

Manual for Development of a Transient
MODFLOW/MT3DMS/SEAWAT Simulation
for the 2001 Tracer Test at the
Boise Hydrogeophysical Research Site

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Abstract

In the summer of 2001 a tracer test was conducted at the Boise Hydrogeophysical Research Site (BHRS), Boise, Idaho using separate injection and pumping wells and a multi-well, packer-port sampling array. A known amount of potassium bromide (KBr) was injected into the ground water and the movement of the plume was monitored via direct water sampling, as well as time-lapse radar tomograms. This report provides a step-by-step tutorial for the set-up and execution of a groundwater flow model and tracer transport model associated with the test. The model incorporates GMS, MODFLOW 2000, and SEAWAT 2000 as well as a set of MATLAB scripts. The results of this model run are compared to the observed data in an effort to correctly identify the hydrogeologic properties of the BHRS shallow aquifer.

Contents

Abstract	2
List of Figures	5
List of Tables	8
List of Boxes	8
I: Introduction	9
Major steps.....	12
II: Development of Gravel Bar Model (GBM)	13
Section I: Steady State	13
GMS.....	13
Importing TIFF file.....	13
Picture Transformation	14
Creating the Conceptual Model	16
Creating the Boundary Coverage.....	17
Drawing Model Boundaries.....	19
Creating River Coverage.....	20
Creating the River Arcs	20
Assigning Properties to Boundaries.....	21
Assigning River Conductance.....	22
Assigning River Values	22
Creating Constant Head Boundaries.....	24
Creating the CHB coverage	25
Assigning CHB values.....	25
Creating Layer Coverages.....	28
Creating L1 Coverage.....	28
Creating Polygons.....	30
Assigning Areal Data.....	30
Creating Layer Polygons.....	32
Creating Observation Coverage	33
Adding Wells	33
Creating Observations Coverage	33
Adding Wells as Refining Points.....	34
Creating the 3D Grid.....	36
Creating a New MODFLOW2000 (MF2K) Simulation.....	39
Editing Model Layer Elevations	40
Editing Model Layer Top and Bottom Elevations	40
Editing the .dis File.....	41
Calibration with Steady State Solution.....	43
Section II: Transient Run	48
Creating Transient Model	48
Creating Injection/Pumping Wells.....	49
Assigning Transient Time Steps	51
Creating the .hob and .obs Files.....	53

ReadDis.m.....	54
Running ‘createHOB.m’ MATLAB Script.....	54
Running MF2K.....	55
Output File Information.....	57
MATLAB.....	57
III: Development of 2nd Model: Flow and Transport Model	59
Flow and Transport Model.....	59
Creating a New Grid.....	59
Creating a New MODFLOW Simulation.....	61 6160
Editing Model Layer Elevations.....	61
Constructing the Conceptual Model.....	62
Creating Boundary Coverage.....	62
Drawing in Model Boundaries.....	63
Creating River Coverage.....	64
Creating the GHB coverage.....	65
Creating the CHB coverage.....	68
Assigning Coverage Properties to MODFLOW.....	71
Assigning MODFLOW Stress Periods.....	72
IV: Preprocessing	75
PREPROC.m MATLAB Script.....	75
Running PREPROC.m.....	75
SPLICE3D.m.....	75
V: Final Model Development	76
Creating Input Files.....	76
Creating the Extract.in File.....	76
Running the Model on the Beowulf Cluster in the Computer Science Department at Boise State University.....	77
Creating the Swarm Command File:.....	77
VI: Post Processing	80
obsSWT2K.m MATLAB Script.....	80
VII: References	85

List of Figures

Figure 1: Photograph showing the location of the BHRS.....	10
Figure 2: A) Map view of the well array at the BHRS, B) Well schematic showing inner wells, injection and pumping wells, and radar tomography transects.	11
Figure 3: Units dialog box	13
Figure 4: Dialog box for opening the base image for the GBM	14
Figure 5: Transform option within the directory tree	15
Figure 6: Coordinate Transformation - Step 1 dialog box.....	15
Figure 7: Dialog box showing the appropriate values for coordinate transformation of the image ‘BHRS.TIF’.....	16
Figure 8: Conceptual Model Properties dialog box for basic setup properties of the conceptual model	17
Figure 9: Coverage Setup dialog box for the ‘Boundaries’ conceptual model.....	18
Figure 10: Image of the ‘Boundaries’ coverage arcs which will define the model boundary	19
Figure 11: Coverage Setup dialog box for the ‘River’ coverage.....	20
Figure 12: Location of the ‘River’ arc (arc types already assigned).....	21
Figure 13: Properties dialog box for assigning conductance values to the river arcs.....	22
Figure 14: RS.xls spreadsheet showing river stage values	23
Figure 15: This figure shows the transient river stage values as well as the bottom elevations taken from the ‘RS.xls’ spreadsheet.....	24
Figure 16: Coverage Setup dialog box for the creation of the ‘Constant Head Boundary’ coverage	25
Figure 17: Vertices and arcs to be selected as specified head arcs.....	26
Figure 18: Properties dialog box for specified head arcs selected in Figure 17	27
Figure 19: Head stage values for the Constant Head Boundary arcs, as taken from RS.xls	28
Figure 20: Coverage Setup dialog box for the L1 layer coverage	29
Figure 21: Location of the arcs encompassing the layers of the GBM.....	30
Figure 22: Properties dialog box for the three L1 polygons	31
Figure 23: Coverage Setup dialog box for the L2-L40 layer coverage.	32
Figure 24: Properties dialog box for the L2-L40 polygon.....	33
Figure 25: Coverage Setup dialog box for setting up the Obs coverage	34
Figure 26: OBS.xls spreadsheet with location data of wells	35
Figure 27: Properties dialog box for the 18 refining points of the Obs coverage.....	35
Figure 28: Final location of the 18 refining points representing the wells of the BHRS	36
Figure 29: Dialog box for inputting the size dimensions of the 3D grid.....	37
Figure 30: Location and orientation of the newly created 3D grid for the GBM	37
Figure 31: Final grid size showing the active cells only.....	38
Figure 32: Global Options dialog box	39
Figure 33: Grid Value dialog box for assigning a constant starting head value for the entire grid.....	40
Figure 34: Sample of the values to be copied from the “GBM lyr elev.txt” file (on CD) that are copied to replace the values of the GBM.dis file created by the simulation	41

Figure 35: X-Z profile of the GBM model grid showing correct model layer elevations	42
Figure 37: Map -> Model dialog box	42
Figure 37: GBM model grid with cell types assigned	43
Figure 38: Observations dialog box for GBM model	44
Figure 39: MODFLOW PCG2 Package dialog box showing the appropriate values	45
Figure 40: MODFLOW-2000 run box showing successful completion of the GBM run	46
Figure 41: Plot Wizard – Step 1 of 2 dialog box	47
Figure 42: Plot of Computed vs. Observed Values for heads of the steady state run	47
Figure 43: Coverage Setup dialog box for the Wells coverage	49
Figure 44: Properties dialog box for the injection well (B3) and pumping well (B6)	50
Figure 45: XY Series Editor dialog box showing transient pumping rate of well B6	50
Figure 46: Stress Periods dialog box for the pumping well showing the imported values	51
Figure 47: Error message 1: Error message associated with assigning stress periods to the model	51
Figure 48: MODFLOW Output Control dialog box with the appropriate options selected	52
Figure 49: Error Message 2: GMS error message	52
Figure 50: Example of the ‘input.txt’ file used for ‘createHOB.m’ script	53
Figure 51: Figure produced by createHOB.m script showing the locations of the points	55
Figure 52: Modified GBM.mfn file after removal of double quotes (“) and RVOB, CHOB, and ASP lines	56
Figure 53: MF2K.exe DOS shell screen showing ‘NAME’ file supplied	57
Figure 54: Create Finite Difference Grid dialog box showing appropriate values for the flow and transport model	60
Figure 55: Initial grid location of the smaller flow and transport model	60
Figure 56: SM.dis file showing the newly input values taken from SM grid.txt	61
Figure 57: SM model grid showing the new discretized grid	62
Figure 58: Coverage Setup dialog box for the Boundaries coverage	63
Figure 59: Boundaries arcs for the SM conceptual model (the slight indentation in the northeast corner corresponds to the road leading down to the site, which is higher elevation)	64
Figure 60: Error message 3: Message associated with moving the River coverage to the SM conceptual model	64
Figure 61: SM conceptual model showing the River coverage which was copied from the GBM model	65
Figure 62: Coverage Setup dialog box for the GHB coverage	66
Figure 63: General Head arcs of the SM conceptual model	67
Figure 64: Properties dialog box for the general head arcs showing the conductance values	67
Figure 65: XY Series Editor dialog box for the GHB head stage values imported from the heads.obs file created by ‘readheadobs.m’	68
Figure 66: Coverage Setup dialog box for the CHB coverage	69
Figure 67: Location of specified head arcs of the CHB coverage	70
Figure 68: Properties dialog box of the CHB arcs	70

Figure 69: XY Series Editor for the specified head arcs of CHB coverage showing transient data input.....	71
Figure 70: SM model with only those cells within the boundaries activated	72
Figure 71: modeltime.xls file showing stress period values to be assigned to the SM model.....	73
Figure 72: Stress Periods dialog box for the SM MODFLOW simulation.....	73
Figure 73: Map -> Model options for the SM model	74
Figure 74: Results of executing the Map -> MODFLOW command for the SM model.	74
Figure 75: Screenshot showing command screen for running the SM model on the Beowulf Cluster	79

List of Tables

<i>Table 1: Values for 'River', 'Unit 5' and 'Other' polygons.....</i>	31
<i>Table 2: Output files generated by obsSWT2K.m.....</i>	84

List of Boxes

<i>Box 1: Help instructions for the createHOB.m MATLAB file.</i>	54
<i>Box 2: Help instructions for the readheadobs.m MATLAB script.</i>	58
<i>Box 3: Example of line commands for Extract.in file</i>	77
<i>Box 4: Example of a swarm 'run' file for the Beowulf Cluster</i>	78
<i>Box 5: Example of the 'run' command for starting the model on the Beowulf Cluster ..</i>	78

I: Introduction

Methodology for developing a flow and transport model for the Boise Hydrogeophysical Research Site Tracer/Time-Lapse Imaging Test (TTLT)

The Boise Hydrogeophysical Research Site (BHRS) is located on a gravel bar along the Boise River approximately 10 miles east of Boise, ID (Figure 1). The site consists of 18 wells emplaced between 1997 and 1998. The wells fully penetrate a shallow sand-gravel aquifer to a depth of approximately 20 m. The aquifer material consists mostly of coarse, cobble-and-sand, fluvial deposits which overlie a red clay layer at approximately 20 m depth throughout the site. Nearby local road cuts in similar material provide insight into the heterogeneity and geometry of the different units within the BHRS.

Several studies have been conducted at the BHRS including single-well, cross-well, multi-well, radar and seismic geophysical, and tracer experiments. This paper focuses on modeling the results of a tracer/time-lapse radar tomographic imaging test that was executed during the summer of 2001 (Barrash et al. 2002). Two tracers, bromide (KBr) and uranine, were injected as an “instantaneous” pulse into a single well (B3) and pumping for tracer removal occurred at a separate well (B6). Throughout the movement of the tracers, multilevel sampling was done using a packer-port system emplaced at specified intervals within the observation wells located throughout the well field (Figure 2). The main movement of the tracer was due to a combination of natural gradient between wells B3 and B6 and forced gradient produced by the pumping well located ~7 m down gradient from the injection well. Approximately 1000 gallons of tracer solution (bromide and uranine) of known concentration were injected over a 4 m depth interval at ~29.5 gal/min. Pumping was initiated ~35 minutes after the injection had stopped and proceeded for the duration of the experiment (~16 days). The inner seven wells were pumped at low rates (~5 mL/min) using peristaltic pumps to obtain time-lapse samples. Upon completion of the tracer test, the data were organized into time-concentration plots for analysis (Hausrath et al., 2002).

This report describes the step-by-step set-up and execution for modeling the movement of the bromide tracer through the subsurface for the duration of the test. The model incorporates MODFLOW 2000, MT3DMS, and SEAWAT 2000 and strives to produce an accurate model of the subsurface heterogeneity as shown by the migration of the tracer plume (Nelson, 2007). This report will also serve as a basic tutorial for set-up and initiation of further modeling of the tracer test and of future tests to be conducted at the site.

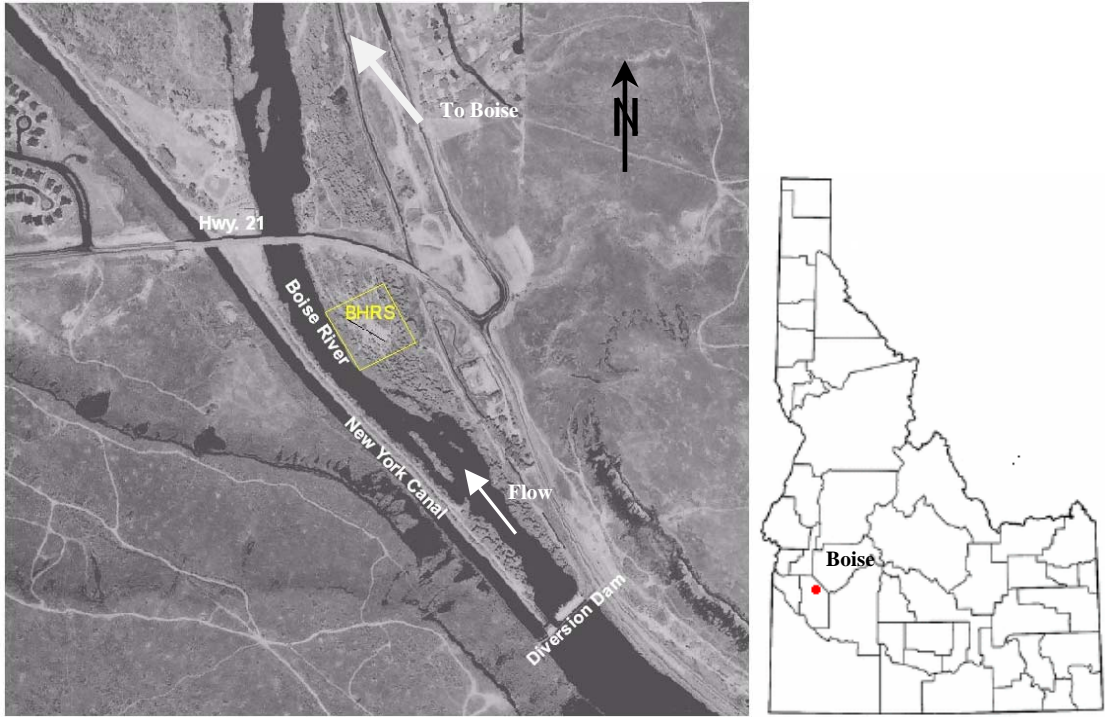


Figure 1: Photograph showing the location of the BHRS

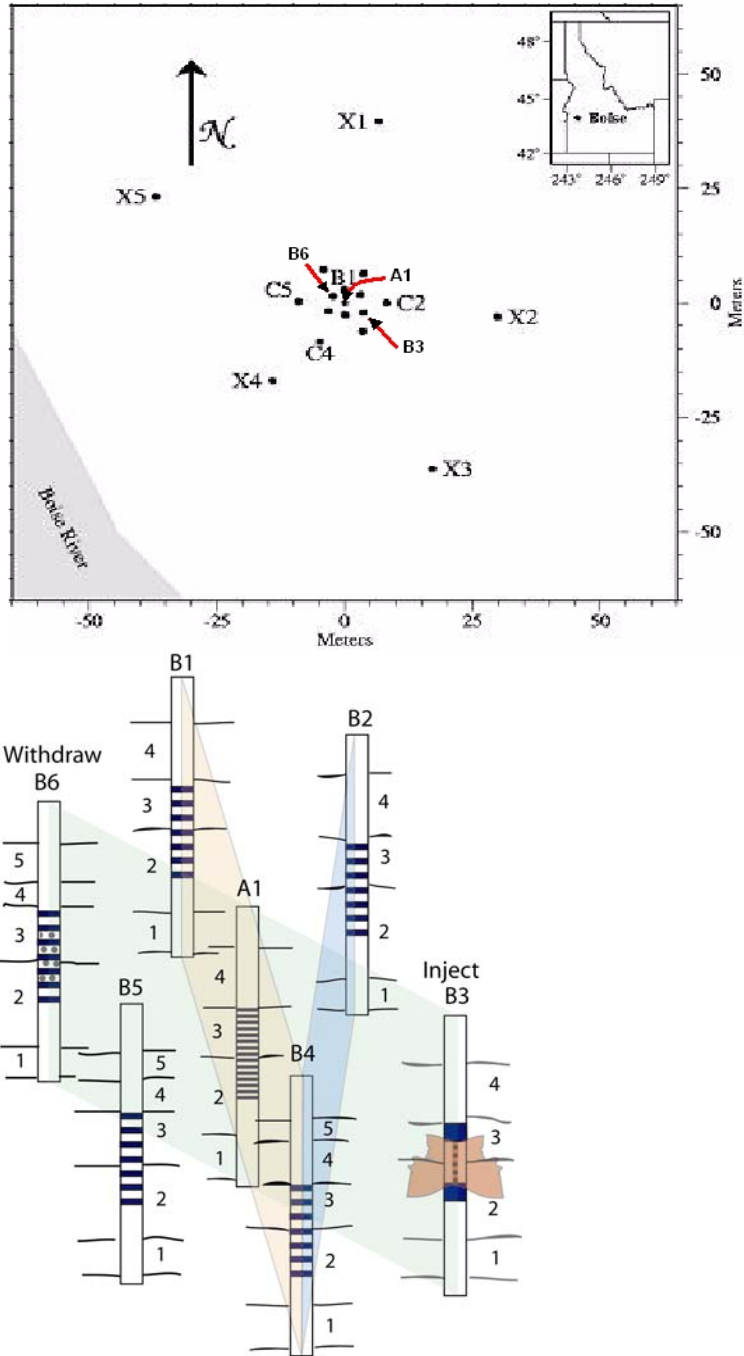


Figure 2: A) Map view of the well array at the BHRS, B) Well schematic showing inner wells, injection and pumping wells, and radar tomography transects.

Major steps

1. Gravel Bar Model

- The Gravel Bar Model (GBM) is run in MODFLOW 2000 to output heads for use as general head, and constant head boundaries of the smaller flow and transport model (discussed below). This model was primarily developed using Groundwater Modeling Systems 5.0 (GMS5).

2. Flow and Transport Model

- A refined flow model of the GBM developed using GMS, Excel, text editors, and MATLAB scripts. The flow model is developed as if it were a MODFLOW 2000 / MT3DMS flow and transport model, but is run using SEAWAT 2000. This can be accomplished because SEAWAT 2000 is a combination of MODFLOW 2000 and MT3DMS with the added capability of handling variable density flow. This model uses the heads generated by the GBM for general head and constant head boundaries; river stage values are also applied. Flow is modeled using the Hydrogeologic Unit Flow (HUF) package or the Layer Property Flow (LPF) package where the modeling domain can be divided into distinct hydrogeologic units, and each unit can be assigned physical properties such as hydraulic conductivity, specific storage and anisotropy. Transport properties are also incorporated through the various MT3DMS packages: advection, dispersion, sources/sinks and mixing, etc.

II: Development of Gravel Bar Model (GBM)

Section I: Steady State

The majority of development of the Gravel Bar Model (GBM) was done using GMS 5.0. It involves intensive use of the map module to draw out boundaries, set up initial head values, and set up the modeling grid. The purpose of this model is to produce head data for use in boundaries of the smaller flow and transport model. The GBM is set up and then run in two sequential steps: first as a steady state model, and then upon successful calibration, as a transient model to generate heads for the transport model.

GMS

Open GMS

From the main toolbar, select *'Edit' – 'units'*

This opens the **'Units'** dialog box

Select **'length'** in meters (m), **'time'** in seconds(s) (Figure 3)

Click *'OK'*

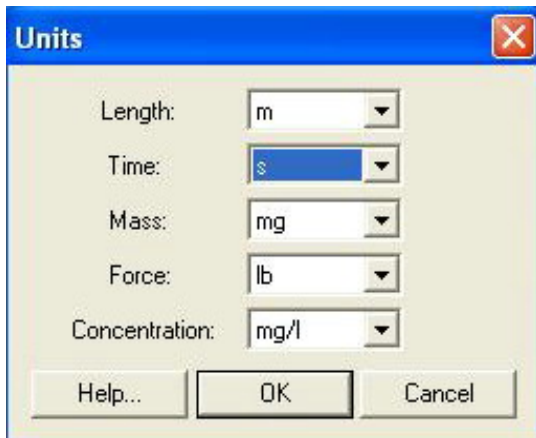



Figure 3: Units dialog box

Importing TIFF file

To form the initial boundaries for the GBM, an aerial photo of the BHRS is imported into GMS as a TIFF image file. Importing this image will allow the boundaries to be drawn in manually around the extent of the gravel bar and along the boundary of the river. The size and shape of the GBM was chosen to represent the entire extent of the gravel bar where the site is located.

Select 'Map' module 
From the main toolbar select 'File' – 'open'
Change 'files of type' to 'JPEG-TIFF Files'
Locate and select 'BHRS.tif' (Figure 4)
Click 'Open'

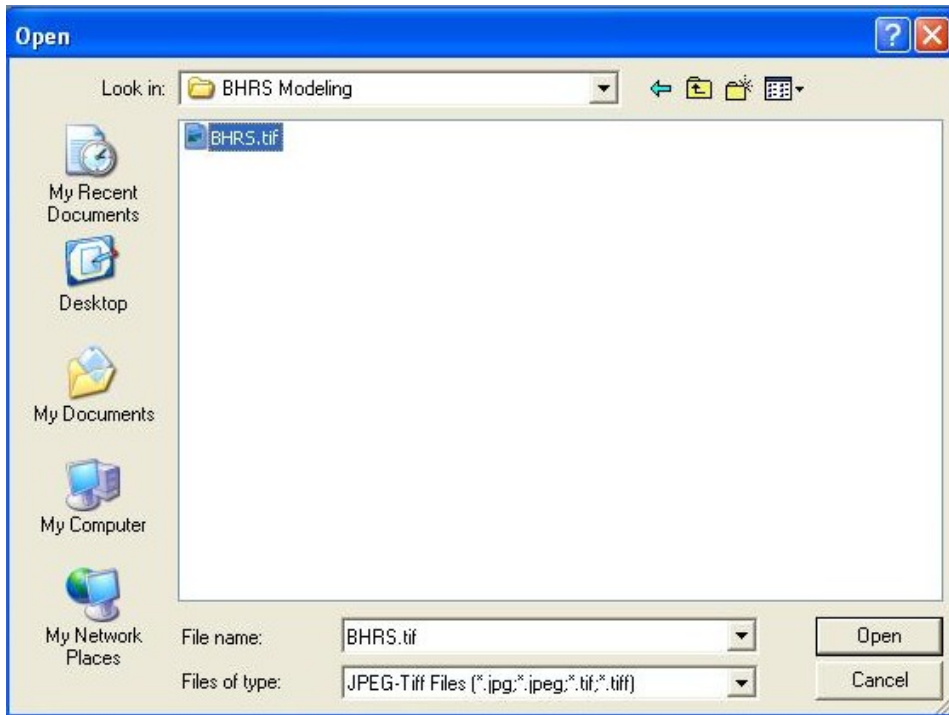


Figure 4: Dialog box for opening the base image for the GBM

Picture Transformation

For the purposes of the tutorial, a local coordinate system will be used; thus it is necessary to transform the image to this coordinate system.

Right click on the image 'BHRS' in the directory tree (Figure 5)
Select 'Transform' to open the 'Coordinate Transformation – Step 1' dialog box (Figure 6)
Select 'Translate, rotate, scale'

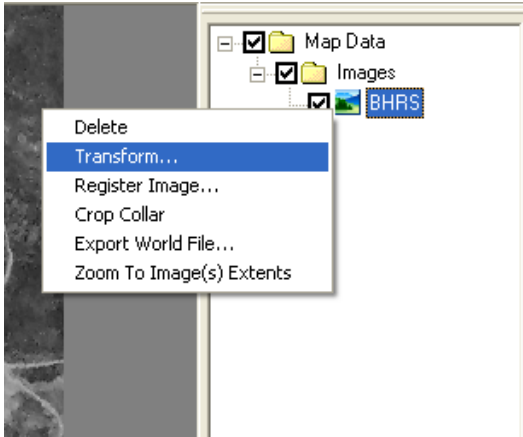


Figure 5: Transform option within the directory tree

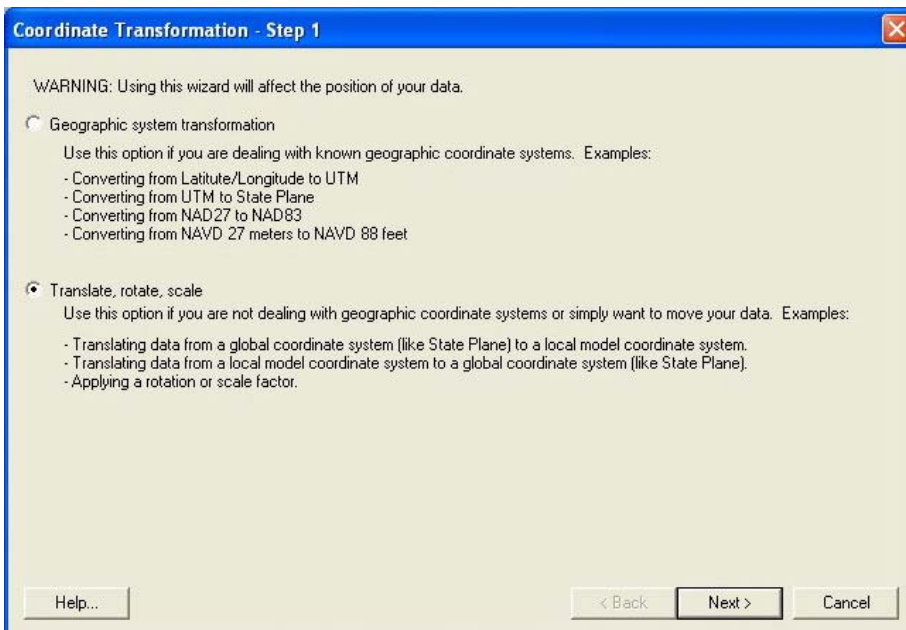


Figure 6: Coordinate Transformation - Step 1 dialog box.

Click 'Next' to continue to 'Coordinate Transformation – Step 2' dialog box (Figure 7)
Input values for X and Y as shown in Figure 7
Click 'Finish'

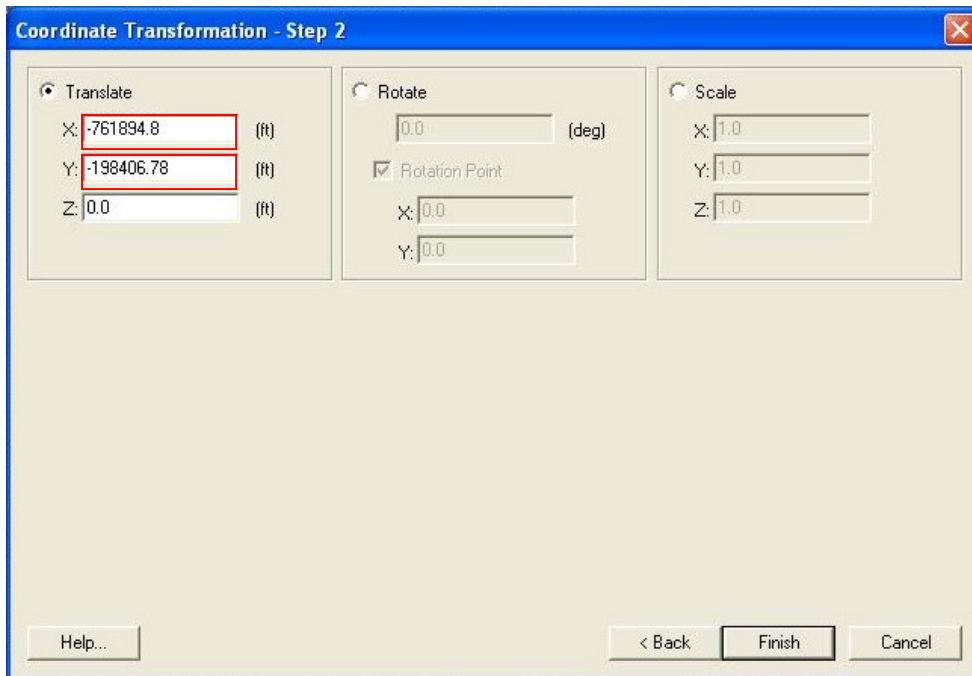



Figure 7: Dialog box showing the appropriate values for coordinate transformation of the image 'BHRS.TIF'.

NOTE:

It may be necessary to re-frame the image , and to adjust the transparency; Right click on 'Images' Folder, select 'Transparency' and adjust the slider as desired, (30% is suggested)

Creating the Conceptual Model

In 'Map' module, Right click on 'Map Data' – select 'New Conceptual Model'
 This opens the 'Conceptual Model Properties' dialog box (Figure 8)

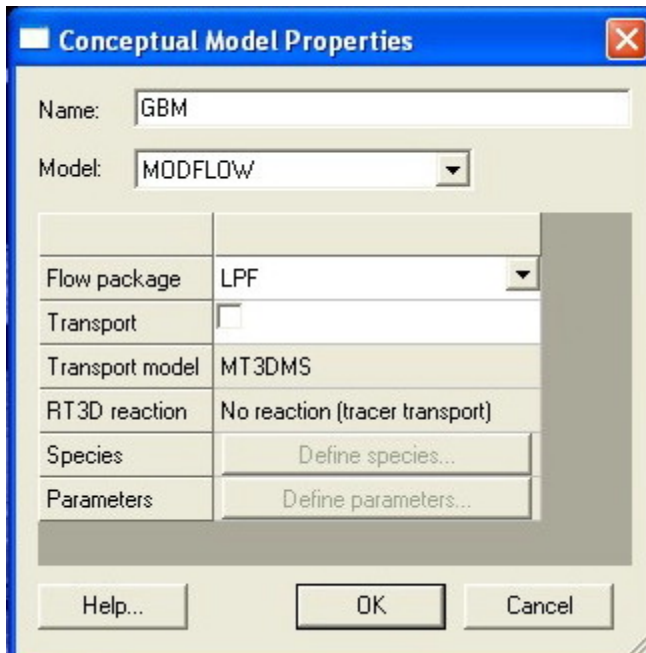


Figure 8: Conceptual Model Properties dialog box for basic setup properties of the conceptual model

Supply a name for the model: “**GBM.**”

Click ‘OK’

Creating the Boundary Coverage

In ‘Map’ module;

Right click the ‘**GBM**’ conceptual model

Select ‘new coverage’ to bring up the ‘**Coverage Setup**’ dialog box (Figure 9)

Supply the name “**Boundaries**”

Set ‘Default layer range’ to “**1-40**”

Check the box ‘Use to define model boundary (active area)’

Set ‘default elevation’ to ‘**18.5**’

Click ‘OK’

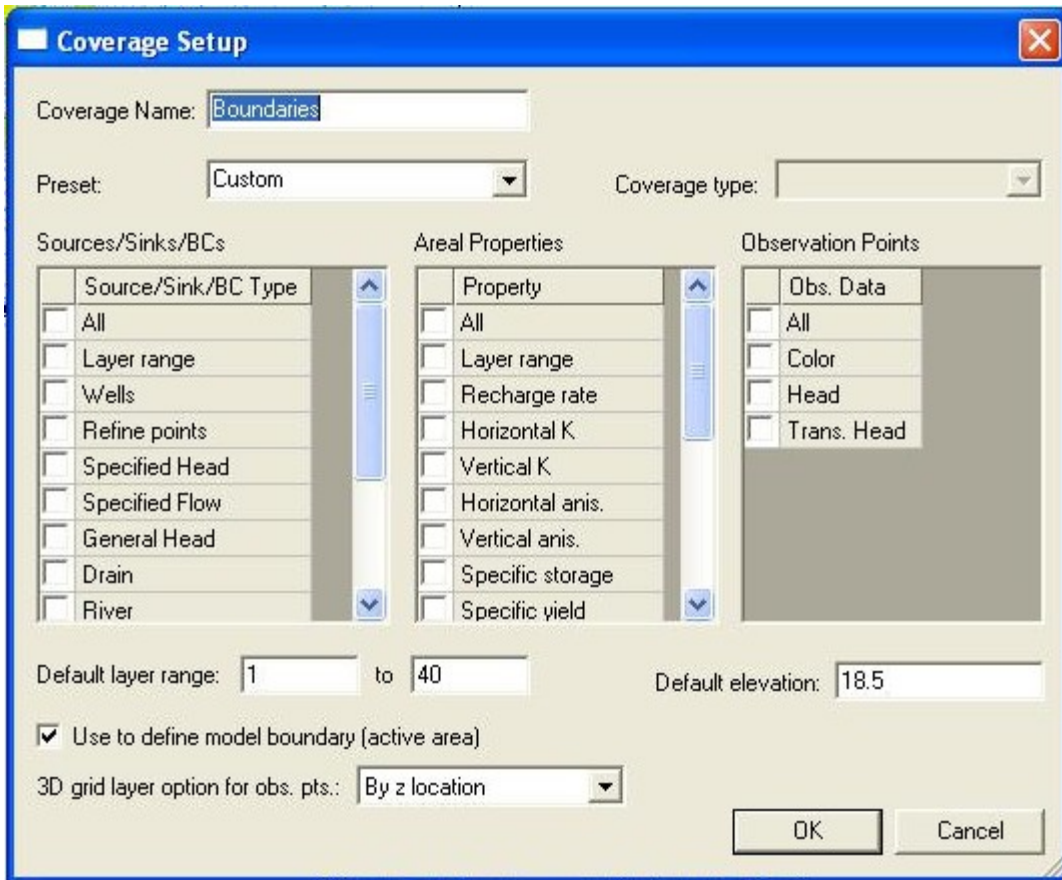


Figure 9: Coverage Setup dialog box for the 'Boundaries' conceptual model.

Drawing Model Boundaries

Select 'Create arc' 

Draw boundary arc as shown in Figure 10.

This boundary is set up around the extent of the gravel bar that will have a direct influence on the BHRS well field. It is bounded by the river to the southwest and the base of a terrace to the east. The upstream and downstream boundaries are where it is surmised that river water enters and exits the site. Flow is to the northwest.

Select 'Feature Objects' – 'Build polygons'

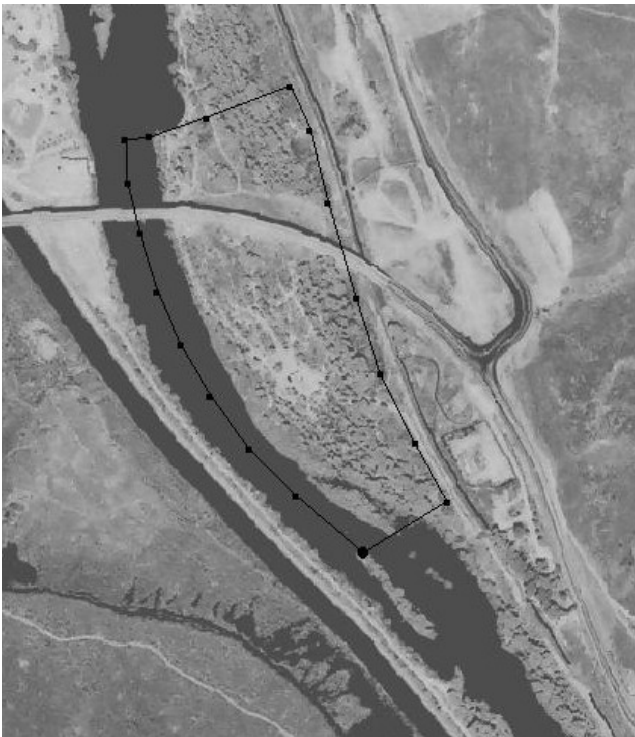


Figure 10: Image of the 'Boundaries' coverage arcs which will define the model boundary

NOTE:

When drawing arcs, it is not necessary to reproduce exactly what is seen in the images, but precision must be taken with different arcs, i.e. the river arc must mimic the boundary arc so appropriate cell types are assigned.

Creating River Coverage

Right click '**GBM**' conceptual model – select '*New coverage*' to open the '**Coverage Setup**' dialog box (Figure 11)

Supply name: "**River**"

Check '*River*' option in **Coverage Setup** dialog box under '*Source/Sink/BC Type*'

Set '*Default layer range*' to "**1-1**"

Uncheck '*Use to define model boundary (active area)*'

Click '*OK*'

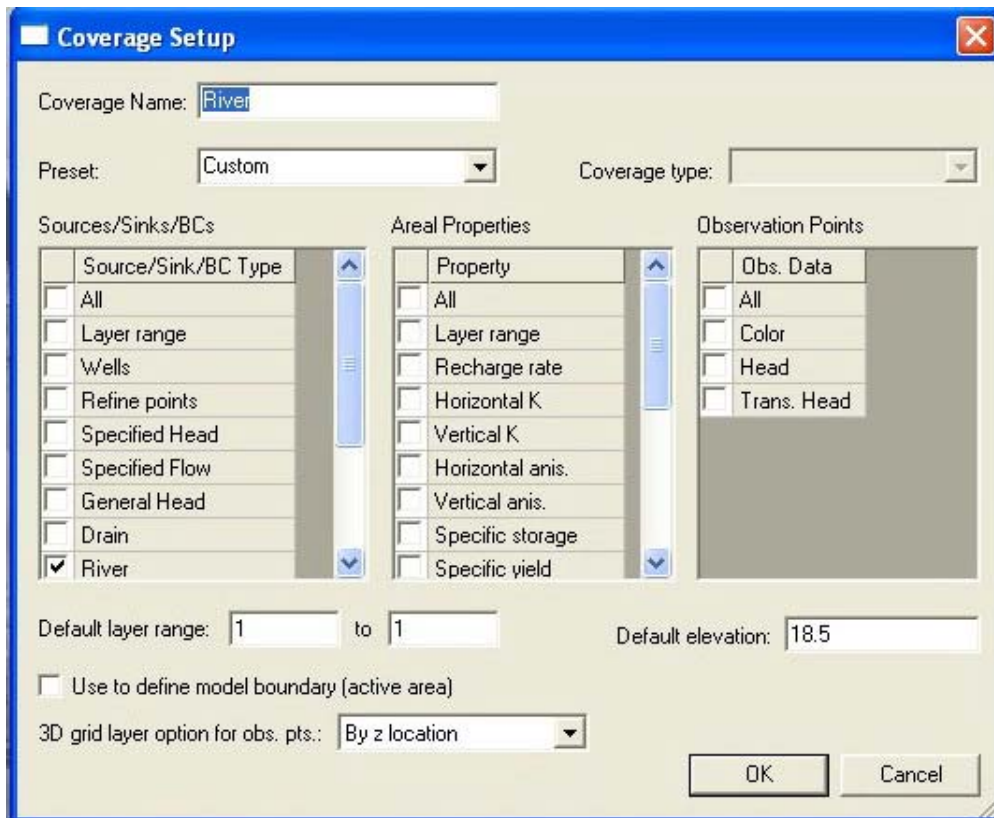



Figure 11: Coverage Setup dialog box for the 'River' coverage

Creating the River Arcs

Make sure '**River**' coverage is active

Click '*Create arc*'

Create river arcs as seen in Figure 12: roughly down the center of the river, over the western edge of the **boundaries** coverage

Click '*Select vertices*' 

Select the vertices to be used as nodes (See note below)

NOTE:

It may not be necessary to select all the vertices of the river to be used as nodes, GMS will interpolate values for the arc based on the upper and lower nodes, so it may only be necessary to use the start and end nodes, depending on the number of river stage measurement locations. For this example, only the start and end nodes are used.

With vertices selected, from the main toolbar - Select 'Feature Objects' - 'Vertices <-> Nodes' (if necessary)

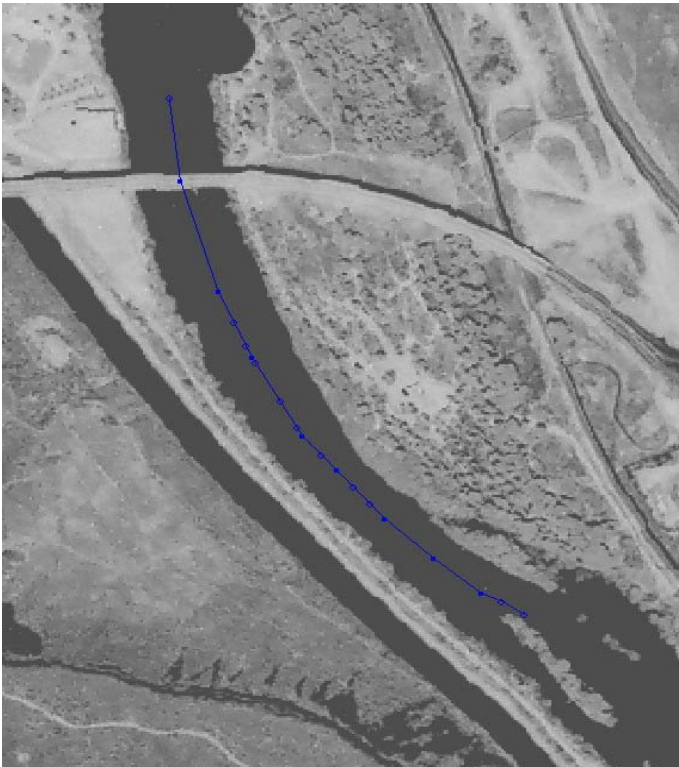


Figure 12: Location of the 'River' arc (arc types already assigned)

Assigning Properties to Boundaries


Transient Constant Head values (head values that remain constant within a stress period, but vary by specified amounts between stress periods) are assigned to the nodes along the gravel bar boundary surrounding the GBM. Transient River Stage values are assigned to the nodes along the river arc to simulate the transient stage levels seen during the TTLT, and constant head values (CHB) are assigned to the upstream and downstream sides of the model (Figure 10). The development of each of these boundaries is discussed separately in the following paragraphs.

Assigning River Conductance

Riverbed conductance is believed to be very high due to the lack of fines (silt and clay particles) in the riverbed. The BHRS is located approximately 4 km downstream of the Lucky Peak Dam, and 0.6 km downstream from a diversion dam. These dams effectively remove the fines from the river leaving the river bed clean and of high permeability. River stage data are input at each node. Stage values are imported from an Excel spreadsheet containing estimates of river stage fluctuations corresponding to the time steps of the tracer test (**RS.xls**, located on the CD). River stage values are estimated from data taken from a transducer placed in the river during the test. GMS interpolates values of river stage for cells located along the arcs between the nodes. River stage values as well as values for the constant head boundary (CHB) are set as transient, which allows for the values to change from stress period to stress period based on preset data.

Assigning River Values

Arcs

In 'Map' module click 'select arcs' 

Select the river arcs, and click 'properties' 

Assign all 'Type' as 'river', and input conductance values of "10" ($\text{m}^2/\text{s}/\text{m}$) for all arcs (see Figure 13).

NOTE:


In this example there is only one arc representing the river.

Click 'OK'



Figure 13: Properties dialog box for assigning conductance values to the river arcs

Nodes

Click 'Select nodes' 

Select the river nodes

Click 'properties'

In the 'Properties' dialog box, assign head stage as 'transient'

Assign transient river stage values for each node based on information found in the 'RS.xls' spreadsheet* (see Figures 14 and 15)

Assign bottom elevations*

Click 'OK'

*NOTE:

Independently determine initial river stage at each river node. The bottom elevation may also vary. For this test, the authors chose the bottom elevation to be about 1.5 m below the initial river stage. The river stage values for the upstream and downstream nodes, for each stress period, were calculated by assigning an initial river stage value in RS.xls (highlighted) and calculating the fluctuation from the initial value. The values to copy would be the 'Time' column and the 'Upstream' and 'Downstream' column. Also note that these values are distinct to this test, and make sure that the "downstream" column is copied to the downstream node and similarly for the upstream node.

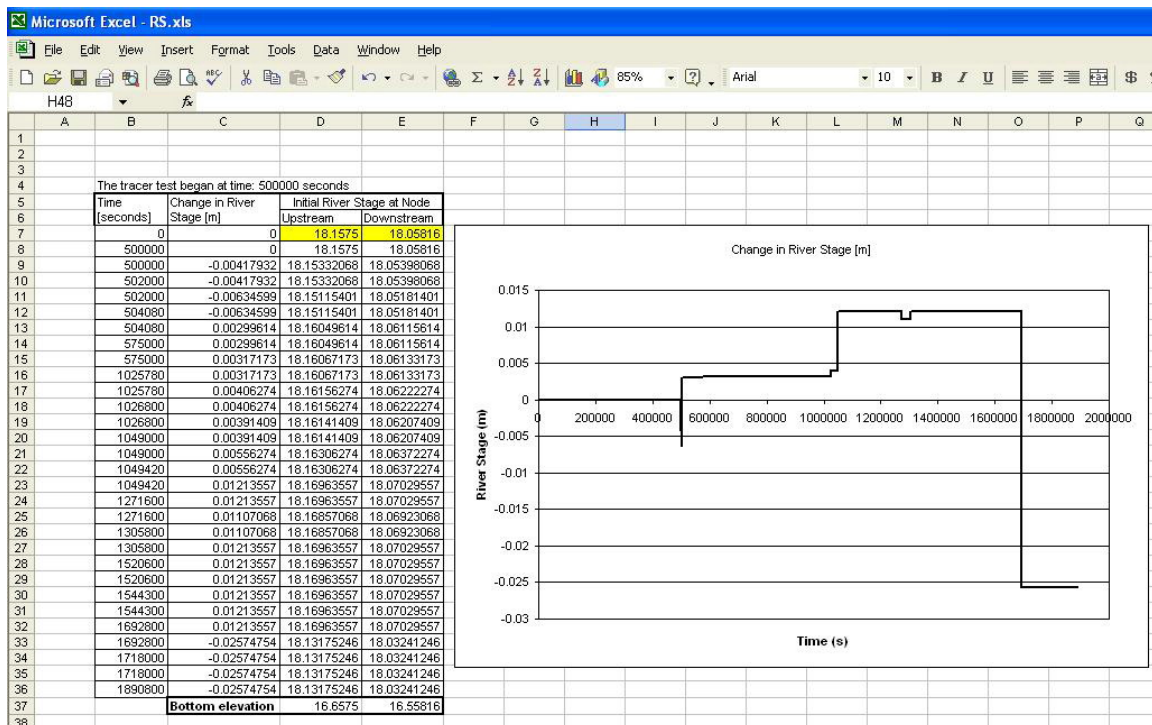


Figure 14: RS.xls spreadsheet showing river stage values

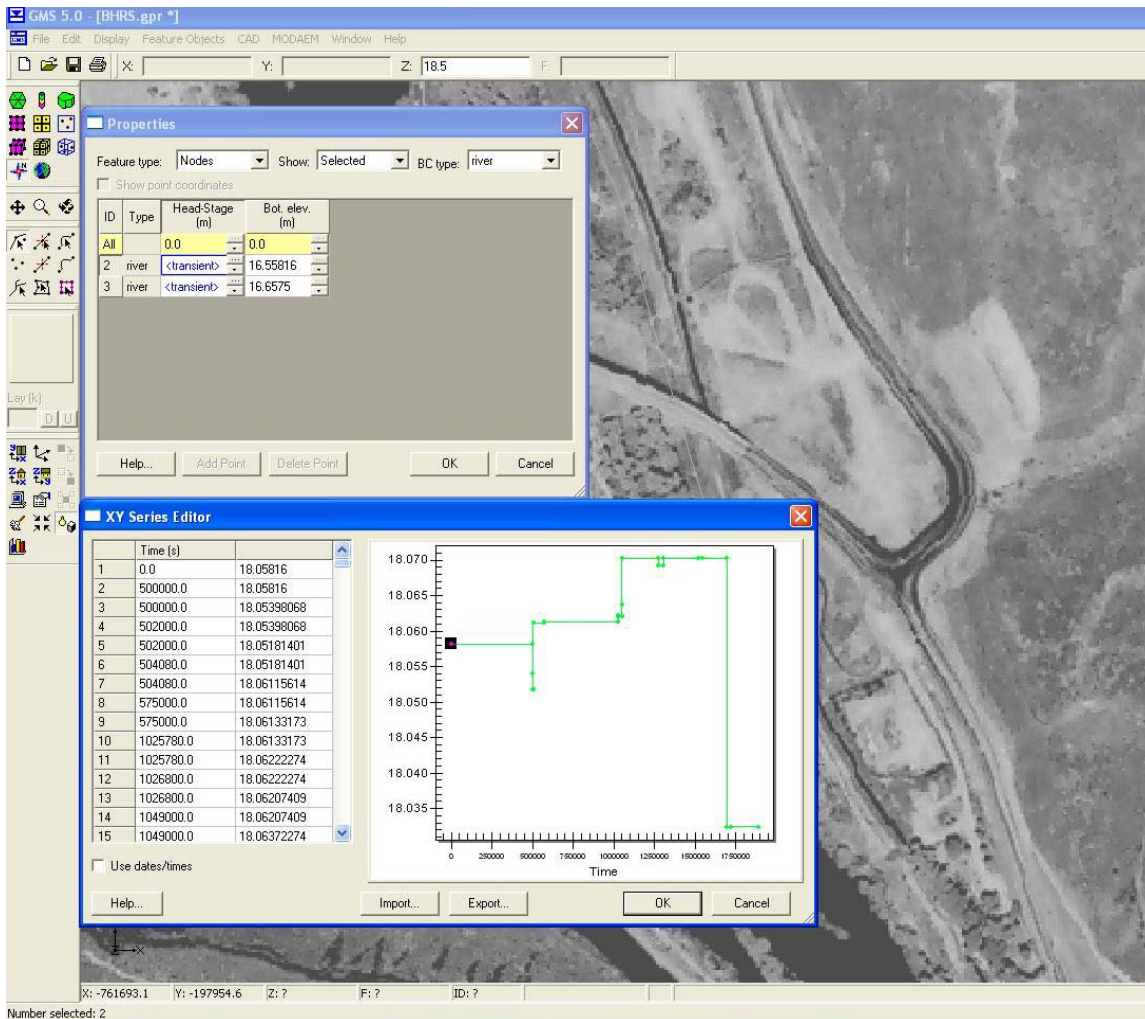


Figure 15: This figure shows the transient river stage values as well as the bottom elevations taken from the 'RS.xls' spreadsheet

Creating Constant Head Boundaries

Transient Constant Head Boundary (CHB)

Values for the Transient Constant Head boundary are set up in a manner similar to those for the River Stage boundary, where initial head values are known and fluctuations in those values are of the same magnitude as fluctuations in the river stage. From the available spreadsheet (**RS.xls**), values for the nodes making up the CHB are copied into GMS. The magnitude of the change in the CHB values can be taken as the same as the upstream and downstream river stage changes. Head values for each stress period are assigned to each node, and again GMS interpolates values along the arcs.

Creating the CHB coverage

Right-click **'Boundaries'** coverage and select *'duplicate'*

Supply name **"CHB"**

Double-click newly formed **'CHB'** coverage to bring up the **'Coverage Setup'** dialog box

Select *'Source/Sink/BC Type'* as *'specified head'*

Uncheck *'Use to define model boundary (active area)'*

Leave *'Default layer range'* and *'Default elevation'* unchanged (Figure 16).

Click *'OK'*

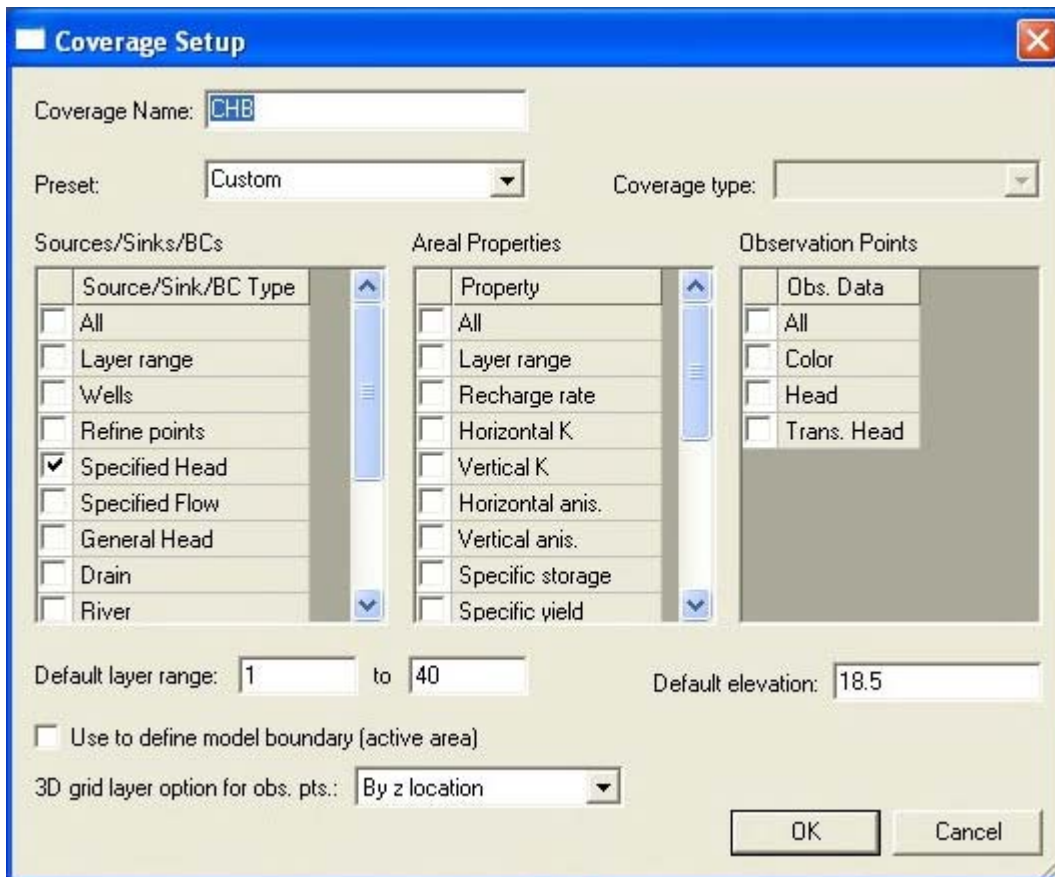



Figure 16: Coverage Setup dialog box for the creation of the 'Constant Head Boundary' coverage

Assigning CHB values

Click *'select vertices'* 

Select the vertices along the boundary to define constant head arcs as shown in red in Figure 17.

NOTE:

*These arcs represent the upstream and downstream river interaction of the model.
The entire upstream side is selected and the part of the downstream side that is covered by the river is selected.*

Select 'Feature Objects' and select 'Vertices<->Nodes'

Click 'select arcs'

Select the CHB arcs as shown in Figure 17

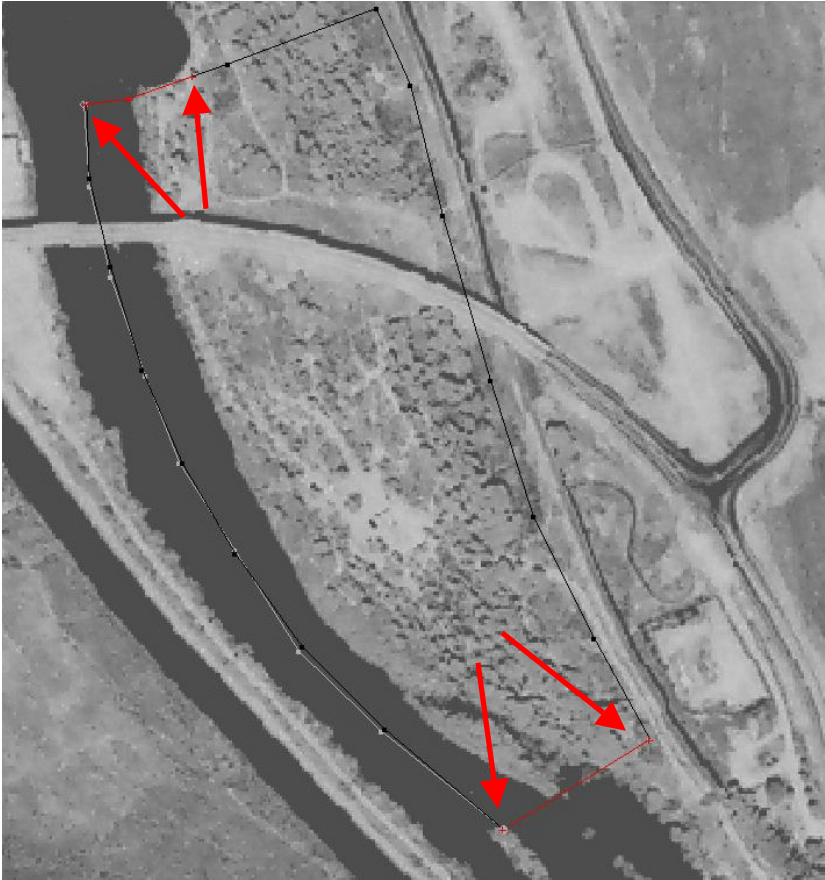


Figure 17: Vertices and arcs to be selected as specified head arcs

Click 'Properties'

Assign type for all arcs as 'specified head' (Figure 18).

Click 'OK'

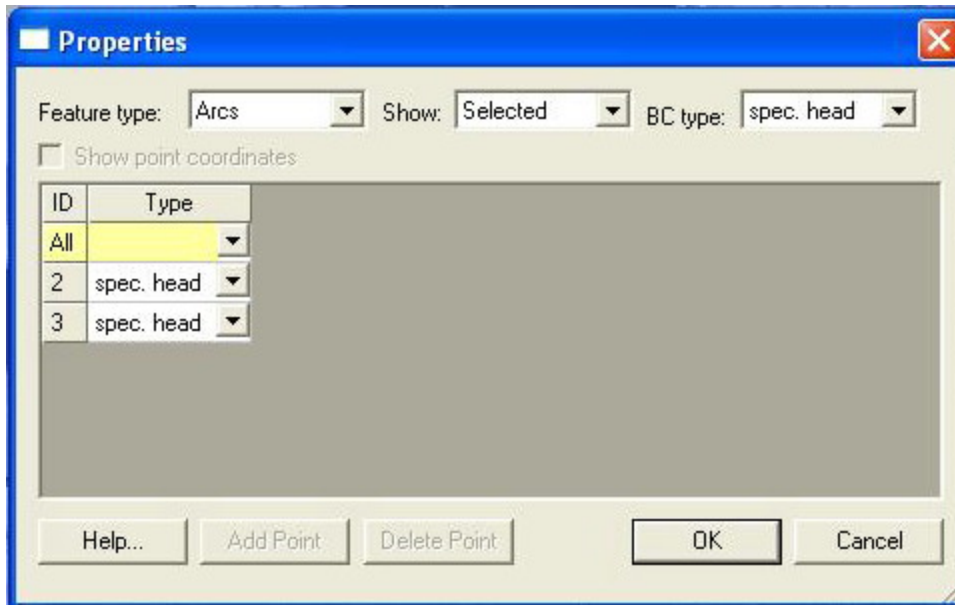


Figure 18: Properties dialog box for specified head arcs selected in Figure 17

Click 'Select nodes'

Select the **CHB** nodes bounding the **CHB** arcs

Click 'Properties'

Change head stage to 'transient' for all

Assign transient head stage values (assumed to be the same as transient river stage changes) from **RS.xls** for upstream and downstream nodes, assuming there is no gradient perpendicular to the river (Figure 19)

Click 'OK'

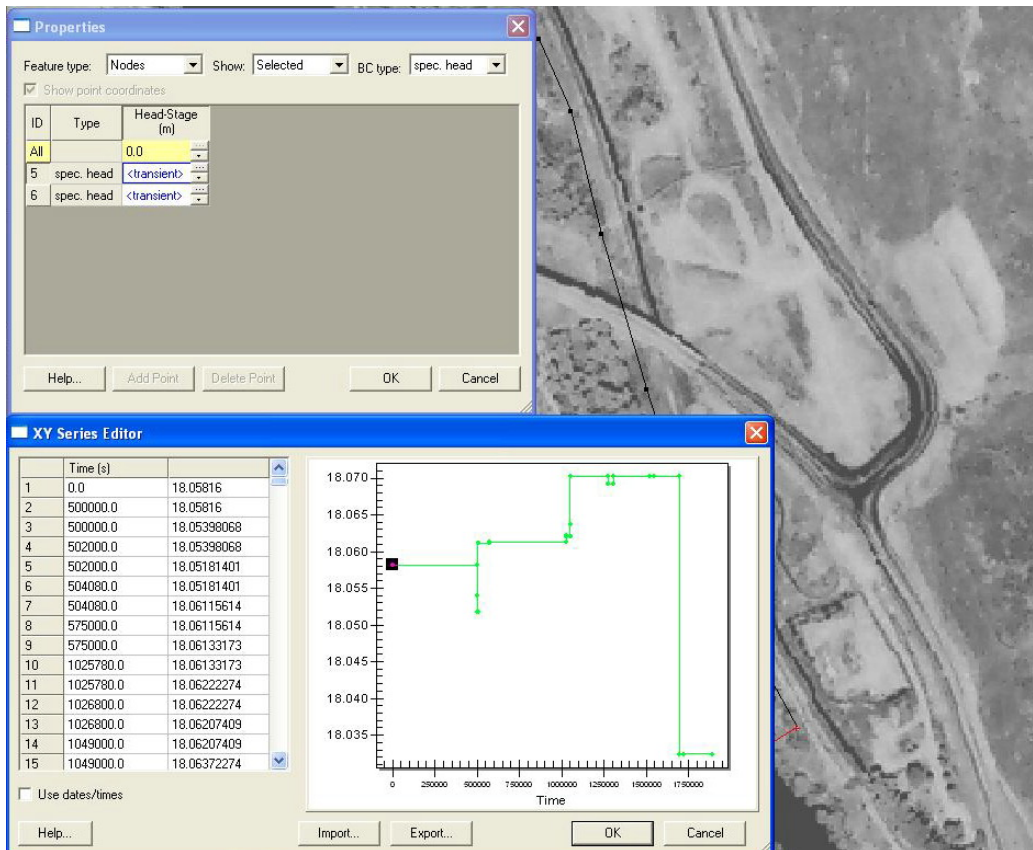


Figure 19: Head stage values for the Constant Head Boundary arcs, as taken from RS.xls

Creating Layer Coverages

Creating L1 Coverage

Right-click '**Boundaries**' coverage - select '*Duplicate*'

Rename "**L1**"

Double-click coverage '**L1**' to open '**Coverage Setup**' dialog box (Figure 20)

Unselect '*Use to define model boundary (active area)*'

Set '*Default layer range*' to "**1-1**"

From the '*Areal Properties*' list, select the following:

'**Horizontal K**'

'**Horizontal anis.**'

'**Vertical anis.**'

'**Specific storage**'

'**Specific yield**'

Leave '*Default elevation*' as shown

Click '**OK**'

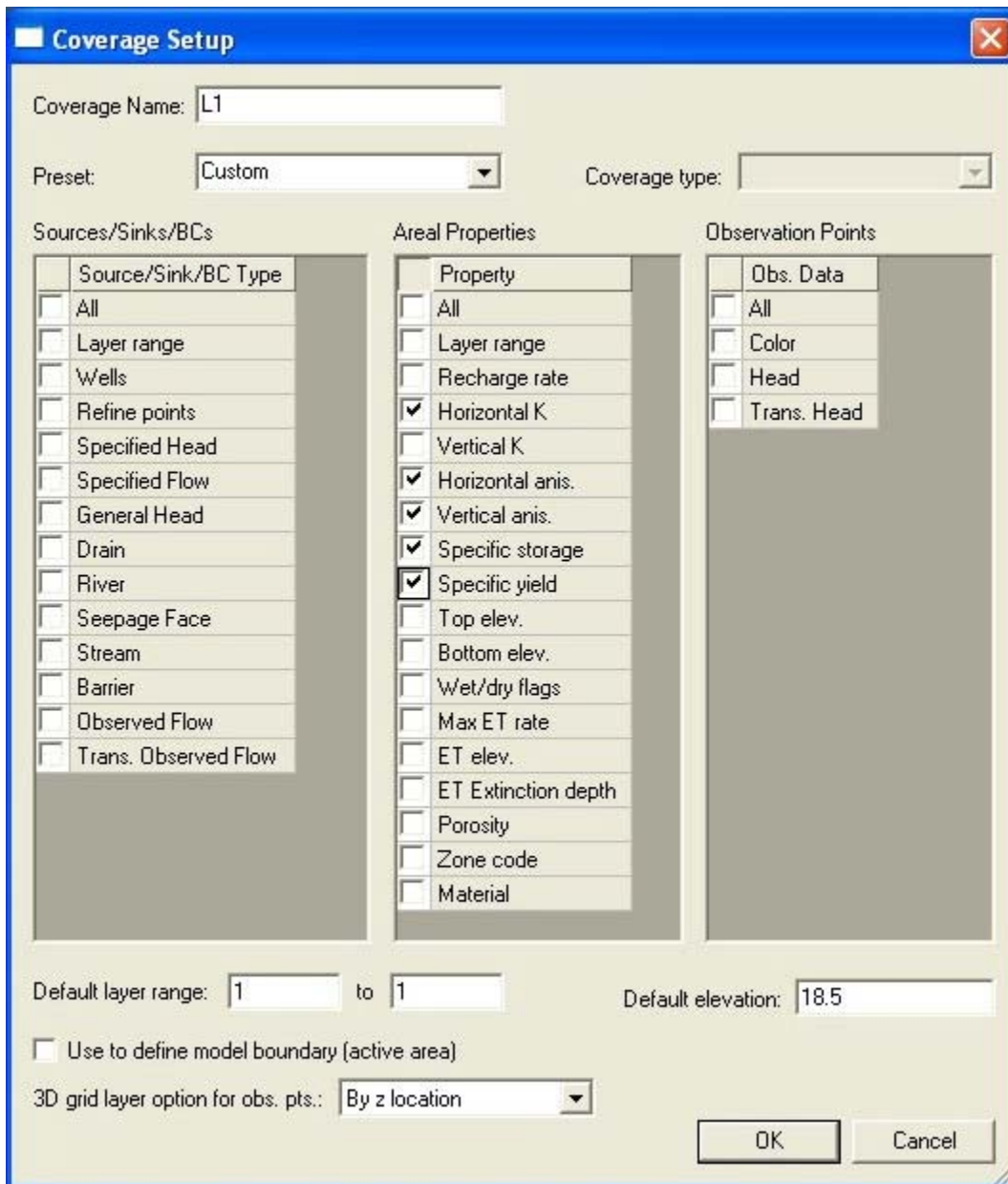


Figure 20: Coverage Setup dialog box for the L1 layer coverage

Click the 'Create arc' tool.

Draw in 'river' and 'unit 5' arcs as shown in Figure 21 by adding arcs, making sure to close all lines such that three polygons are created.




Figure 21: Location of the arcs encompassing the layers of the GBM

Creating Polygons

From the main toolbar, select '*Feature objects*' – '*Build polygons*'

The **GBM** now consists simply of 3 distinct hydrogeologic units: a river unit, a “Unit 5” in the middle (which is a pinching sand layer inferred from previous observations and developed to account for the observation of increased flow from the river), and a third unit in the northeast which includes the rest of the cells and is set up as a single unit with hydrologic values averaged throughout the gravel bar.

Assigning Areal Data

Click '*select polygon*' tool. 

Hold '**shift**' key and select all three polygons.

Click '*Properties*' to bring up '**Properties**' dialog box, assign polygon values as shown in Table 1 and in Figure 22

Click '*OK*'

Polygon	Property				
	Horizontal Conductivity	Horizontal Anisotropy	Vertical Anisotropy	Specific Storage	Specific Yield
River (Arc 1)	10.0	1.0	1.0	0.000045	1.0
Unit 5 (Arc 2)	0.001	1.0	1.0	0.000045	0.425
Other (Arc 3)	0.000305	1.0	1.0	0.000045	0.21

Table 1: Values for 'River', 'Unit 5' and 'Other' polygons

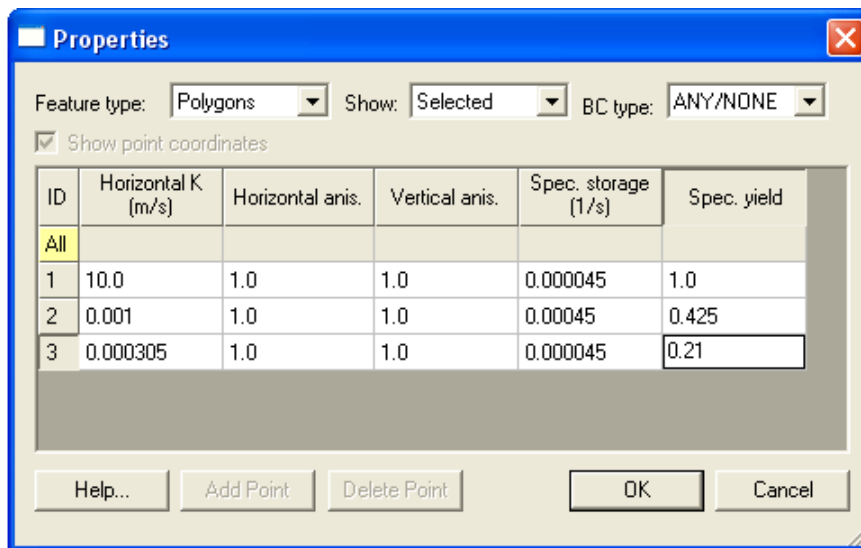


Figure 22: Properties dialog box for the three L1 polygons

Right-click 'Boundaries' coverage – select 'Duplicate'

Rename to "L2-L40"

Double-click 'L2-L40' coverage to open 'Coverage Setup' dialog box (Figure 23).

From the 'Areal Properties' list, select the following:

'Horizontal K'

'Horizontal anis.'

'Vertical anis.'

'Specific storage'

'Specific yield'

Unselect 'Use to define model boundary (active area)'

Change 'Default layer range' to "2-40"

Click 'OK'

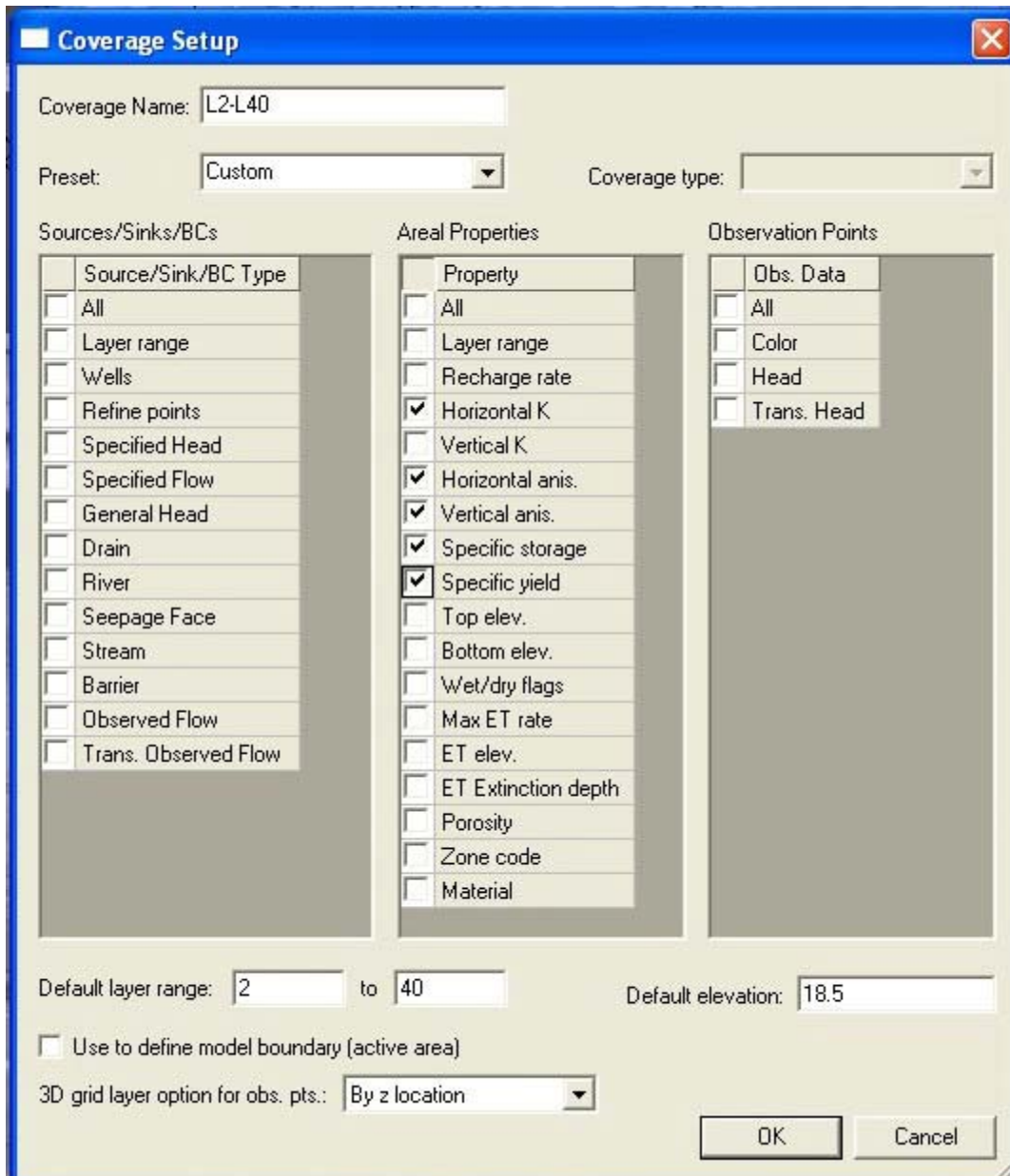



Figure 23: Coverage Setup dialog box for the L2-L40 layer coverage.

Creating Layer Polygons

Select 'Feature Objects' – 'Build polygons'

Click 'Select polygon' tool 

Double-click 'L2-L40' polygon

Click 'Properties'

Assign values same as 'Other' layer from Table 1 and seen in Figure 24.

Click 'OK'

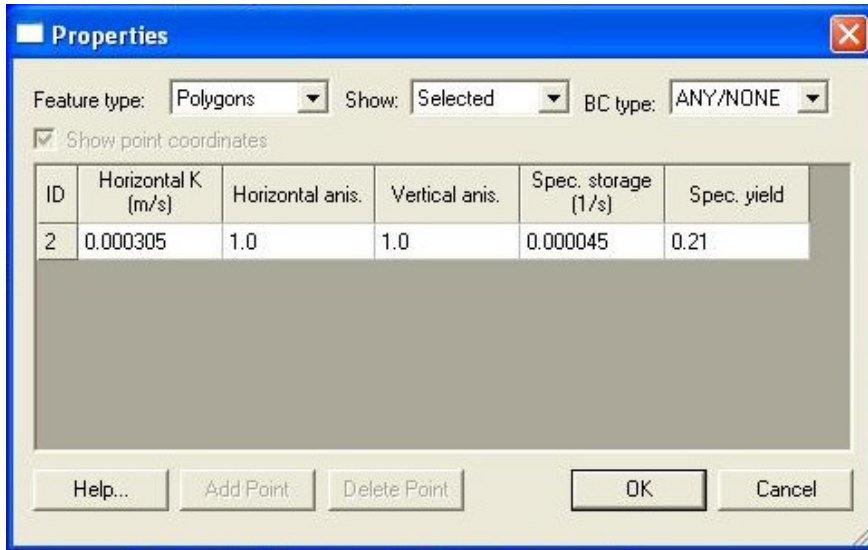


Figure 24: Properties dialog box for the L2-L40 polygon

Creating Observation Coverage

Adding Wells

The wells of the BHRS (A1, B-, C-, and X-rings) are incorporated into the model in GMS using their geospatial data (Easting, Northing and model elevation). The wells are set to be treated by GMS as refining points from which to initiate grid development. The well locations are assigned a specific cell size, and the grid is extended out from those points with increasing size until a maximum cell size of 20 m is met. The denser grid arrangement near the wells allows for more accurate data to be obtained during the model run. The wells also act as observation points for head values throughout the model run. This way the produced values can be compared to the actual values measured during the TTLT.

Creating Observations Coverage

Right-click 'GBM' conceptual model – select 'New coverage'.

This opens the Coverage setup dialog box (Figure 25).

Supply name "Obs"

Check 'head' and 'refining points' from the 'Obs. Data' and 'Sources/Sinks/BCs' columns, respectively

Set 'Default layer range' to "1-40"

Uncheck 'Use to define model boundary (active area)'.

Change '3D grid layer option for obs. pts.' to 'By layer number'.

Change 'Default elevation' to "18.5"

Click 'OK'

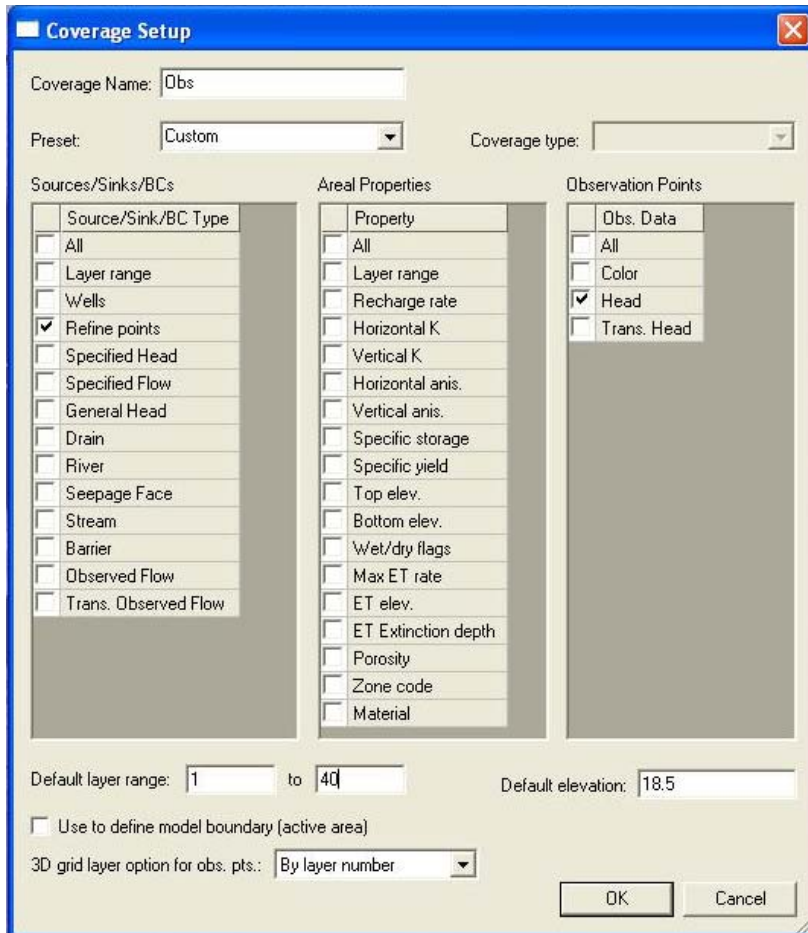



Figure 25: Coverage Setup dialog box for setting up the Obs coverage


Adding Wells as Refining Points

Click 'Create points' tool 

Anywhere on the map, create **18** points

NOTE:

The spatial data of these points will be adjusted in the properties box from values located in "Obs.xls"

Click 'Select Points/Nodes' tool 

Select all 18 points – easily done by drawing a box around all 18.

Click 'Properties' to open the 'Properties' dialog box

Check 'Show point coordinates' – check all as 'Refine'

Change 'base size' to **0.2**, 'Bias' to **1.25**, and 'Max size' to **20** for all points

Open the 'Obs.xls' document and copy 'well ID', and 'x-y data', from Obs.xls to the "Name", "X", "Y" columns for all points (Figure 26).

	A	B	C	D	E	F	G	H	I
1	Well	X	Y	Obs Head value [m]					
2	A1	10000.04	10000.02						
3	B1	9999.77	10002.94						
4	B2	10002.98	10001.96						
5	B3	10003.76	9998.1						
6	B4	10000.27	9997.39						
7	B5	9996.96	9998.13						
8	B6	9997.66	10001.32						
9	C1	10003.3	10006.61	18.063					
10	C2	10008.18	10000.54	18.066					
11	C3	10003.86	9994.02	18.072					
12	C4	9995.71	9991.3	18.072					
13	C5	9990.91	9999.76	18.063					
14	C6	9995.48	10007.03	18.06					
15	X1	10004.41	10040.04	18.036					
16	X2	10030.04	9998.74	18.082					
17	X3	10019.26	9964.87	18.097					
18	X4	9986.93	9982.25	18.072					
19	X5	9961.84	10021.09	18.048					
20									
21									
22									

Figure 26: OBS.xls spreadsheet with location data of wells

Set **Z** value to “12.0”

Select only the C and X wells as ‘*obs pt*’ from the ‘*Type*’ column

Copy the ‘*obs. head values*’ from Obs.xls to ‘**Obs. Head**’ column for C- and X- wells. (Figure 27)

ID	Name	X	Y	Z	Refine	Base size (m)	Bias	Max size (m)	Type	Layer	Obs. Head	Obs. Head interval	Obs. Head conf(%)	Obs. Head std. dev	Computed Head	Residual Head
114	A1	10000.04	10000.02	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	NONE	1	0.0	1.0	95	0.51021		
115	B1	9999.77	10002.94	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	NONE	1	0.0	1.0	95	0.51021		
116	B2	10002.98	10001.96	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	NONE	1	0.0	1.0	95	0.51021		
117	B3	10003.76	9998.1	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	NONE	1	0.0	1.0	95	0.51021		
118	B4	10000.27	9997.39	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	NONE	1	0.0	1.0	95	0.51021		
119	B5	9996.96	9998.13	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	NONE	1	0.0	1.0	95	0.51021		
120	B6	9997.66	10001.32	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	NONE	1	0.0	1.0	95	0.51021		
121	C1	10003.3	10006.61	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.063	1.0	95	0.51021		
122	C2	10008.18	10000.54	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.066	1.0	95	0.51021		
123	C3	10003.86	9994.02	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.072	1.0	95	0.51021		
124	C4	9995.71	9991.3	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.072	1.0	95	0.51021		
125	C5	9990.91	9999.76	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.063	1.0	95	0.51021		
126	C6	9995.48	10007.03	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.06	1.0	95	0.51021		
127	X1	10004.41	10040.04	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.036	1.0	95	0.51021		
128	X2	10030.04	9998.74	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.082	1.0	95	0.51021		
129	X3	10019.26	9964.87	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.097	1.0	95	0.51021		
130	X4	9986.93	9982.25	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.072	1.0	95	0.51021		
131	X5	9961.84	10021.09	12.0	<input checked="" type="checkbox"/>	0.2	1.25	20.0	obs. pt	1	18.048	1.0	95	0.51021		

Figure 27: Properties dialog box for the 18 refining points of the Obs coverage

Click ‘**OK**’

Final well placement should resemble Figure 28.



Figure 28: Final location of the 18 refining points representing the wells of the BHRS

Creating the 3D Grid

Be sure to have the 'Obs' coverage selected in the directory tree.

From the main toolbar, select 'Feature objects' – 'Map<->3D grid'

This will bring up the 'Create Finite Difference Grid' dialog box (Figure 29)

Input values of X-Dimension origin, X-Dimension Length, Y-Dimension Origin, Y-Dimension Length, Z-Dimension Length, Number Cells, and Rotate about Z-axis as shown in Figure 29.

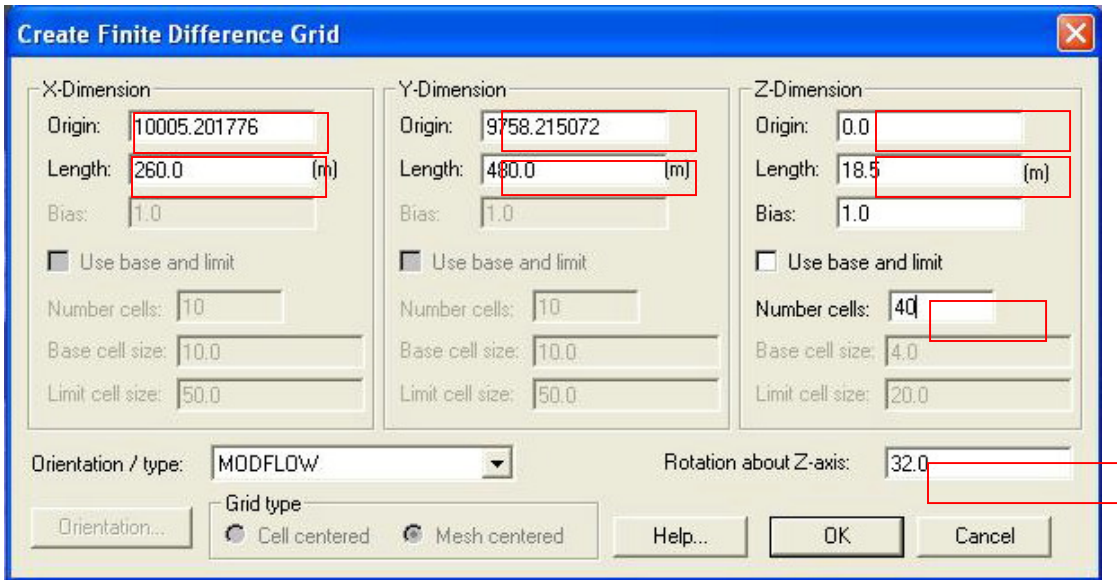


Figure 29: Dialog box for inputting the size dimensions of the 3D grid

Click 'OK'.

Grid should be created resembling Figure 30.

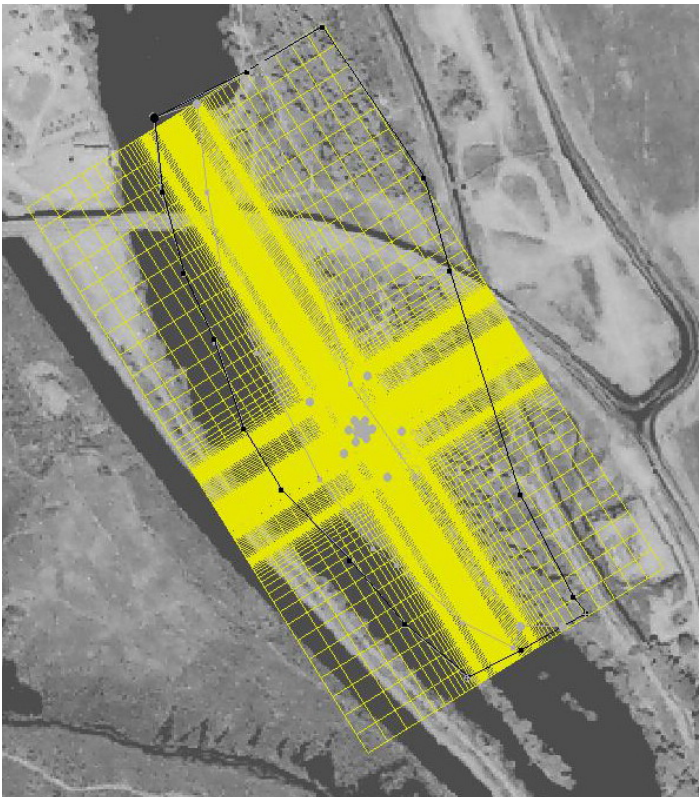


Figure 30: Location and orientation of the newly created 3D grid for the GBM

From the main toolbar, select ‘*Feature objects*’ – ‘*Activate cells in coverage*’ to show only the cells bounded by the GBM **Boundaries** coverage (Figure 31).

NOTE:

*If incorrect cells are displayed you can adjust the locations of vertices and nodes of the boundary coverage to activate or inactivate the appropriate cells; this is done through the ‘*Select vertices*’ or ‘*Select nodes*’ tools and clicking and dragging the vertices/nodes to the correct locations. Once the vertices are adjusted, polygons must be recreated, and steps for creating the grid must be redone (Creating Boundary Coverage). Likewise if the boundary coverage is not encompassed by the modeling grid, the values from Figure 29 can be adjusted.*

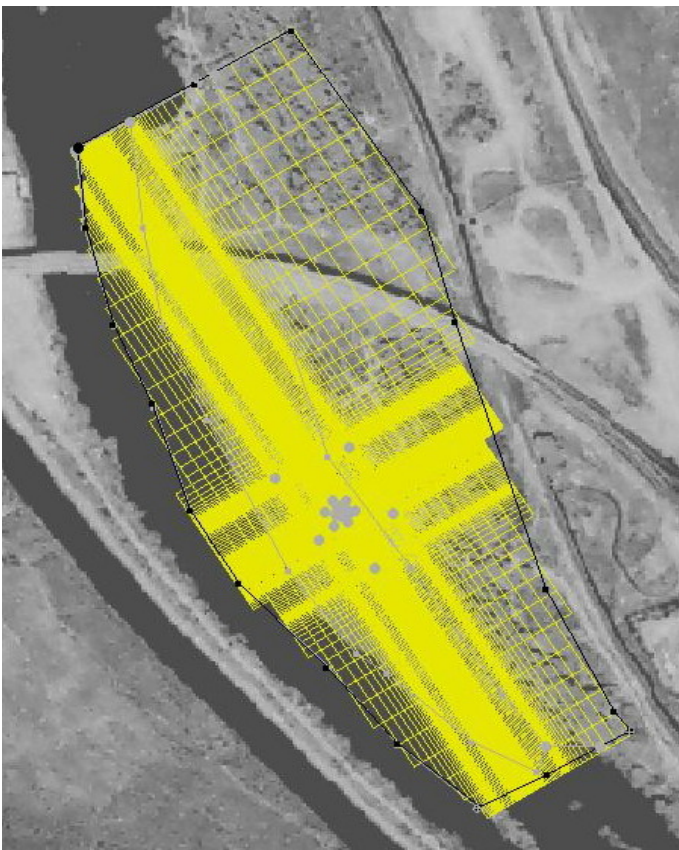



Figure 31: Final grid size showing the active cells only

Creating a New MODFLOW2000 (MF2K) Simulation

Click '3D grid' module 

From the main toolbar, select 'MODFLOW' – 'New simulation'

This will bring up the 'Global Options' dialog box (Figure 32)



Figure 32: Global Options dialog box

Select 'Starting heads' to open the **Starting Heads** dialog box.

Select 'Constant->Grid' - assign "18" for the *Constant Value for Grid* (Figure 33).

Click 'OK'.

Click 'OK' to exit 'Starting Heads' dialog box.

Click 'OK' to exit 'Global Options' dialog box.

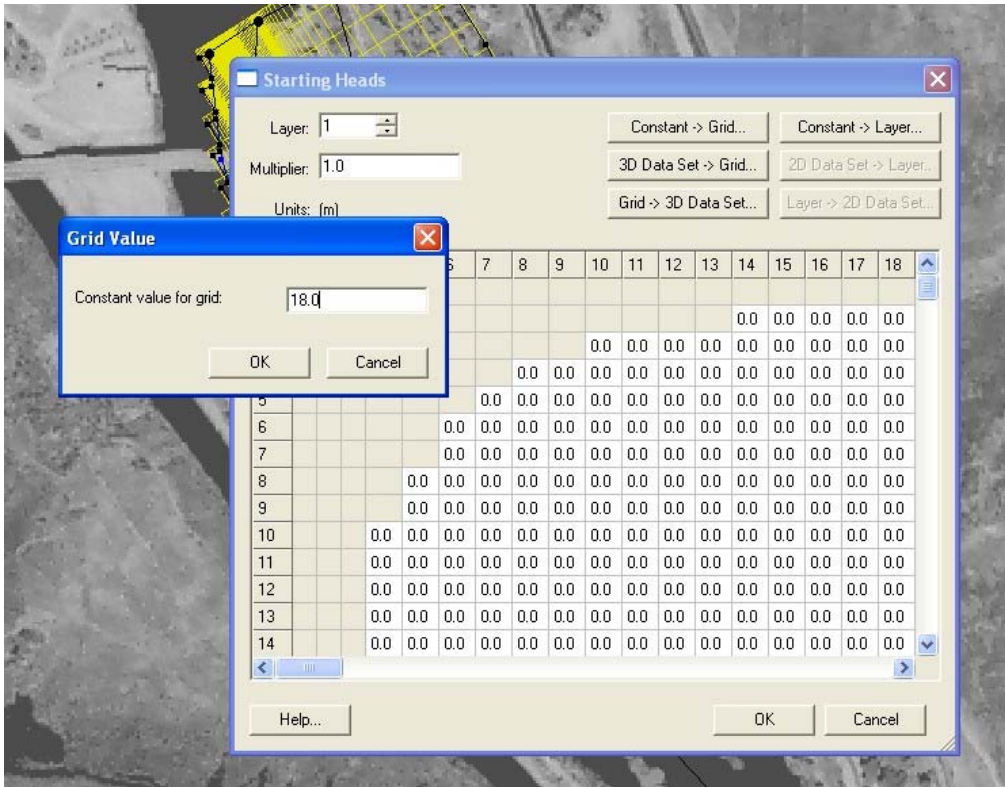


Figure 33: Grid Value dialog box for assigning a constant starting head value for the entire grid

Save Project

Select 'File' – 'save'
Exit GMS

Editing Model Layer Elevations

Editing Model Layer Top and Bottom Elevations

The discretization file (.dis) is opened in a text editor and '**Top**' and '**BOTM**' (MODFLOW 2000 array names in the discretization file) are adjusted. Top and bottom model layer elevations are set to match the sampling zones of well A1 (A1-A20) during the TTLT. Model layer 10 corresponds to the top sampling zone: A20. Over the sampling intervals in well A1 (20 in all), the model cell heights are each set to correspond to the height of one sampling zone (0.25 m). Above and below the extent of the sampling zone (20 x 0.25m zones in all), the cell height increases by 1.2 times the previous cell height. The discretization file is then saved and the coverages in the Map module containing the river, CHB, and hydrogeologic properties (K, Ss, Sy, etc) are mapped to MODFLOW.

Editing the .dis File

Exit GMS

Navigate to the saved project files – open ‘**GBM.dis**’ in text editor

Replace ‘**Top**’ and ‘**BOTM**’ values of ‘**GBM.dis**’ file (lines 14 - 54) with values from ‘**GBM lyr elev.txt**’ file (on CD) (Figure 34).

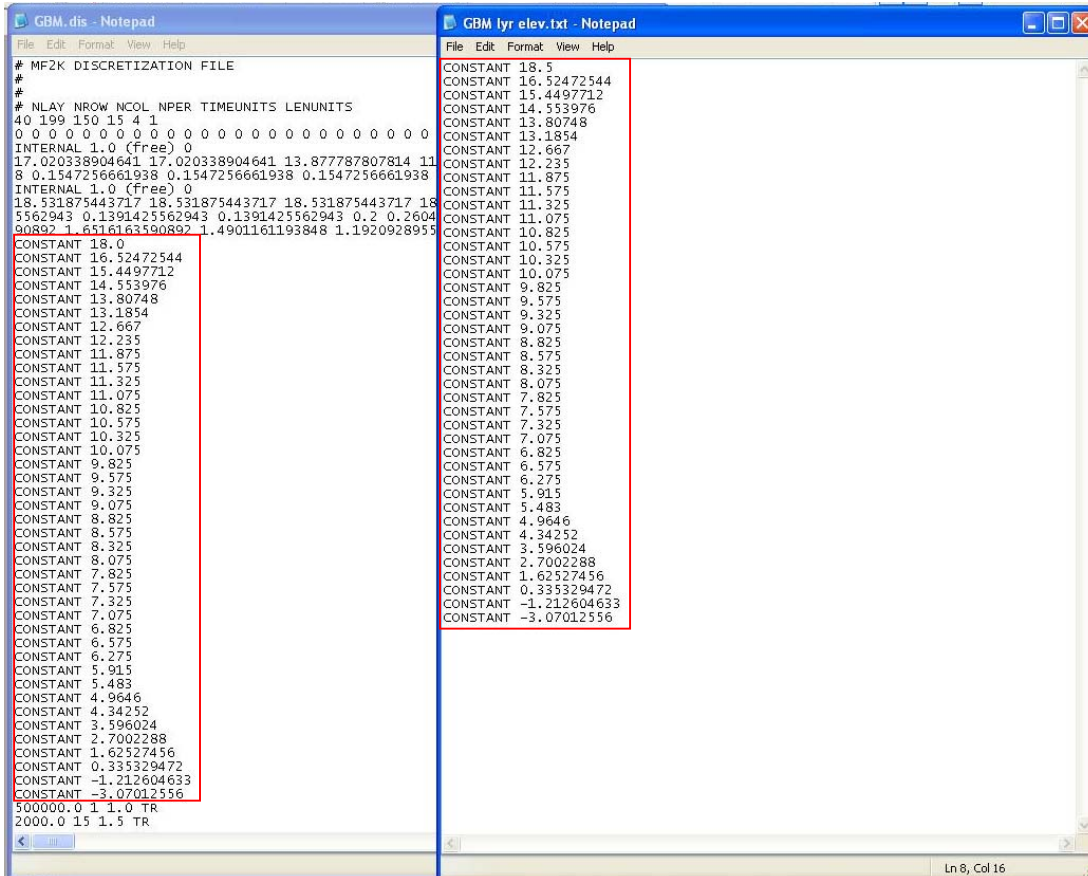


Figure 34: Sample of the values to be copied from the “GBM lyr elev.txt” file (on CD) that are copied to replace the values of the GBM.dis file created by the simulation

Save and close the **GBM.dis** file

Open GMS

Open the **GBM.gpr** model file to check the values of layer elevations (Figure 35)

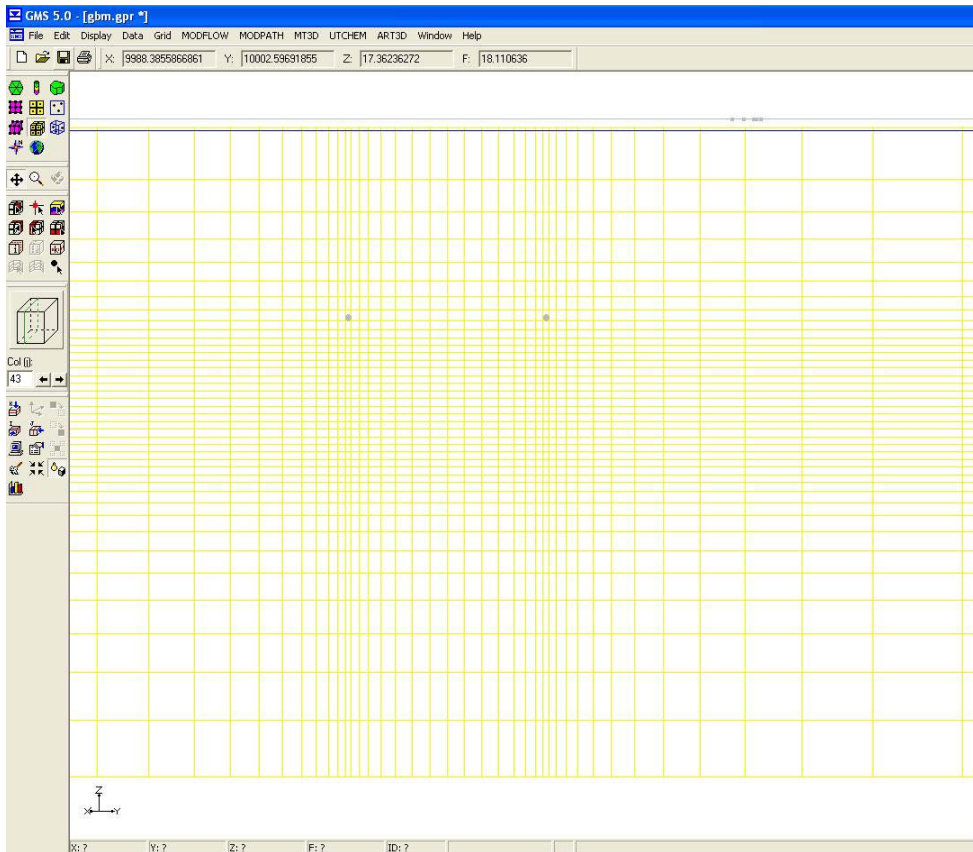


Figure 35: X-Z profile of the GBM model grid showing correct model layer elevations

In 'Map' module select 'Feature Objects' – 'Map<->MODFLOW' to open the **Map <-> Modflow** dialog box (Figure 36)

Select 'All applicable coverages' to apply the new layer elevations to the 3D grid.



Figure 36: Map -> Model dialog box

Click 'OK'.

Grid cells types are now assigned (Figure 37).

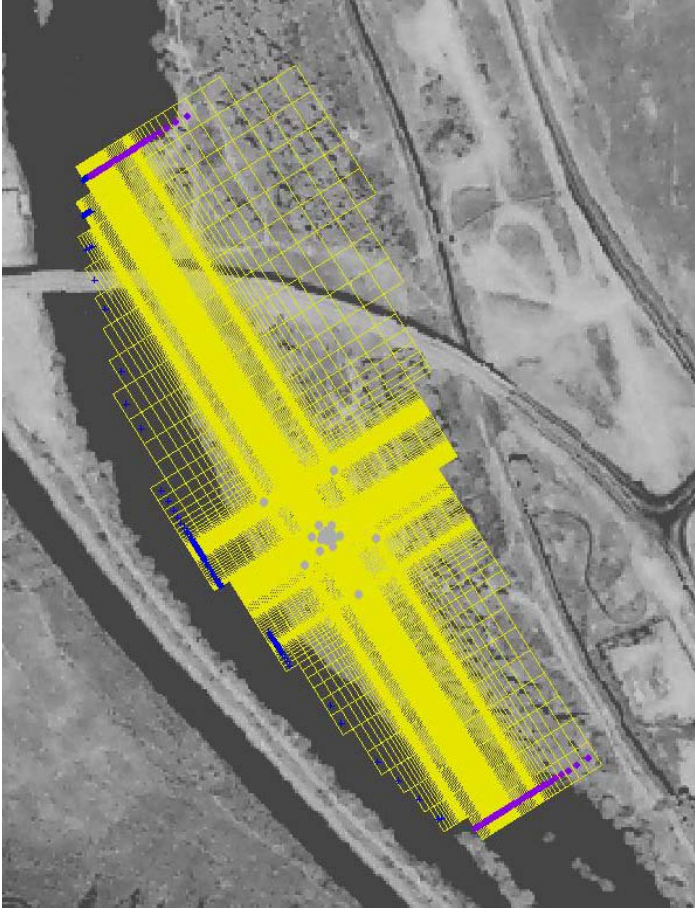



Figure 37: GBM model grid with cell types assigned

Calibration with Steady State Solution

Select '3D grid' module  – select 'MODFLOW' – 'Observations' to open the **Observations** dialog box (Figure 38)

Check 'Obs' coverage from *Coverages (head observations)* if not already selected

Click 'OK'

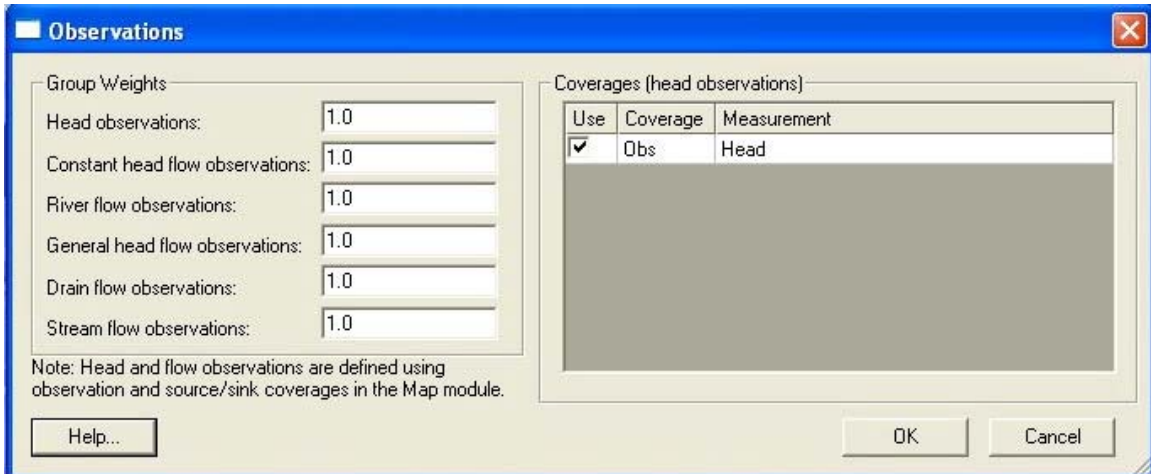


Figure 38: Observations dialog box for GBM model

Click 'MODFLOW' – 'PCG2 package' to open the **MODFLOW PCG2 Package** dialog box (Figure 39)

Change the following values:

'Max inner iterations' to **300**

'Head change criterion for convergence' to **0.0001**

'Residual criterion for convergence' to **0.0001**

Click 'OK'

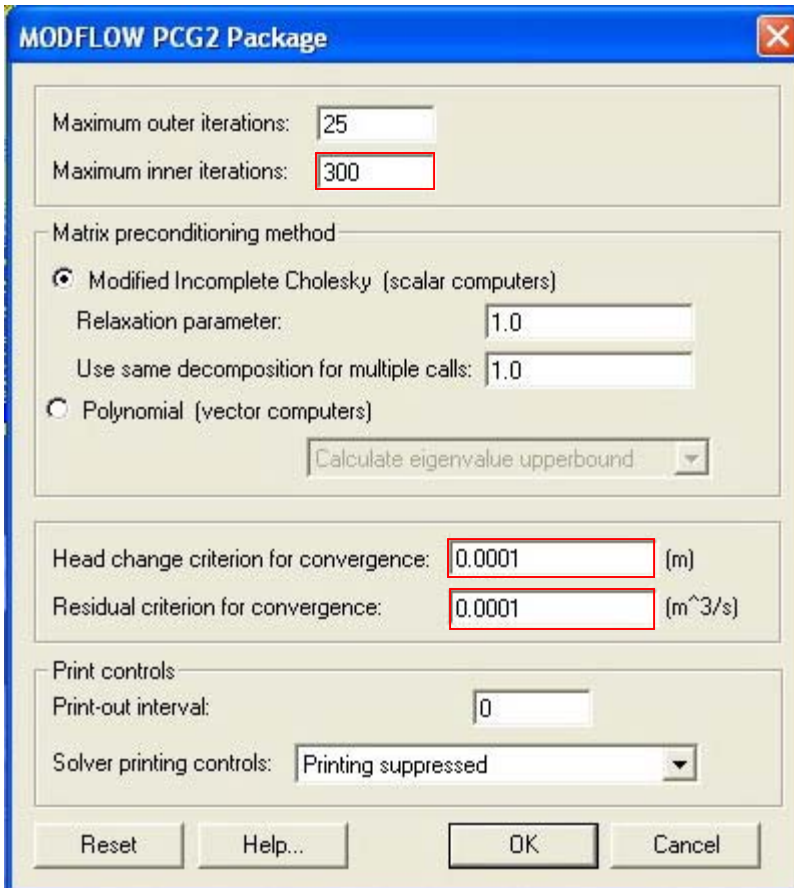


Figure 39: MODFLOW PCG2 Package dialog box showing the appropriate values

Save

Click 'MODFLOW' – 'Run MODFLOW' to run MODFLOW-2000 (Figure 40).

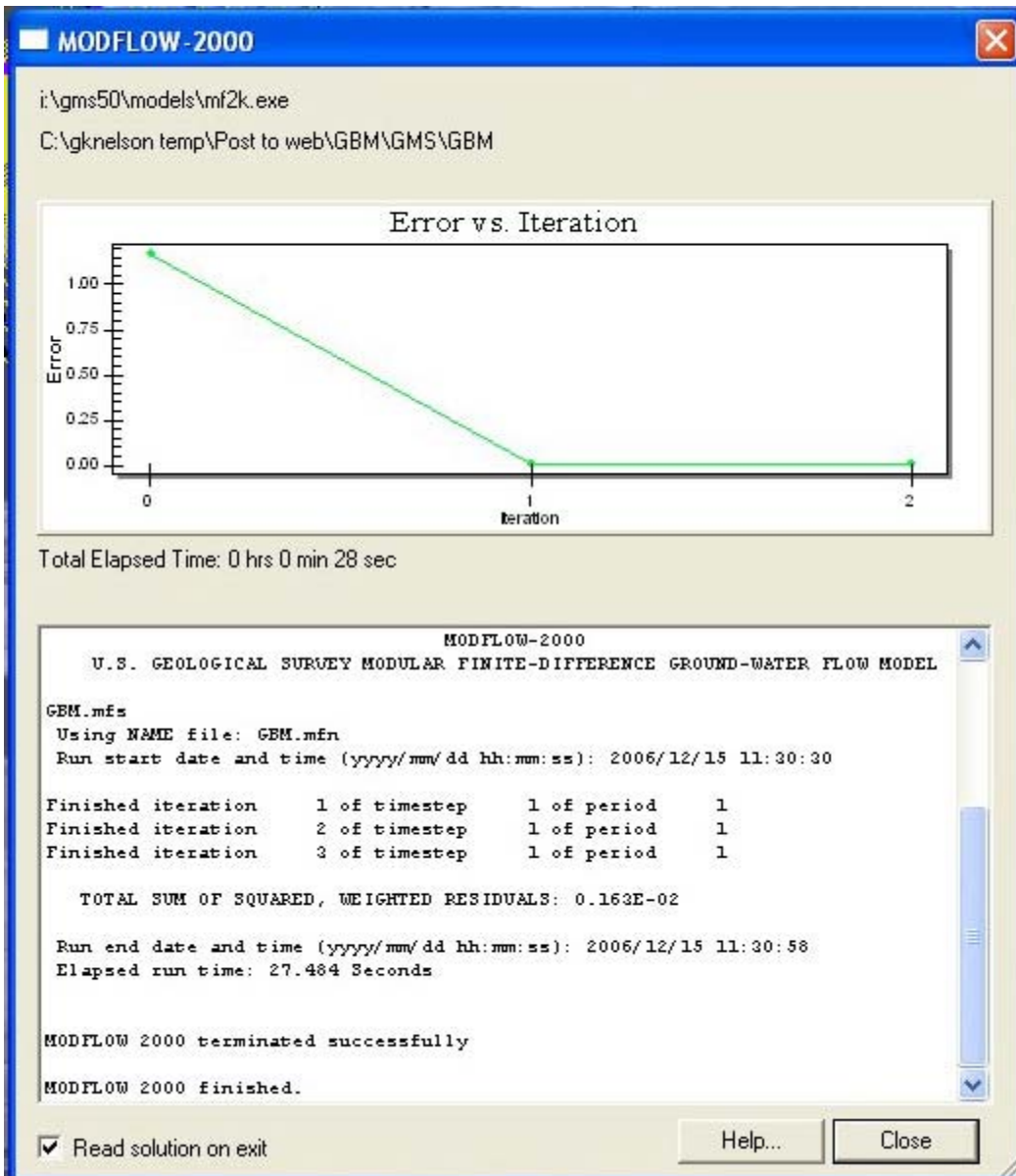


Figure 40: MODFLOW-2000 run box showing successful completion of the GBM run

Select 'Close' after successful completion to map head data to GMS.

Click 'Plot wizard'  to open the **Plot Wizard – Step 1 of 2** dialog box (Figure 41)

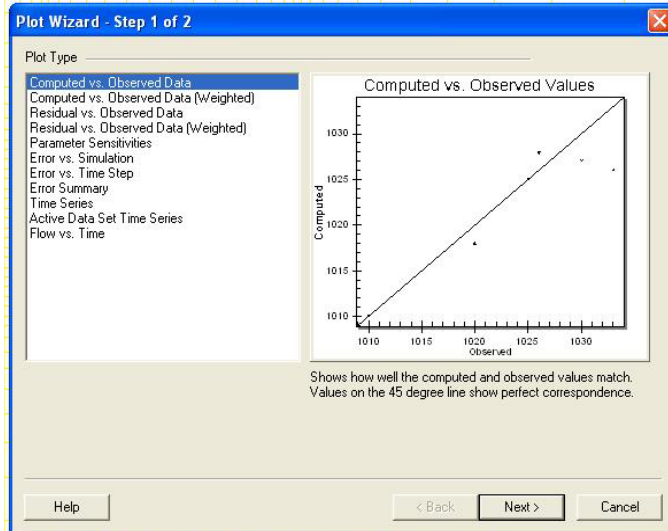


Figure 41: Plot Wizard – Step 1 of 2 dialog box

Select ‘Computed vs. Observed Data’ – Click ‘Next’ - then ‘Finish’. A plot similar to Figure 42 should be seen.

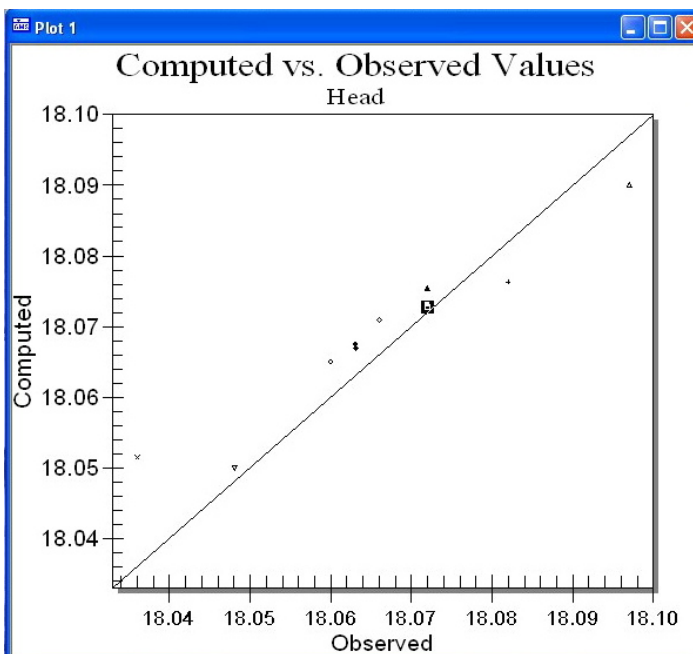


Figure 42: Plot of Computed vs. Observed Values for heads of the steady state run

NOTE:

If you are not satisfied with computed vs. observed correlation, adjust the initial head and river stages accordingly and rerun the steady state simulation.

Proceed upon successful calibration!

Section II: Transient Run

Development of Gravel Bar Model (GBM) Section II: Transient Run

The next step is to run the GBM to obtain new initial head values throughout the grid. The steady state results are read into GMS and the corresponding potentiometric surface is displayed. At this point the contours are compared to the measured head values within the wells. If they compare reasonably, the steady-state results are used as the initial head values for the transient simulation. If they do not match reasonably, the boundary conditions (CHB values and River Stage values) are adjusted and the steady state model is run again until favorable results are gained. The following time information is entered: number of stress periods, number of time steps per stress period, and the multiplier for the time steps in each stress period. The transient data are then re-mapped to MODFLOW (well, river, and CHB values). Information on the length of each stress period, the number of time steps, and the multiplier is copied straight from the 'Obs.xls' file which contains the necessary information. The simulation is then re-saved and GMS is closed.

Creating Transient Model

Click 'Map' Module

Right-click on '**GBM**' conceptual model – select '*New coverage*'.

This opens the '**Coverage Setup**' dialog box (Figure 43)

Name the coverage '**Wells**'.

Check '*Wells*' from the '*Source/Sink/BC Type*' menu.

Set '*Default layer range*' to "**1-40**"

Uncheck '*Use to define model boundary (active area)*'.

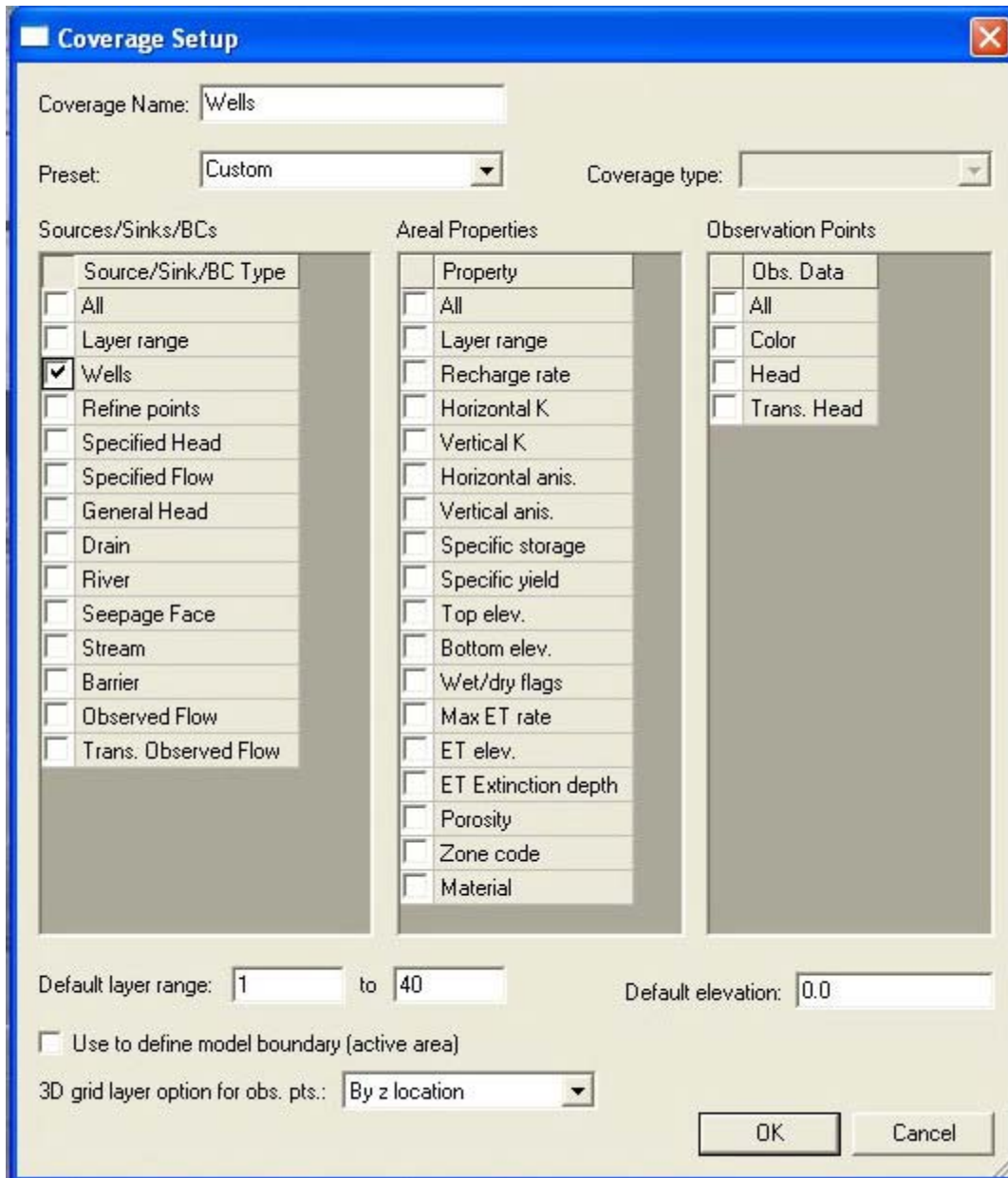


Figure 43: Coverage Setup dialog box for the Wells coverage

Creating Injection/Pumping Wells

Create 2 points using the 'Create points' tool.

Select both points using the 'Select points/nodes' tool

Click 'Properties' to open the **Properties** dialog box (Figure 44).

Check 'Show point coordinates'.

Insert values for 'Name', 'X', 'Y', from **Obs.xls** for wells B3 and B6, set 'Z' value to "20.0" (Figure 44).

Change 'Type' to "Well"

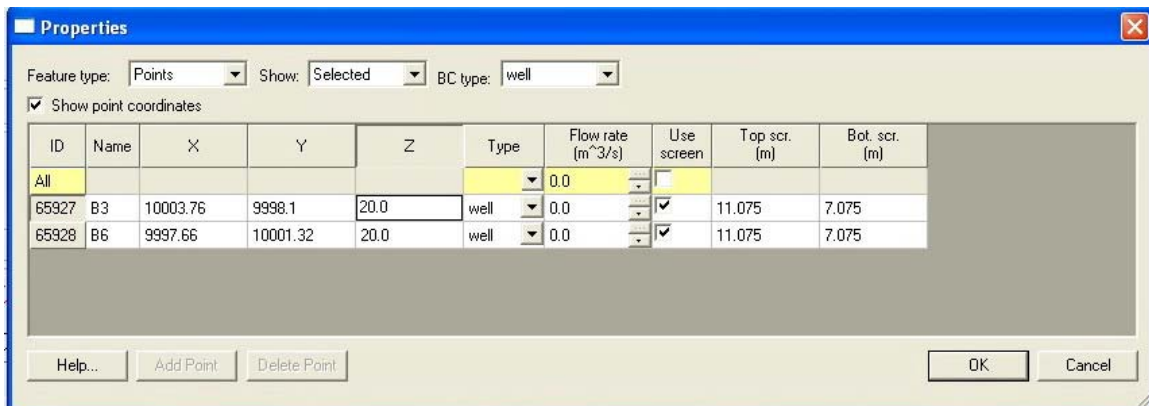


Figure 44: Properties dialog box for the injection well (B3) and pumping well (B6)

Under 'Flow rate' assign 'transient' to both wells and check 'Use screen'. Insert values for 'Top scr.' (11.075), and 'Bot scr.' (7.075) for both wells. Input the transient flow rate values for both wells from worksheets 'B3 injection' and 'B6 pumping' of OBS.xls as seen in Figure 45. Click 'OK' to exit both the XY Series Editor and Properties dialog box.

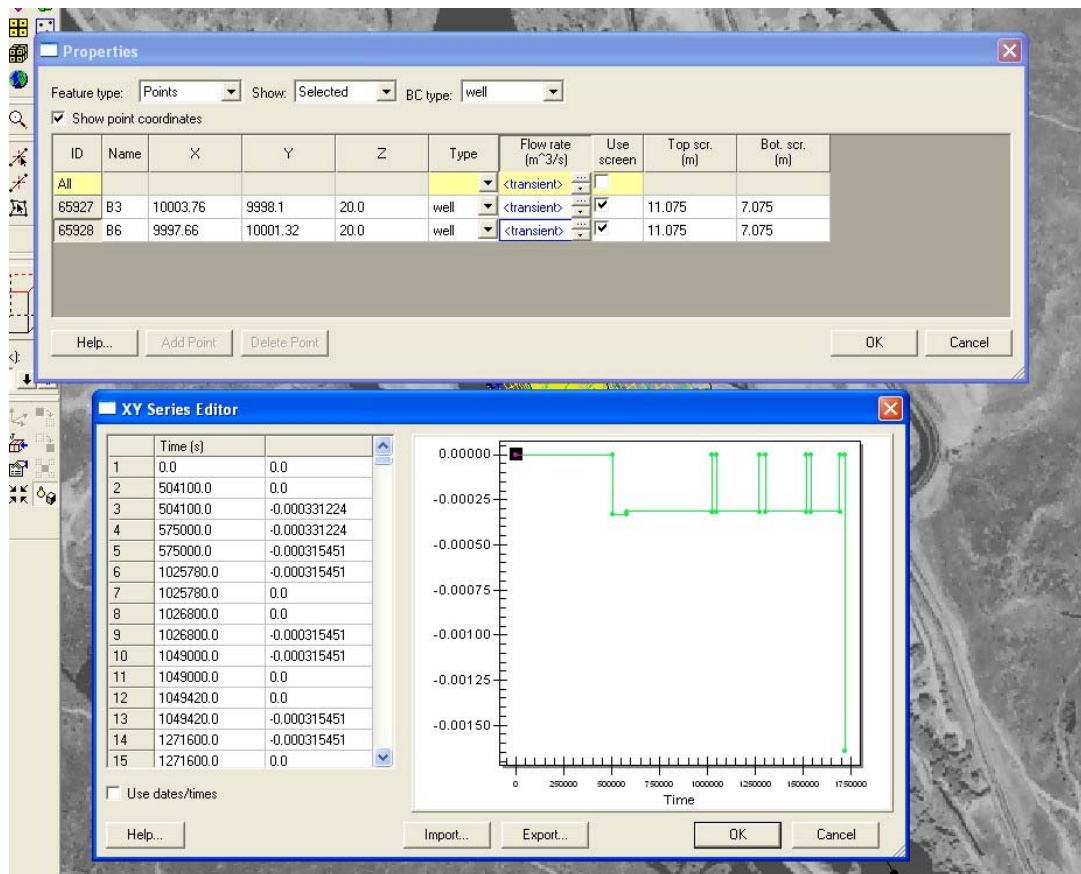


Figure 45: XY Series Editor dialog box showing transient pumping rate of well B6

Assigning Transient Time Steps

Click '3D grid' module

Select 'MODFLOW' – 'Global Options'.

Under 'Model type' check 'Transient'.

Click 'Stress Periods' to open up the 'Stress Periods' dialog box. (Figure 46)

Copy 'Length', 'Num Time Steps', and 'Multiplier' from 'Modeltime.xls' to the 'Stress Periods' dialog box.

Click 'OK' to close both boxes.

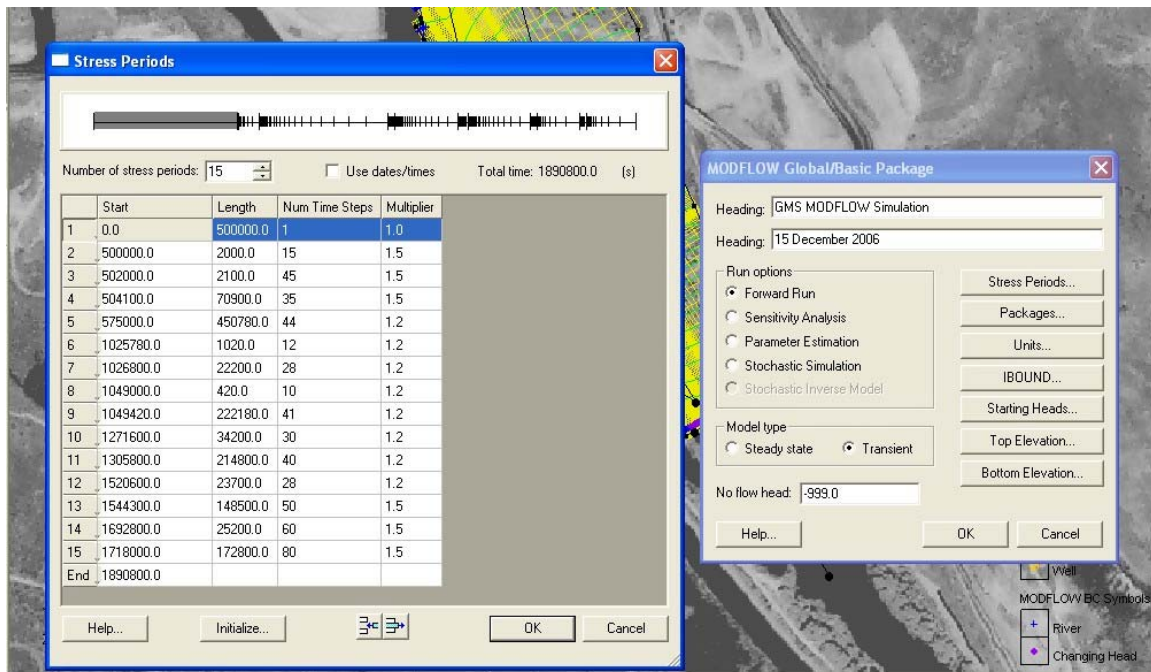


Figure 46: Stress Periods dialog box for the pumping well showing the imported values

Click 'Map' module

Select 'Feature Objects' – 'Map<->MODFLOW'.

Select 'All applicable coverages'.

*If an error message like the one in Figure 47 appears, click 'OK'



Figure 47: Error message 1: Error message associated with assigning stress periods to the model

Click '3D grid' module

Select 'MODFLOW' – 'Output Control' to open the 'Output Control' dialog box.

Select only the following options and unselect any others (Figure 48):

-Output at every time step

-Save heads to *.hed file

-Global output file

-List output file

-Enable saving of computed flows for all source/sink objects.

Click 'OK'.

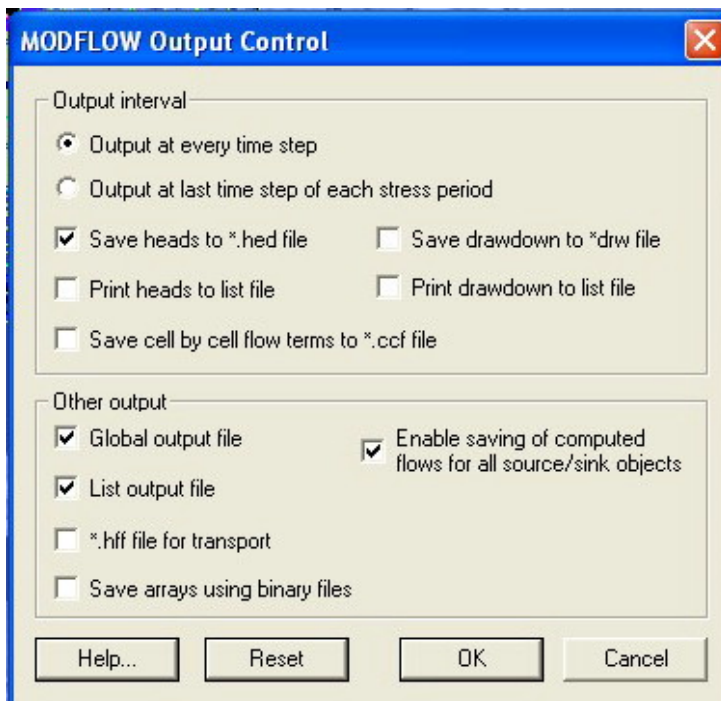


Figure 48: MODFLOW Output Control dialog box with the appropriate options selected

Save the project.

If the following error message appears (Figure 49), click 'OK'

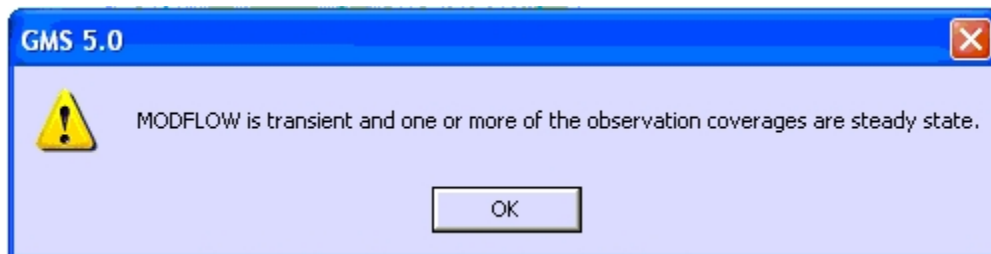
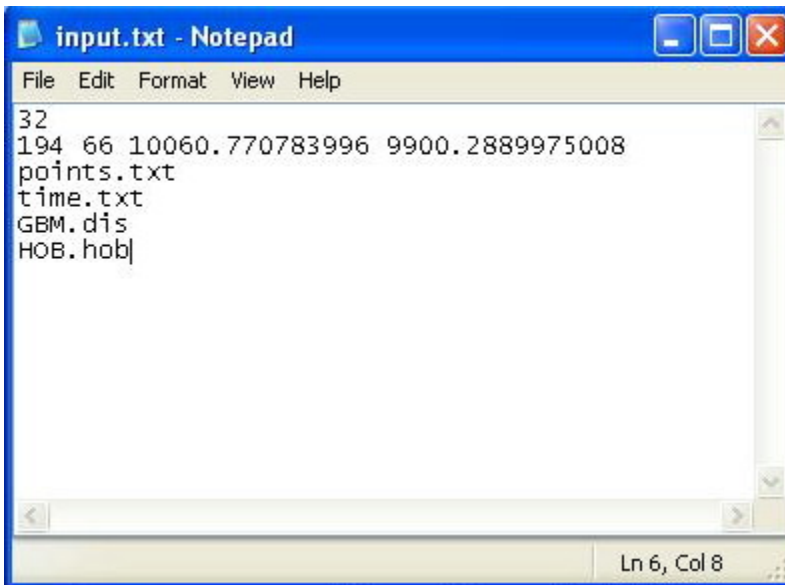


Figure 49: Error Message 2: GMS error message

Close GMS.

Creating the .hob and .obs Files

Both the HOB and the OBS files should be created outside of GMS. The HOB and OBS files are created to allow for direct head measurements to be extracted at specific locations (as opposed to the center of the cell). The OBS file can be created in any text editor, following MODFLOW 2000 instructions, to output a *.*_os* file upon completion of the model run. The HOB file can be created using the '**createHOB.m**' MATLAB script. This script uses an 'input.txt' file which gives instructions on: angle or grid orientation, center grid cell dimensions, time steps, points (locations where heads will be returned), the *.*dis* file from the model, and the name of the file to be produced. Another MATLAB script '**ReadDis.m**' outputs values for the points at times specified. Below is an example of the 'input.txt' file (Figure 50). The points file can be adjusted to include, change, or extrude points as appropriate. Examples of the 'input.txt', 'points.txt' and 'time.txt' files are located on the CD and can be adjusted for each use, although 'points' must fall within the SM boundary and 'times' must match the time steps of the model. For instructions on using this script open MATLAB and set the current directory to the directory containing '**createHOB.m**' and type "**help createHOB**" at the MATLAB command prompt. It will list a set of instructions for the file. For completeness they are also listed in Box 1:



```
input.txt - Notepad
File Edit Format View Help
32
194 66 10060.770783996 9900.2889975008
points.txt
time.txt
GBM.dis
HOB.hob
Ln 6, Col 8
```

Figure 50: Example of the 'input.txt' file used for 'createHOB.m' script

ReadDis.m

ReadDis is a function that reads in the MODFLOW discretization file and returns the X locations of the grid, the column widths, the Y locations of the grid, the row widths, the elevations of the grid cell centers (allowed to vary from cell to cell), the top and bottom layer elevations (also allowed to vary from cell to cell), and the stress period information (T).

This function reads in an input file. If the name of the input file is not passed to the file, the default name of 'input.txt' is used. The input file has six lines to it. (1) lists the angle from east to the grid rows (increasing j). (2) has 4 values listing the i and j values of grid cell center, and the Easting and Northing coordinates of the same cell center. (3) lists the name of the points file which has 1 header row, and 5 columns of data - HOBID, Easting, Northing, Top of screened elevation, and bottom of screened elevation. (4) Lists the name of the observation time file which has one header row and then one column of data containing the times at which you want head observations; these times should be in the same units as those of the MODFLOW simulation and should be time since the beginning of stress period 1. (5) Lists the name of the MODFLOW discretization file; the discretization file must have exactly 4 header lines; the Top and BOTM arrays must be either constant or internal.

Box 1: Help instructions for the **createHOB.m** MATLAB file.

NOTE:

It is important to note at this point that the purpose of development of this larger Gravel Bar Model is to generate head values that will be used in the smaller flow and transport model as head inputs for General Head Boundaries and Constant Head Boundaries. If the user does not know where they wish to have these head values located, they are advised to skip to the beginning of the “Development of the 2nd Model: Flow and Transport Model” section and work through until they know where they would like to have heads saved. At that point, the user can return to this point and proceed. The desired locations can be entered as points in the point file for 'createHOB.m'; 'createHOB.m' and an example of the HOB.hob and OBS.obs files are on the CD.

Running 'createHOB.m' MATLAB Script

Open MATLAB

Type “**createHOB('input.txt')**” on MATLAB command line; ‘**input.txt**’ refers to the input file for the model being run. The script will run and a .hob file will be created along with a .jpg image showing the location of the points (Figure 51).

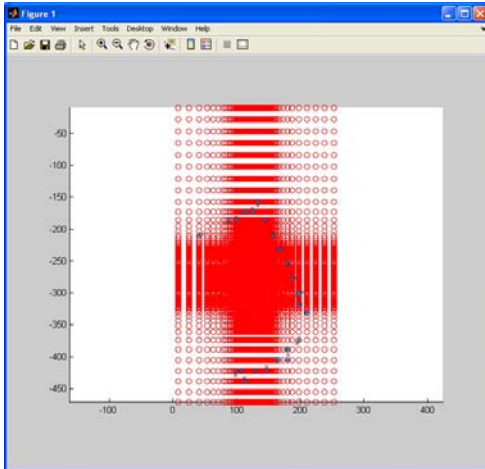


Figure 51: Figure produced by createHOB.m script showing the locations of the points

Once the .hob and .obs files are created, they are saved to a common directory where the GBM model will be run.

Running MF2K

Running MODFLOW 2000 outside of GMS

Copy the necessary MODFLOW files to the common directory ('run directory') from the directory where the GMS files were saved.

Below are the file extensions of all of the file types to copy to the run directory.

.ba6
.chd
.dis
.lpf
.mfn
.oc
.riv
.wel
.pcg or .gmg (depending on which solver is used)
.hob*
.obs*

* hob and obs files are files created outside of GMS as described above.

Copy **MF2K.exe** program (located on the CD) into run directory.

Editing the MODFLOW Name File

The MODFLOW name file created by GMS needs to be modified for it to be used outside of the GMS user interface. Therefore there are certain formatting and name changes that must be done so that the same name file can be run exclusively by MF2K.exe.

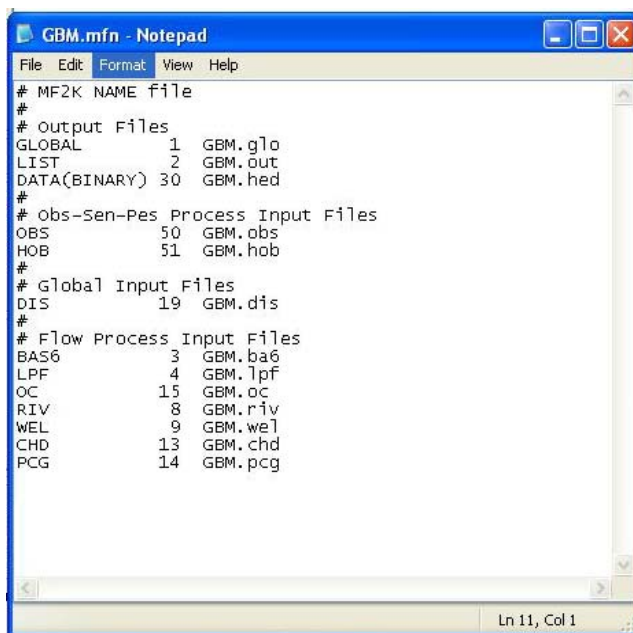
From the **run directory** open '**GBM.mfn**' in text editor

Remove all double quotes (“

Change *.hob and *.obs file names to the names of the files the user created (likely from createHOB.m, for simplicity they can be named “GBM”).

Remove '**RVOB**', '**CHOB**' and '**ASP**' lines from **GBM.mfn** (Figure 52)

Save and Close **GBM.mfn**.



```
# MF2K NAME file
#
# output Files
GLOBAL      1  GBM.glo
LIST        2  GBM.out
DATA(BINARY) 30 GBM.hed
#
# Obs-Sen-Pes Process Input Files
OBS         50  GBM.obs
HOB         51  GBM.hob
#
# Global Input Files
DIS         19  GBM.dis
#
# Flow Process Input Files
BAS6        3  GBM.ba6
LPF         4  GBM.lpf
OC          15  GBM.oc
RIV         8  GBM.riv
WEL         9  GBM.wel
CHD        13  GBM.chd
PCG        14  GBM.pcg
```

Figure 52: Modified GBM.mfn file after removal of double quotes (“) and RVOB, CHOB, and ASP lines

Running MODFLOW

Open '**MF2K.exe**' from the run directory. This opens up a DOS shell where the user is prompted for the name file: “**GBM.mfn**” (Figure 53).

```

c:\ H:\BHR5\Test 2 3-26\Run\mf2k.exe
                                MODFLOW-2000
U.S. GEOLOGICAL SURVEY MODULAR FINITE-DIFFERENCE GROUND-WATER FLOW MODEL
                                Version 1.17.02 02/14/2007

Enter the name of the NAME FILE:
GBM.mfn
Using NAME file: GBM.mfn

Run start date and time (yyyy/mm/dd hh:mm:ss): 2007/03/26 15:23:26

```

Figure 53: MF2K.exe DOS shell screen showing 'NAME' file supplied

Upon completion, MODFLOW 2000 will output a `*._os` file which contains head data at the points specified by the HOB.hob file.

Output File Information

MATLAB

The `._os` output file contains head values that will be used in the smaller flow and transport models as general head boundaries and constant head boundaries. If 'createHOB.m' was used to create the HOB file, then the MATLAB script 'readheadobs.m' can be used to organize the data. To run this script the `._os` and the 'points.txt' file from 'createHOB.m' are copied to the common directory along with 'readheadobs.m' and the files are called for at the MATLAB command line:

```
readheadobs('._os file, points file')
```

NOTE:

The readheadobs.m MATLAB script calls for the `._os` file having the name "GBM._os." If the original model was saved as "GBM", there will not be a problem. If not, rename the outputted `._os` file to "GBM._os."

The script simply reads in the head values and for each observation point saves the times and calculated head values to an output file in two columns – i.e. there are two columns in the file for each observation point: (1) time; and (2) head. For completeness the instructions for the file are listed in Box 2.

This function reads in the '_os' MODFLOW file and creates a file with one line of header. It needs the points file from 'createHOB.m' and uses this to name the points. The output file has two columns for every point - one for the time and one for the calculated head. The default heads file name is GBM._os. The function takes two input files: the first is the name of the _os file and the second is the points file used in createHOB.m.

Box 2: *Help instructions for the **readheadobs.m** MATLAB script.*

Once the head.obs file is created by **readheadobs.m** the information can be copied into an Excel spreadsheet and organized to be used later.

III: Development of 2nd Model: Flow and Transport Model

This second model is developed as a smaller model to decrease computational time while still encompassing the entire volume of the tracer plume. This ‘flow and transport’ model uses head data acquired from running **GBM** and produced by ‘**readheadobs.m**’. This model will be incorporated into SEAWAT 2000 which will be set up to model the transport of the bromide tracer during the TTLT.

Steps

1. Develop Model Boundaries and Grid
2. Run the PREPROC.m MATLAB script to create needed SEAWAT 2000 input files.
3. Write remaining files using a text editor

Flow and Transport Model

Start GMS

Open ‘**GBM.gpr**’

Save as ‘**SM.gpr**’

**This allows for the information from the GBM model to be used in developing the flow and transport model without duplicating each step.*

If the error message seen in Figure 49 appears, click ‘OK’

Creating a New Grid

Click ‘3D Map’ module

Click ‘Grid’ – ‘Create Grid’ to open the ‘**Create Finite Difference Grid**’ dialog box.

Click ‘OK’ to the two messages regarding creating a new grid.

Input grid values for *X-Dimension origin, X-Dimension Length, X-Dimension Number cells, Y-Dimension Origin, Y-Dimension Length, Y-Dimension Number cells, Z-Dimension Length, Z-Dimension Number Cells, and Rotate about Z-axis* as seen in Figure 54



Figure 54: Create Finite Difference Grid dialog box showing appropriate values for the flow and transport model

Click 'OK'

Figure 55 shows the initial grid location of the smaller flow and transport model.

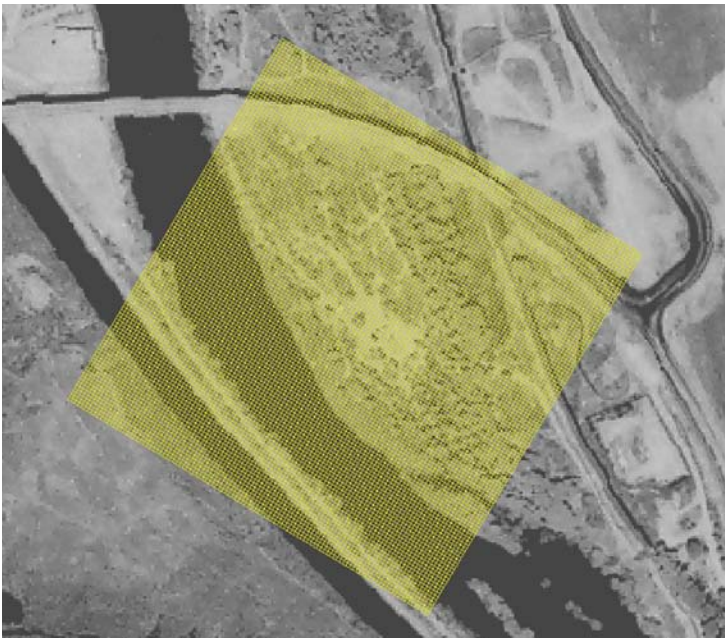


Figure 55: Initial grid location of the smaller flow and transport model

Save **SM.dis** and Close both files.

Re-open GMS.

Open '**SM.gpr**'

The grid similar to Figure 57 should appear.



Figure 57: SM model grid showing the new discretized grid

Constructing the Conceptual Model

Click '*Map*' module

Right-click '*Map Data*' – select '*New conceptual model*' to open the *New Conceptual Model* dialog box.

Name the model "**SM**"

Click '*OK*'

Creating Boundary Coverage

Right-click '**SM**' – select '*New Coverage*' – name "**Boundaries**"

Check 'Use to define model boundary (active area)' and set 'Default layer range' to "1-40" (Figure 58).

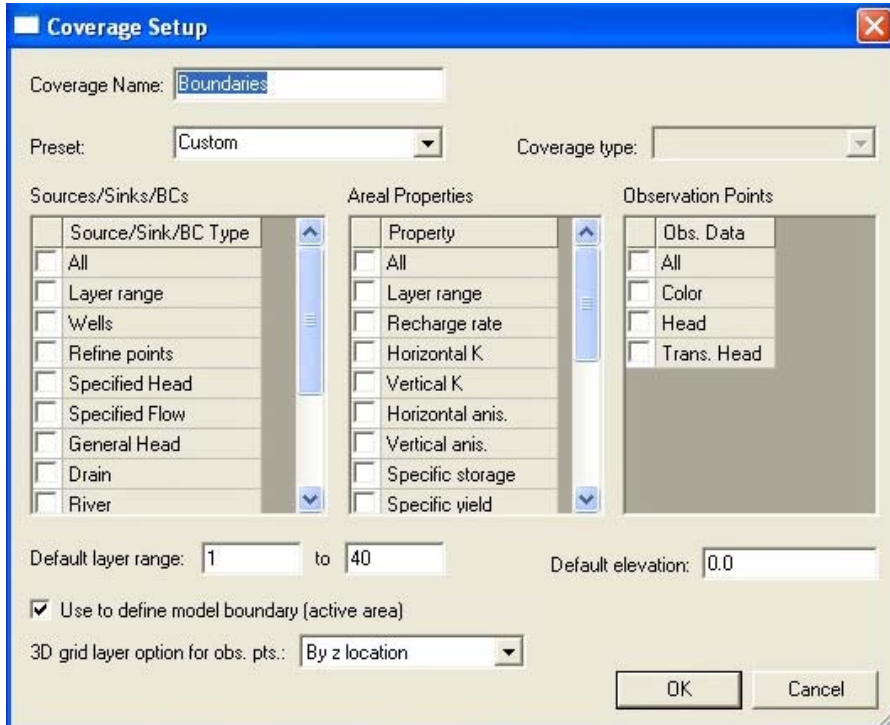


Figure 58: Coverage Setup dialog box for the Boundaries coverage

Drawing in Model Boundaries

Click 'Create arc' tool.

Create arcs around the modeling domain boundary similar to those seen in Figure 59.

NOTE:

When constructing the SM Boundaries coverage, it must be made large enough to incorporate the points set up in the 'createHOB.m' script.



Figure 59: Boundaries arcs for the SM conceptual model (the slight indentation in the northeast corner corresponds to the road leading down to the site, which is higher elevation)

Click 'Feature Objects' – 'Build polygons'

Creating River Coverage

Copy the '**River**' coverage from the **GBM** conceptual model to the **SM** conceptual model. This should be done by *right-clicking* on the '**River**' coverage and selecting '*Duplicate*' then dragging the '**Copy of River**' down to the **SM** model. Click 'OK' to the error message (Figure 60)

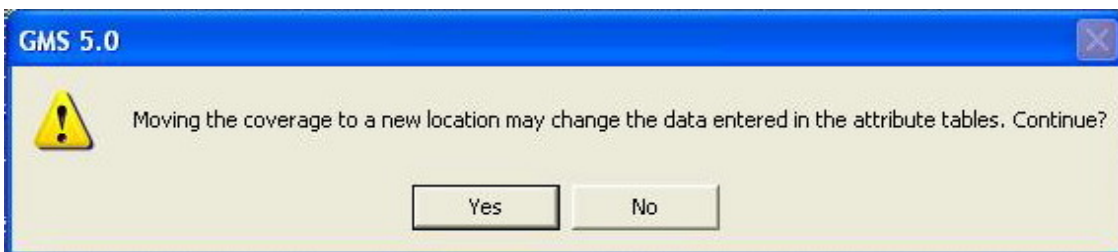


Figure 60: Error message 3: Message associated with moving the River coverage to the SM conceptual model

Figure 61 shows the SM conceptual model with the River coverage copied from the GBM model.



Figure 61: SM conceptual model showing the River coverage which was copied from the GBM model

Creating the GHB coverage

Right-click 'SM' conceptual model – select 'New coverage' to open the '**Coverage Setup**' dialog box (Figure 62). Name the coverage "**GHB**"
Check 'General Head' from 'Source/Sink/BC Type'
Set the 'Default layer range' to "**1-40**"
Uncheck 'Use to define model boundary (active area)'
Click 'OK'.

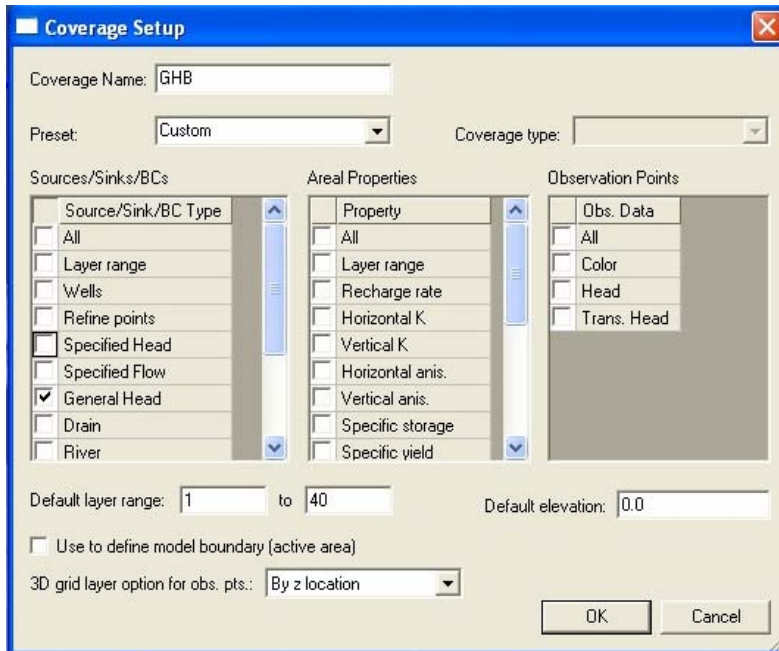


Figure 62: Coverage Setup dialog box for the GHB coverage

The GHB arcs (Figure 63) will be associated with the head values output from the transient GBM model and are defined by the points.txt file supplied to **createHOB.m**. Therefore, the arcs created for both the **GHB** coverage and the **CHB** (described later) should connect the points used.

Click 'Create points' tool

Create the same number of points as were identified in the **points.txt** file, which will be used as general head points.

Click 'select points/nodes' tool

Select the newly created points and assign X-Y data from the **points.txt** file using the "properties" button.

Click 'Create arcs' tool

Create arcs connecting these points to be used for the GHB coverage

Click 'Select arcs' tool.

Select only the arcs that will define the general head boundary (Figure 63).

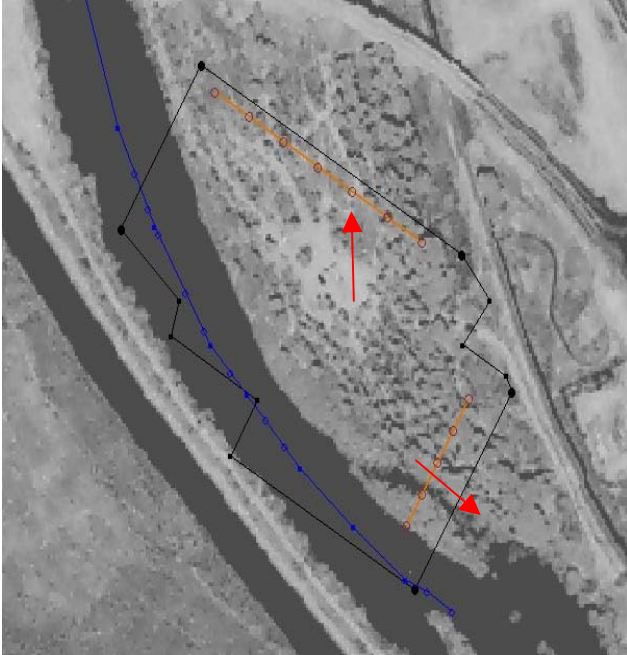


Figure 63: General Head arcs of the SM conceptual model

Click 'Properties' to open the **Properties** dialog box (Figure 64).

Change all 'Type' to 'general head'

Assign conductance as determined by where the observation points are located in relation to cell centers. For simplicity a value associated with the average conductivity of the GBM was used (L2-L40 coverage) (Figure 64).

Click 'OK' to exit the **Properties** dialog box.

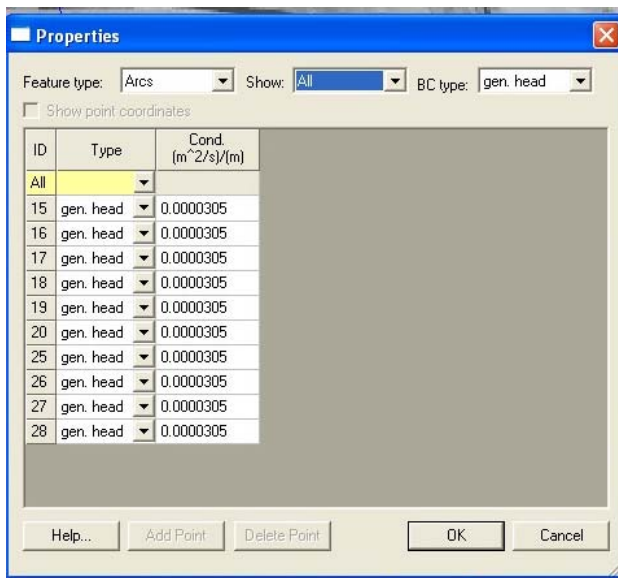


Figure 64: Properties dialog box for the general head arcs showing the conductance values

Click 'Select nodes' tool.

Select the general head nodes – click 'Properties' to open the **Properties** dialog box.

Assign 'Head Stage' as 'transient'

Input appropriate values (Time and Head) from file created by **readheadobs.m** (Figure 65).

Click 'OK' to exit the dialog boxes.

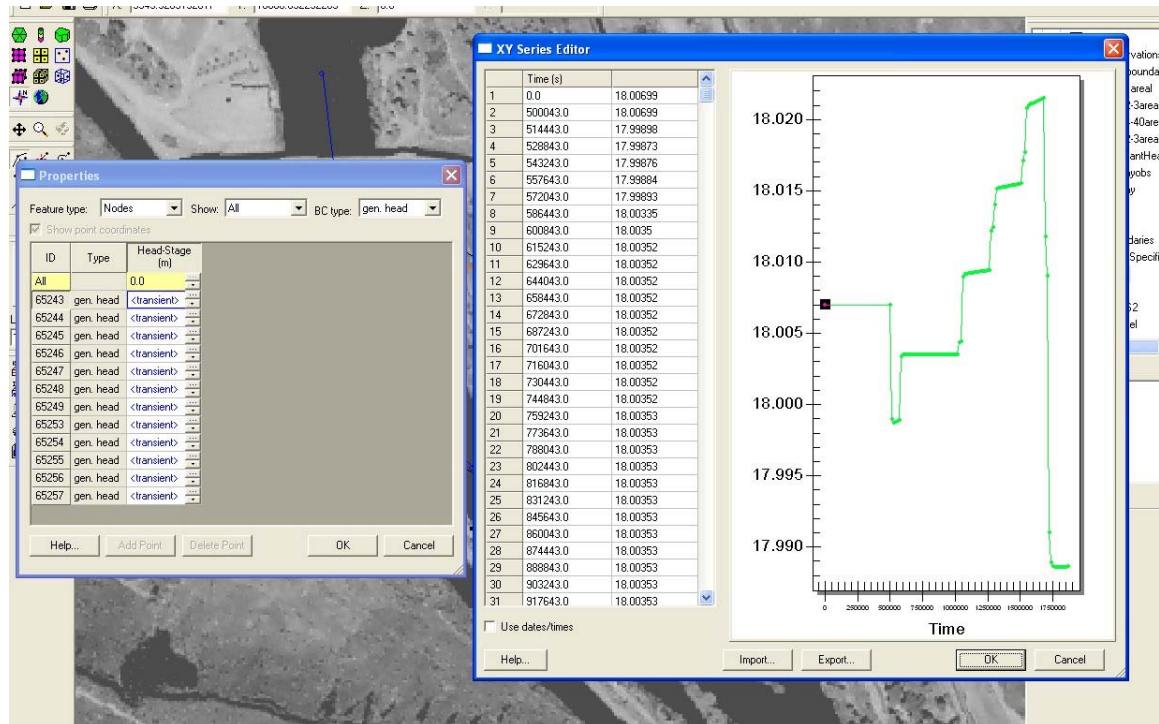


Figure 65: XY Series Editor dialog box for the GHB head stage values imported from the heads.obs file created by 'readheadobs.m'

Creating the CHB coverage

Right-click 'SM' conceptual model – select 'New coverage' to open the **Coverage Setup** dialog box.

Name the coverage "CHB".

Under 'Sources/Sink/BC Type' check 'specified head'

Set 'Default layer range' to "1-40".

Uncheck 'Use to define model boundary (active area)'. (Figure 66)

Click 'OK'.

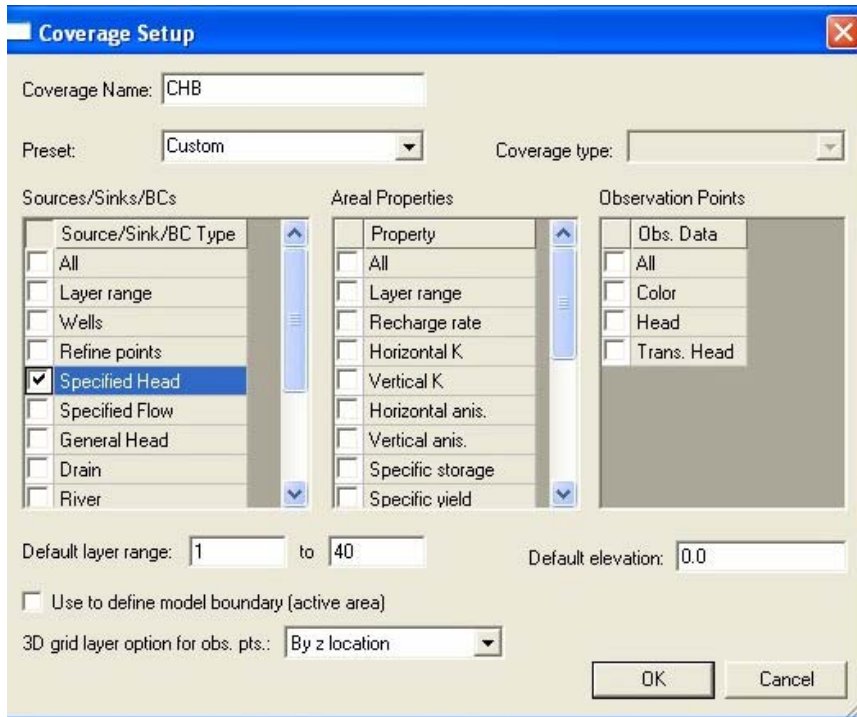


Figure 66: Coverage Setup dialog box for the CHB coverage

This coverage is also set up to use the values produced by **createHOB.m** and so should be set up in the same manner as the **GHB** coverage.

Click 'Create points' tool

Create the same number of points as were identified in the **points.txt** file as constant head points (Figure 67).

Click 'select points/nodes' tool

Select the newly created points and assign X-Y data from the **points.txt** file.

Click 'Create arcs' tool

Create arcs connecting these points to be used for the CHB coverage (Figure 67)

Click 'Select arcs' tool.

Select all of the arcs that will define the constant head boundary (Figure 67)

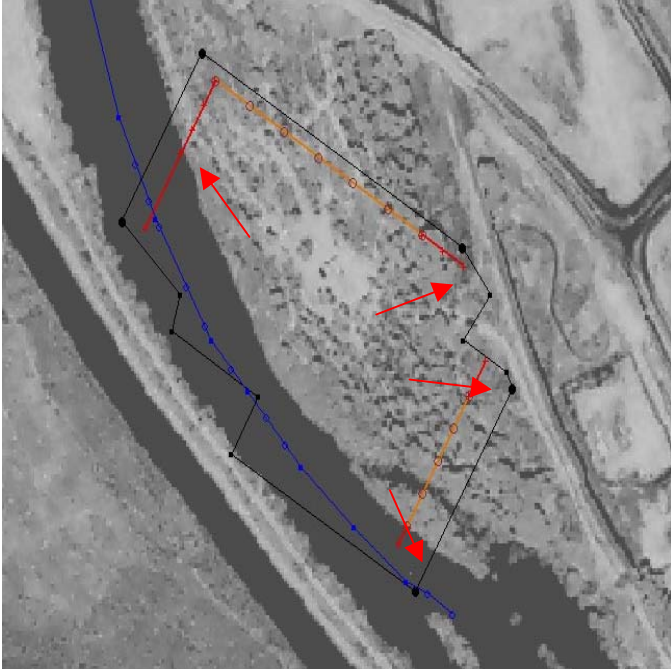


Figure 67: Location of specified head arcs of the CHB coverage

Click 'Properties' to open the **Properties** dialog box (Figure 68)
 Change all 'Type' to 'specified head'
 Click 'OK' to exit the **Properties** dialog box.
 Click 'OK'.

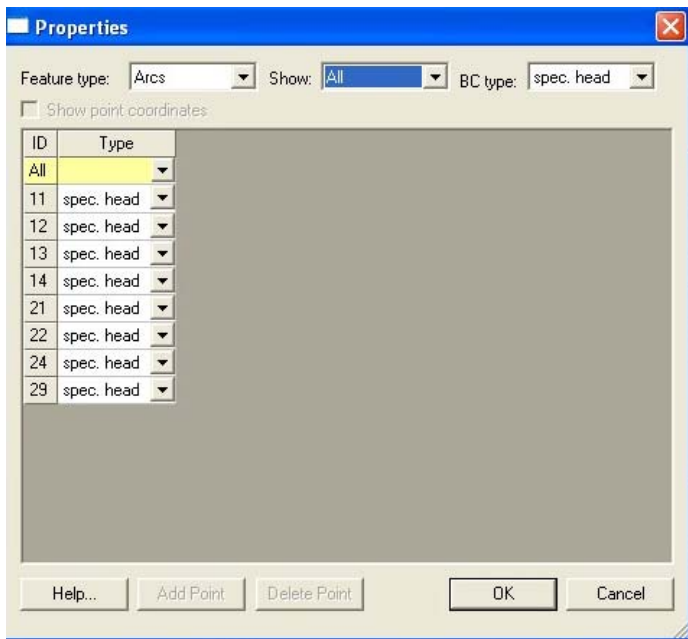


Figure 68: Properties dialog box of the CHB arcs

Click 'Select nodes' tool.

Select all specified head nodes – click 'Properties'.

In the **Properties** dialog box, assign 'Head Stage' as 'transient' (Figure 69).

Input values for appropriate cells from **head.obs** file created by **readheadobs.m**.

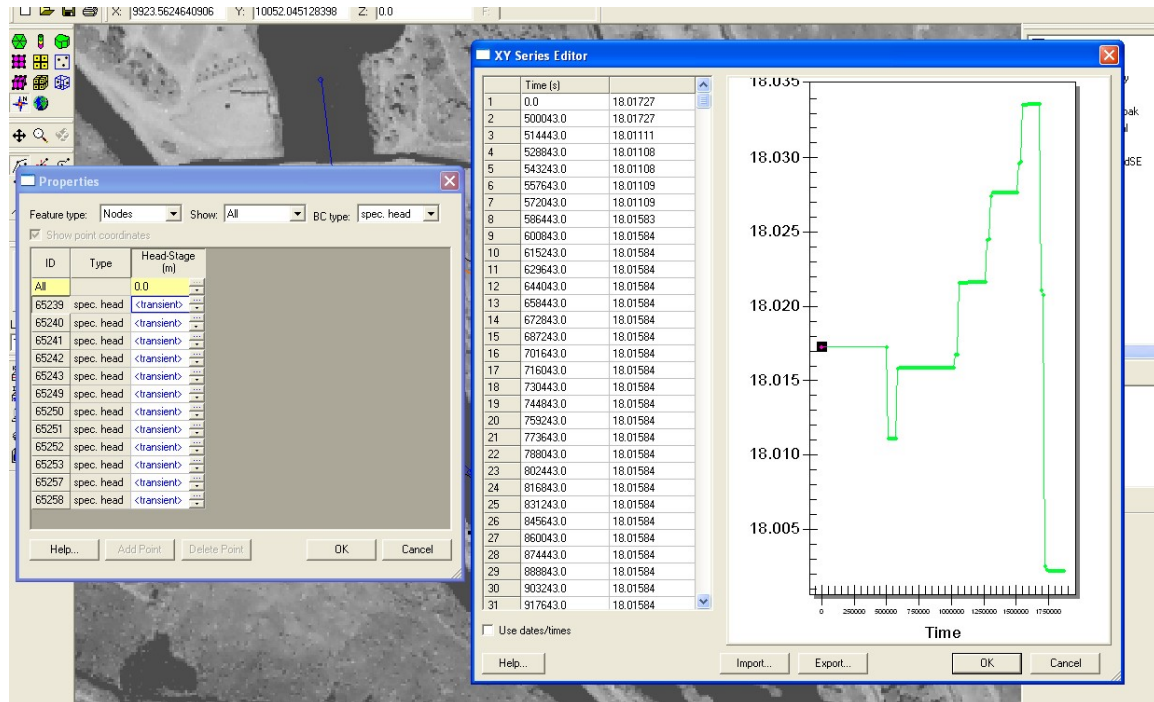


Figure 69: XY Series Editor for the specified head arcs of CHB coverage showing transient data input

Click 'OK' to close both dialog boxes

Assigning Coverage Properties to MODFLOW

NOTE:

Make sure that only the coverages of the **SM** conceptual model are visible by checking all coverages under **SM** conceptual model and un-checking all under **GBM** conceptual model.

Select the **SM - boundaries** coverage – making it the active coverage

Select 'Feature objects' – 'Activate cells in coverage'. This will activate only the cells encompassed by **boundaries** (Figure 70).

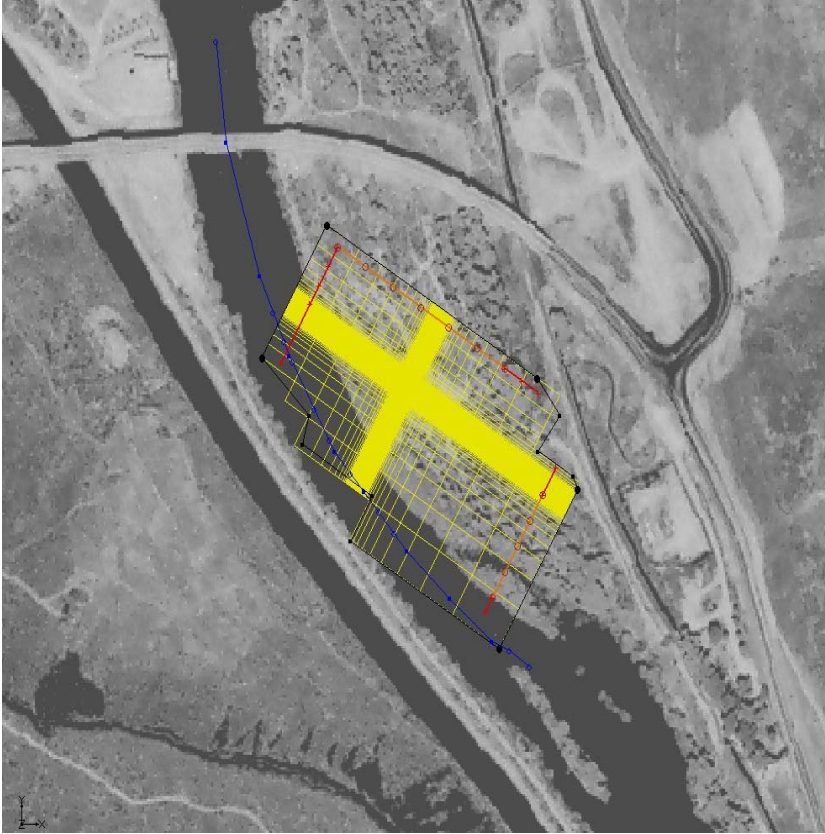


Figure 70: SM model with only those cells within the boundaries activated

Identify inactive cell indices for future use in PREPROC.m MATLAB script. Inactive cells are those whose IBOUND values are zero. The IBOUND array can be opened from the 3D Grid module – MODFLOW – Global Options and clicking the IBOUND button.

Assigning MODFLOW Stress Periods

Click '3D grid' module

Select 'MODFLOW' – 'Global Options'

Click '**transient**'

Click 'Stress Periods' to open the **Stress Periods** dialog box.

Input values for stress periods from '**modeltime.xls**' as seen in Figures 71 and 72.

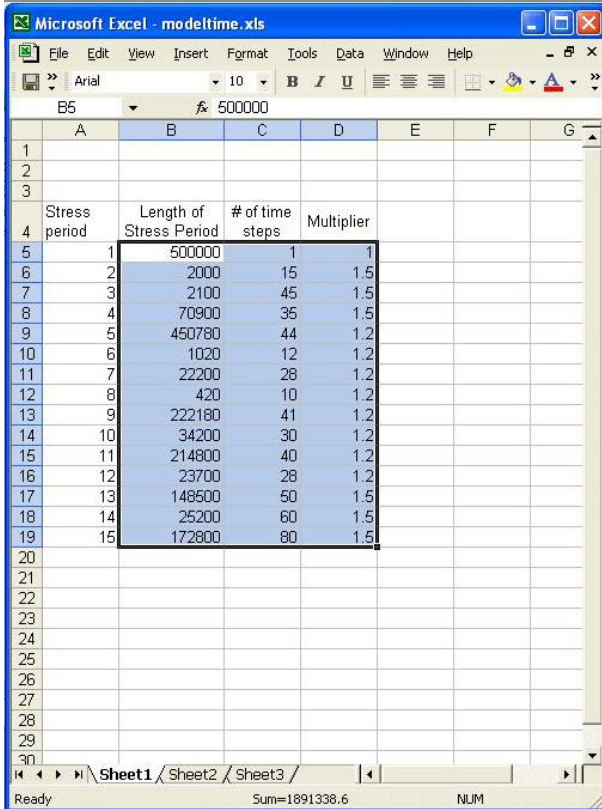


Figure 71: modeltime.xls file showing stress period values to be assigned to the SM model

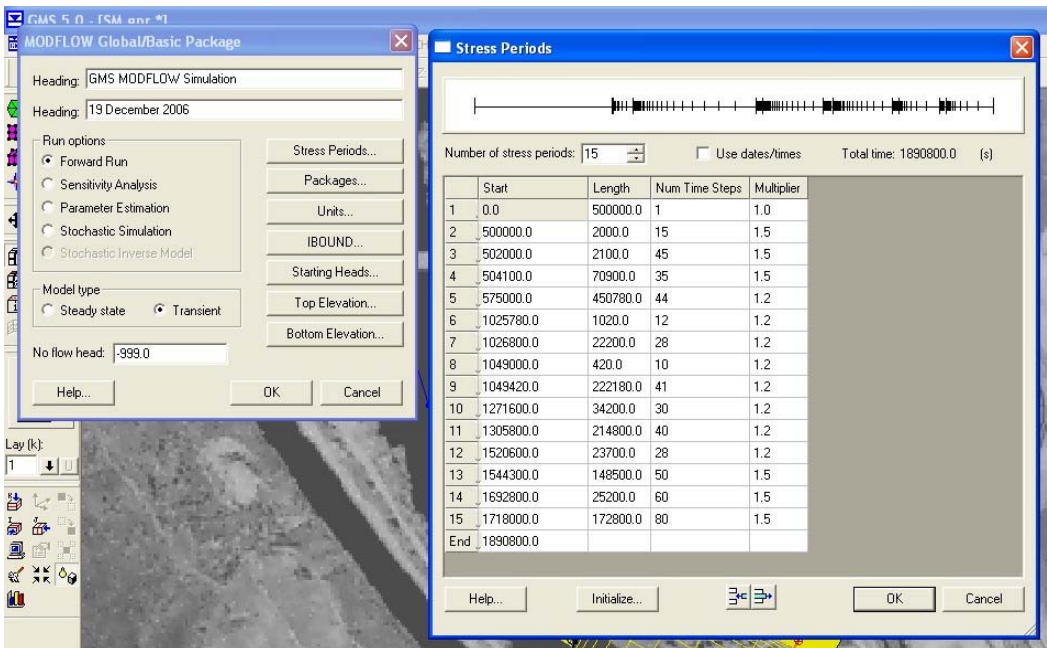


Figure 72: Stress Periods dialog box for the SM MODFLOW simulation

Click 'OK' to close both dialog boxes.

Click 'Map' module.

*Make sure all SM coverages are visible

Click 'Feature objects' – 'Map to MODFLOW'

Select 'All visible coverages' from the **Map -> Model** dialog box (Figure 73)

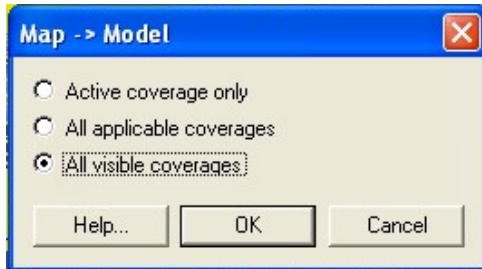


Figure 73: Map -> Model options for the SM model

Click 'OK'.

Cells should now be assigned as in Figure 74



Figure 74: Results of executing the Map -> MODFLOW command for the SM model

NOTE:

If **Error Message 1** (Figure 47) appears, **Save** the project.

If **Error Message 2** (Figure 49) appears, click 'OK'

Exit GMS

Copy the **.chd**, **.dis**, **.ghb**, **.riv** files into the run directory (the directory that will hold all of the input files for a given flow and transport model).

IV: Preprocessing

PREPROC.m MATLAB Script.

The MATLAB PREPROC.m script was developed to facilitate the creation of many of the MODFLOW 2000, MT3DMS, and SEAWAT 2000 input files that would be difficult or time consuming to create in GMS or in a text editor. The script takes an input file that contains flags and names of other input files needed to create the model input files. The reader is referred to the documentation of the PREPROC (**'preproc documentation.pdf'**) (on the CD) for more information on using this script. Most of the examples provided can be used for this model, and changes can be made at the user's discretion.

Running PREPROC.m

This is done by making the MATLAB path directory the directory containing PREPROC.m and all of the needed script input files (listed below) and typing 'PREPROC' at the MATLAB command prompt.

PREPROC.m can create the following files:

.ba6	basic flow file
.btn	basic transport file
.tob	transport observation file
.lpf or .huf	flow file
.wel	well file
.hbf	horizontal barrier flow file

SPLICE3D.m

SPLICE3D.m is another MATLAB script developed to splice together output from a set of realizations of GSLIB's SGSIM (Sequential Gaussian Simulation) program. Again the reader is referred to the documentation of the script (**'Splice3d.m documentation vs. 2.0 12-13-06.pdf'**, included on the CD) for instructions on its use. The output from this script can be directly input into PREPROC.m.

V: Final Model Development

The last stage in model development incorporates additions needed for running in SEAWAT 2000. This step includes production of the files associated with MT3DMS for transport. Development of the files for use in this model is primarily done using a text editor and following the directions in either the MT3DMS manual or the SEAWAT 2000 manual.

Creating Input Files

In a text editor or spreadsheet editor, create the following files according to MODFLOW 2000, MT3DMS, or SEAWAT 2000 input instructions:

.vdf	variable density flow file (SEAWAT 2000)
.swn	SEAWAT name file (SEAWAT 2000)
.ssm	source/sink mixing package file (MT3DMS)
.dsp	dispersion package file (MT3DMS)
.adv	advection package file (MT3DMS)
.gmg or .pcg	flow solver package file (MODFLOW 2000) *The authors suggest the GMG solver because it is more likely to converge.
.gcf	conjugate gradient transport solver package file (MT3DMS)
.oc	output control file (MODFLOW 2000) – you can create this file in GMS and edit for transport steps that you want saved.

Creating the Extract.in File

This file is used by Tom Clemo's **Extract** program (see Box 3 and CD). This file lists cell indices for which head values will be extracted from the binary head file created by MODFLOW.

Extract file has 10 lines:

1	Comment: must begin with #
2	Kind of data: must be 1
3	MODFLOW head file
4	Binary file: options are .false. (not a binary file), .true. (binary file)
5	Number of records: number of times heads are saved to MODFLOW head file.
6	Number of layers in MODFLOW model
7	Kind of output: must be 1
8	Output file name
9	Number of cells that you want head data from (0 yields all)
10	Layer, row, column: this row is repeated for each cell listed on line 9

*Box 3: Example of line commands for **Extract.in** file*

Running the Model on the Beowulf Cluster in the Computer Science Department at Boise State University

The input files will need to be copied to your account on the cluster. Make sure that the files are all formatted for 'Unix'.

Creating the Swarm Command File:

NOTE:

*'#' sign denotes comment line anywhere in the file
Each line should be a PBS command*

Due to file size constraints on personal hard drive space on the Computer Science Department cluster, files should be copied to a Temp directory on the Beowulf cluster and the simulation should be run from the Temp directory.

After the simulation is run, the Extract program needs to be run from the Temp directory, and then output files can be copied to your personal directory. All of this is done through the 'swarm' script (Box 4), an example of which is on the CD.

Below is an example of a swarm 'run' file.

```
# copy input files to the temp directory
cp -r /home/gknelson/seawat/Variable_density/MODELS/DK /tmp
cp /home/gknelson/seawat/Variable_density/MODELS/CommonFiles/* /tmp/DK/
# change directory to the temp directory
cd /tmp/DK/

# run seawat
swt2k /tmp/DK/SWT.nam

# run extract
extract
# copy output files to destination directory.
cp /tmp/DK/Cwells /home/gknelson/seawat/Variable_density/MODELS/DK/CwellDK;
cp /tmp/DK/Concobs.ocn
    /home/gknelson/seawat/Variable_density/MODELS/DK/ConcDK.ocn;
cp /tmp/DK/Concobs.mfx
    /home/gknelson/seawat/Variable_density/MODELS/DK/ConcDK.mfx;
```

Box 4: Example of a swarm 'run' file for the Beowulf Cluster

Due to large memory requirements and long run times, several swarm command options are utilized. An example command line run is shown below (Box 5).

```
swarm -f run -b 8 -n 1 -l walltime=500:00:00
```

Description:

-f run	swarm file option
-b 8	8 commands will be run from each node
-n 1	one processor per node will be used
-l walltime=500:00:00	500 hours will be allotted to run the simulation

Box 5: Example of the 'run' command for starting the model on the Beowulf Cluster

Run Seawat2000 through swarm (Figure 75).

```
gknelson@beowulf:~  
Connection to beowulf.boisestate.edu closed.  
gknelson@MG208-GNELSON1 ~  
$ ssh -Y gknelson@beowulf.boisestate.edu  
gknelson@beowulf.boisestate.edu's password:  
Warning: No xauth data; using fake authentication data for X  
11 forwarding.  
Last login: Tue Dec 19 13:09:18 2006 from mg208-gnelson1.boisestate.edu  
-----  
Boise State Beowulf Cluster  
Send email to amit@cs.boisestate.edu or lhindman@onyx.boisestate.edu for  
questions.  
-----  
[gknelson@beowulf ~]$ swarm -f run -b 8 -n 1 -l walltime=500:00:00
```

Figure 75: Screenshot showing command screen for running the SM model on the Beowulf Cluster

VI: Post Processing

Upon completion of running SEAWAT 2000 for the flow and transport model, SEAWAT 2000 will output an observed concentration file (**.ocn**), and a mass flux file (**.mfx**) which contain information on concentrations and mass flux at the points designated by the **.tob** file. '**Extract.in**' is run after SEAWAT and it outputs a file with the head data for the specified locations found by SEAWAT. These files are then used as inputs into the **obsSWT2K.m** MATLAB script which will produce several charts and metrics used to evaluate the results.

Metrics

Metrics are used to provide a qualitative representation of the accuracy of the produced results. Based on the work by Schiebe and Chien (2003) the most influential properties by which to evaluate the effectiveness of this type of model are:

1. Time to arrival of center of mass
2. Time to peak concentration
3. Value of peak concentration
4. Time to early arrival (rising limb)
5. Time to late arrival (falling limb)
6. Effective dispersivity (degree of spreading)
7. Total mass

obsSWT2K.m MATLAB Script

Once the simulation runs have completed, copy the output files (**.ocn**, **.mfx**, and output file from **Extract**) and **obsSWT2K.m** to an analysis directory.

*If you use the same grid, .oc file, extract.in, and .tob file as in the example on the CD, the MATLAB script 'obsSWT2K.m' can be used to post-process the files. This script will create the following files (Table 2):

File Name	Contents
Average_hydraulic_gradient_from_B3_to_A1.jpg	Plot of the average hydraulic gradient between B3 and A1.
Calculated_Semi_Analytical_Fit.jpg	Plot of the semi-analytical fit to the breakthrough curves calculated in the sampling zones A1-1 through A1-12.
Observed_Semi_Analytical_Fit.jpg	Plot of the semi-analytical fit to the breakthrough curves observed in the sampling zones A1-1 through A1-12.
SWT2K_B3_Obs_Vs_Pre_Head_Change.jpg	Observed versus Calculated head change for well B3.
SWT2K_B3_Pred_and_Obs_Head_Change.jpg	Observed and predicted head change in B3.
SWT2K_C1_Obs_Vs_Pre_Head_Change.jpg	Observed versus Calculated head change for well C1.
SWT2K_C1_Pred_and_Obs_Head_Change.jpg	Observed and predicted head change in C1.
SWT2K_C2_Obs_Vs_Pre_Head_Change.jpg	Observed versus Calculated head change for well C2.
SWT2K_C2_Pred_and_Obs_Head_Change.jpg	Observed and predicted head change in C2.
SWT2K_C3_Obs_Vs_Pre_Head_Change.jpg	Observed versus Calculated head change for well C3.
SWT2K_C3_Pred_and_Obs_Head_Change.jpg	Observed and predicted head change in C3.
SWT2K_C4_Obs_Vs_Pre_Head_Change.jpg	Observed versus Calculated head change for well C4.
SWT2K_C4_Pred_and_Obs_Head_Change.jpg	Observed and predicted head change in C4.
SWT2K_C5_Obs_Vs_Pre_Head_Change.jpg	Observed versus Calculated head change for well C5.
SWT2K_C5_Pred_and_Obs_Head_Change.jpg	Observed and predicted head change in C5.
SWT2K_C6_Obs_Vs_Pre_Head_Change.jpg	Observed versus Calculated head change for well C6.
SWT2K_C6_Pred_and_Obs_Head_Change.jpg	Observed and predicted head change in C6.
File Name	Contents
SWT2K_3D_plumecentroid.jpg	3D plot of the path of the plume centroid
SWT2K_Mapview_plumecentroid.jpg	Mapview plot of the path of the plume centroid.
SWT2K_XZ_plumecentroid.jpg	Cross section plot of the plume centroid path where the cross-section is along the B3-B6 plane.
SWT2K_YZ_plumecentroid.jpg	Cross section plot of the plume centroid path where the cross-section is perpendicular to the B3-B6 plane.
SWT2K_PlumeSlice_0.18056_and_3.4722.jpg	Plots of the plume slices at two times (0.18056 days and 3.4722 days) at model elevations: 5.2238, 6.095, 7.7, 9.2, and 11.45 meters. To get elevation above sea level add 830.
SWT2K_PlumeSlice_6.9676_and_12.9745.jpg	Plots of the plume slices at two times (6.9676 days and 12.9745 days) at model elevations: 5.2238, 6.095, 7.7, 9.2, and 11.45 meters. To get elevation above sea level add 830.
SWT2K_TotalMass.jpg	Plot of the calculated total mass in the system.
COBS_Concentration_SEAWAT.dat	First column of this file is time since injection began (days). The subsequent columns contain the calculated concentration data at the locations stated in the first row (the header row). Where and L refers to locations south of the B3-B6 plane and R refers to locations north of the B3-B6 plane. The numbers after R or L refer to how far offset from A1 perpendicular to the B3-B6 plane the observation was taken at – multiples of 0.4 m (example A1R3-6 is the calculated concentration from the same elevations as sampling zone A1-6, but offset 1.2 meters north – perpendicular to the B3-B6 plane from well A1).

COBS_Norm_Conc_SEAWAT.dat	Has the same columns as COBS_Concentration_SEAWAT.dat except the concentrations are normalized to the initial concentration (7.56 g/l).
Mbarxyz_SEAWAT.dat	This file has 4 columns where the first is time since injection began (days), the second through the fourth are the grid coordinates for the calculated center of mass.
Conc_NormObs_and_NormCalc_SEAWAT.txt	First column is the time since injection began (days). The subsequent columns contain the concentrations at the locations denoted in its header (row one). The concentrations are the measured concentrations if denoted by an Obs in the header. The concentrations are normalized to the maximum concentration measured or calculated at that location.
Conc_Obs_and_Calc_SEAWAT.txt	This file contains the same info as that of Conc_NormObs_and_NormCalc_SEAWAT.txt but the concentrations are normalized to the initial concentration of the injectate.
Fitting_Metric_Obs_and_Calc.txt	Contains the 'Goodness of fit' metrics for the simulation. First column is the sampling zone of A1. Columns 2 through 8 contain the metrics for the observed data and columns 9 through 15 contain the metrics for the calculated data. The metrics are: Time to center of mass of the BTC. Peak Concentration. Time to Peak concentration. Time to rising limb (7.5% of the initial concentration). Time to falling limb (7.5% of the initial concentration). Mass under the BTC. Disspersivity.
Fitting_Metric_Observed	Contains the same info as Fitting_Metric_Obs_and_Calc.txt except no metrics for the calculated.
SWT2K_slice_data_layer_7.txt	This file contains the data necessary to plot a plume slice in layer 7. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
SWT2K_slice_data_layer_10.txt	This file contains the data necessary to plot a plume slice in layer 10. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
SWT2K_slice_data_layer_13.txt	This file contains the data necessary to plot a plume slice in layer 13. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.

SWT2K_slice_data_layer_16.txt	This file contains the data necessary to plot a plume slice in layer 16. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
SWT2K_slice_data_layer_19.txt	This file contains the data necessary to plot a plume slice in layer 19. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
SWT2K_slice_data_layer_22.txt	This file contains the data necessary to plot a plume slice in layer 22. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
SWT2K_slice_data_layer_25.txt	This file contains the data necessary to plot a plume slice in layer 25. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
SWT2K_slice_data_layer_28.txt	This file contains the data necessary to plot a plume slice in layer 28. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
SWT2K_slice_data_layer_31.txt	This file contains the data necessary to plot a plume slice in layer 31. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
SWT2K_slice_data_layer_33.txt	This file contains the data necessary to plot a plume slice in layer 33. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.

SWT2K_slice_data_layer_35.txt	This file contains the data necessary to plot a plume slice in layer 35. The columns of the file are: K I J Easting_[m] Northing_[m] Elevation_[m] Grid_Easting_[m] Grid_Northing_[m] Grid_Elevation_[m] Time_0.18056 Time_3.4722 Time_6.9676 Time_12.9745. The time columns contain the calculated concentrations at that time.
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Table 2: *Output files generated by obsSWT2K.m*

Output files generated by **obsSWT2K.m** can be used in Excel or Grapher for review, analysis, and plotting.

VII: References

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