HST3D Example Problem 1

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HST3D Example Problem 1

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.

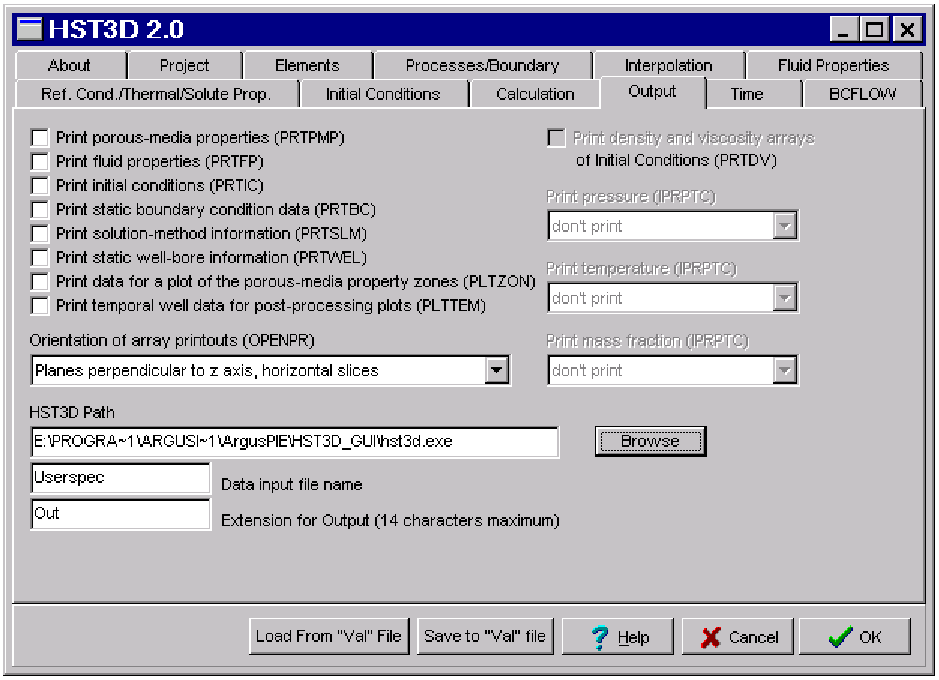
In this example we will recreate Kipp's example of a saltwater intrusion into a coastal aquifer (Kipp, 1997, p. 94). This model is 14,400 feet long, 9600 feet wide and 200 feet thick. The aquifer is homogeneous but anisotropic. Aquifer parameters are as follows.

Horizontal permeability:	7.754e-9 $ft.^2$
Vertical permeability:	7.754e-10 $ft.^2$
Longitudinal dispersivity:	150 ft.
Transverse dispersivity:	30 ft.
Porosity:	0.2
Vertical compressibility:	0.
Distribution coefficient:	0.
Freshwater density:	62.42 lb/ft^3
Saltwater salinity:	35.7 parts per thousand
Fluid density at maximum solute mass fraction:	63.98 lb/ft^3
Number of nodes in the X direction:	62
Number of nodes in the Y direction:	19
Number of nodes in the Z direction:	11

Non-Spatial Data - Output Tab

We will begin by creating a new HST3D model by selecting "New HST3D Project" from the PIE's menu. After we select a Cartesian coordinate, the Edit Project Info Dialog box appears. Lets switch to the Output tab first.

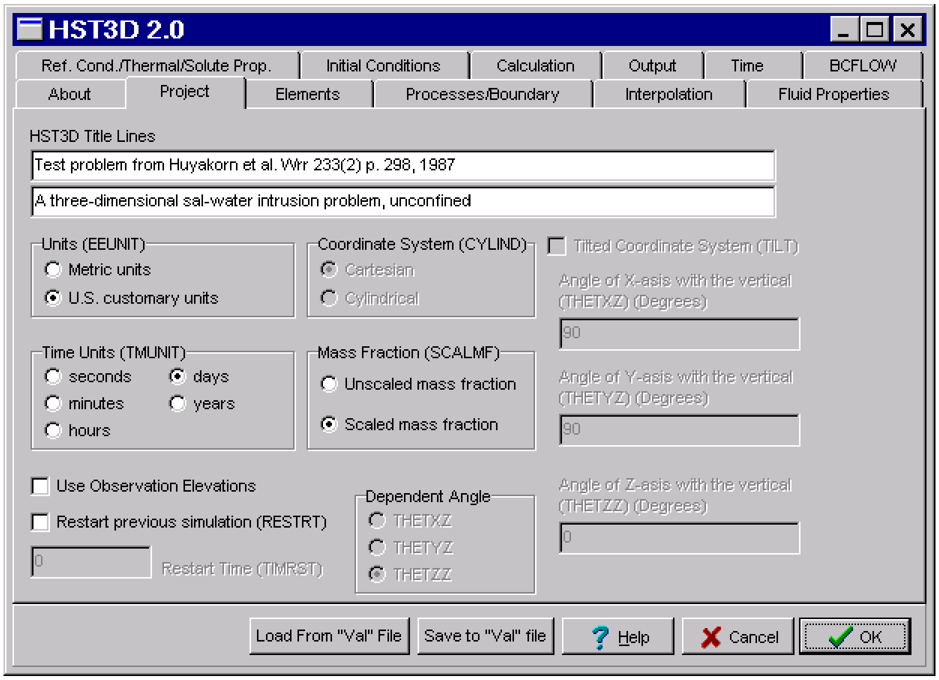
Enter the correct path for HST3D on your system. You don't have to type it, you can click on the "Browse" button to select the file on your hard drive.



Once you have the correct path, click on the "Save to 'Val' file" button and accept the default name and path of the file. This will set the default values of all the data in the Edit Project Info dialog box including the correct path. Now whenever you start a new HST3D Project, you will automatically start up with the correct path for HST3D. You can use the same procedure to set the default values of all the items in the Edit Project Info dialog box.

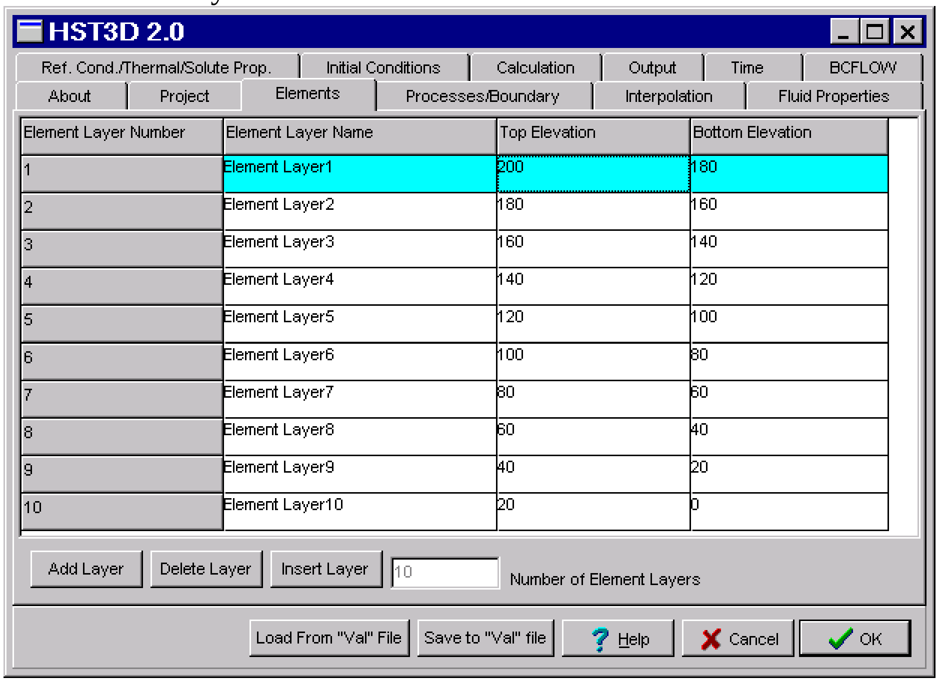
Non-Spatial Data - Project Tab

For this example, we will use U.S. customary units, a time unit of days and scaled mass fractions. HST3D requires that all data be in either metric units or U.S. customary units. You can not have some data in metric units and other data in U.S. customary units. However, HST3D interface comes with a PIE that provides functions that can convert from metric units to U.S. customary units and vice versa.



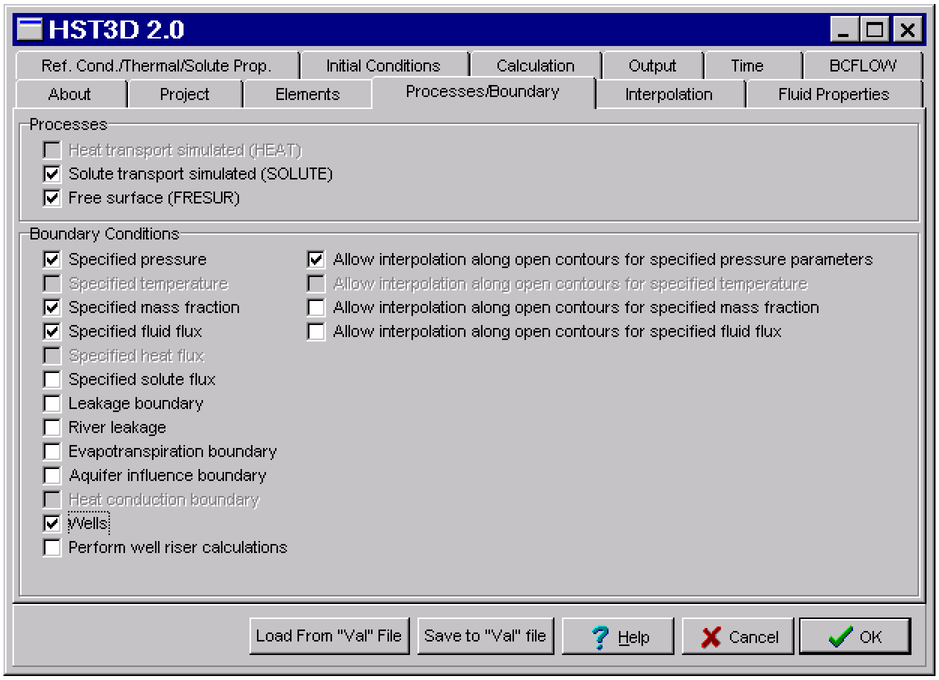
Non-Spatial Data - Elements Tab

Next, we go to the Elements tab where we set the vertical discretization. Our model has eleven node layers in the vertical direction. This corresponds to 10 element layers. We will click on the "Add Layer" button until there are 10 element layers. We will then edit the top and bottom elevations so that the elevations range from 200 at the top of the uppermost layer to 0 at the bottom of the bottommost layer.



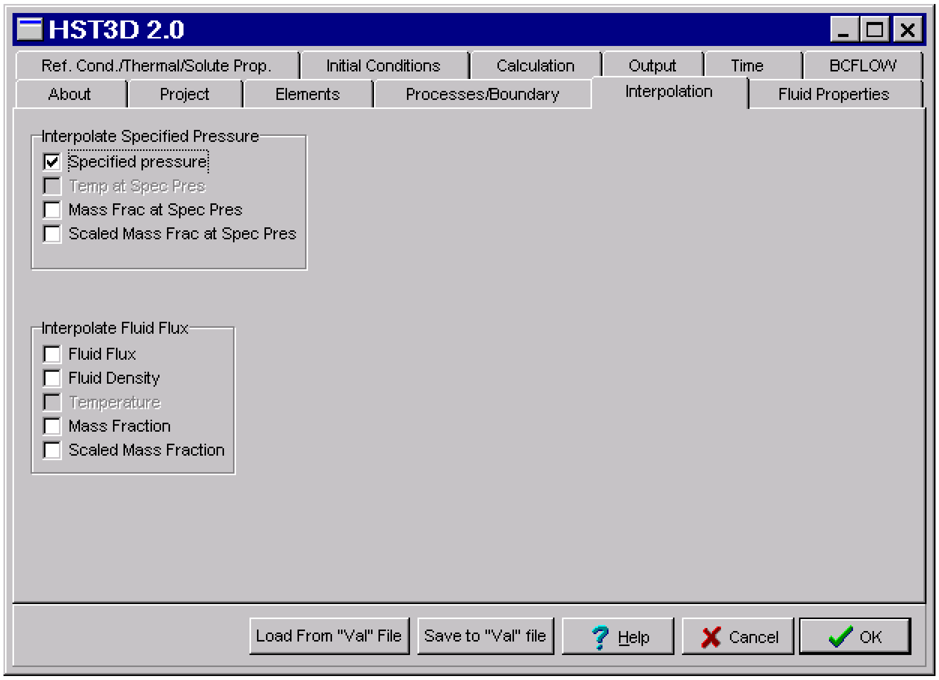
Non-Spatial Data - Processes/Boundary Tab

On the "Processes/Boundary" tab, we will select the options we need for the model. We will select Solute transport, Free Surface, Specified pressure, Specified mass fraction, Specified fluid flux, Wells, and Allow interpolation along open contours for specified pressure parameters.



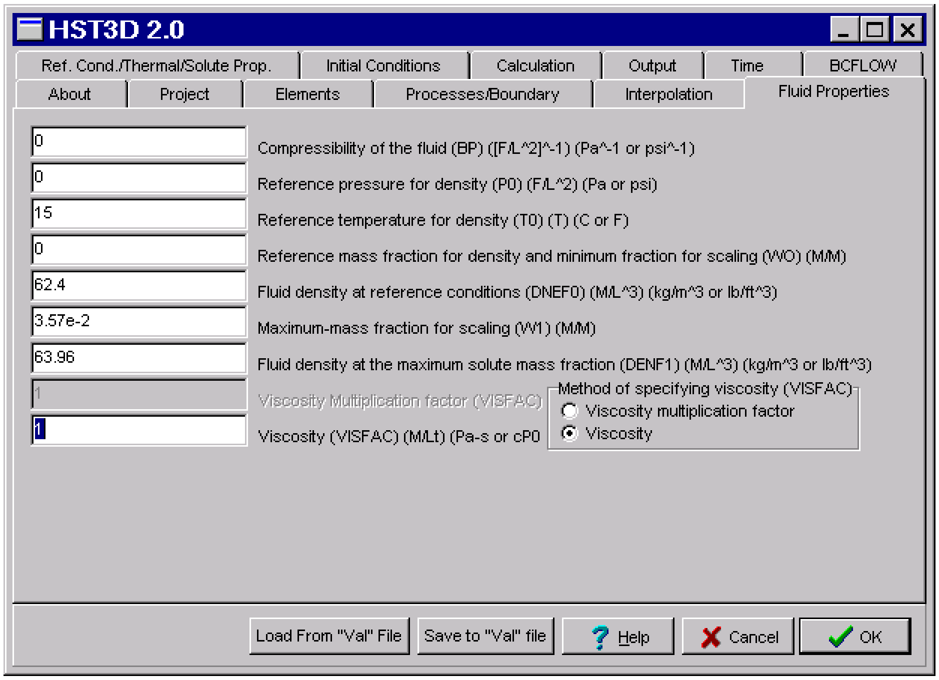
Non-Spatial Data - Interpolation Tab

We will need to interpolate the specified pressure parameter so on the Interpolation tab, we will select "Specified Pressure". (These check boxes were disabled until we selected " Allow interpolation along open contours for specified pressure parameters" on the Processes/Boundary tab.



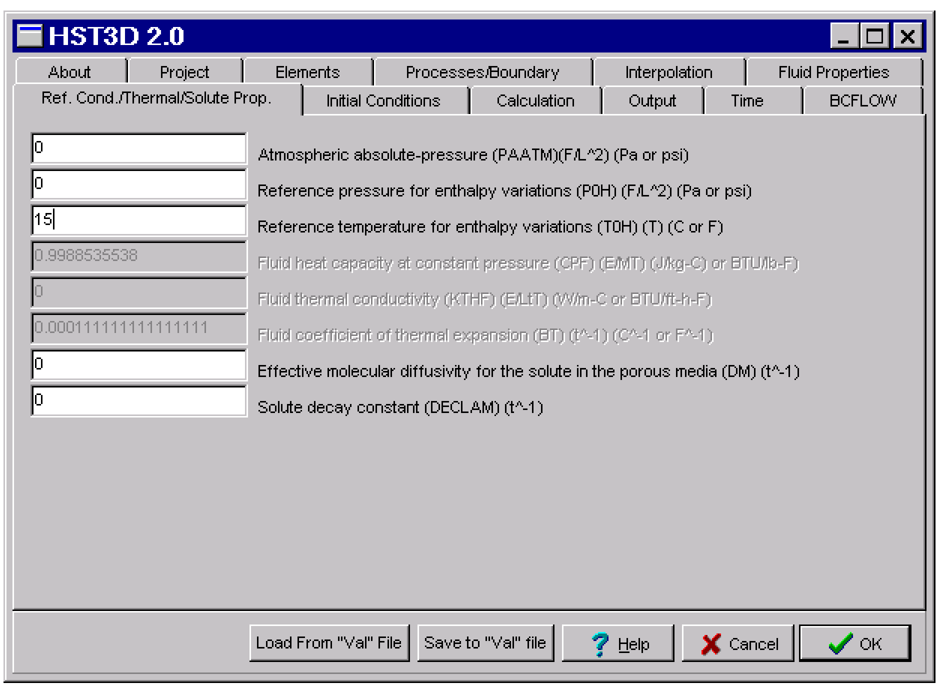
Non-Spatial Data - Fluid Properties Tab

On the Fluid Properties tab, we will set values of the different items as shown below.



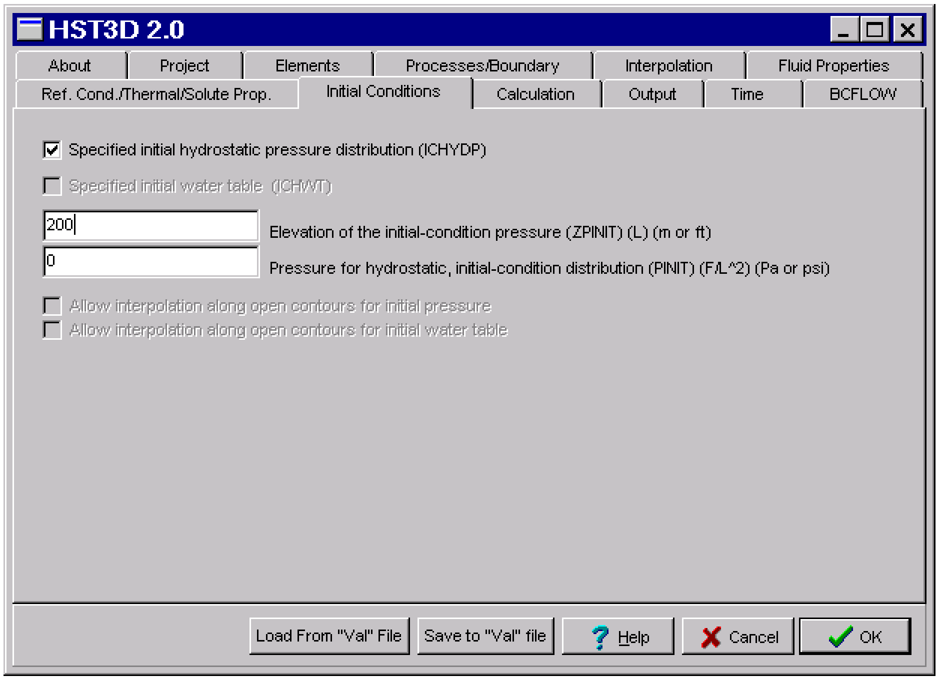
Non-Spatial Data - Ref. Cond./Thermal/Solute Prop. Tab

We will set the reference temperature for enthalpy variations to 15.



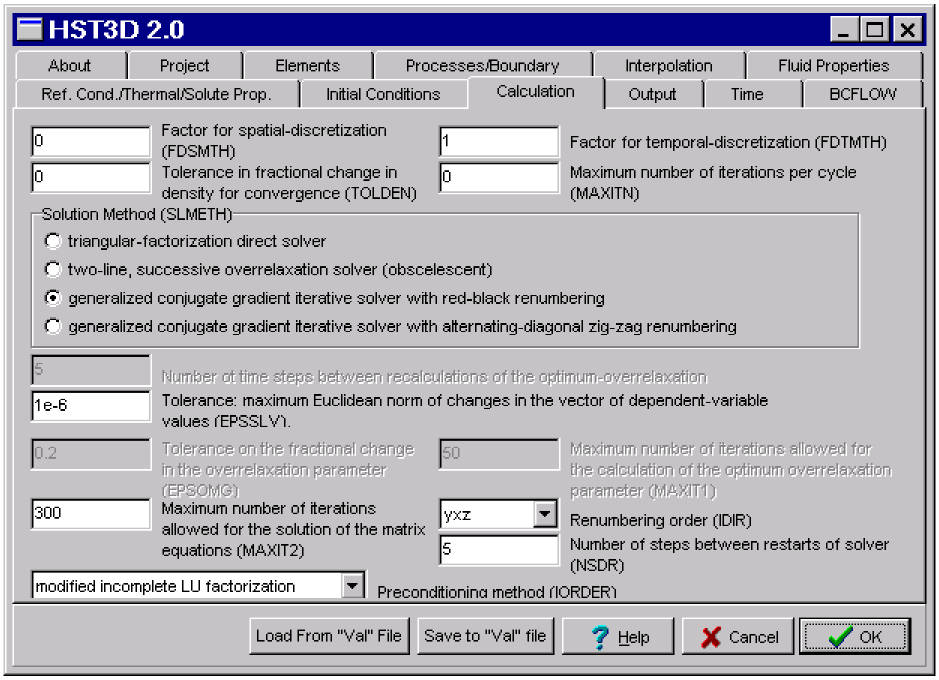
Non-Spatial Data - Initial Conditions Tab

We will use a specified initial hydrostatic pressure distribution. The elevation at which we will specify the pressure is 200 (the top of the model). The pressure there will be 0.



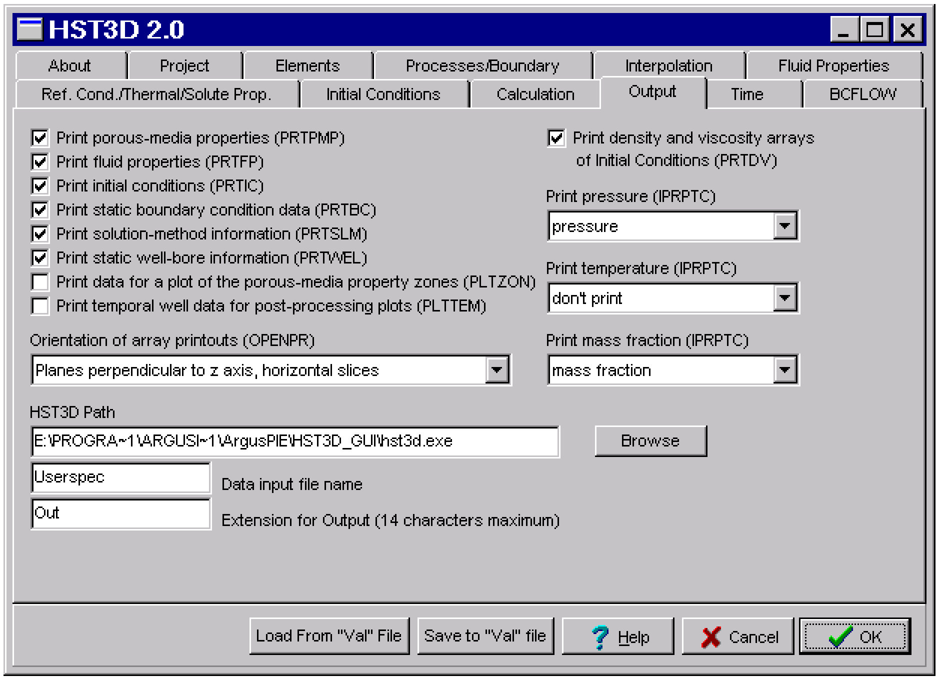
Non-Spatial Data - Calculation Tab

We will set the calculation information as illustrated below. In some cases, we have used a value of 0. This causes HST3D to set these variables to the default value.



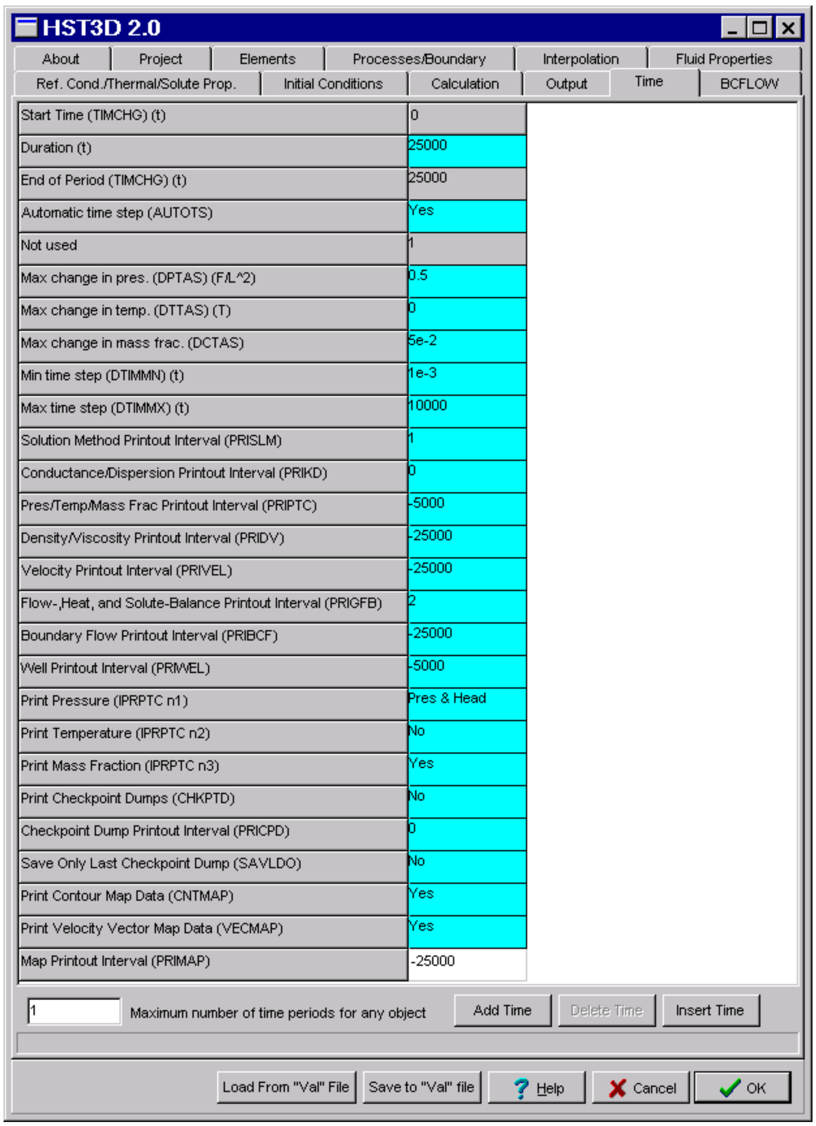
Non-Spatial Data - Output Tab (again)

Next we need to decide what sort of output we want. The following are good choices for this problem. However, you should make sure that you have the correct path for HST3D on your system if you have not done so already.



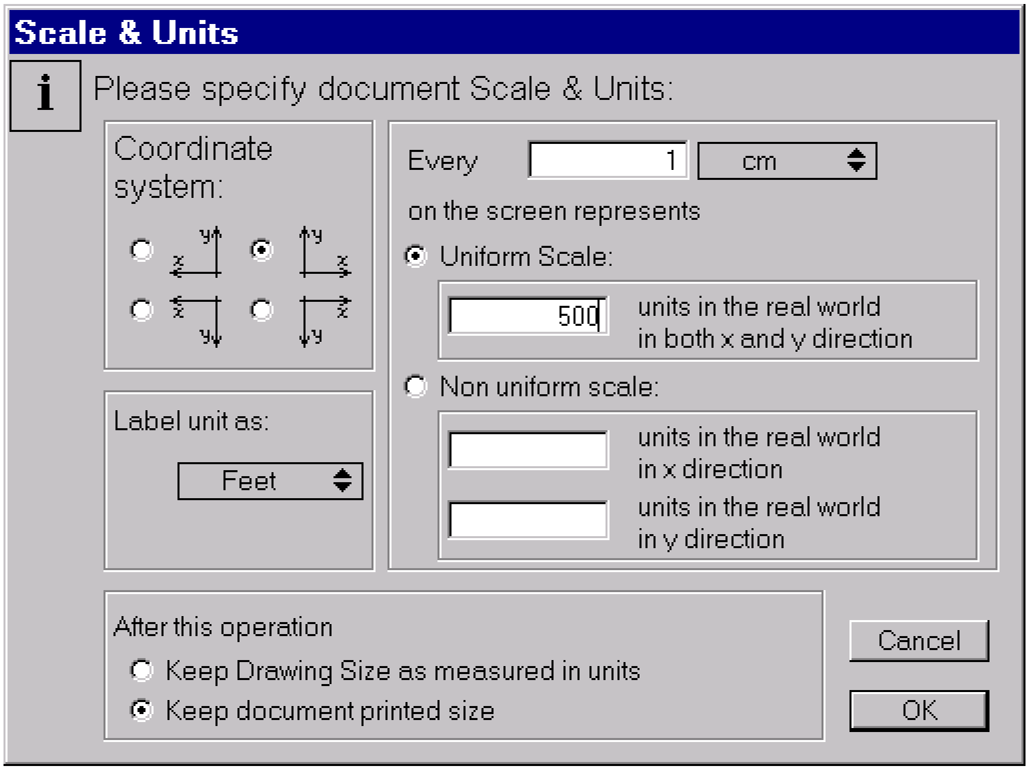
Non-Spatial Data - Time Tab

Finally we set the time parameters. In this case I have resized the Dialog box so that all the data to be entered is visible at once but you could also use the scroll bars to move up or down. We enter a duration for the first (and only) time period of 25000 days. (It is days rather than some other time unit because that is the time unit we selected on the project tab.) We have used negative numbers for some of the printout intervals such as the Well Printout interval. The minus 5000 there indicates that we should print well data every time the model reaches an even multiple of 5000 days. If we had used a positive 5000, that would have meant to write output every time the time the time step number was an even multiple of 5000. For example, a **-30** would indicate that data should be printed at 30, 60, 90… **days.** A **+30** would indicate that we wished to print data at **time step numbers** 30, 60, 90….



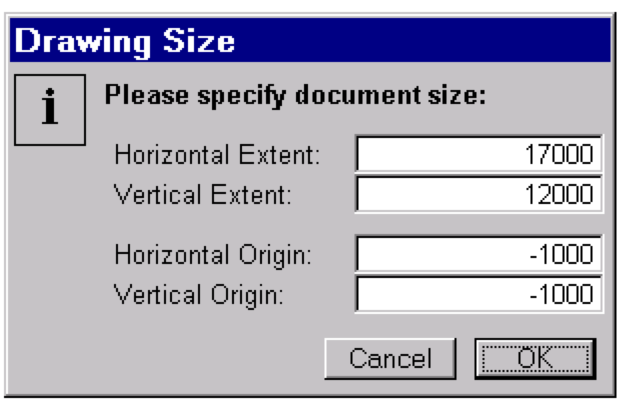
Scale and Units

After clicking the OK button the PIE will create the proper layer structure for the choices we have made. Next we need to change the drawing size to be large enough to fit the model. In this case, the easiest way to do this is to select "Special|Scale and Units". We can set the units to feet and the uniform scale factor to 500. When we click OK the drawing area will be big enough.



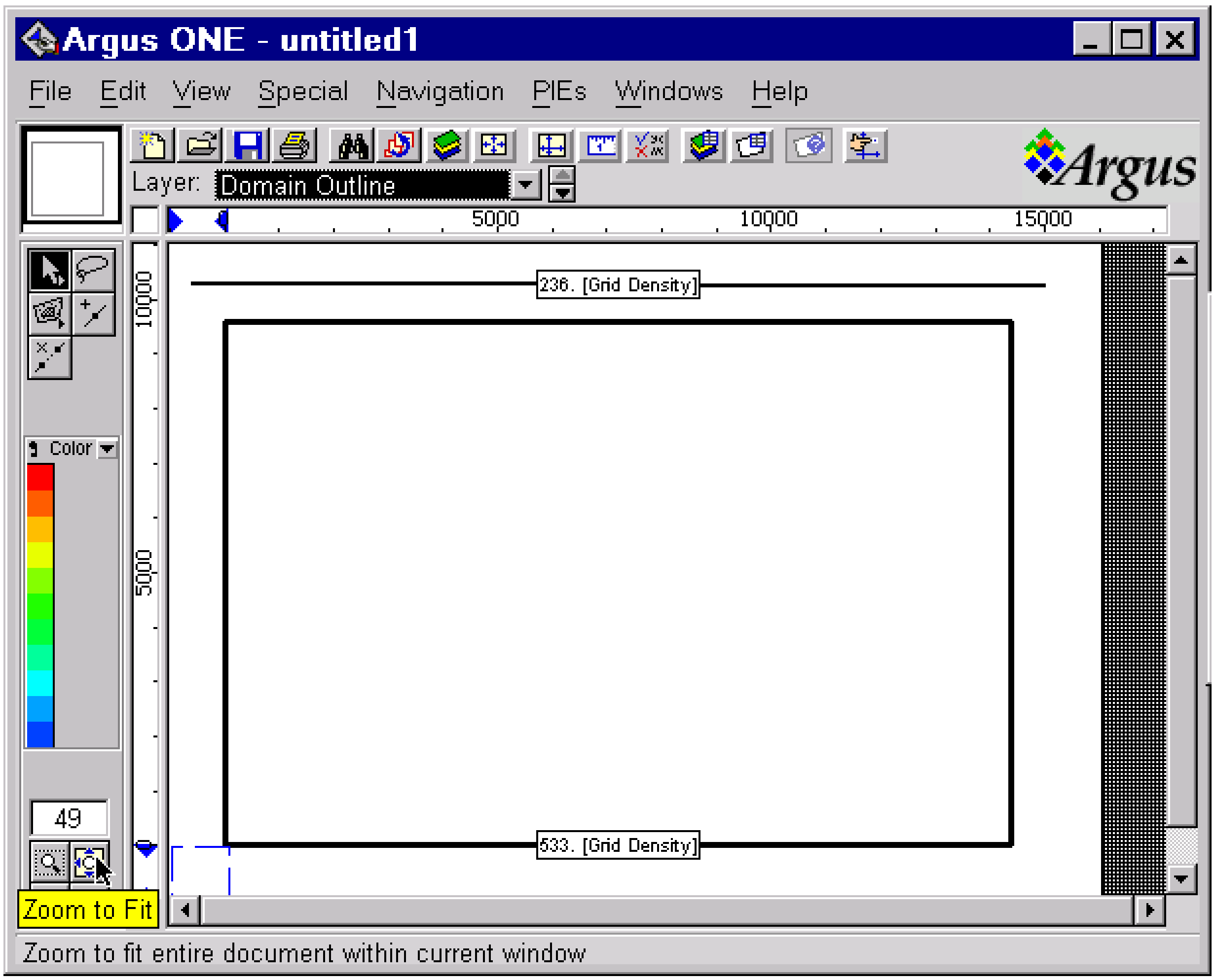
Drawing Size

It is also convenient to set the drawing area to slightly different values. We can set the origin of the drawing to (-1000,-1000) and make it slightly larger so that it is easy to put the lower left corner of the model on (0,0).



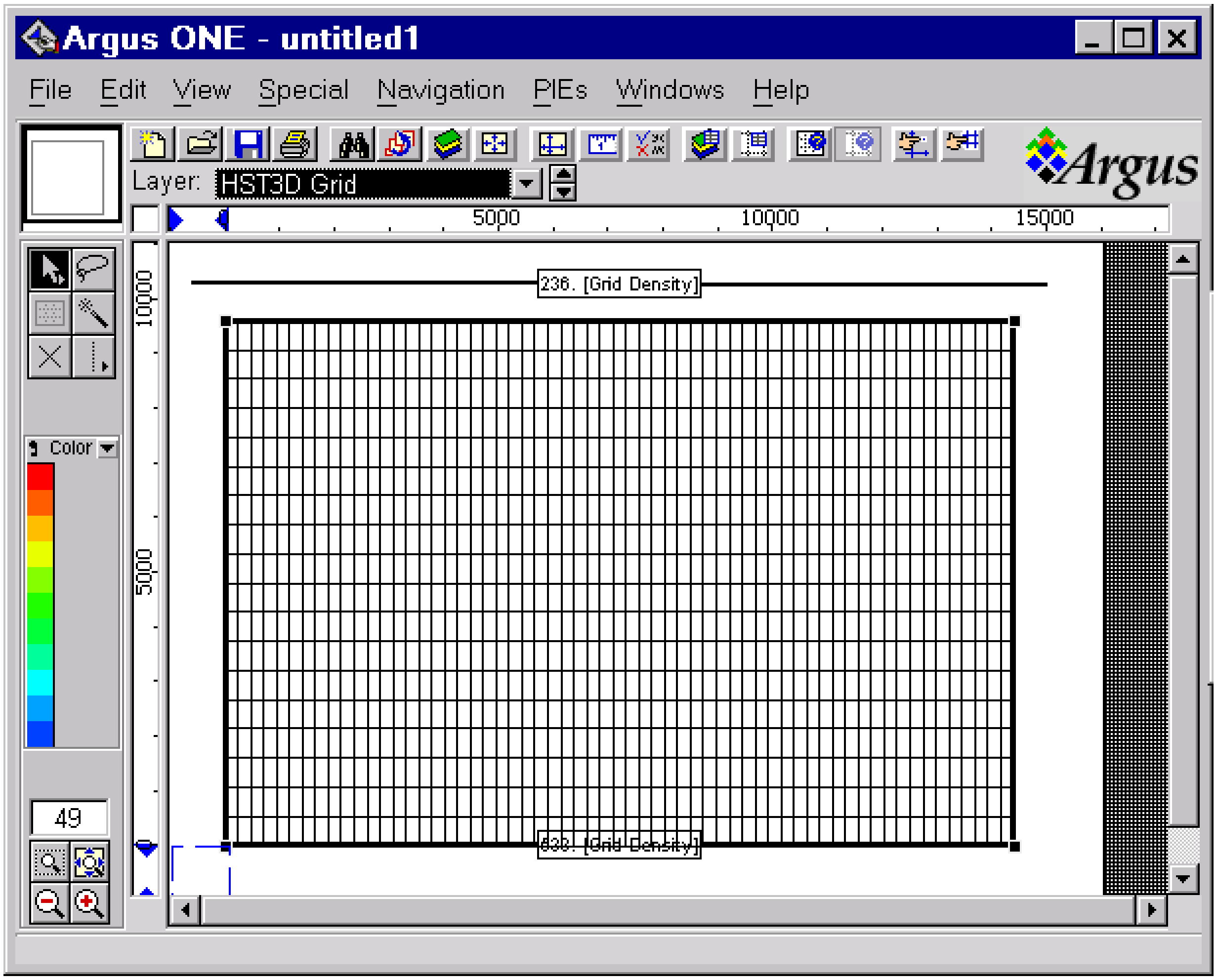
Domain Outline and Grid Density

Next, we'll draw the domain outline. It should extend from (0,0) on the lower left to (14400,9600) on the upper right. One way to make it exactly rectangular is to use the rectangle tool on the Maps layer and then copy the rectangle to the domain outline. If you are concerned about making the domain outline exactly the right size, select "File|Import|Edit Contours" to edit the positions of the nodes. You can assign the Domain Outline layer a grid density of 533. This will be the default grid size. In this case we want the grid density to be smaller in the x direction so on the Grid Density layer, we'll place another contour outside the domain outline with a grid density of 236. It will be placed so that it controls the grid density in the X direction.



Creating the Grid

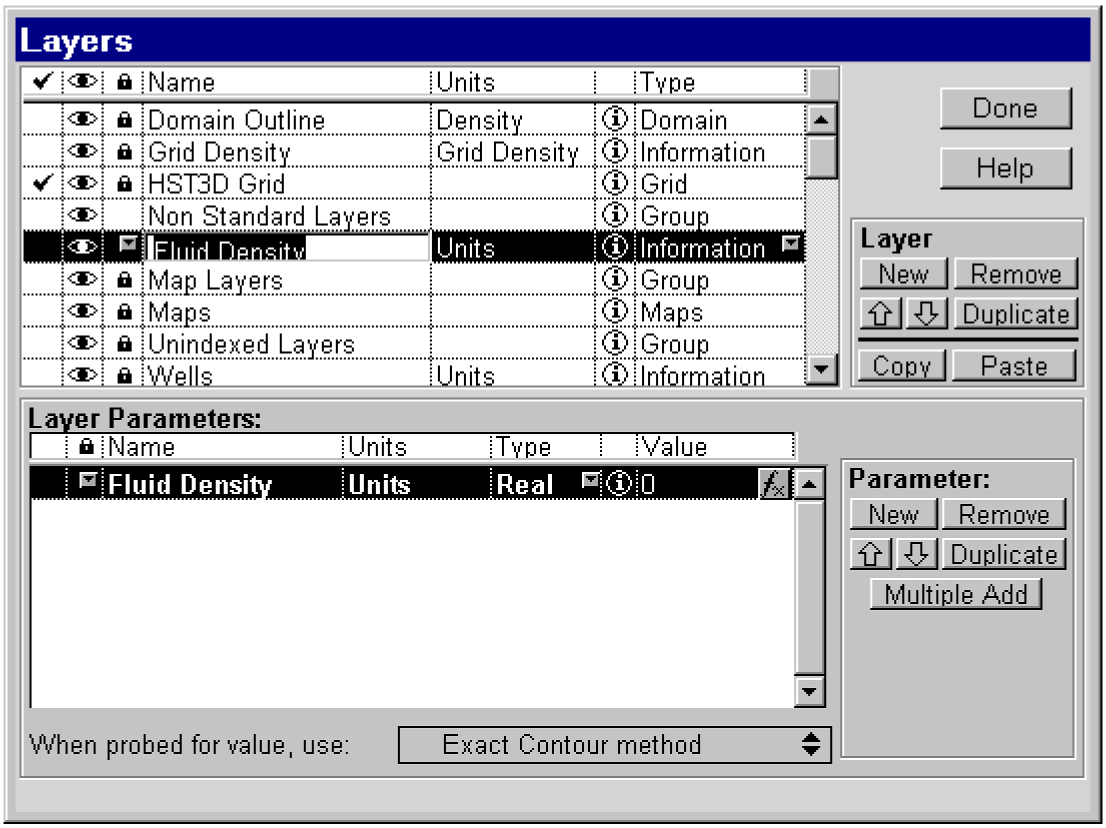
Next we can click with the magic wand tool anywhere inside the domain outline and create the grid. This is a grid of HST3D elements. The HST3D nodes will be at the corners of the elements.



Specified State Boundaries - Creating New Layers

Next we will set the specified pressure boundaries. We will use expressions to simplify the calculating the pressure from the head and fluid density. Because we will assume that there is no vertical variation in Fluid Density, we will create a single layer to represent fluid density.

First we will create a new group layer called "Non_Standard Layers to separate our newly created layers from those created by the PIE. To create the new layer select "View|Layers" and switch to the Maps layer in the upper half of the dialog box. Click the New button in the upper half of the dialog box to create a new layer. In the "Type" column in the upper half of the dialog box, change the layer type from "Information" to "Group". Change the name of the new layer to "Non_Standard Layers". Create another new information layer underneath the new group layer and label it "Fluid Density". Change "when probed for value" from "Nearest Contour method" to "Exact Contour method".

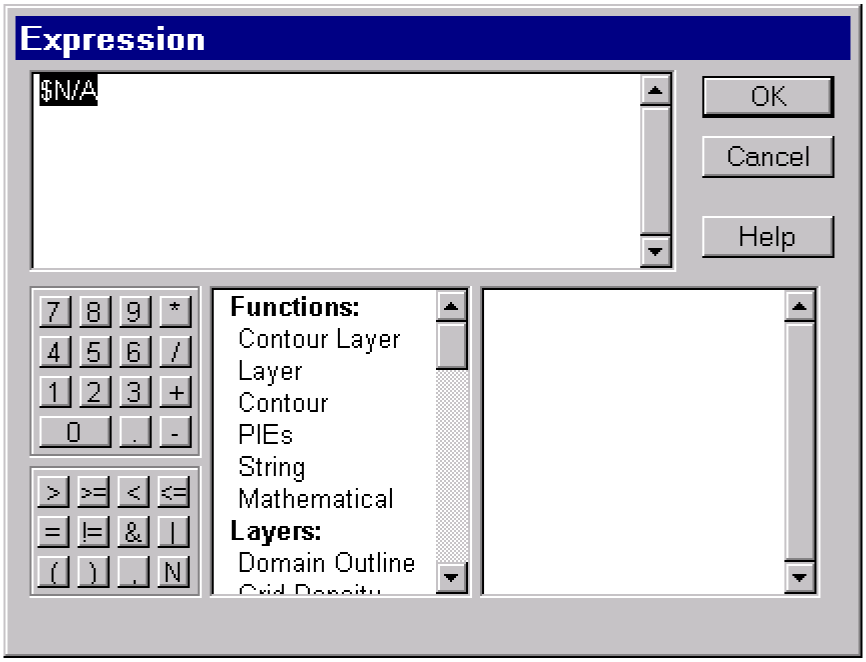


Specified State Boundaries - Adding New Parameters

We will also add parameters to the Specified State layers. Click on the Specified State NL1 layer and add two new parameters named Added Head and End Added Head. The expression for Added Head should be 0. The expression for End Added Head should be $N/A (not available).

Specified State Boundaries - Setting Expressions

You Add a new parameter by clicking the "New" Button on the lower half of the Layers dialog box. Click the f_x button next to the parameter to set the expression. This will bring up the expression editor. A quick way to enter the $N/A expression is to click the N button.



Click OK when you are finished with the expression editor. Then add similar parameters to all the other Specified State layers.

Now we are going to need to calculate the specified pressure distribution. On the sea boundary on the right, we have a hydrostatic pressure distribution. We know what sea level is so we need to calculate the pressure from the known head (= 0 = sea level). The relationship is

$$h = \frac{p}{\rho g} + z$$

$$p = (h - z)\rho g$$

where
h = head,
p = pressure,
ρ = fluid density,
g = gravitational acceleration, and
z = elevation.

For sea level, z = 0 for the top node layer. For the lower node layers, we can calculate z from the grid geometry:
z = HST3D Grid.Elevation NL1 - HST3D Grid.Elevation NL[i]
where
HST3D Grid.Elevation NL1 = the elevation of the top layer of nodes and

HST3D Grid.Elevation NL[i] = the elevation of the i'th layer of nodes.

For the fresh-water boundary on the left, it is a little more complicated because the head in the top Node layer is not 0. Instead it varies from 5 in the south to 4 in the north and there is a similar variation in all other node layers to maintain a hydrostatic pressure distribution. We will use two new parameters to specify the additional head that we can't calculate from the grid geometry alone. These parameters are "Added Head" and "End Added Head". In the top node layer, "Added Head" will represent the head at one end of an open contour. "End Added Head" will represent the heat at the other end. In lower node layers we will use the same values for "Added Head" and "End Added Head" but we will account for the elevation difference as we did on the sea boundary.

We now have all the information we need to calculate the pressure. Because the pressure will vary along some open contours, we will use two parameters for the pressure, Pressure NL[i] and End Pressure NL[i]. These two parameters are created by the HST3D PIE. If End Pressure NL[i] is "$N/A" (not available), the pressure will be uniform along the contour.

An expression for the h-z term in our previous equation for calculating the pressure ($p = (h - z)\rho g$) would be:

Added Head + HST3D Grid.Elevation NL1 - HST3D Grid.Elevation NL[i].

We will just multiply this by ρg to determine the pressure. This would give use the following

(HST3D Grid.Elevation NL1 - HST3D Grid.Elevation NL[i] + Added Head) * Fluid Density

We are using US customary units for which the density is a weight density rather than a mass density so g is already incorporated "Fluid Density". This gives us a pressure in pounds per square foot. To convert to psi (pounds per square inch), we must divide by 144. The final expressions for Specified State NL[i]. Specified Pressure1 and Specified State NL[i]. End Specified Pressure1 are:

(HST3D Grid.Elevation NL1 - HST3D Grid.Elevation NL[i] + Added Head) * Fluid Density/144

and

(HST3D Grid.Elevation NL1 - HST3D Grid.Elevation NL[i] + End Added Head) * Fluid Density/144

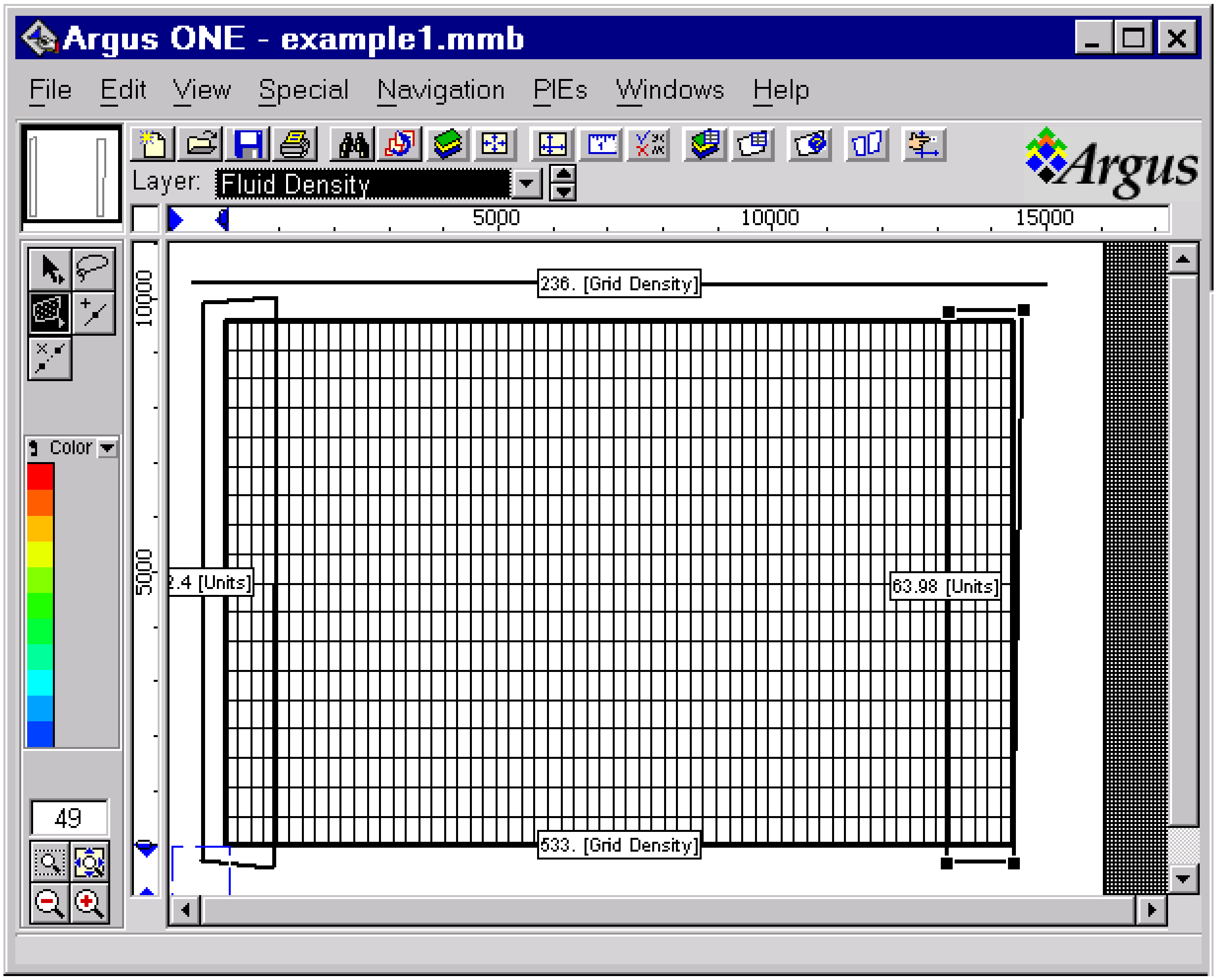
where i is the index of the layer. Thus for layer 9, the expression for specified pressure would be

(HST3D Grid.Elevation NL1 - HST3D Grid.Elevation NL9 + Added Head) * Fluid Density/144

Enter these expressions for all the Pressure NL[i] and End Pressure NL[i] parameters. When you have finished adding all the expressions, click the "Done" button on the Layers dialog box.

Specified State Boundaries - Fluid Density

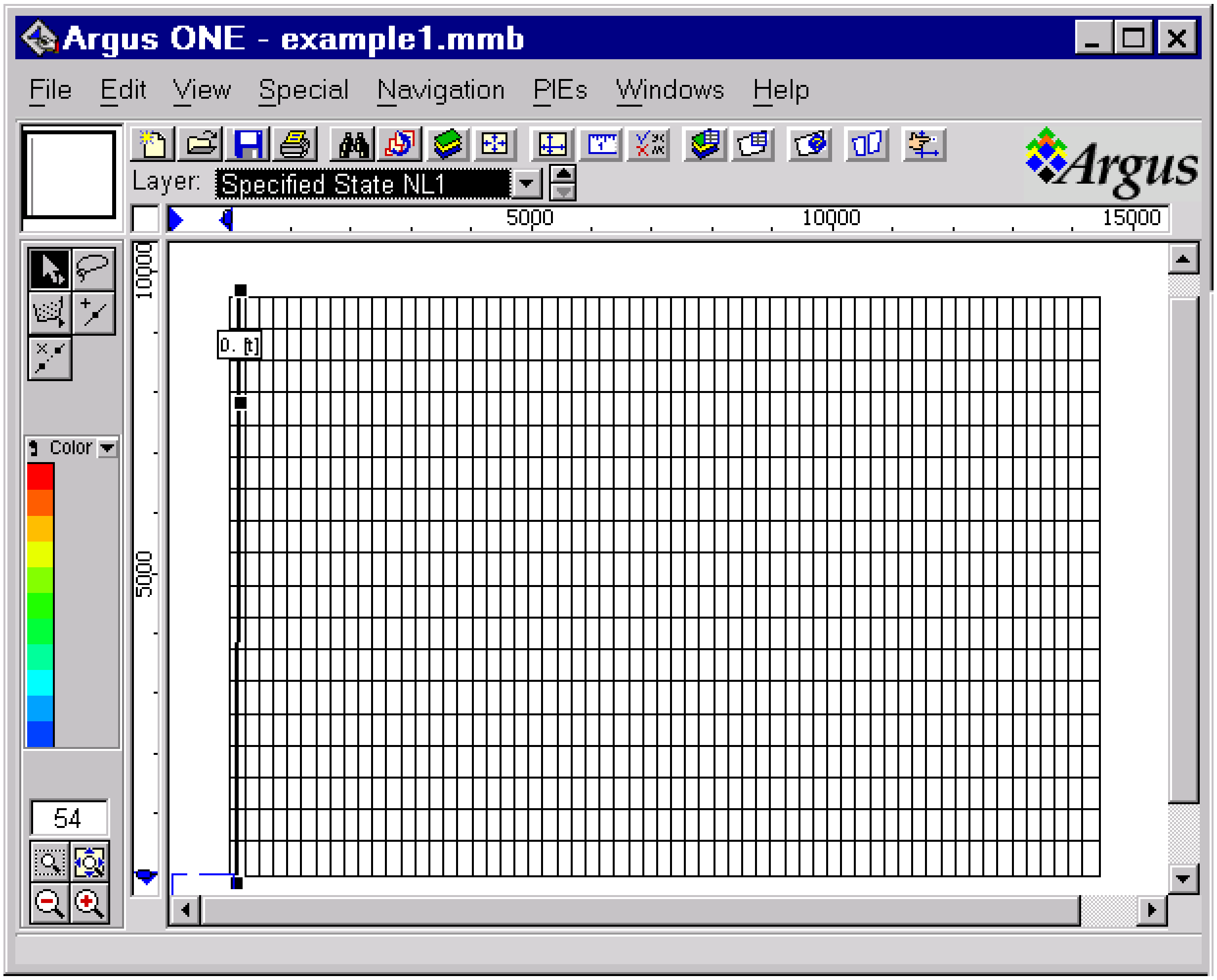
Next we will specify the Fluid Density. We will be having specified pressure boundaries on the left and right sides of the model so we only will be using the fluid density there. In this case, the easiest way to specify fluid density is to just outline the areas we want to specify with closed contours.



The water on the left side of the model is fresh water with a density of 62.42 lb/ft^3. On the right side, the sea water has a density of 63.98 lb/ft^3.

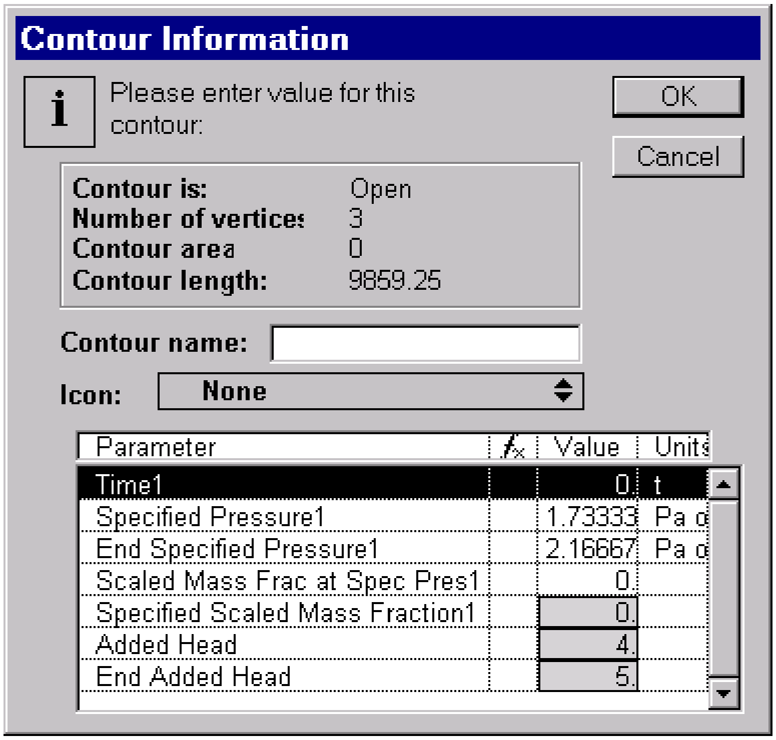
Specified State Boundaries - Adding Contours

Next we will add the specified state boundary conditions. On the left side, we need a specified pressure boundary that will vary along its length. The head will be 4 ft. at the top left corner and 5 ft. at the bottom left corner. Draw a contour starting near the upper left corner of the grid and extending to near the lower left corner. Make sure that the direction of the contour is correct. "Added Head" will apply to the beginning of the contour. If you start the contour at the top, "Added Head" should be 4. If you start it as the bottom, "Added Head" should be 5.



Specified State Boundaries - Assigning Contour Values

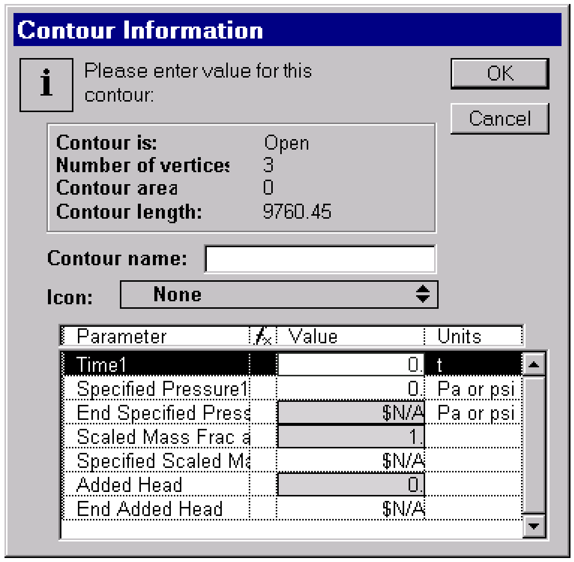
When you are finished drawing the contour, set Added Head to 4 and End Added Head to 5. This will make the specified Pressure1 and End Specified Pressure1 parameters different and the value exported to HST3D will be interpolated between these two values. Because this is a freshwater boundary, the scaled mass fraction parameters should both be 0. You can accept the default values of Time1, Specified Pressure1 and End Specified Pressure1. The latter will appear as $N/A until you have changed "End Added Head" and clicked on the OK button.



You can copy this contour to all the other Specified Pressure layer. After copying it you will have to delete the values of Specified Pressure1 and End Specified Pressure1 so that the default values are used.

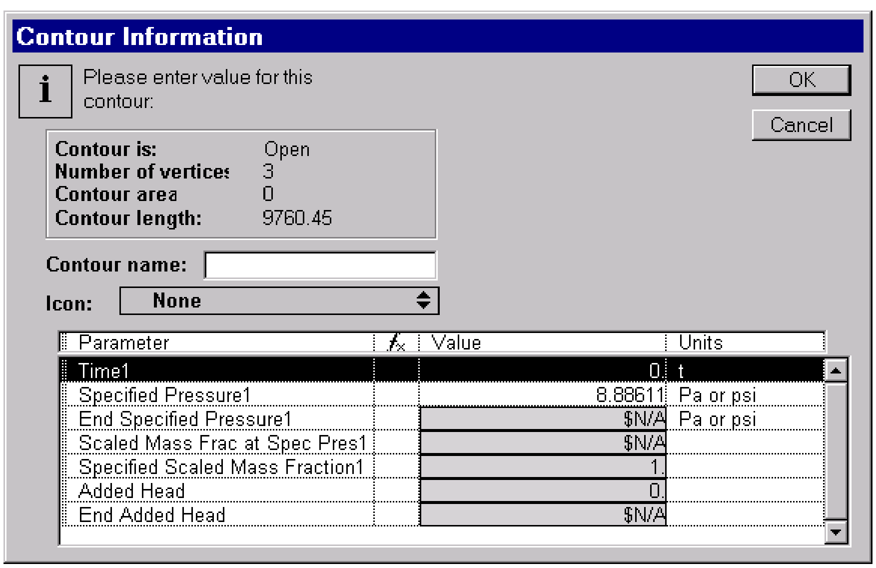
Specified State Boundaries - Specified Pressure Boundary

We will create a similar boundary on the right hand side of the model. For the top layer, this will be a specified pressure boundary. We won't interpolate along the contour this time so we can leave the End Added Head parameter at $N/A. This will make the End Specified Pressure1 parameter equal to $N/A as well. The added head parameter will be 0. The Scaled Mass Fraction at Spec Pres1 parameter should be set to 1.



Specified State Boundaries - Specified Mass Fraction Boundary

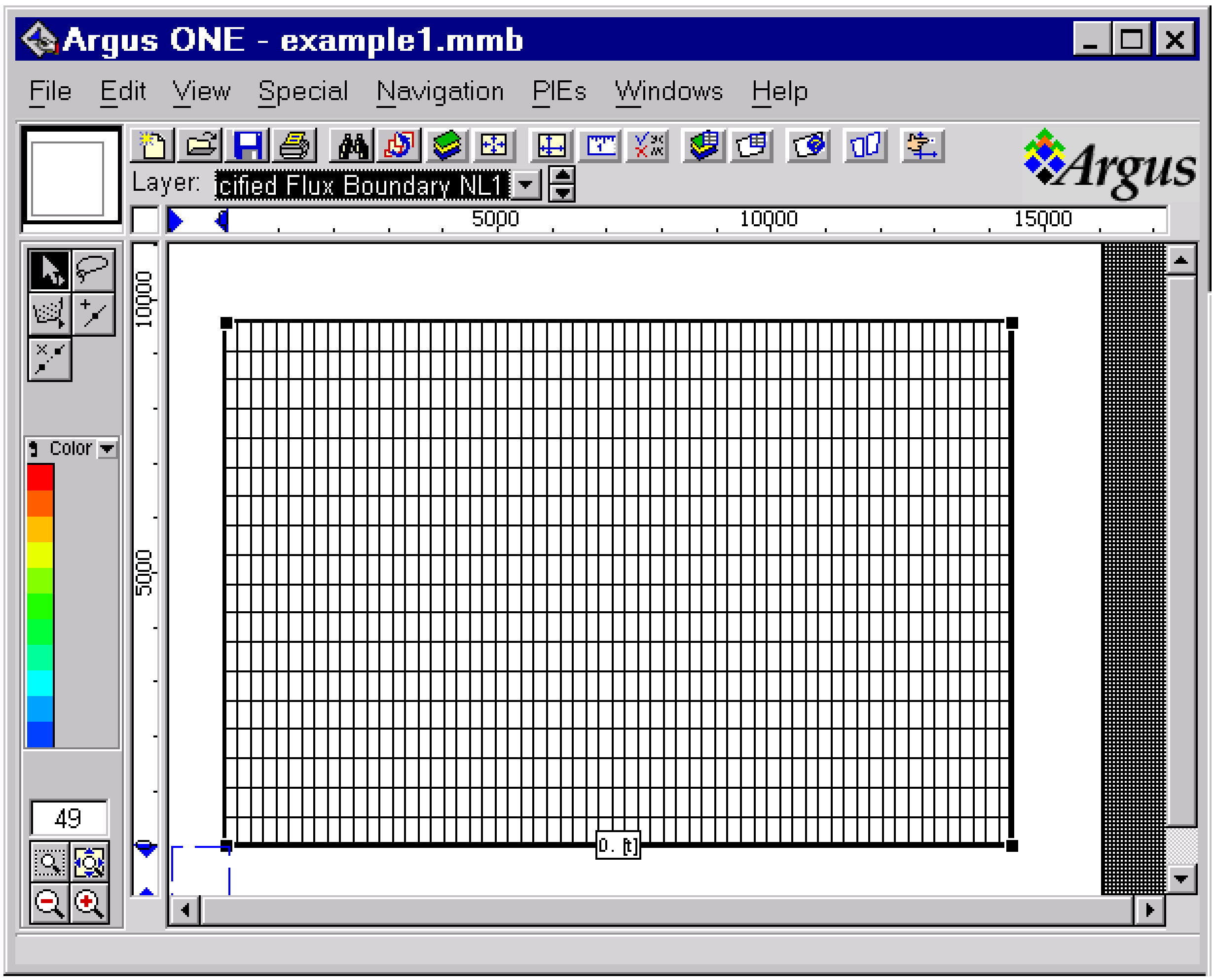
On all the other layers, there is also a specified pressure boundary on the right hand side but it is also a specified mass fraction boundary. As shown below for Specified Pressure NL2.



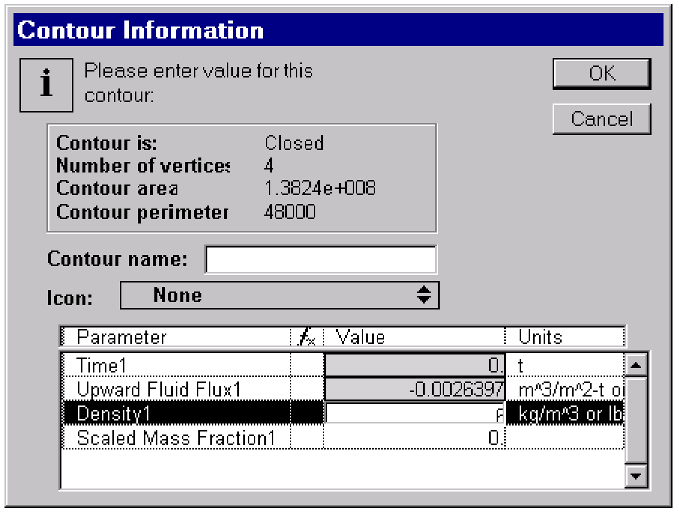
The initial scaled mass fraction on all layers should be 0. The easiest way to do this is to copy the domain outline to the Initial mass fraction layer and assign the copied contour a value of 0. This can then be copied to the remaining Initial mass fraction layers.

Specified Flux Boundary

Finally we will have a specified flux boundary on the top surface. We can copy the domain outline to the Horizontal Specified Flux Boundary NL1 layer. HST3D doesn't allow both a specified state and specified flux boundary in the same cell. If your model is set up to assign both a specified state and specified flux boundary to the same cell, the PIE will only use the specified state boundary for that cell and ignore the specified flux.

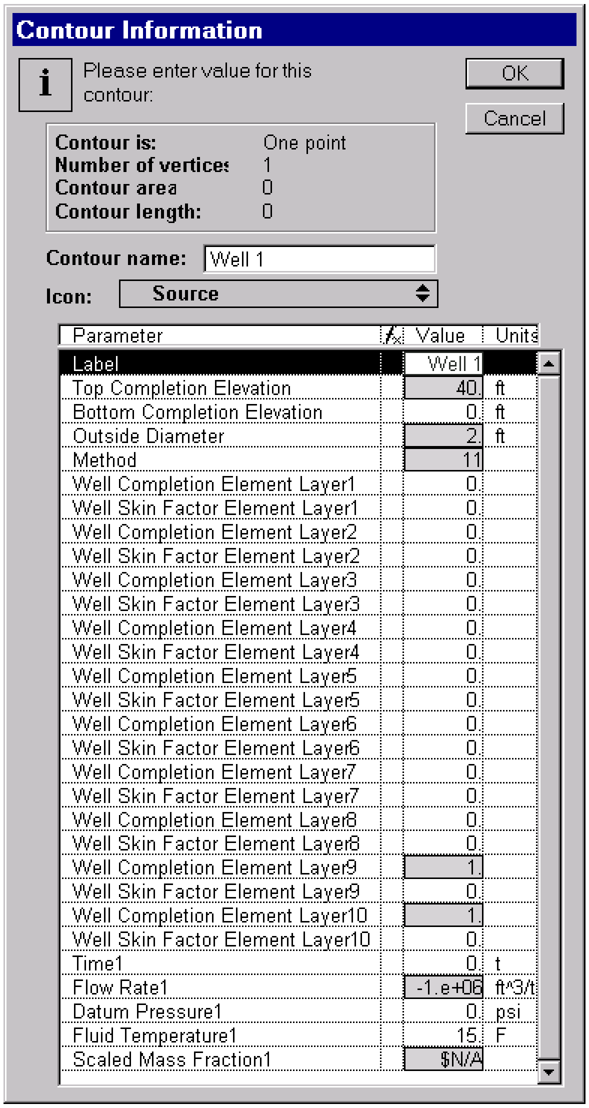


The flux is downward rather than upward so we use a negative value for the flux rate. The flux rate is set at -0.0027397 ft^3/ft^2-day. The density is set at 62.42 lb/ft^3 and the scaled mass fraction is set at 0.



Wells

Next we need to enter the wells for the model. There are two wells. The first well is at (4800, 2400) and the second is at (7200,6240). Both wells have outside diameters of 2 feet. Use method 11 (Specified well-flow rate with allocation by mobility). The first well extends from 0 to 40 feet. The second extends from 160 to 200 feet. The first well has a pumping rate of 1 x 10^6 ft^3/day. The second has a pumping rate of 0.5 x 10^6 ft^3day. The well completion factors for the elements within the screened intervals is 1.0.



Contour Information

Please enter value for this contour:

OK

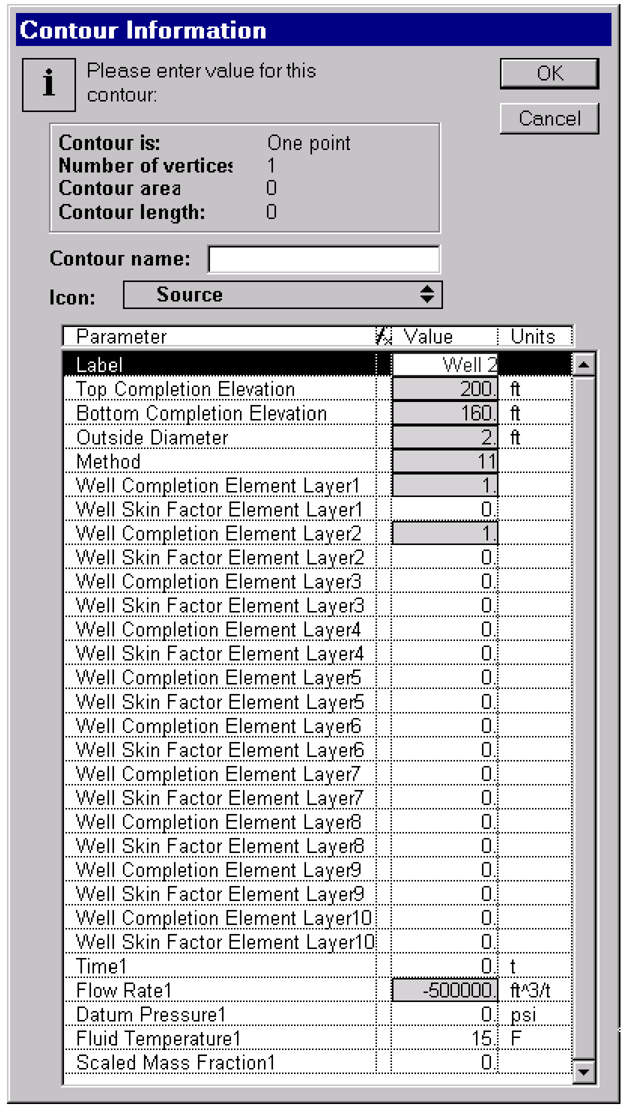
Cancel

Contour is: One point
Number of vertices 1
Contour area 0
Contour length: 0

Contour name: Well 1

Icon: Source

Parameter	Value	Units
Label	Well 1	
Top Completion Elevation	40	ft
Bottom Completion Elevation	0	ft
Outside Diameter	2	ft
Method	11	
Well Completion Element Layer1	0	
Well Skin Factor Element Layer1	0	
Well Completion Element Layer2	0	
Well Skin Factor Element Layer2	0	
Well Completion Element Layer3	0	
Well Skin Factor Element Layer3	0	
Well Completion Element Layer4	0	
Well Skin Factor Element Layer4	0	
Well Completion Element Layer5	0	
Well Skin Factor Element Layer5	0	
Well Completion Element Layer6	0	
Well Skin Factor Element Layer6	0	
Well Completion Element Layer7	0	
Well Skin Factor Element Layer7	0	
Well Completion Element Layer8	0	
Well Skin Factor Element Layer8	0	
Well Completion Element Layer9	1	
Well Skin Factor Element Layer9	0	
Well Completion Element Layer10	1	
Well Skin Factor Element Layer10	0	
Time1	0	t
Flow Rate1	-1.e+06	ft^3/t
Datum Pressure1	0	psi
Fluid Temperature1	15	F
Scaled Mass Fraction1	$N/A	



Contour Information

Please enter value for this contour:

OK

Cancel

Contour is: One point
Number of vertices 1
Contour area 0
Contour length: 0

Contour name:

Icon: Source

Parameter	Value	Units
Label	Well 2	
Top Completion Elevation	200	ft
Bottom Completion Elevation	160	ft
Outside Diameter	2	ft
Method	11	
Well Completion Element Layer1	1	
Well Skin Factor Element Layer1	0	
Well Completion Element Layer2	1	
Well Skin Factor Element Layer2	0	
Well Completion Element Layer3	0	
Well Skin Factor Element Layer3	0	
Well Completion Element Layer4	0	
Well Skin Factor Element Layer4	0	
Well Completion Element Layer5	0	
Well Skin Factor Element Layer5	0	
Well Completion Element Layer6	0	
Well Skin Factor Element Layer6	0	
Well Completion Element Layer7	0	
Well Skin Factor Element Layer7	0	
Well Completion Element Layer8	0	
Well Skin Factor Element Layer8	0	
Well Completion Element Layer9	0	
Well Skin Factor Element Layer9	0	
Well Completion Element Layer10	0	
Well Skin Factor Element Layer10	0	
Time1	0	t
Flow Rate1	-500000	ft^3/t
Datum Pressure1	0	psi
Fluid Temperature1	15	F
Scaled Mass Fraction1	0	

Aquifer Properties

We have now finished entering the boundary conditions but we still need to enter the aquifer properties. The easiest way to do this is to set the default values for all the properties in the element layers.

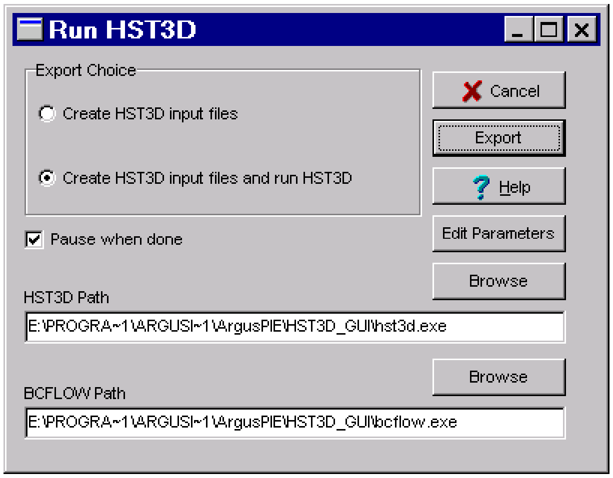
We may want to change these properties later so we will use expressions to link parameters so that if we want to go back and change a the properties, we will only have to change it in one place.

For Permeability Element Layer1.kx, we will set the permeability as 7.754e-9. For Permeability Element Layer1.**ky**, we will set the expression as **kx**. Thus any change in kx will automatically be reflected in ky. For Permeability Element Layer1.**kz**, we will set the expression as **kx**/10. For Permeability Element Layer2.kx through Permeability Element Layer11.kx, we will set the expression to Permeability Element Layer1.kx. Similarly, the expressions for Permeability Element Layer2.ky through Permeability Element Layer11.ky will be Permeability Element Layer1.ky and the expressions for Permeability Element Layer2.kz through Permeability Element Layer11.kz will be Permeability Element Layer1.kz.

The vertical compressibility of water needs to be set to 0 in the same way. (Set it to 0 on Vertical Compressibility Element Layer1 and link the remaining layers to Vertical Compressibility Element Layer1.) We also need to set the longitudinal dispersivity to 150 and the transverse dispersivity to 30 for all the element layer. The default values for the remaining parameters are those needed for the model so we won't need to modify them. If we did need to modify them, we could link them the same way we did the permeability parameters so that we could change the values throughout the model by changing a single value.

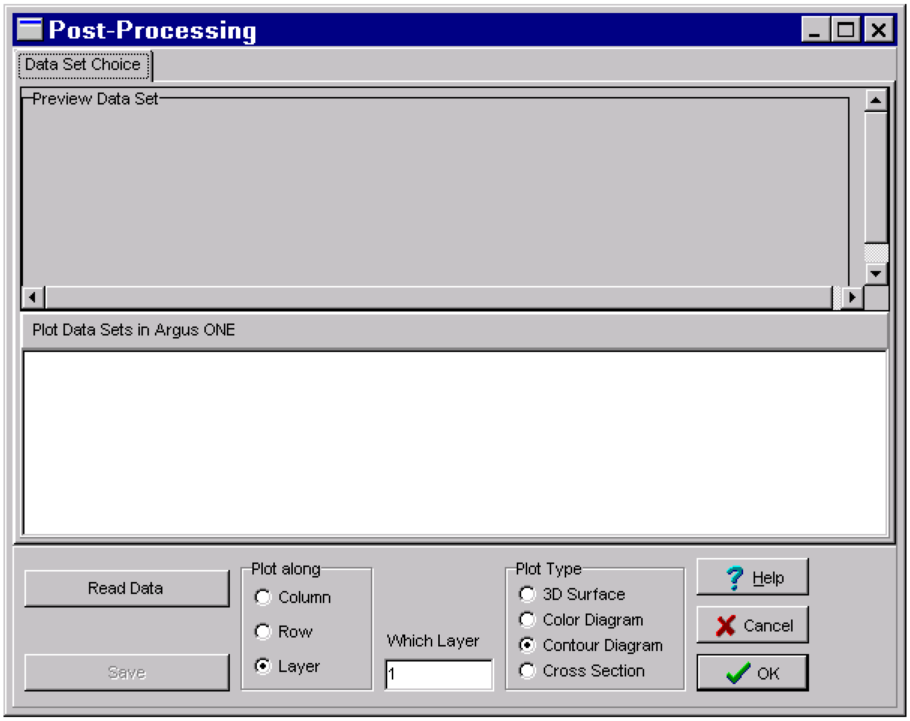
Run HST3D

We have now completely defined the model and are ready to run it. Switch to the HST3D Grid layer and select "Run HST3D". The Run HST3D dialog box will appear. Select "Create HST3D input files and run HST3D". If the path for HST3D is not correct for your system, edit the path so that it is correct or click the Browse button next to the HST3D Path and select HST3D on you computer. Click Export to begin exporting the HST3D input files. HST3D will be started as one of the last steps in the export process. If you have a big model that will use a lot of memory, you may run into a problem: HST3D won't start. If that happens, save the Argus ONE model, shut down Argus ONE and other programs to free up memory and then run HST3D. You can run HST3D by double clicking on the file named "RunHST3D.BAT" in the directory in which you created the HST3D input files. If you know that this will be a problem, you may choose just to create HST3D input files and then run the model yourself by double clicking on "RunHST3D.BAT" or starting it from a DOS window.

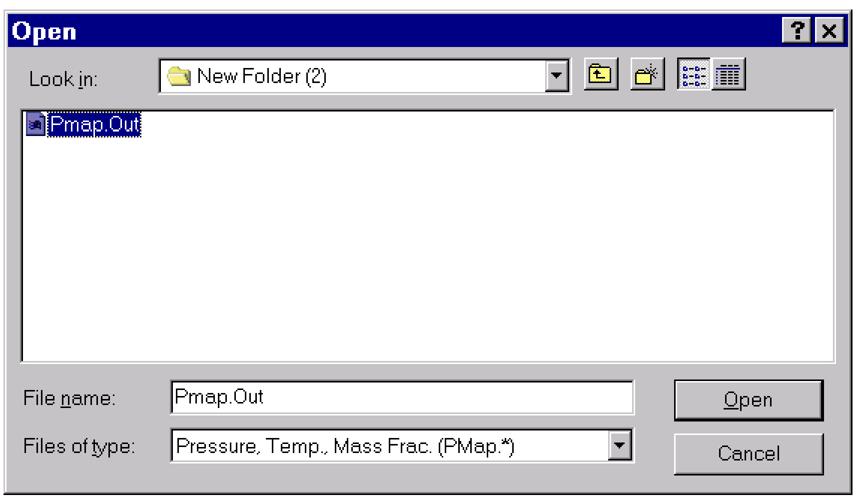


Viewing Results

When HST3D has finished running, you can use Argus ONE to view the results. Select "PIEs|HST3D Post-processing…". The HST3D Post-processing dialog box will appear.



Click the Read Data dialog box and select either a PMAP, PMAP2, or VMAP file for post-processing. In this case we will read the PMAP file.



The Post-processing PIE will read the data in the file and display the captions it read from the file. You can preview the data for any data set by selecting it in the Preview Data Set box at the top of the Post-processing dialog box. The data will appear on the Data tab. Select one or more data sets to import into Argus ONE the direction of the plot (along a column, row, or layer), the type of plot and your choice of column, row or layer from which to import data.. In this case we will read the data for mass fractions for layer 1 and create a contour diagram. Click the OK button and the post-processing diagram will be created.