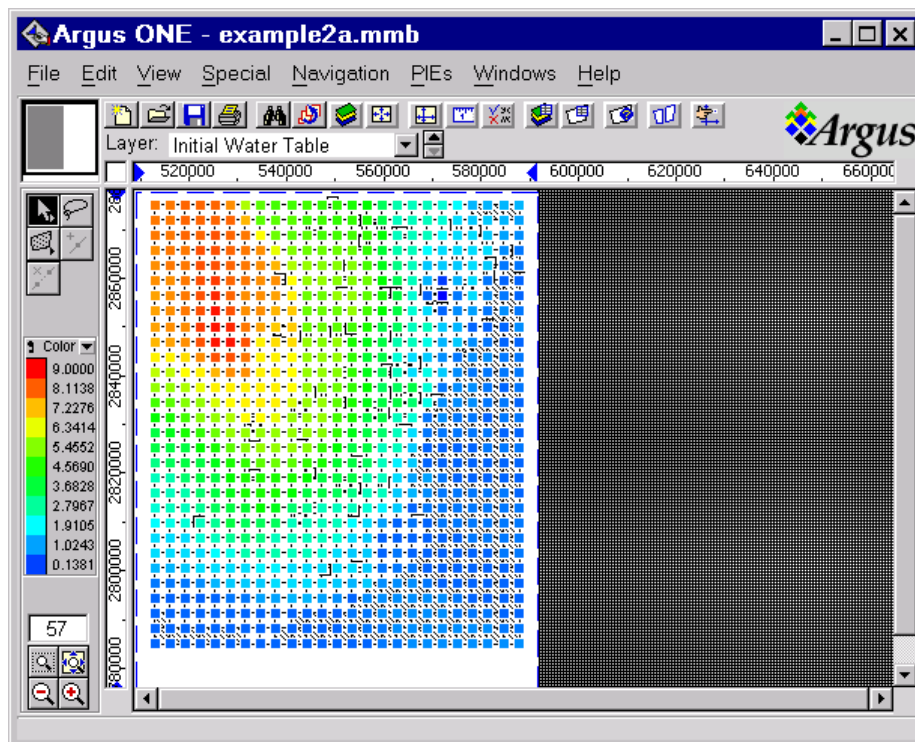
### Specifying the Initial Mass Fraction

We could use this same technique to specify the initial mass fraction. However, we wish to specify a uniform initial mass fraction of 0 so it is easier just to draw a contour around all the grid cells and give it a value of 0.
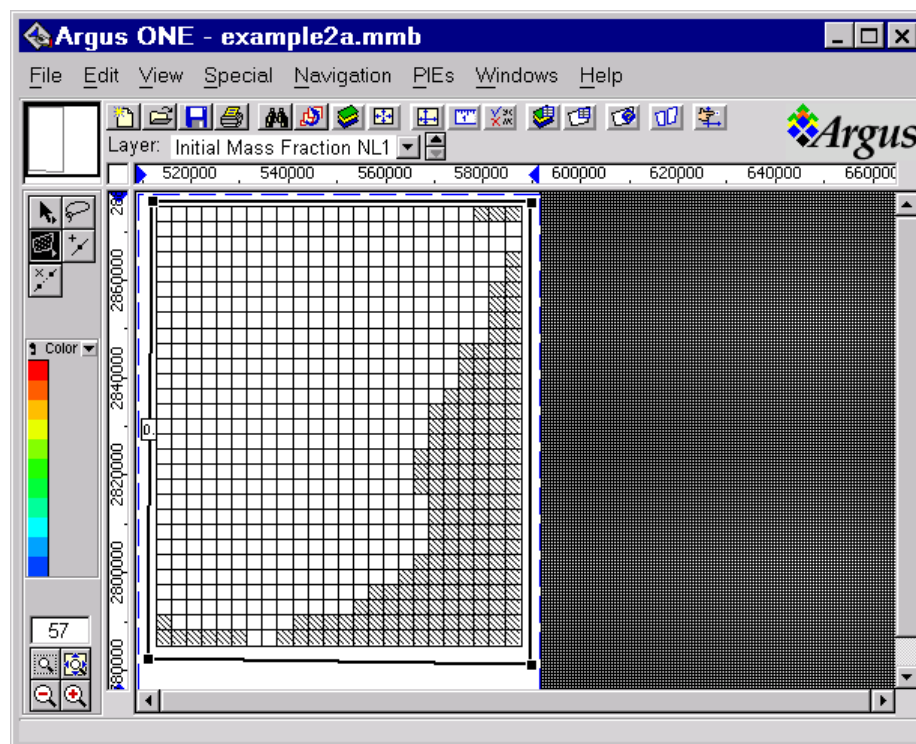


### Specified Pressure and Concentration Boundaries

The next thing to do is to add in the specified pressure and specified concentration boundaries along the coastline. The easiest way to specify the location of the boundary is to go to the domain outline line layer, use the lasso tool to select the portion of the domain outline that defines the coastline, and copy it to the clipboard. You can then paste it on all the Specified State NL[i] layers. After you have finished copying it on to all the Specified State NL[i] layers, you will need to go back and change the values associated with the contour. You will need to change Time1 to 0 for each of the contours you pasted. The default value of Time1 is 0 but that value was overridden by the 3000 from the Domain Outline layer. You can either type in 0 in place of 3000 or just delete the 3000. Next, we need to specify the pressure at each of these boundaries. On each Specified State NL[i] we will set the expression for the pressure to an expression of the form "(-HST3D Grid.Elevation NL[i])*63.98/144". HST3D Grid.Elevation NL[i] is the elevation of the node layer i. 63.98 is the specific weight of seawater in $lb/ft^3$. You divide by 144 to convert the pressure from $lb/ft^3$ to psi. This works in the special case where the pressure is 0 at an elevation of 0. If the pressure was 0 at some different elevation, you would need a formula of the form "(Zero Pressure Elevation-HST3D Grid.Elevation NL[i])* fluid specific weight/144 if you were using English units.

For all of the contours you pasted, you have to override the default value of "Scaled Mass Frac at Spec Pres1" and assign it a value of 1. For all but Specified State NL1, you must also override "Specified Scaled Mass Fraction1" and assign it a value of 1. This is like the Huyakorn example problem from the HST3D documentation.

We will also import another specified pressure boundary. On Specified State NL1, select File|Import Specified State NL1|Text File and select the file " Specified State NL1.exp". This file contains the location of a canal. We will assign different pressures to the upstream and downstream ends of it. Assign "Specified Pressure1" a value of -1.72 and End Specified Pressure1 a value of -3.11. Assign "Scaled Mass Frac at Spec Pres1" a value of 0. The specified pressures are derived from typical heads at the upstream and downstream end of the canal.
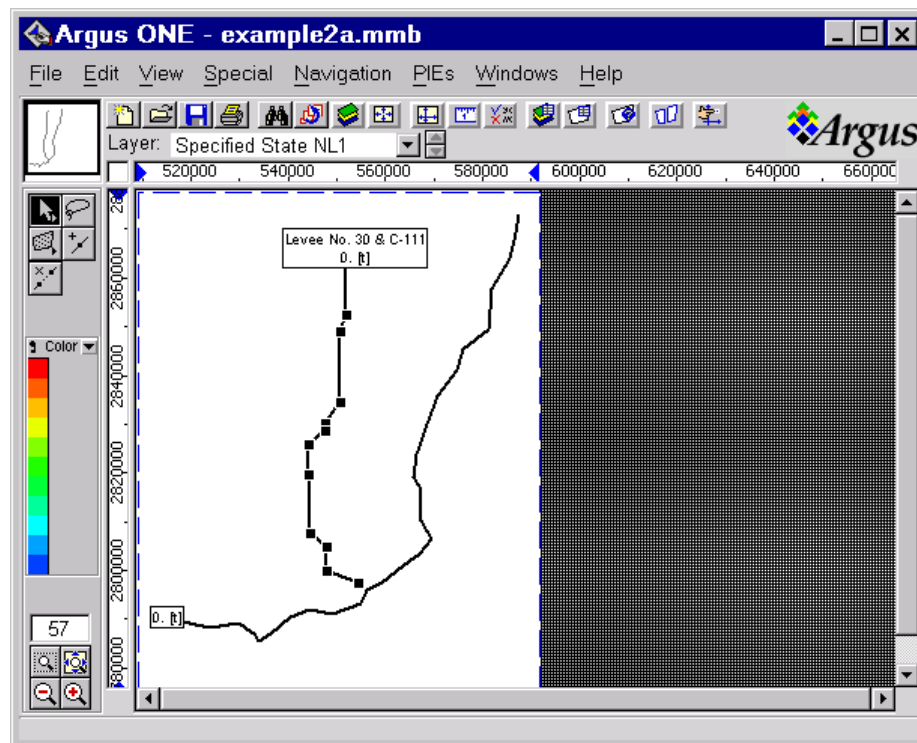
### Specified Flux Boundary

Finally we will specify recharge on the "Horizontal Specified Flux Boundary NL1" layer. This layer is for flux boundaries that are horizontal. The flux is normal to the boundary and thus is vertical. Draw a contour surrounding the active area and assign it the following values

| Time1 | 0 |
|---|---|
| Upward Fluid Flux1 | -0.001 |
| Density1 | 62.4 |
| Scaled Mass Fraction1 | 0 |
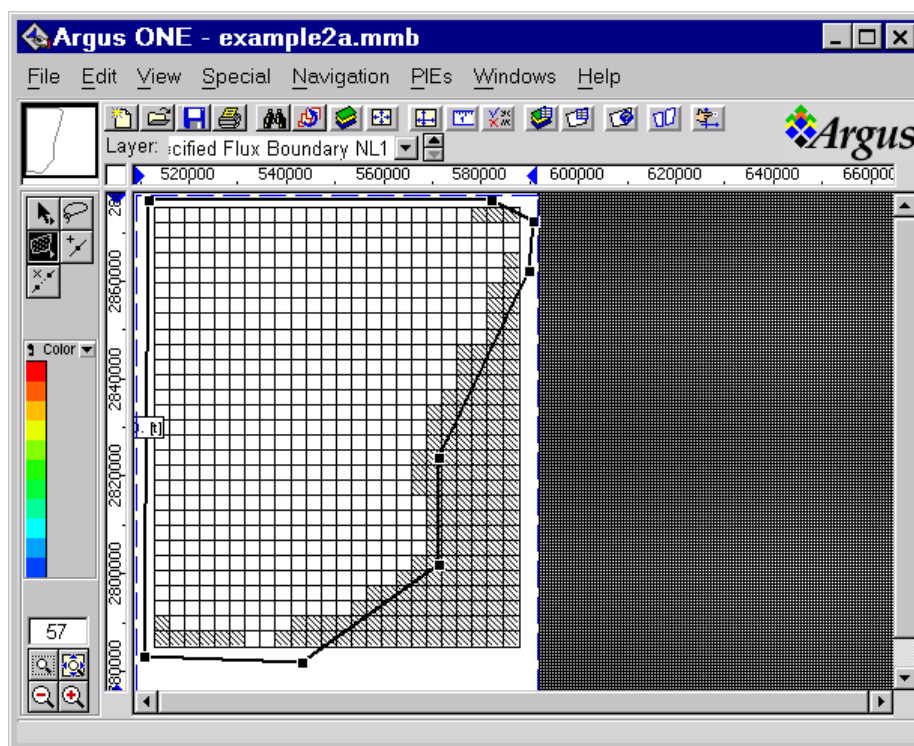


You can't have any other sort of boundary in cells that have specified state boundaries so at first it might appear that drawing the horizontal flux boundary to include cells that are also specified state boundaries would cause a problem. However, the HST3D GUI takes care of this for you. It checks each cell to make sure it is not a specified state boundary before assigning it as a specified flux boundary.

### Adding a Well

Finally, we will add a well to the model. Put the well in the prominent drawdown area in the northeastern section of the model.
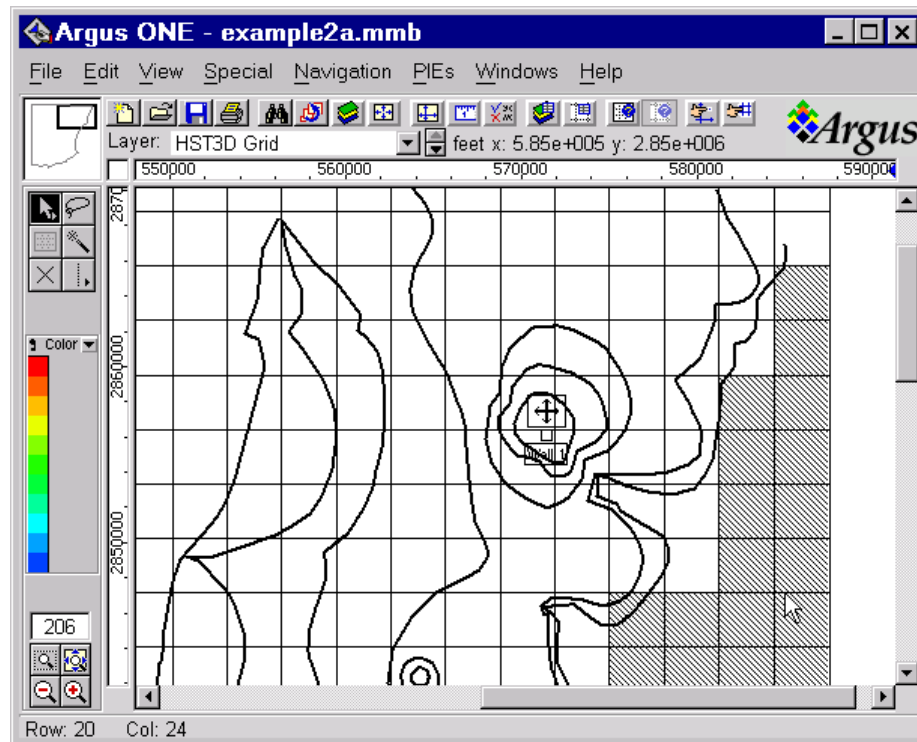


We will use expressions to assign the top and bottom completion elevations to the top of the model and the bottom of the Biscayne aquifer respectively. These expressions are as follows:

HST3D Grid.Elevation NL1

Biscayne Aquifer bottom

The outside diameter of the well is 2 and we will assign a method of 11 (specified flow rate with allocation by mobility). The well completion is 1 for element layers 1 to 5 and 0 for the other layers. The well skin factor is 0 for all layers. Time1 is 0, The flow rate is -1.3e7 ft$^3$/day, the datum pressure1 is 0, the fluid temperature1 is 68 F, and the scaled mass fraction1 is 0.

### *Running the Model*

This completes the data entry for this version of the model. Let's try running it. To run the model select PIEs|Run HST3D. The Run Dialog box will appear. Make sure the path for HST3D is correct and select Create HST3D input files and run HST3D. Then click on the Export button.
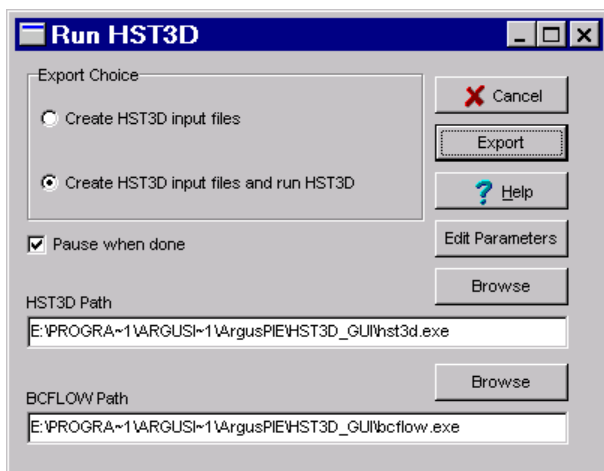


You will need to select the directory in which you run the model. When you have done that, the Argus ONE will begin exporting the model input file. This can take a while. While the export is going on, two progress bars will appear. Argus ONE generates one. It allows you to cancel the export at any time but gives no indication of how long the export process will take.
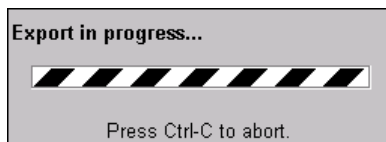


The PIE generates the other progress bar. It gives an estimate of how much longer the export process will take. If you want to cancel the export process, move the PIE-generated progress bar aside and use the Argus ONE progress bar to cancel the export.

**Export Progress** ✕

Phase 2: Exporting Data Set 2.12

Elapsed Time: 00:00:39 | Estimated Time Remaining: 00:00:31
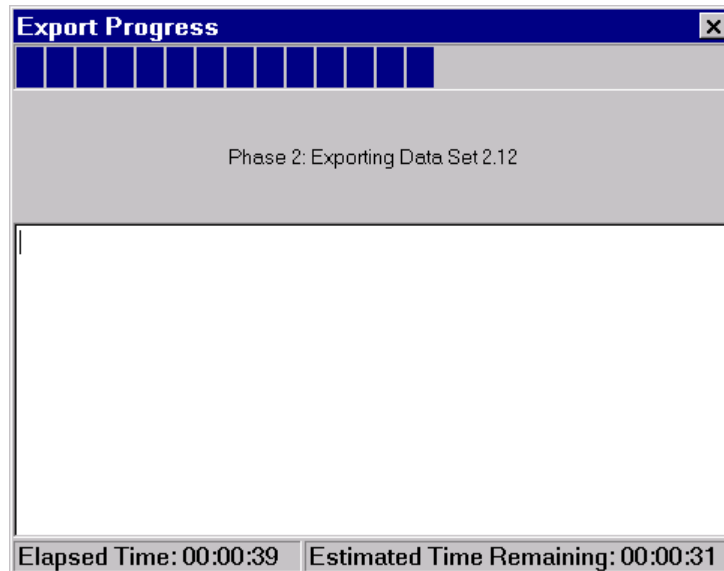
When the export process is done, the HST3D GUI will start HST3D. HST3D requires a lot of memory so it may not be able to start. You can get a variety of messages including one that says the program is not a valid Windows program. In reality, the program is valid, you just need to free up more memory to run it. One way to free-up memory is to save your Argus ONE model and shut down Argus ONE. Then in the directory in which you saved the HST3D input file there will be a file named RunHST3D.bat. Double click that file and it will start HST3D.

```
Command Prompt - runhst3d                                    _ □ ✕

        No. of solver iterations, Relative residual:    1  8.7660863E-10

        Equation no. 3, Mass Fractions       ; Iteration no. 2

        No. of solver iterations, Relative residual:    1  8.3544093E-15
             Maximum density change from solute: DENCHC   4.48846E-13

   Time ............................   3.000E-05  (d  )

   Maximum change in pressure ................   2.5292E+00   (psi) at location
( 5.812E+05, 2.850E+06, -270.   )(ft)
   Maximum change in scaled mass fraction ....  1.0000E+00     (-) at location
( 5.875E+05, 2.872E+06, -19.0   )(ft)

   Time step no.      2

   Current time step length ..........   3.000E-05  (d  )

        Equation no. 1, Pressures          ; Iteration no. 1

        No. of solver iterations, Relative residual:    1  1.1267786E-10

        Equation no. 3, Mass Fractions      ; Iteration no. 1
```

## *Viewing Model Results*

Next, we can look at the result of our model. Select "PIEs|HST3D Post-processing". The Post-processing dialog box will appear.
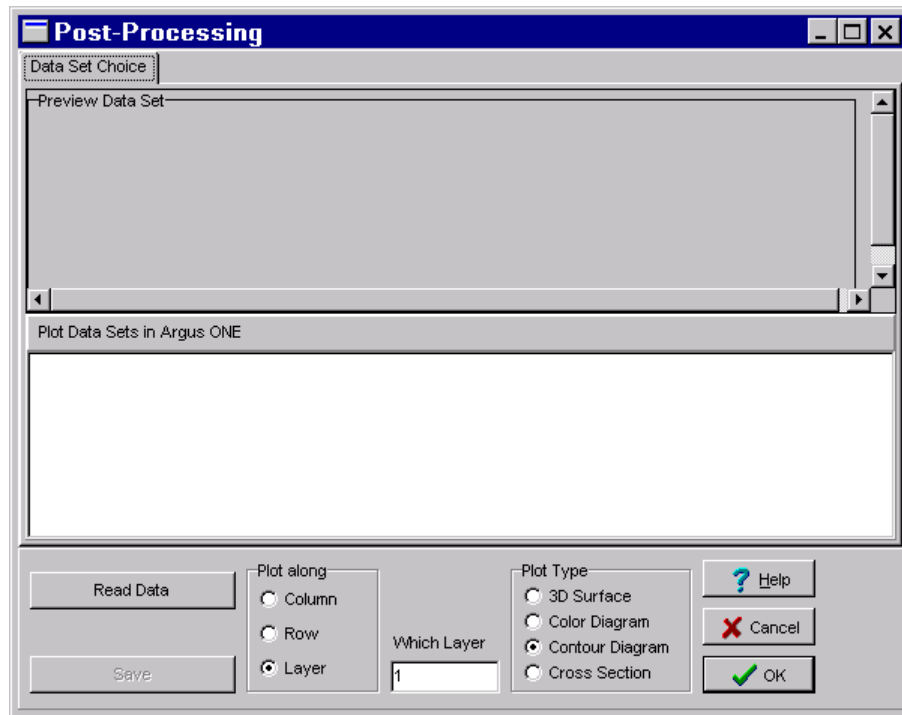
Click the "Read Data" button and then select the HST3D output file of your choice. There are three types of output files read by the post processing PIE; Pmap files (pressure, temperature, and mass fraction), Pmap2 files (potentiometric head and density), and Vmap files (velocities in the X- Y- and Z-directions).
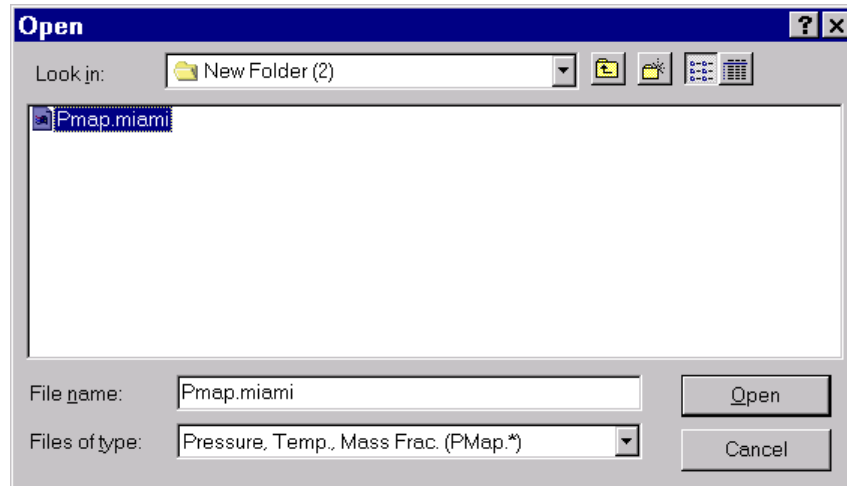
In this case, select the Pmap file. The HST3D GUI will read the file and display the data sets it contains.
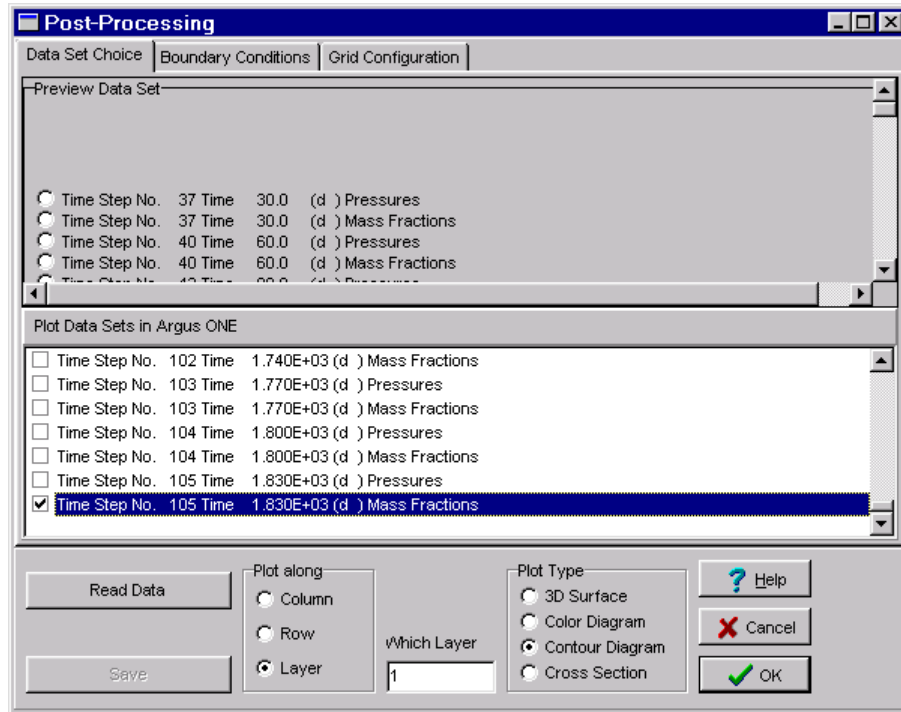


If you wish, you may preview a data set by selecting it in the list of radio buttons top half of the dialog box. You will create a post processing plots of all the data sets you select in the list of check boxes in the lower half of the dialog box. You can also look at the boundary conditions and grid configuration. In this case, select the last data set. We will plot a contour diagram of the top layer (layer 1). Click the OK button after you have selected the data set.

After you click OK, the postprocessing chart will appear. (This map has been edited and so will appear slightly from what appears initially.  To reproduce this map, make the layer containing the map the active layer, double click on the map, change the contouring algorithm to "Linear", uncheck the "Calculate automatically" check box and change the Maximum to 1 and the Delta to 0.1.)
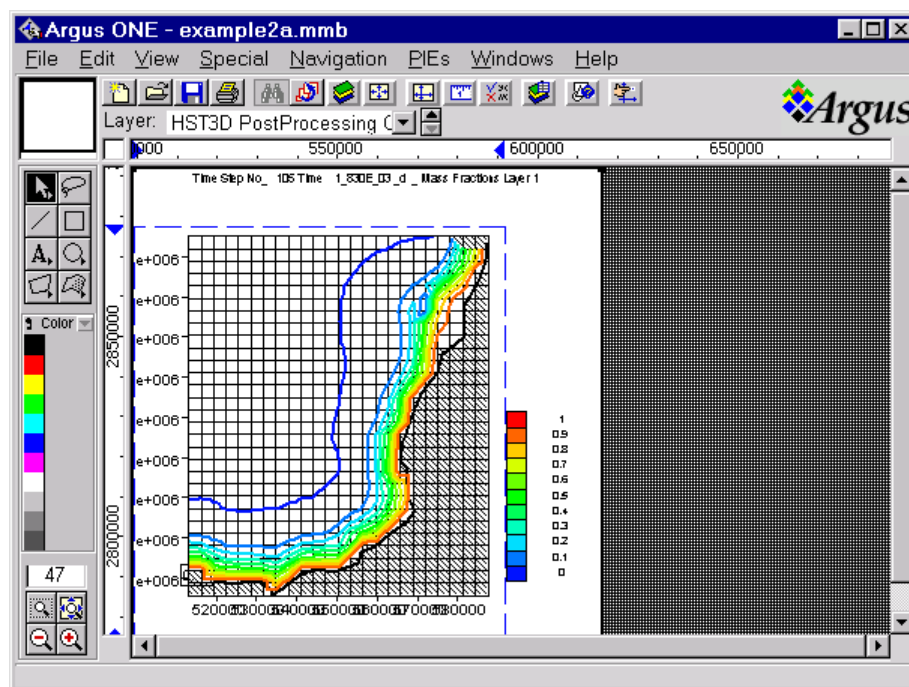


### Creating and Running a Transient Model

Thus far, none of the boundary conditions changed over time. Our next step will be to introduce temporal variation. A word of warning however, When you have a lot of time periods or layers in a model, the current version of Argus ONE (4.2.0p) can take an extremely long time to remove layers or parameters. If you change your options in such a way that layers or parameters will be removed from the model, you may find that Argus ONE will appear to "freeze-up" while it attempts to remove the layers or parameters. You may get impatient and decide to terminate Argus ONE thus loosing any changes you have made in your file. Thus, it is a good idea to save your work before you make such changes. For example, if you have a leakage boundary condition and decide to remove it in the Edit project dialog box, it would be a good idea to save your work if you have a lot of layers and time periods in the model. I have found that if I have more than 100 time periods in a model, Argus ONE is quite slow about removing layers but not so slow that I decide to quit the model rather than wait it out. If I have 150 time periods and try to remove a layer, I get tired of waiting before Argus ONE has finished. Thus, for me, 100 time periods is the maximum number of time periods I would normally choose to use. You may wish to experiment to see what you can tolerate.

In addition, if you have many time periods, the size of the output files may become large.

With that said, lets save our work now before continuing because we will soon increase the number of time periods to 156. Before increasing the number of time periods, you may wish to check that you have not selected any options in the Edit Project Info dialog box that you don't

46

want. After changing the number of time periods, it may be impractical to change some options. You may also wish to save a copy of the model with a new name so that you have a back-up copy that does not have so many time periods. When you have lots of layers and/or parameters, Argus ONE needs a very long time for to process the deletions.

When you have checked that you have all the right options in the Edit Project Info dialog box and have saved a back-up copy of the model, select PIEs|Edit Project Info and go to the Time tab. We will be having monthly time steps. Because some months will be 31 days long, we will want to change some of the variables on the time tab from 30 to 31 days. Change the following variables.

| Variable | Old Value | New Value |
|---|---|---|
| Max time step (DTIMMX) (t) | 30 | 31 |
| Pres/Temp/Mass Frac Printout Interval (PRIPTC) | -30 | -31 |
| Flow-Balance Printout Interval (PRIGFB) | -30 | -31 |
| Specified-Value Flow Printout Interval (PRIBCF) | -30 | -31 |
| Well Printout Interval (PRIWEL) | -30 | -31 |
| Map Printout Interval (PRIMAP) | -30 | -31 |

Select OK to close the Edit Project Info dialog box.

## Importing Transient Data

Next, you need to open one of the two Excel[TM] files that contain the data we will import. Lets start with start_pressure.xls. This contains the heads in the upstream end of the canal that we imported into Specified State NL1. We need to convert these heads to pressures and then import them into the model. The Excel[TM] file already has formulas to perform these conversions. As illustrated below, We subtract 9 from the elevation (because 9 is the elevation of NL1 where the boundary is applied) This gives the distance from the head in the canal to the node layer. We multiply that distance by the specific weight of water (62.4 lb/ft$^3$) to get the pressure in lb/ft$^2$. We divide by 144 to convert the pressure to psi (lb. per square inch).



Microsoft Excel - start_pressure.xls

File  Edit  View  Insert  Format  Tools  Data  Accounting  Window
Help

B52  =  =+(B18-9)*62.4/144

| | A | B | C | D | E | F | G | H | |
|---|---|---|---|---|---|---|---|---|---|
| 48 | 1997 | 3361 | 2914 | 2735 | 2794 | 2347 | 4376 | 4555 | 44 |
| 49 | | | | | | | | | |
| 50 | S32_H_DBKEY_06897 | | | | | | | | |
| 51 | YEAR | JAN | FEB | MAR | APR | MAY | JUN | JUL | AU |
| 52 | 1985 | -1.25667 | -1.25667 | -1.25667 | -1.25667 | -1.25667 | -1.25667 | -1.25667 | -1. |
| 53 | 1986 | -1.38667 | -1.45167 | -1.41267 | -1.22633 | -1.677 | -1.45167 | -1.729 | -2. |
| 54 | 1987 | -1.35633 | -1.37367 | -1.30433 | -1.34767 | -1.38667 | -1.59033 | -1.56 | -1. |
| 55 | 1988 | -1.16567 | -1.26967 | -1.23067 | -1.352 | -1.417 | -1.417 | -1.37367 | -1. |
| 56 | 1989 | -1.41267 | -1.73333 | -1.94567 | -2.42233 | -2.405 | -2.34433 | -2.015 | -2. |
| 57 | 1990 | -1.95433 | -2.12333 | -2.32267 | -2.34 | -2.48733 | -2.21867 | -2.07567 | -1. |
| 58 | 1991 | -2.171 | -1.976 | -2.236 | -2.11033 | -2.002 | -1.63367 | -1.26533 | -1. |
| 59 | 1992 | -1.45167 | -1.47333 | -1.612 | -1.60767 | -1.93267 | -1.859 | -1.25667 | -1. |
| 60 | 1993 | -1.17433 | -1.17867 | -1.16567 | -1.20467 | -1.33467 | -1.27833 | -1.31733 | -1. |
| 61 | 1994 | -1.339 | -1.34767 | -1.235 | -1.248 | -1.365 | -1.38233 | -1.391 | -1. |
| 62 | 1995 | -0.819 | -1.26967 | -1.17867 | -1.09633 | -1.16133 | -1.09633 | -1.04 | -0. |
| 63 | 1996 | -1.079 | -1.17433 | -1.222 | -1.30867 | -1.34333 | -1.18733 | -1.053 | -1. |
| 64 | 1997 | -1.25233 | -1.31733 | -1.34333 | -1.33467 | -1.39967 | -1.105 | -1.079 | -1. |

S32_H_DBKEY_06897

Ready

Next select the data (including the two title lines) and copy it to the clipboard. Then select New|Workbook to create a new workbook. Select "Edit|Paste Special|Values" to paste the data into the new workbook.

**Microsoft Excel - start_pressure.xls**

File  Edit  View  Insert  Format  Tools  Data  Accounting  Window  Help

A50 = S32_H_DBKEY_06897

| | A | B | C | D | E | F | G | H | I | J | K | L | M |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 48 | 1997 | 3361 | 2914 | 2735 | 2794 | 2347 | 4376 | 4555 | 4495 | 5510 | 5033 | 5003 | 5689 |
| 49 | | | | | | | | | | | | | |
| 50 | S32_H_DBKEY_06897 | | | | | | | | | | | | |
| 51 | YEAR | JAN | FEB | MAR | APR | MAY | JUN | JUL | AUG | SEP | OCT | NOV | DEC |
| 52 | 1985 | -1.25667 | -1.25667 | -1.25667 | -1.25667 | -1.25667 | -1.25667 | -1.25667 | -1.235 | -1.22633 | -1.21333 | -1.20467 | -1.32167 |
| 53 | 1986 | -1.38667 | -1.45167 | -1.41267 | -1.22633 | -1.677 | -1.45167 | -1.729 | -2.25333 | -1.768 | -1.32167 | -1.34767 | -1.39533 |
| 54 | 1987 | -1.35633 | -1.37367 | -1.30433 | -1.34767 | -1.38667 | -1.59033 | -1.56 | -1.56 | -1.59033 | -1.313 | -1.23933 | -1.144 |
| 55 | 1988 | -1.16567 | -1.26967 | -1.23067 | -1.352 | -1.417 | -1.417 | -1.37367 | -1.00967 | -1.09633 | -1.11367 | -1.27833 | -1.339 |
| 56 | 1989 | -1.41267 | -1.73333 | -1.94567 | -2.42233 | -2.405 | -2.34433 | -2.015 | -2.07133 | -1.80267 | -1.62933 | -1.74633 | -1.82867 |
| 57 | 1990 | -1.95433 | -2.12333 | -2.32267 | -2.34 | -2.48733 | -2.21867 | -2.07567 | -1.833 | -1.68567 | -1.61633 | -1.846 | -2.17967 |
| 58 | 1991 | -2.171 | -1.976 | -2.236 | -2.11033 | -2.002 | -1.63367 | -1.26533 | -1.248 | -1.404 | -1.26967 | -1.34333 | -1.404 |
| 59 | 1992 | -1.45167 | -1.47333 | -1.612 | -1.60767 | -1.93267 | -1.859 | -1.25667 | -1.196 | -1.13533 | -1.144 | -1.09633 | -1.144 |
| 60 | 1993 | -1.17433 | -1.17867 | -1.16567 | -1.20467 | -1.33467 | -1.27833 | -1.31733 | -1.34333 | -1.313 | -1.21333 | -1.131 | -1.27833 |
| 61 | 1994 | -1.339 | -1.34767 | -1.235 | -1.248 | -1.365 | -1.38233 | -1.391 | -1.17433 | -1.00533 | -0.83633 | -0.68467 | -0.72367 |
| 62 | 1995 | -0.819 | -1.26967 | -1.17867 | -1.09633 | -1.16133 | -1.09633 | -1.04 | -0.936 | -0.88833 | -0.78 | -1.24367 | -1.04433 |
| 63 | 1996 | -1.079 | -1.17433 | -1.222 | -1.30867 | -1.34333 | -1.18733 | -1.053 | -1.027 | -1.118 | -1.014 | -1.24367 | -1.261 |
| 64 | 1997 | -1.25233 | -1.31733 | -1.34333 | -1.33467 | -1.39967 | -1.105 | -1.079 | -1.08767 | -0.94033 | -1.00967 | -1.014 | -0.91433 |
| 65 | | | | | | | | | | | | | |

S32_H_DBKEY_06897

Ready                    Sum=25663.69433

Next select File|Save As to open the save dialog box. Save the file as a tab-delimited text file by select "Text (Tab delimited) (*.txt)" in the "Save as type" combo box.

Follow a similar procedure with the other Excel$^{TM}$ file named end_pressure.xls, which represents the head at the downstream end of the canal.

You should now have two tab-delimited text files named start_pressure.txt and end_pressure.txt each containing 13 years or monthly pressures at the upstream or downstream end of the canal. We will import these data into the existing canal contour. You can now close Excel and go back to Argus ONE. Select Edit Project Info and go to the Time tab. Change "Maximum number of time periods to be used for any object" to 156 which is the number of data values in each text file and select OK. You may have to wait a little while as Argus ONE adds the new parameters to the existing layers. This takes about a minute on my computer.

When Argus ONE is done adding parameters, make Specified State NL1 the active layer and select the canal contour. Double click on the canal contour to inspect its parameter values. It should have 156 sets of parameters values; one for each time period. Most of the parameters will have default values of $N/A.

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Cut the contour to the clipboard again. Now select PIEs|Import Monthly Data. Select the current layer from the dialog box (Specified State NL1).
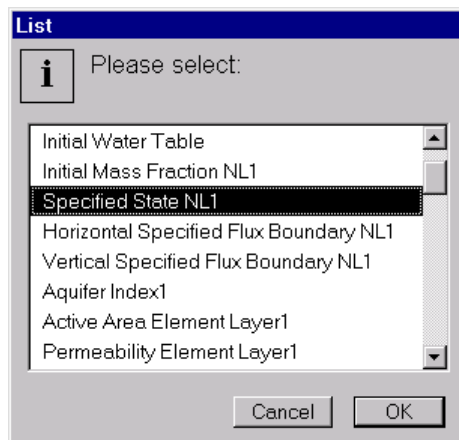


We will import the data for the starting pressures so select "Specified Pressure" in the top half of the dialog box and click the OK button.
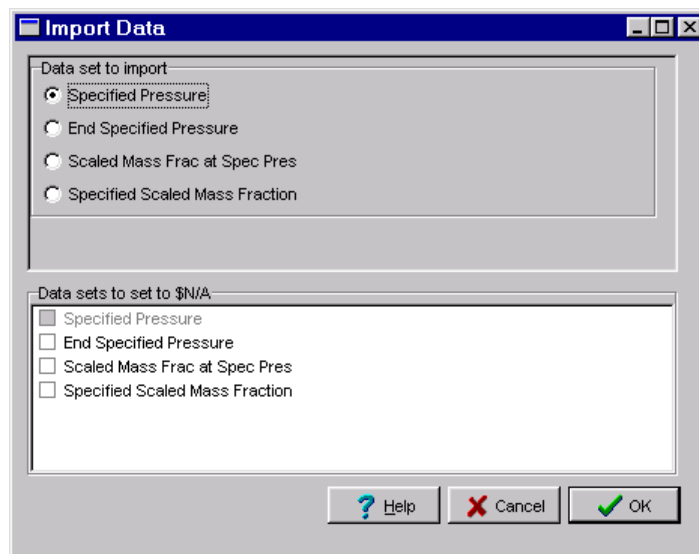


An open file dialog box will appear. Select the start_pressure.txt file and click OK. The Canal contour will reappear on the layer with the time and Specified Pressure parameters set to the correct values. We will do almost the same thing for the "End Specified Pressure" parameter, which represents the pressure at the downstream end of the contour. (Argus ONE will interpolate between the Specified Pressure and End Specified Pressure parameters when exporting data for this contour to HST3D).

Cut the contour to the clipboard again. This time select "End Specified Pressure" in the top half of the dialog box and "Specified Scaled Mass Fraction" in the lower half of the dialog box.
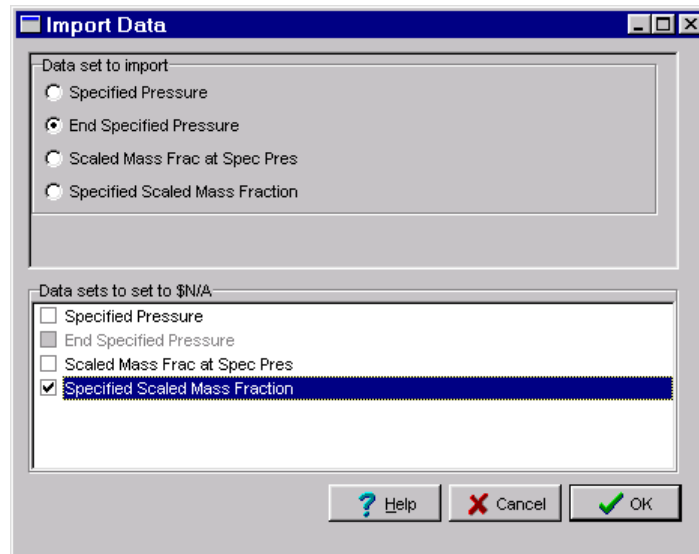


Click OK and import the end_pressure.txt file. Now double-click on the canal contour and you'll see that the "Specified Scaled Mass Fraction" parameters have all been assigned values of $N/A (= not available). This means that this boundary is not a specified concentration boundary.

You can now run the model again. However, you may choose not to do so. Exporting the data set may take a while (about 15 minutes) and running the model will take hours. You will need a large amount of free disk space to store the output files (about 500 Mb). You may instead just choose to look at the output as shown below.
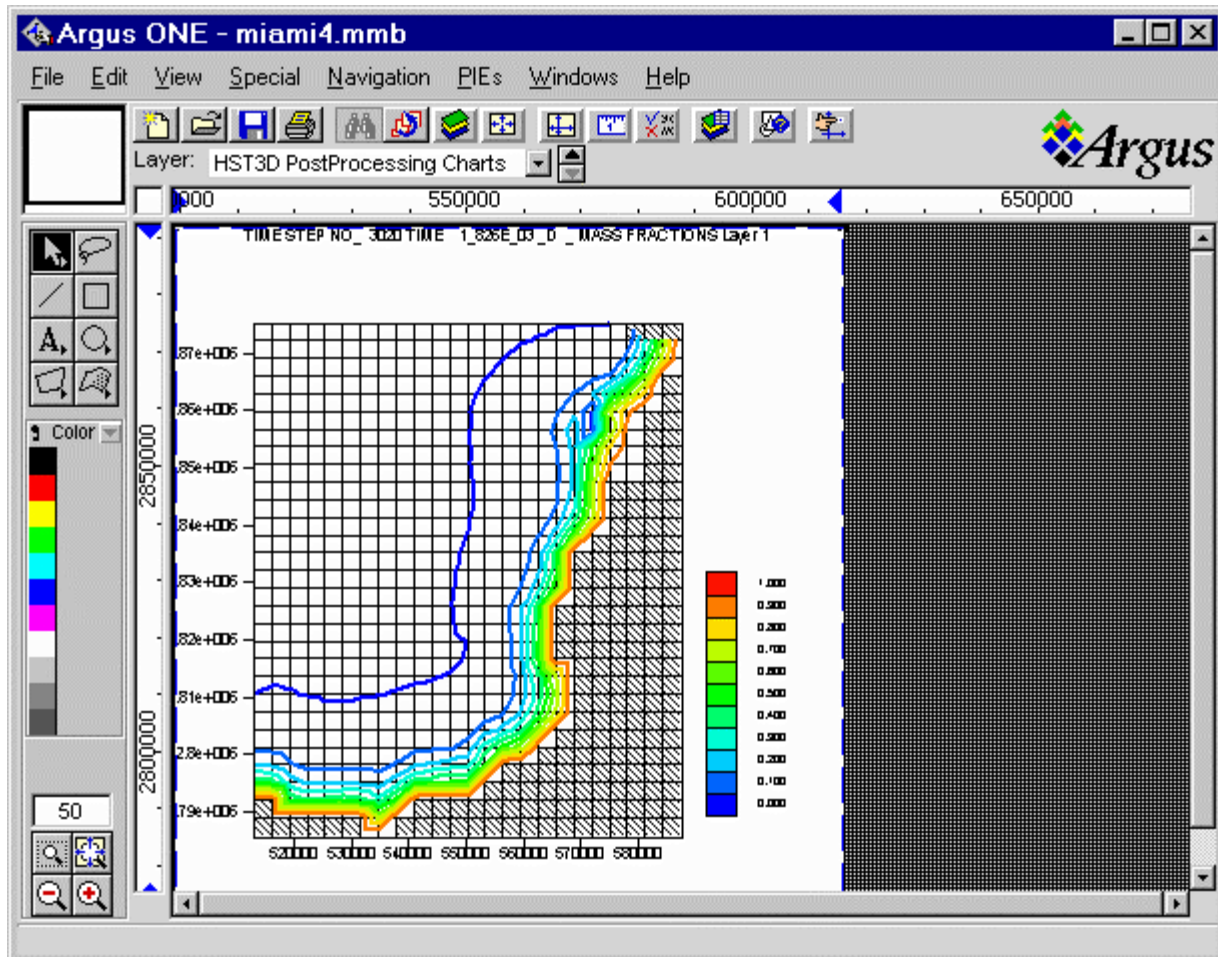


You may notice that this bears a striking resemblance to the output from the model with only a single time period. In this case including the temporal variation did not greatly alter the final result. If you examine the data that we imported, you will see that the pressures don't vary by a large amount and thus they had a small effect on the outcome. In this case, we gained little by including the monthly data. In fact, the only reason for including monthly data in this model was that the people providing the funds for the model required monthly time periods! In this simplified example, at least, monthly time periods do not appear to be justified.

This model could be improved in several ways.

- First, the northern and western model boundaries arbitrary. It would be better to choose natural boundaries such as the outcrop of the Biscayne aquifer.
- The longitudinal and transverse dispersivity values are not based on any data. Instead, they are numbers picked out of thin air. Thus, a more realistic model would need values that have a better basis in fact.

- The model coordinates we used in this model should have been metric units because those are the actual units of the base map. We pretended that they were English units to show how to unit conversions in English units but that does not represent the real situation.
- We did not include all the canals that exist in the model area. We need to include more of them.
- We could use an Aquifer-Influence boundary to model the effects of surrounding aquifers. It is not clear to me whether or not this would be required in this case.
- We do not use precise data for the pumpage from the well field nor did we model all the wells in the model area. We could improve the model by using better pumpage values.
- We did not check to see if the spatial and temporal discretization were satisfactory.
- We did not have good data on the permeability of the Surficial aquifer.
- We used generalized values of porosity, dispersivity and vertical compressibility without any good data to back-up these values.

With all these limitations, its clear that this model is not adequate for predicting the actual behavior of the Biscayne aquifer although it might represent a starting point for such a model. Of course, it was never intended to provide an adequate model. Instead, it was intended to demonstrate how to use the HST3D GUI and it does fulfill that goal.