Model for investigating the impacts of groundwater abstraction on river flows User's manual for the ZOOM_IGARF spreadsheet tool and numerical model

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Contents

FIGURES

TABLES

Executive Summary

This document provides the information required by a user to apply the spreadsheet tool ZOOM_IGARF to run the groundwater flow model ZOOMQ3D and other associated utilities for the investigation of the impact of groundwater abstraction on river flows. This tool has been developed to improve the techniques available to Environment Agency hydrogeologists involved in involved in assessing the impact of groundwater abstraction on river flows.

The existing tools developed by the Agency as part of the Impacts of Groundwater Abstraction on River Flows (IGARF) project (NC/00/28) are adequate for up to about 50% of abstraction licence assessments. However, it is recognised by the developers that the existing IGARF analytical models do not produce results with sufficient confidence where:

- The particular hydrogeological setting significantly influences the impact of an abstraction and generic tools such as IGARF 1 are inadequate.
- The groundwater level falls below the bed of the river and away from hydraulic contact with the river.
- A more accurate spatial or seasonal distribution of the impacts on both flow and groundwater level is important, for example when the effects of several abstractions must be considered.
- There is a variation of hydraulic conductivity with depth as in most Chalk and limestone catchments.
- The regional context is important for estimating the local impact, which is often true for wetland sites.

Such features are represented in the many regional groundwater models that the EA has developed, however, these cannot be run quickly, i.e. within the time constraints of a licensing officer. The cost of developing a regional groundwater model, where one does not currently exist, is approximately £200k to £300k. Consequently, a tool is required to assess the impact of groundwater abstraction on river flow, which is relatively easy and quick to use but which incorporates some of the complex features that can be simulated by regional groundwater models. The Excel spreadsheet, ZOOM_IGARF has been developed for this purpose. This simple spreadsheet tool is used as pre and post-processor for the groundwater flow model ZOOMQ3D with which a user can construct models including, for example, multiple dendritic river catchments. It is then possible to run the model and process the output to analyse the impact of an abstraction borehole on one or more reaches of a river within a catchment. The benefit of the use of Excel is that its application requires little prior knowledge of the structure of the input and output of the flow model, ZOOMQ3D.

1 Introduction

The Excel workbook "ZOOM_IGARF.xls" has been developed to enable the rapid assessment of the impact of an abstraction borehole on river baseflow using the numerical groundwater flow model, ZOOMQ3D. The spreadsheet provides clear and simple methods to (i) construct the input files required by the flow model (ii) run the flow model and (iii) analyse its output. Whilst the flow model can provide information on the variation of groundwater head and river baseflow over-time, the spreadsheet modelling process has been designed to quantify and plot the amount of water that an abstraction borehole draws from a river reach or multiple reaches. The rate at which the abstraction borehole reduces the flow in a reach of a river after it starts to pump is termed the *depletion rate*. An example of the output of the spreadsheet modelling process is shown in Figure 1 in which the depletion rate is calculated for two river reaches for a single abstraction borehole.

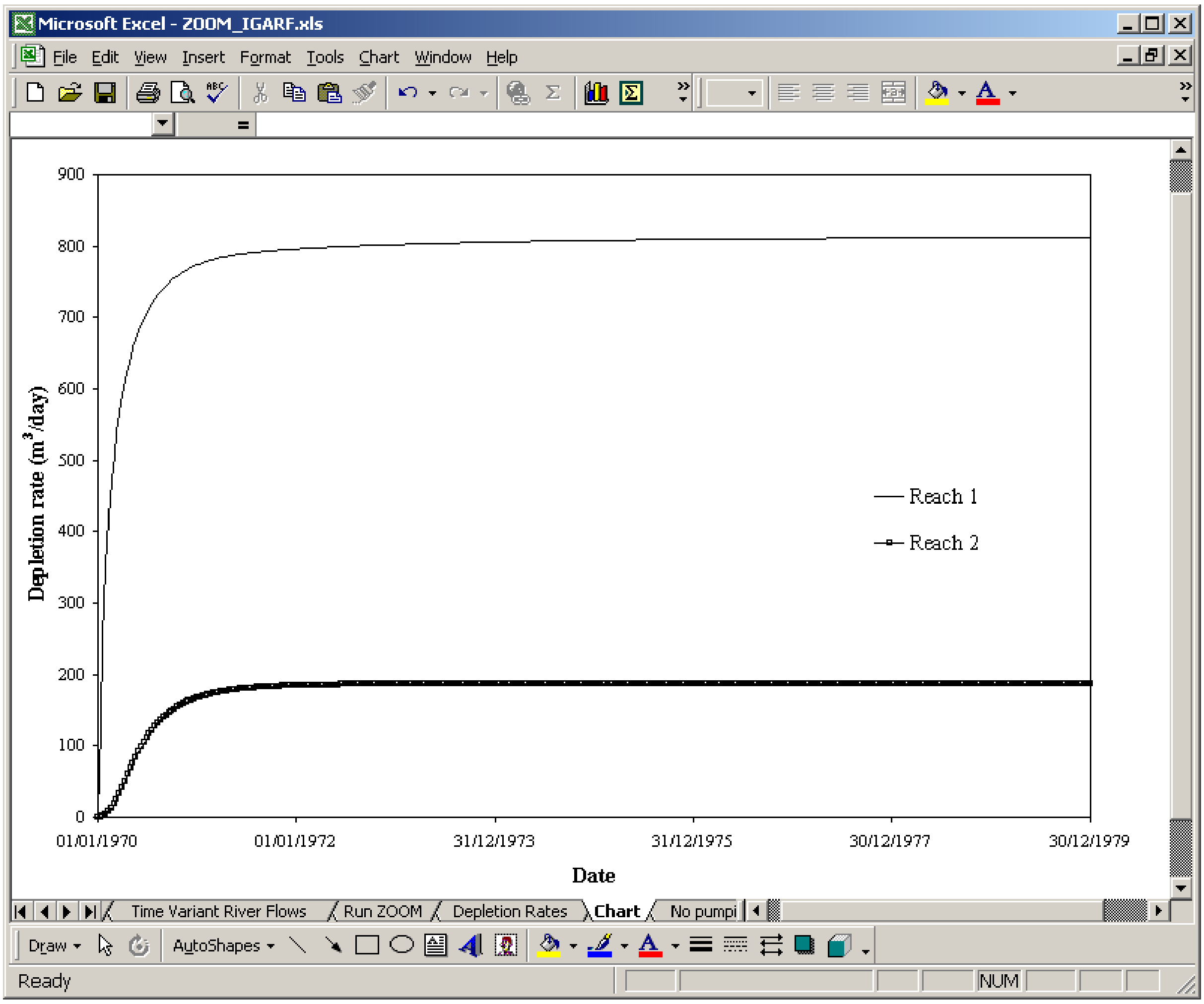


Figure 1 Example depletion rate curves plotted using the Excel spreadsheet

The aim of the Excel workbook is to prepare the input files of the numerical groundwater model ZOOMQ3D and analyse the impact of abstraction on river baseflow by running the flow model. The number of input files required to define the structure of the numerical model varies with its complexity. This depends on the conceptual model used to represent the aquifer system. This spreadsheet tool produces the basic files required by ZOOMQ3D to simulate the impact of abstraction on a groundwater system. For example, ZOOMQ3D is capable of simulating groundwater flow in three dimensions in heterogeneous aquifers, but the Excel workbook only allows the consideration of homogeneous aquifers using one layer of finite-difference nodes. This level of complexity has been deemed adequate for the assessment of the impact of the abstraction using this tool given the likely restricted amount of time available during a licence assessment. Additional complexity can be introduced into the model by manually editing the model text input files produced by the spreadsheet tool. However, this requires a more detailed knowledge of the ZOOMQ3D input files structure.

Each worksheet of the Excel workbook deals with one specific type of model data. The input data varies from that which is spatially varying such as the physical structure of the model to temporally varying information such as pumping rate. The worksheets of the Excel workbook are organised so that if they are followed from left to right, the process of constructing and running the model is undertaken.

2 Installing the workbook

The workbook “ZOOM_IGARF.xls” can be copied into any user defined directory. The Microsoft Excel program must be available on the user’s machine and should allow the use of macros. The user has to ensure that the “Analysis ToolPak” and the “Analysis ToolPak VBA” are selected within Excel from the <Tools> <Add-Ins> menu. Some of the worksheets in the Excel file launch external executable files. These are:

- ZOOMQ3D.EXE
- ZETUP.EXE
- CREATE_RIVER_SPLINES.EXE
- MODIFY_MODEL_RIVERS.EXE

These executables should be copied into a folder called “ZOOM_IGARF” under the root directory of a drive chosen by the user, for example drive “c”.

3 Using the spreadsheet tool

3.1 LAYOUT OF THE EXCEL WORKBOOK

The Excel workbook “ZOOM_IGARF.xls” is composed of seventeen worksheets which are arranged in the following order from left to right:

1. Help
2. Project Details
3. Create Base Grid
4. Boundary Definition
5. Rivers
6. Clock & SOR
7. Regional Parameters
8. Fixed Heads & Leakage
9. Boundary Condition
10. Monitoring Points
11. Abstraction
12. Initial River Flows
13. Time Variant River Flows
14. Run ZOOM
15. Depletion Rates
16. No Pumping Results
17. Pumping Results

Each of the worksheets is clearly laid out. By progressing through the worksheets in this order and entering data where required, the user constructs and runs the flow model, ZOOMQ3D. The spreadsheet then calculates and plots the rate of depletion of river baseflow due to groundwater abstraction for the selected river reaches.

3.2 HELP WORKSHEET

The first worksheet of this tool “Help” instructs the user of how to install and use the spreadsheet tool (Figure 2). It summarises the procedure for determining the impact of an abstraction borehole on a reach, or multiple reaches of a river.

3.3 PROJECT DETAILS WORKSHEET

This sheet allows the user to write descriptive information such as the purpose of the model run, the name of the modeller and the date the work was undertaken. The user can record any other information that is deemed relevant here.

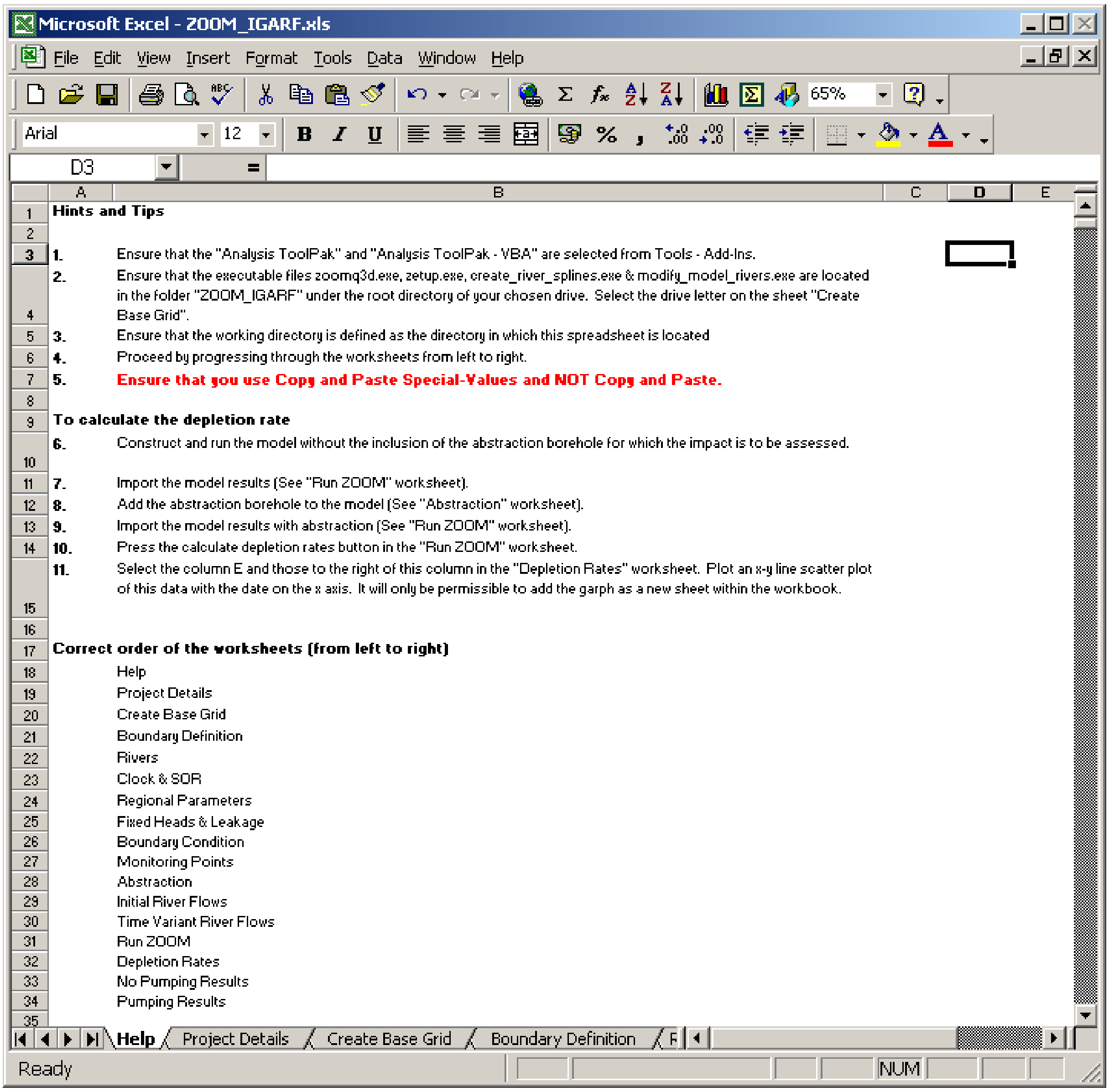


Figure 2 The "Help" worksheet

3.4 CREATE BASE GRID WORKSHEET

This worksheet is used to specify the working directory, and to define the size and structure of the mesh (Figure 3).

- To set the working directories:
  - Cell F3: Enter the working directory of the project. This must be the path of the directory where the Excel workbook is located.
  - Cell I3: Enter the letter of the drive under which the directory "ZOOM_IGARF" is located. Refer to Section 2.

ZOOMQ3D allows the use of one coarse grid and as many sub-grids (refined grids) as required (Figure 4). The mesh is regular but the cells composing it do not have to be square i.e. a different mesh spacing can be used in the x and y directions. This worksheet maintains this functionality. The required information entered as follows:

- Base grid information;
  - Cell B6: Enter the x co-ordinate of the lower left corner of the base grid (m).
  - Cell C6: Enter the y co-ordinate of the lower left corner of the base grid (m).
  - Cell B8: Enter the x co-ordinate of the upper right corner of the base grid (m).
  - Cell C8: Enter the y co-ordinate of the upper right corner of the base grid (m).
  - Cell D8: Enter the cell size. This worksheet allows the creation of square meshes only so the value entered here represents the dimensions of the cells in the x and y directions. The values of Cells B10 and C10 are updated automatically.
- Sub-grid information:

  Proceed by pressing the buttons to add or remove sub-grids. The numbers of sub-grids is shown in Cell B18 and the cells required to set the sub-grids characteristics are automatically highlighted from Cell B20 onwards. For each sub-grid, enter the following data:

  - Cell B(19+i): Enter the x co-ordinate of the lower left corner of the ith sub-grid (m).
  - Cell C(19+i): Enter the y co-ordinate of the lower left corner of the ith sub-grid (m).
  - Cell D(19+i): Enter the x co-ordinate of the upper right corner of the ith sub-grid (m).
  - Cell E(19+i): Enter the y co-ordinate of the upper right corner of the ith sub-grid (m).
  - Cell F(19+i): Enter the number of divisions, i.e. the number of refined grid intervals per coarse grid interval, in the x direction
  - Cell G(19+i): Enter the number of divisions, i.e. the number of refined grid intervals per coarse grid interval, in the y direction

  where $i = 1 \to n$ and n is the total number of sub-grids.

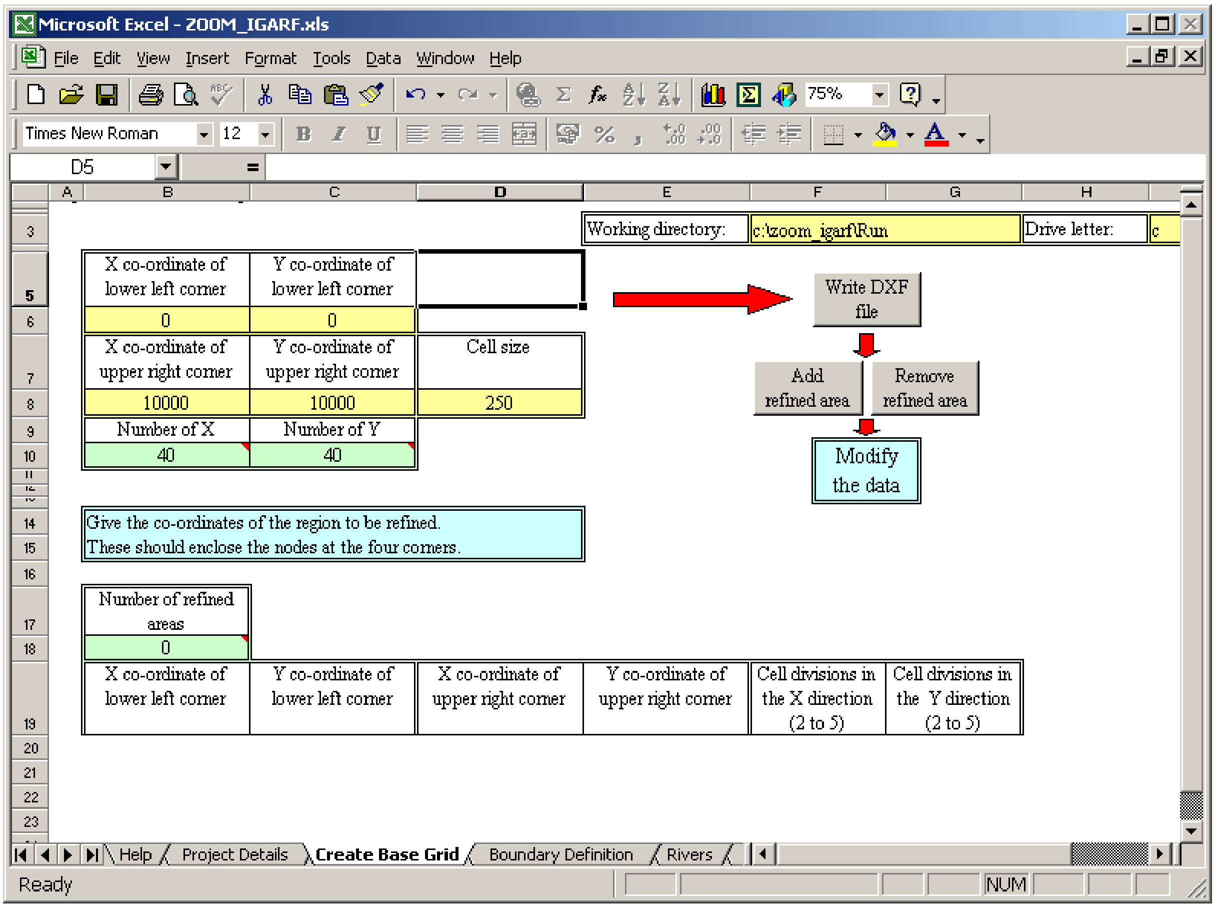


Figure 3 The "Create Base Grid" worksheet

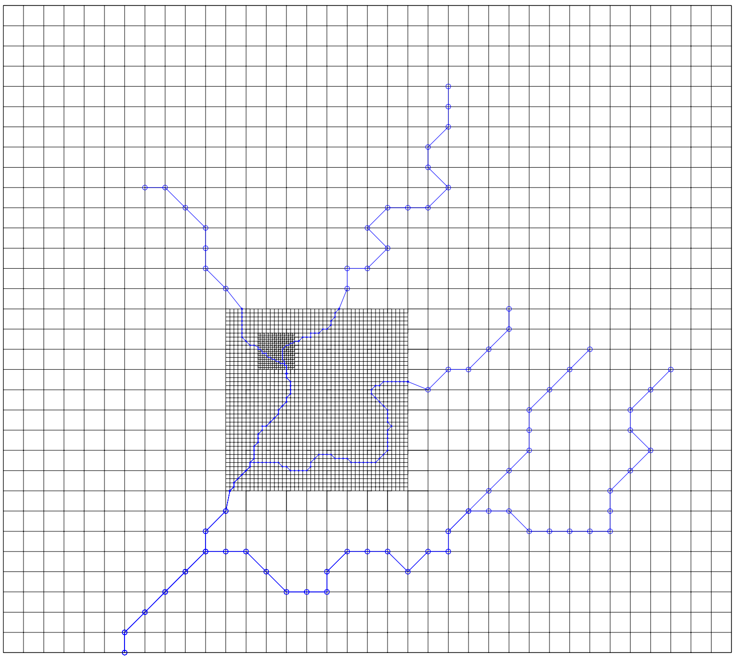


Figure 4 Example of a refined model mesh

3.5 BOUNDARY DEFINITION WORKSHEET

This worksheet allows the user to define a simple rectangular boundary or to prepare a text file that describes a complex boundary that has been constructed in ArcView.

- To prepare a simple rectangular boundary, press the “Produce a simple rectangular boundary” button (Figure 8). A rectangular boundary will be generated. This boundary is created based on the values specified in Cells B10 and C10 of the “Create Base Grid” worksheet.
- To define a more complex boundary it is necessary to use ArcView and perform the following procedure:
  - Press the “Write DXF file” button in the “Create Base Grid” worksheet.
  - This will create a file called “basegridsquare.dxf”.
  - Create an ArcView project and add the following extensions: “Cad Reader” and “Spatial analyst”.
    - Add “basegridsquare.dxf” to the ArcView project as a theme by selecting “View->Add Theme” from the menu.
    - If you already have a shape file of your model boundary then use this for the next operation, otherwise create a new polygon theme and draw the model boundary. This must be contained within the limit of the dxf file just added (Figure 5).
    - Ensure your boundary theme is selected i.e. the active theme.
    - Select “Theme->Convert to grid” from the menu
    - Select a name for your new grid theme and press “OK”
    - Set the “Output Grid Cell Size” (Figure 6) to “As Specified Below” and set the value in the edit box next to the “Cell Size” to the same value specified in the Excel sheet, Cell D8 of “Create Base Grid Worksheet” (Figure 3).
    - Select “Same as Basegridsquare.dxf” for the output extent (Figure 6). The number of rows and columns in the ArcView active dialog box should be updated and should be equal to the values given in Cells B10 and C10 of the “Create Base Grid” worksheet (Figure 3). Press “OK” in answer to the subsequent messages. A new theme will be added to the view (Figure 7).
    - Choose “File->Export data source” from the menu. Choose ASCII raster. Select the newly created grid theme and then a name for the output asc file.
  - Open the exported ASCII data in a new Excel workbook.
  - Ignore the first six rows containing the header lines of the ASCII file and copy the other cells containing data, starting from Cell A7, and paste them in the “Boundary Definition” worksheet starting from Cell A6.
  - Press the “Format boundary” button then the “Produce boundary file” button (Figure 8).

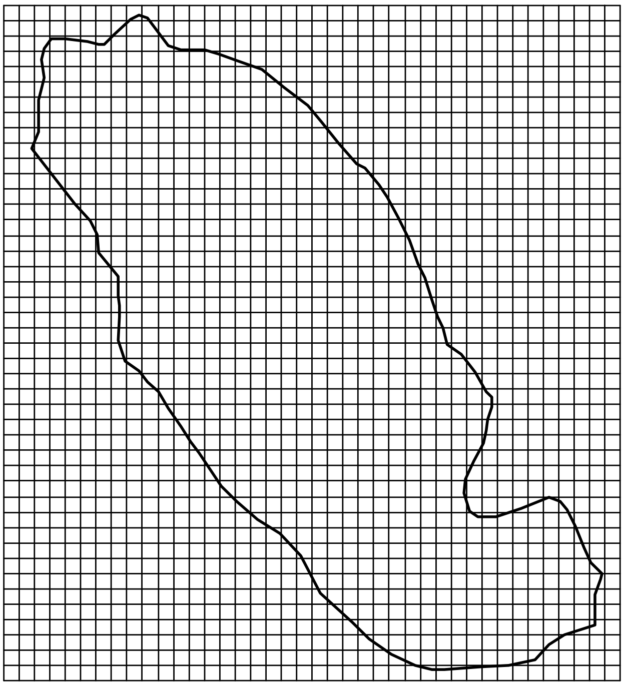


Figure 5 Example DXF file of model grid imported into ArcView and a polyline theme of the aquifer boundary

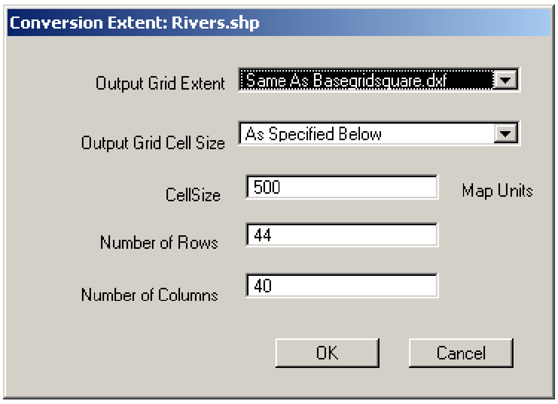


Figure 6 Dialog box used during conversion of polyline boundary theme to a grid

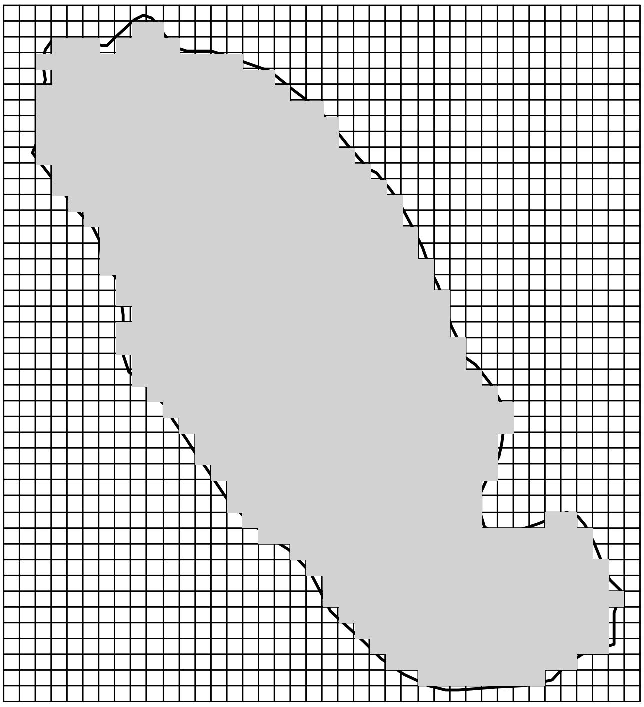


Figure 7 The gridded boundary theme after conversion using ArcView

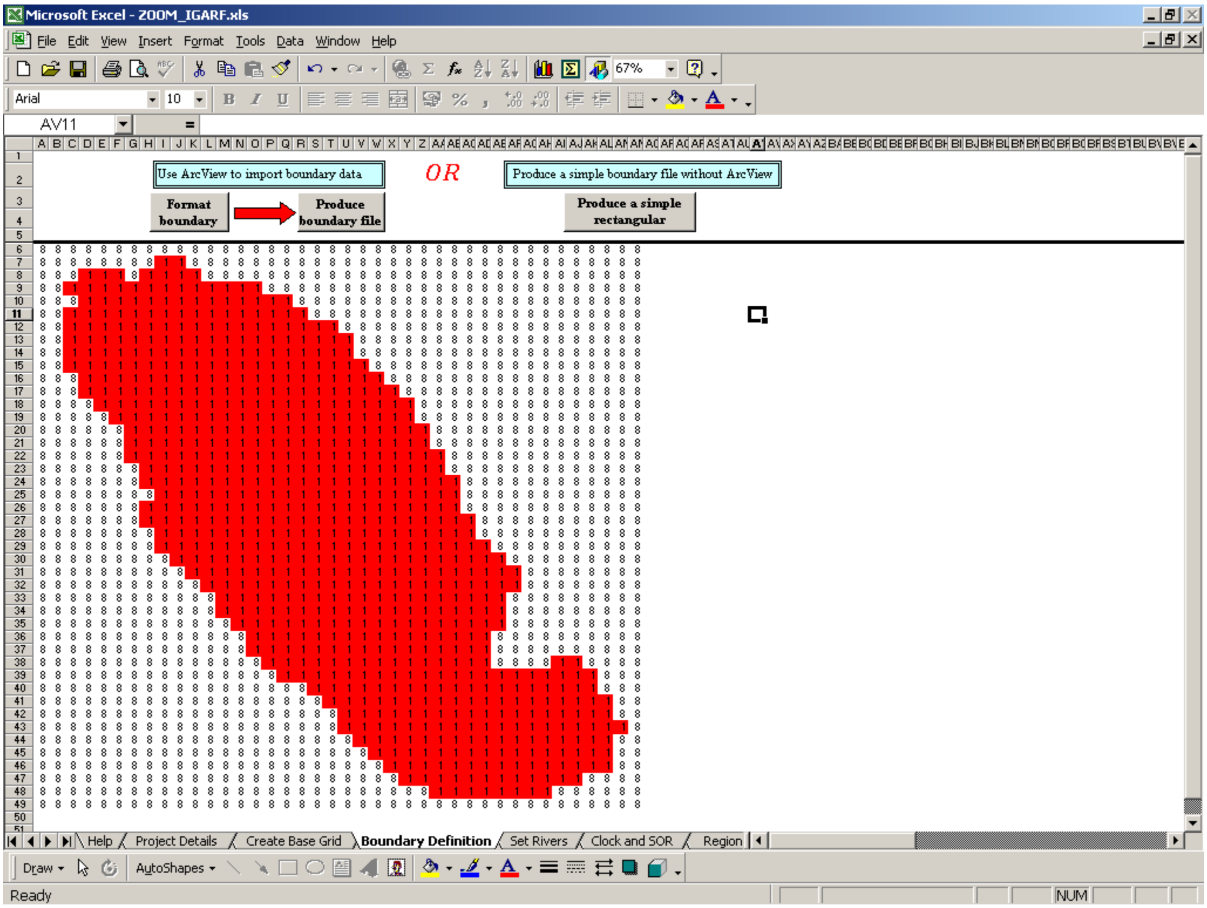


Figure 8 The "Boundary Definition" worksheet

3.6 RIVERS WORKSHEET

This worksheet allows the user to construct simple straight-line rivers or to run the CREATE_RIVER_SPLINES application to create more complex create rivers.

- To create simple straight rivers:
  - Use the buttons “Add river” and “Remove river” to add and remove rivers. The number of rivers is adjusted automatically in Cell C18 (Figure 9).
  - Set the characteristics of the rivers in the activated cells from B22 onwards. Each row of data starting from Row 22 corresponds to one river. The data included in these cells are:
    - Cell B(21+i): This cell holds an integer representing the river number. This value is written automatically when a river is added.
    - Cell C(21+i): Enter the x co-ordinate of the downstream end of the i^{th} river (m).
    - Cell D(21+i): Enter the y co-ordinate of the downstream end of the i^{th} river (m).
    - Cell E(21+i): Enter the stage of the downstream end of the i^{th} river (m).
    - Cell F(21+i): Enter the x co-ordinate of the upstream end of the i^{th} river (m).
    - Cell G(21+i): Enter the y co-ordinate of the upstream end of the i^{th} river (m).
    - Cell H(21+i): Enter the stage of the upstream end of the i^{th} river (m).
    - Cell I(21+i): Enter the bed conductivity of the i^{th} river (m day^{-1}).

where $i = 1 \rightarrow n$ and *n* is the total number of rivers.

- The CREATE_RIVER_SPLINES interface allows the user to create a complicated network of rivers. Press the button “Run river interface” to launch this application. For a full description of how to use this application refer to Section 4.3.2.

After defining the rivers, the structure of the numerical model can be built. The application ZETUP, which is a pre-processor for the flow model, is used to construct the model grids and rivers. To run this application, press the button “Run ZETUP”. Two operations are performed:

1. Before ZETUP is run, a text file is created for each river defined in the model. These text files are given the name “River##_SplinePts.dat” where ## represents the ID number of the river. ZETUP reads these files to create the model rivers i.e. the numerical representation of the rivers on the finite difference mesh.
2. A DOS box is opened and ZETUP is run. ZETUP reads an ASCII text file produced by the Excel spreadsheet and creates the finite difference mesh as illustrated in Figure 10. ZETUP then asks the user if rivers are to be included in the model.
   - Type ‘y’ for yes if rivers are included in the model and ‘n’ for no if not.
   - Write the name of the river data file “River##_SplinePts.dat” where ## should be 01 for the first river file, 02 for the second river file etc.
   - Repeat the above two steps for all the rivers.

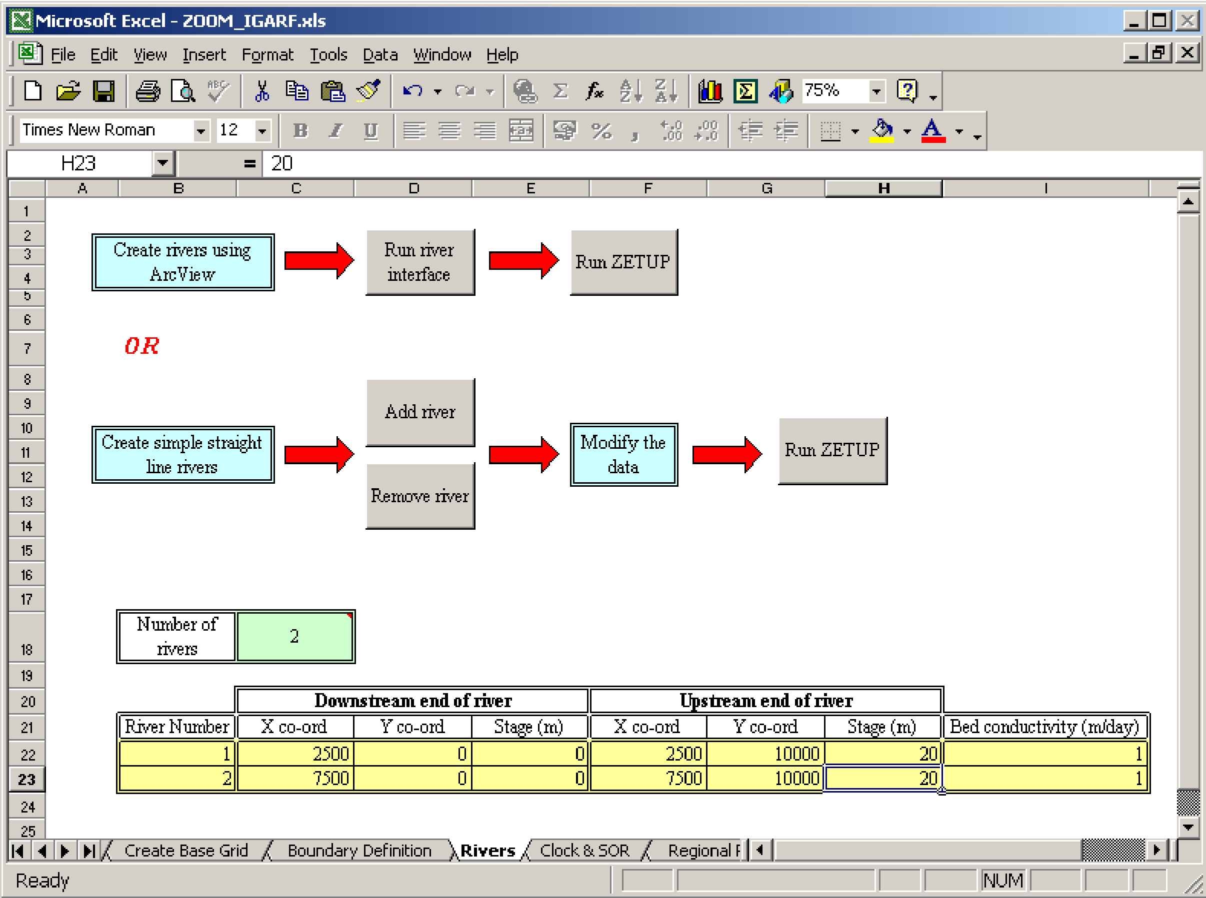


Figure 9 The "Rivers" worksheet

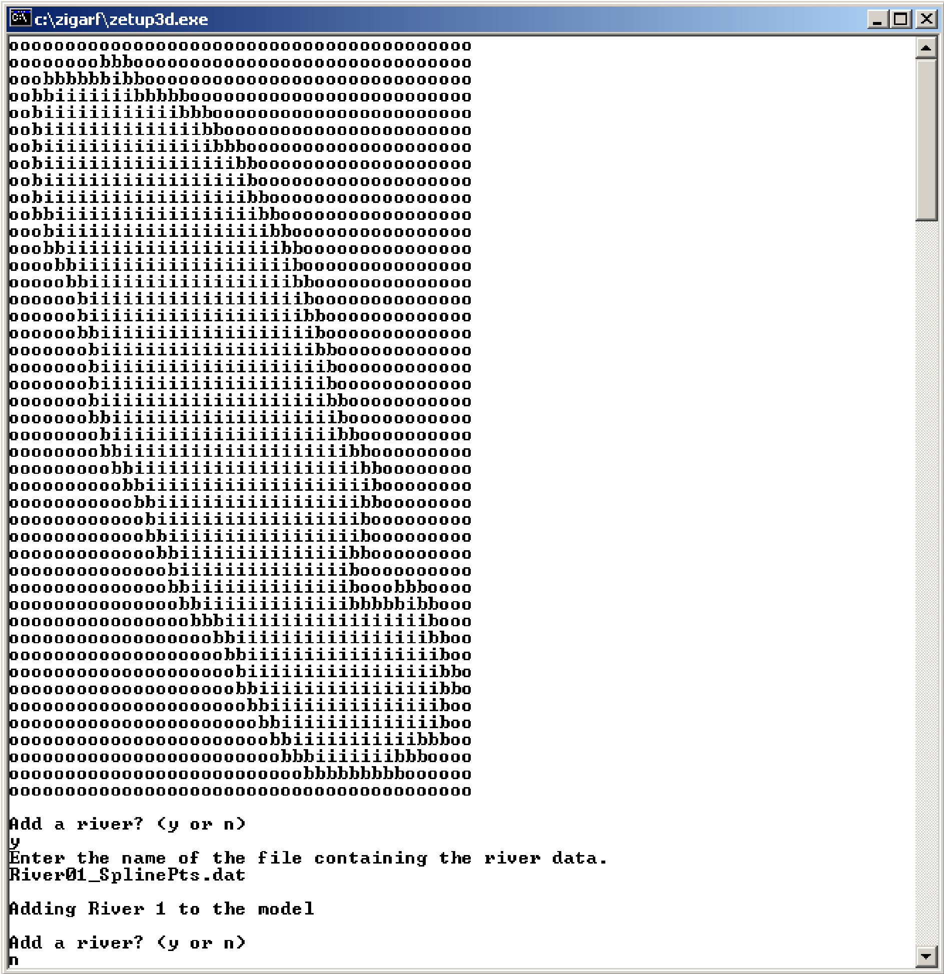


Figure 10 Example output during execution of ZETUP from “Rivers” worksheet

3.6.1 River-aquifer interaction

In ZOOMQ3D river-aquifer interaction is represented as a linear head-dependent leakage mechanism. The rate of leakage depends on the difference between groundwater head and river stage and is expressed by:

$$Q_z = \frac{K_z}{B} \cdot W \cdot L \cdot (h_a - h_r)$$

where

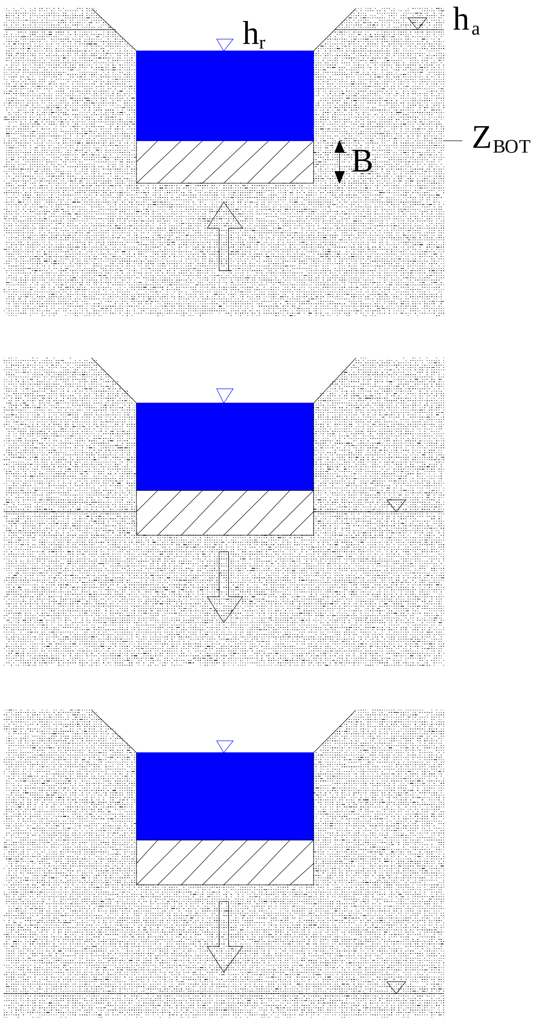
- Q_z is the leakage rate ($m^3 day^{-1}$),
- K_z is the vertical hydraulic conductivity of the river bed ($m\ day^{-1}$),
- B is the thickness of the river bed (m),
- W is the width of the river (m),
- L is the length of the river reach (m),
- h_a is the head in the aquifer (m) and,
- h_r is the river stage (m).

Therefore, when the groundwater head is above the river stage groundwater discharges to the river. As the groundwater head falls below the river stage, the river starts to lose water to the aquifer until a limiting rate is reached. The above equation is modified when the head in the aquifer falls below the base of the river bed, $(Z_{BOT} - B)$, where Z_{BOT} is the elevation of the bed of the river. Under these conditions, the driving head is equal to the difference between the river stage and the base of the river bed, $\left(Z_{BOT} - B\right)$. The leakage from the river under perched conditions is therefore defined as:

$$Q_z = K_Z^E \cdot W \cdot L \cdot \left[\left(Z_{BOT} - B\right) - h_r\right]$$

Figure 11 shows the relationship between groundwater head and river leakage applied in ZOOMQ3D.

The Excel spreadsheet “ZOOM_IGARF.xls” and associated utilities produce a simplified river input file for the flow model. In this file some of the river parameters are set to unity to simplify the representation of the river. In this case, river aquifer interaction is represented by the equations shown in Table 1.



a) Influent river

$$Q_z = \frac{K_Z^I}{B} \cdot W \cdot L \cdot (h_a - h_r)$$

b) Effluent river. Groundwater head above the base of the river bed, $(Z_{BOT} - B)$, but below river stage

$$Q_z = \frac{K_Z^E}{B} \cdot W \cdot L \cdot (h_a - h_r)$$

c) Effluent river. Groundwater head below base of the river bed, $(Z_{BOT} - B)$

$$Q_z = K_Z^E \cdot W \cdot L \cdot [(Z_{BOT} - B) - h_r]$$

Q_z is the flow rate ($m^3 day^{-1}$) from the aquifer to the river,

K_Z^E is the vertical hydraulic conductivity of the river bed ($m\ day^{-1}$) under effluent river conditions,

K_Z^I is the vertical hydraulic conductivity of the river bed ($m\ day^{-1}$) under influent river conditions,

Z_{BOT} is the elevation of the bed of the river,

B is the thickness of the river bed (m),

W is the width of the river (m),

L is the length of the river reach (m),

h_a is the head in the aquifer (m) and,

h_r is the river stage (m).

Figure 11 Representation of river aquifer interaction in ZOOMQ3D

Table 1 Simplified representation of river-aquifer interaction in ZOOM_IGARF

Flow equation	**Assumptions**
$Q_z = K_Z \cdot L \cdot (h_a - h_r) \cdot$ for $h_a > h_r - 1$	River width (W) = 1 m Bed thickness (B) = 1 m K_Z has the same value for influent and effluent conditions. $(Z_{BOT} = h_r) \Rightarrow (Z_{BOT} - B) = h_r - 1$
$Q_z = -K_Z \cdot L$	River width (W) = 1 m Bed thickness (B) = 1 m K_Z has the same value for influent and effluent conditions $(Z_{BOT} = h_r) \Rightarrow (Z_{BOT} - B) = h_r - 1$

An example relationship between groundwater head and river leakage is shown in Figure 12 for a given river stage and river bed hydraulic conductivity.

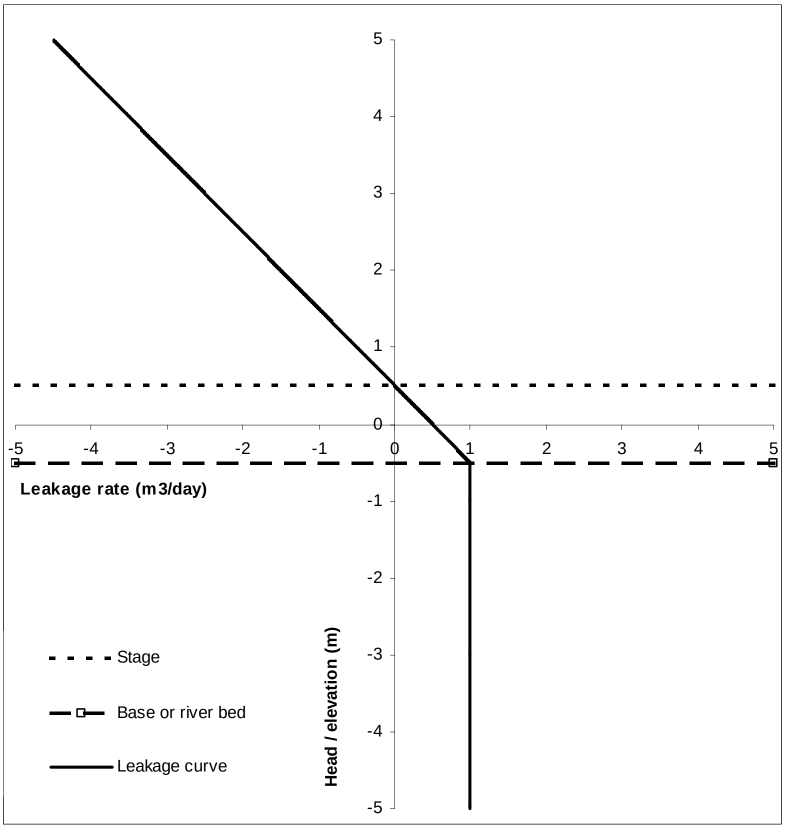


Figure 12 Example relationship between groundwater head and river leakage in ZOOM_IGARF

3.7 CLOCK & SOR WORKSHEET

This worksheet is used to specify the number of years to be simulated (Cell D4) and the year the simulation starts (Cell D5). The user can also specify if this run is a continuation from a previous simulation (Refer to Appendix A, Section A3.3 for more details). If this model is being re-run set Cell D6 to "t" for true and if it is a new run set Cell D6 to "f" for false (Figure 13).

The Successive Over Relaxation (SOR) method is used to solve the numerical equations. This is an iterative technique which converges towards the solution. The iteration procedure is stopped when a specified level of accuracy has been achieved. The parameter that controls the convergence of the numerical solution is defined in Cell D11. A value greater than or equal to 1.0 but less than 2.0 must be used. The maximum number of iterations is specified in Cell D12. This parameter represents the number of iterations after which the model progresses to the next time step if the convergence criterion is not satisfied. ZOOMQ3D writes convergence information after a certain number of iterations to a text file (Refer to Appendix A, Sections A3.10). This number is specified in Cell D13.

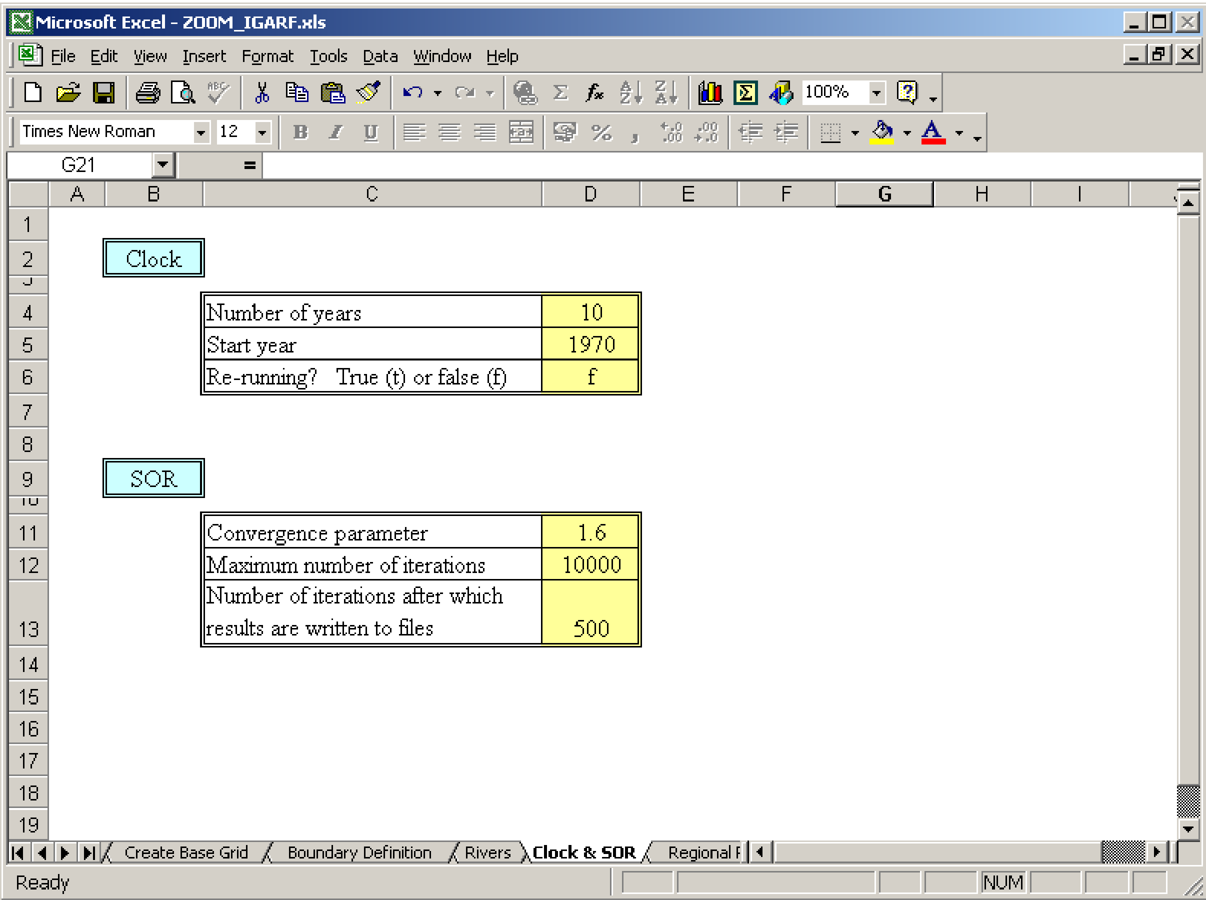
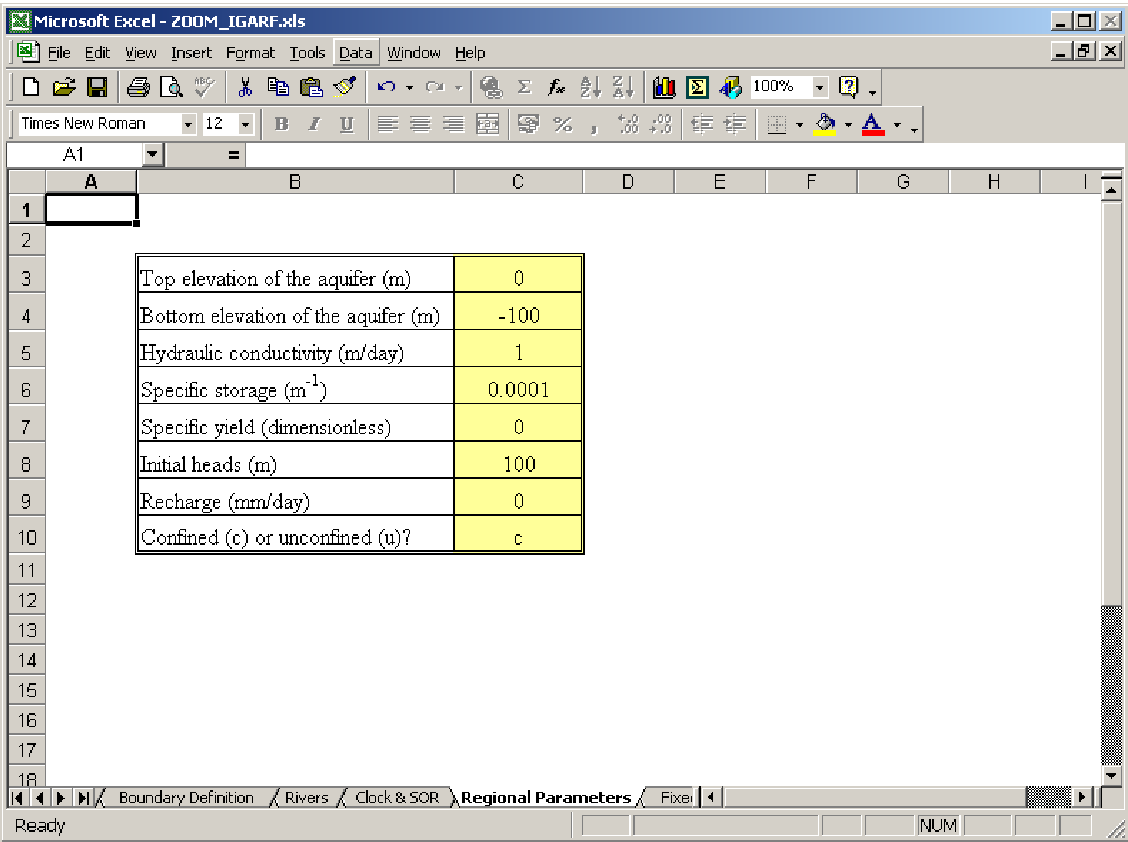


Figure 13 The "Clock & SOR" worksheet

3.8 REGIONAL PARAMETERS WORKSHEET

As discussed previously, the Excel workbook only allows the construction of a numerical model with one layer. This layer is homogeneous and recharge can only be distributed uniformly across it. The aquifer parameter values are specified in this worksheet. These values are assigned to all the finite-difference nodes in the model. These parameters values are defined using the following cells (Figure 14):

- Cell C3: Set the elevation of the top of the aquifer (m).
- Cell D3: Set the elevation of the base of the aquifer (m).
- Cell E3: Set the horizontal hydraulic conductivity of the aquifer (m day^{-1}).
- Cell F3: Set the specific storage of the aquifer (m^{-1}).
- Cell G3: Set the specific yield of the aquifer.
- Cell H3: Set the initial heads at the start of the simulation (m). To use this value, the flag in Cell D6 of the "Clock & SOR" worksheet should be set to 'f'.
- Cell I3: Set the recharge rate (mm day^{-1}).
- Cell J3: A flag to specify if the model is simulating a confined (c) or an unconfined (u) aquifer.



Top elevation of the aquifer (m)	0
Bottom elevation of the aquifer (m)	-100
Hydraulic conductivity (m/day)	1
Specific storage (m^{-1})	0.0001
Specific yield (dimensionless)	0
Initial heads (m)	100
Recharge (mm/day)	0
Confined (c) or unconfined (u)?	c

Figure 14 The "Regional Parameters" worksheet

3.9 FIXED HEADS & LEAKAGE WORKSHEET

This worksheet is used to specify any fixed head nodes *inside* the model boundary and any head dependent leakage nodes within the model (Figure 15). Fixed heads may be required, for example, to represent large surface water features such as a lake and leakage nodes could be used to represent spring discharges.

- To specify the fixed head nodes:
    - Use the buttons "Add a fixed head node" or "Remove a fixed head node" to add or remove fixed head nodes. The number of the fixed head nodes is adjusted automatically in Cell B5.
    - Set the location of the fixed head nodes in the cells located in Columns B, C and D. Set the fixed head values (m) in the cells of Column E, that is:
        - Cell B(6+i): A value of 1 should be entered in this cell. This is the layer number where the node is located. Since only one layer is allowed, this cell should only hold a value of 1.
        - Cell C(6+i): Enter the x co-ordinate of the i^{th} fixed head node (m).
        - Cell D(6+i): Enter the y co-ordinate of the i^{th} fixed head node (m).
        - Cell E(6+i): Enter the value of the fixed head (m).

where $i = 1 \rightarrow n$ and n is the total number of fixed head nodes.

Leakage nodes allow the discharge or the recharge of water to the aquifer system based on the difference between its elevation and the groundwater head multiplied by a vertical conductance term. This conductance term is conceptualised as being equivalent to the vertical hydraulic conductivity (m day^{-1}) of the material separating the aquifer from the leakage node divided by its thickness (m).

- To include leakage nodes:
    - Use the buttons "Add a leakage node" or "Remove a leakage node" to add or remove leakage nodes. The number of the leakage nodes is adjusted automatically in Cell H5.
    - Set the location of the leakage nodes in the cells located in Columns H, I, J and K. The layer number must be set to 1 as only one layer model can be created. The elevation (Z) of the node is required to calculate the flow discharging from or leaking into the aquifer.
    - Two values of the vertical conductance term must be defined; one when the leakage node is effluent and one when it is influent. These values are defined in the cells of Columns L and M respectively. The following is an explanation of the cells used to set the leakage node parameters:
        - Cell H(6+i): A value of 1 should be entered in this cell. This is the layer number where the node is located. Since only one layer is allowed in the model, this cell should only hold a value of 1.
        - Cell I(6+i): Enter the x co-ordinate of the i^{th} leakage node (m).
        - Cell J(6+i): Enter the y co-ordinate of the i^{th} leakage node (m).
        - Cell K(6+i): Enter the z value of the i^{th} leakage node (m).
        - Cell L(6+i): Enter value of the vertical conductance term of the i^{th} leakage node when the flow is discharging from the aquifer (day^{-1}).
        - Cell M(6+i): Enter value of the vertical conductance term of the i^{th} leakage node when there is leakage into the aquifer (day^{-1}).

where $i = 1 \rightarrow n$ and n is the total number of leakage nodes.

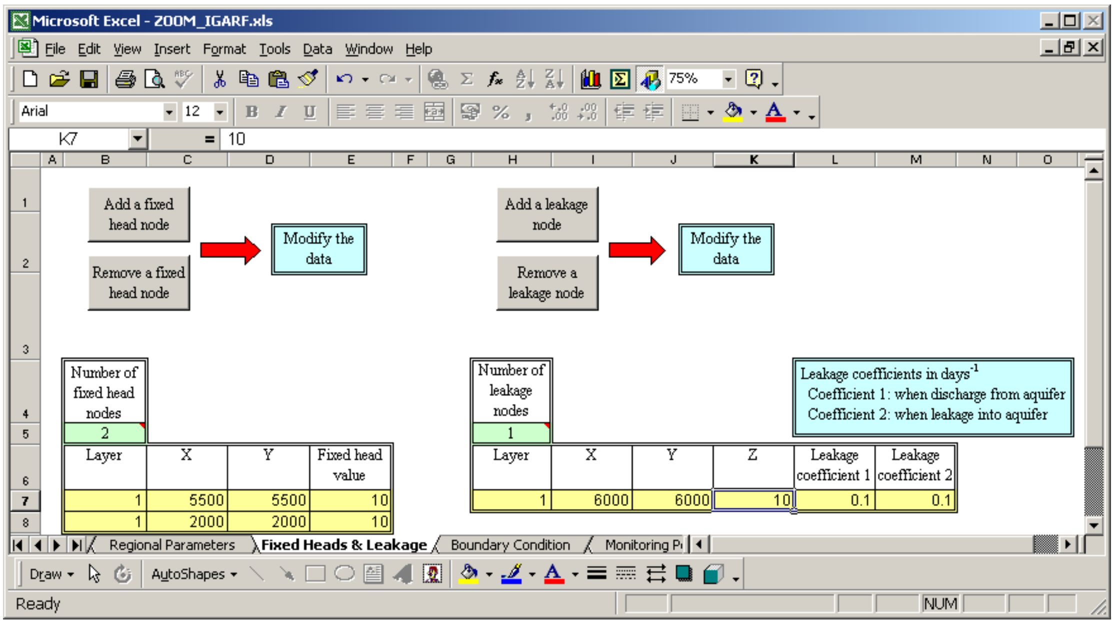


Figure 15 The "Fixed Heads & Leakage" worksheet

3.10 BOUNDARY CONDITION WORKSHEET

This worksheet is used to specify the boundary condition at the nodes located *at the edge of* the model. A fixed head value or a fixed inflow rate can be specified at these nodes. To define an impermeable boundary at a node a specified flow of zero is specified. The length of this worksheet depends on the size of the model and the shape of its boundary (Figure 16). The worksheet must, therefore, be formatted first. Proceed as follows:

- Press the button "Get boundary conditions". The worksheet will be formatted automatically based on the original file produced by ZETUP.
- For each node set the flag in the cell of Column C to 'f' for fixed head and 's' for specified flow.
- For each node set the value of the inflow in m^3day^{-1} in the cell of Column D if a specified flow is selected or the value of the fixed head in metres if a fixed head is selected. An outflow at the boundary can be specified by using a negative flow rate.

Hint: To edit more than one cell at once: 1) select the required cells by holding the "Shift" key down and click on the first and the last cells if the cells are contiguous or by holding the "Ctrl" key down and click on the required cells if they are not contiguous, 2) enter the required value in the formula bar, 3) press "Ctrl+Enter".

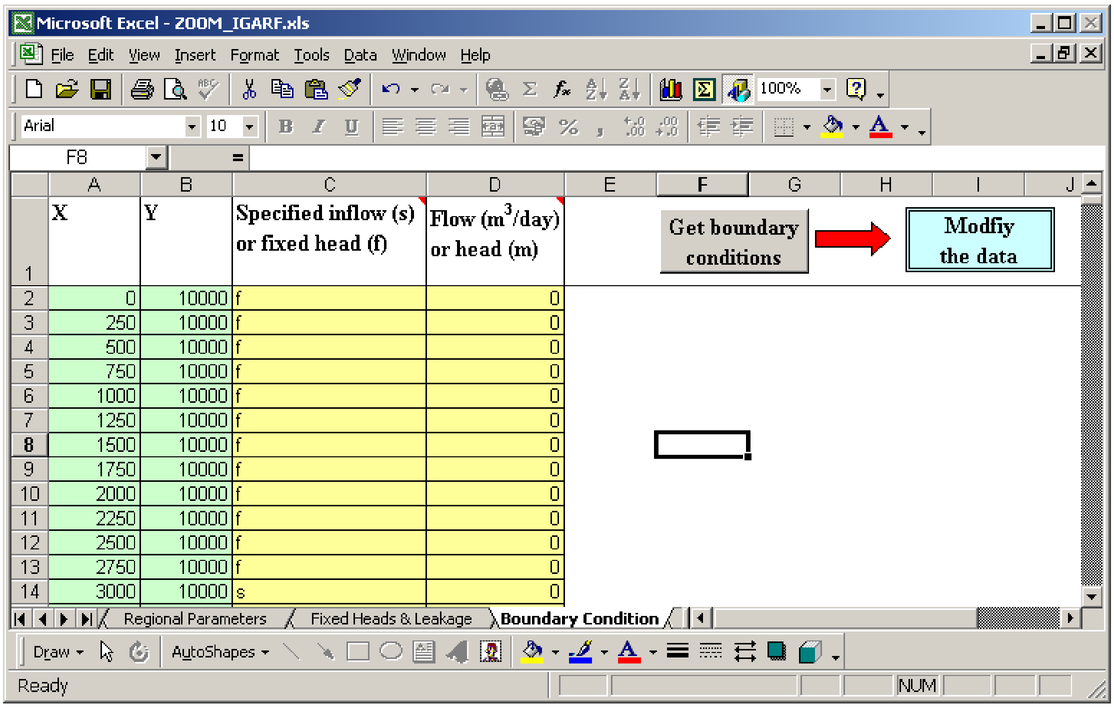


Figure 16 The “Boundary Condition” worksheet

3.11 MONITORING POINTS WORKSHEET

This worksheet is used to specify the nodes where the variation of groundwater head over time is monitored. In addition, the baseflow in the river can be monitored by defining one or more gauging stations along the river. Lastly, and most importantly, sections of the rivers can be defined for which the impact of an abstraction well is calculated over time. This impact is referred to as a “depletion rate” (Figure 17).

- To specify the nodes where the groundwater head variations with time are monitored (i.e. observation well nodes):
  - o Use the buttons “Add an observation well” or “Remove an observation well” to add or remove observation wells. The number of the observation wells is adjusted automatically in Cell B5.
  - o Set the monitoring start and end times in Cells B7 and C7 respectively. These are specified as years. For example, if only one year is simulated, e.g. 1970, set both cells to 1970.
  - o Set the location of the observation wells:
    - ▪ Cell B(8+i): Enter the x co-ordinate of the i^{th} observation well (m).
    - ▪ Cell C(8+i): Enter the y co-ordinate of the i^{th} observation well (m).

where $i = 1 \rightarrow n$ and n is the total number of observation wells.

The model text output file “obswells.out” contains the variation of head over time at each of the nodes specified. This file is described in Section A3.1, Appendix A.

- To specify the location of the river baseflow gauging stations:
  - o Use the buttons “Add a river gauging station” or “Remove a river gauging station” to add or remove river gauging stations. The number of the river gauging stations is adjusted automatically in Cell H5.

- o Set the monitoring start and end times in Cells H7 and I7 respectively.
- o For each gauging station:
  - ▪ Cell H(8+i): Enter the river number where the i^{th} gauging station is located. (Refer to Section 4.2 for details of river node numbering).
  - ▪ Cell I(8+i): Enter the node number which represents the i^{th} gauging station. (Refer to Section 4.2 for details of river node numbering).

where $i = 1 \rightarrow n$ and n is the total number of gauging stations.

The model text output file “gauging_stations.out” contains the variation of river flow over time at each of the specified gauging station nodes. This file is described in Section A3.4, Appendix A.

- To specify the river reaches where depletion rates are calculated:
  - o Use the buttons “Add a river reach to monitor” or “Remove a river reach to monitor” to add or remove river reaches. The number of the river reaches is adjusted automatically in Cell M5.
  - o For each river reach:
    - ▪ Cell M(6+i): Enter the river number to which the i^{th} river reach belongs.
    - ▪ Cell N(6+i): Enter the number of the upstream node of the i^{th} river reach. This will be higher than the number of the node at the downstream end of the reach. (Refer to Section 4.2 for details of river node numbering).
    - ▪ Cell O(6+i): Enter the number of the downstream node of the i^{th} river reach. This will be lower than the number of the node at the upstream end of the reach. (Refer to Section 4.2 for details of river node numbering).

where $i = 1 \rightarrow n$ and n is the total number of river reaches.

The output file showing the river baseflow accretion profiles is described in Section A3.5 in Appendix A.

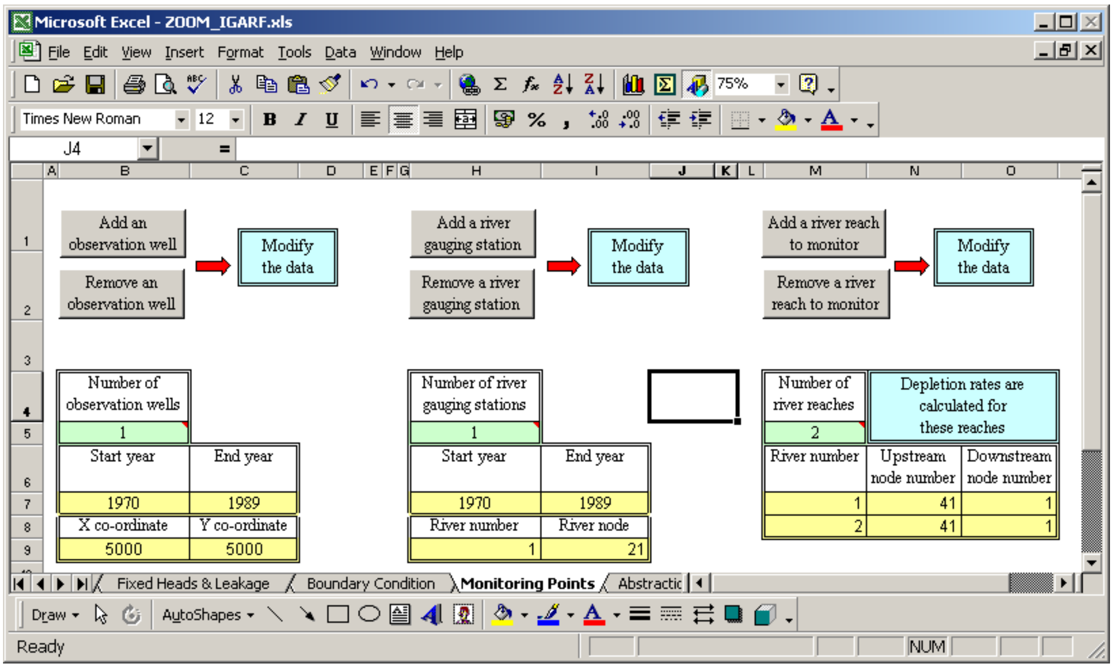


Figure 17 The “Monitoring Points” worksheet

3.12 ABSTRACTION WORKSHEET

This worksheet is used to specify the location of the abstraction wells and their pumping rates. The number of simulation years and the start date of the simulation are read automatically from the “Clock & SOR” worksheet. The first step is to format the worksheet (Figure 18) based on the time parameters which are read in “Clock & SOR” worksheet. Proceed as follows:

- Press the button “Format sheet” to format the sheet.
- Change the number of abstraction wells by pressing the “Add abstraction well” button to add an abstraction well or by pressing the “Remove abstraction well” to remove an abstraction well.
- The number of abstraction wells will change automatically in Cell F2.
- Enter the following information for each abstraction well:
    - Cell A(13+i): This cell gives the number of the i^{th} pumping well. This cell cannot be edited.
    - Cell B(13+i): Enter the x co-ordinate of the i^{th} abstraction well (m).
    - Cell C(13+i): Enter the y co-ordinate of the i^{th} abstraction well (m).
    - Enter the monthly pumping rate (m^3day^{-1}) in Column G onwards. Column G relates to the well specified in Cell A14, Column H relates to the well specified in Cell A15 and so on.

where $i = 1 \rightarrow n$ and n is the total number of abstraction wells.

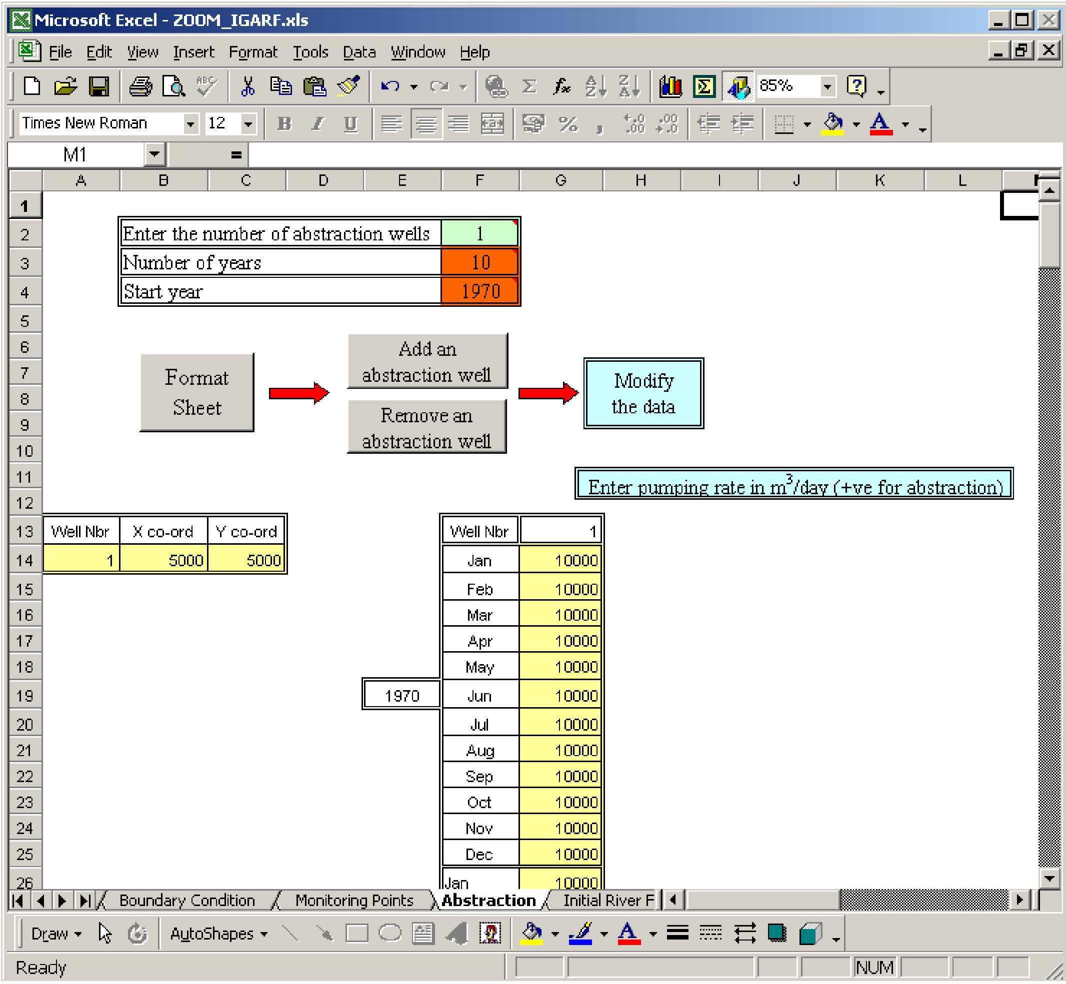


Figure 18 The "Abstraction" worksheet

3.13 INITIAL RIVER FLOWS WORKSHEET

The initial *baseflow* (not total flow) at each of the river nodes is set in this worksheet. This requires a file created by ZETUP to be imported into the Excel worksheet first. This is achieved by pressing the "Import data from ZETUP" button. The number of rivers is adjusted automatically in Cell A10 and information is copied into the cells of Columns A, B, C and D starting from Row 12. The information is composed of blocks of data that are separated by dashed lines (an example of this line is shown in Row 11 of Figure 19). Each block corresponds to one river, the number of which is given in the first cell in Column A after the dashed line (Cell A12 for example). The first cell in Column B after the dashed line gives the number of nodes in the river. The initial flow at each node of the rivers can then be entered in the corresponding cell of Column D (Figure 19).

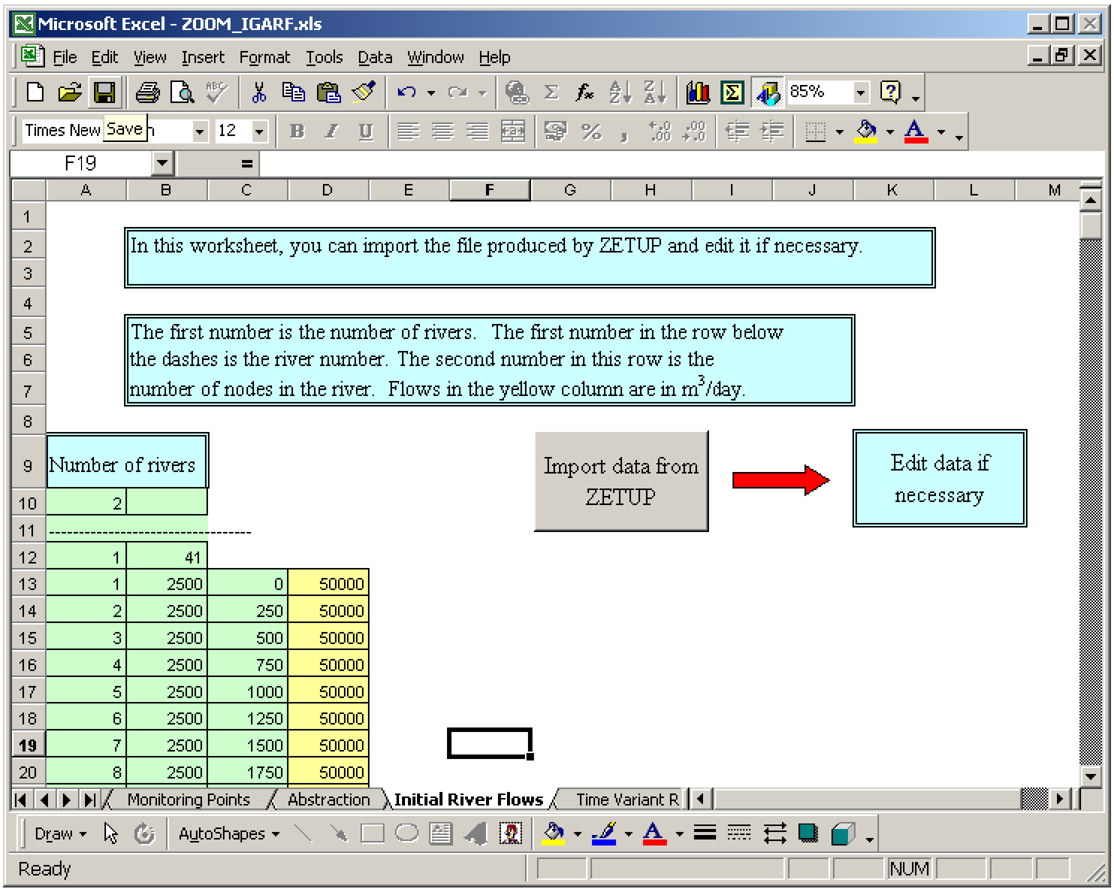


Figure 19 The "Initial River Flows" worksheet

3.14 TIME VARIANT RIVER FLOWS WORKSHEET

This worksheet allows the user to specify time variant discharges to a river. The flow can be specified at one or at several nodes of a river. For each node defined, the variation of flow with time must be specified during the simulation period. The worksheet must first be formatted based on the length of the simulation (Figure 20). Proceed as follows:

- Press the button "Format sheet" to format the sheet.
- Press "Add specified flow node" button or the "Remove specified flow node" button to add or remove specified flow nodes.
- New cells in Columns A, B and C are highlighted or made blank. In addition, cells in columns starting from Column G will be highlighted or made blank. Edit the cells as follows:
    - Cell A(13+i): This cell gives the number of the i^{th} node. This cell cannot be edited.
    - Cell B(13+i): Enter the river number to which the required node belongs.
    - Cell C(13+i): Enter node number that represents the specified flow node in this river.
    - Enter data in the yellow cells in the columns after Column F. Enter the monthly specified flow ($m^3 day^{-1}$) in the appropriate columns. Column G relates to the node specified in Cell A14, Column H relates to the node specified in Cell A15 and so on.

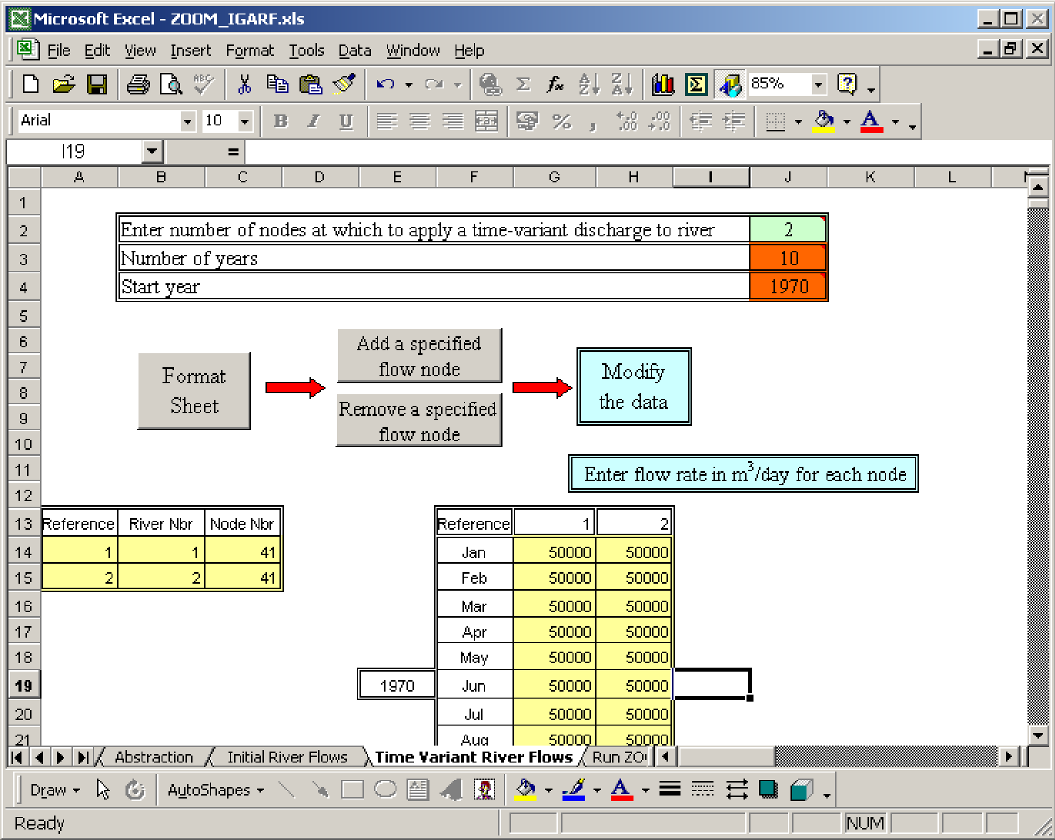


Figure 20 The "Time Variant River Flows" worksheet

3.15 RUN ZOOM WORKSHEET

This worksheet is used to run (i) the application MODIFY_MODEL_RIVERS to change river characteristics and (ii) the flow model ZOOMQ3D to simulate the aquifer system constructed using the other worksheets. The Excel worksheet is also used to import the model results and to calculate the depletion rates (Figure 21).

- To modify the river characteristics, press the button "Modify model river parameters". Refer to Section 5 for details on how to use this application.
- To run ZOOMQ3D press the "Run ZOOM" button. A DOS box will be launched and ZOOMQ3D will produce a solution. The time required to produce the solution depends on the length of the simulation period, the size of the model, the convergence criterion and the speed of the user's computer.
- To calculate the depletion rates the user must proceed as follows:
  - Run the model without the inclusion of the pumping well for which the impact is to be quantified.
  - Press the button "Import results with no abstraction". The results will be copied to the "No Pumping Results" worksheet automatically.
  - Run the model including the abstraction well under investigation.
  - Press the button "Import results with abstraction". The results will be copied to the "Pumping Results" worksheet automatically.
  - Press the button "Calculate depletion rates" and the "Depletion Rates" worksheet will be updated automatically.

- In the “Depletion Rates” worksheet, select Column E and those to the right of it. Create an x-y scatter plot of the depletion rates (Figure 22). For each river reach defined in the “Monitoring Points” worksheet one column of data will have been written to the right of Column E in the “Depletion Rates” worksheet. Note that a message will pop up preventing the addition of the graph to the active worksheet. Proceeding by pressing OK will allow the insertion of the graph as a new worksheet.

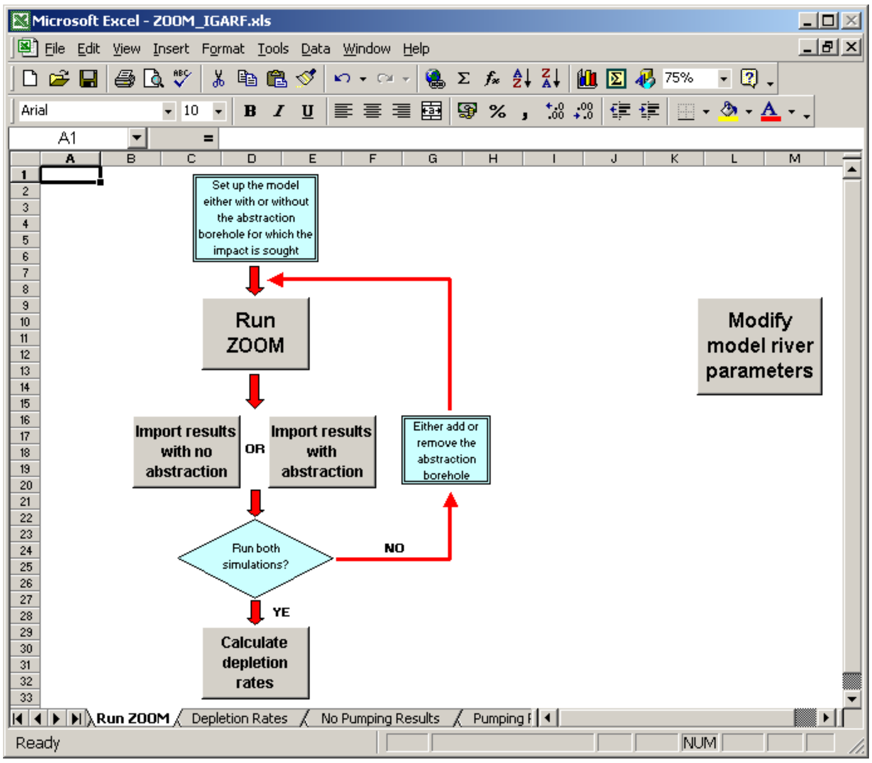


Figure 21 The “Run ZOOM” worksheet

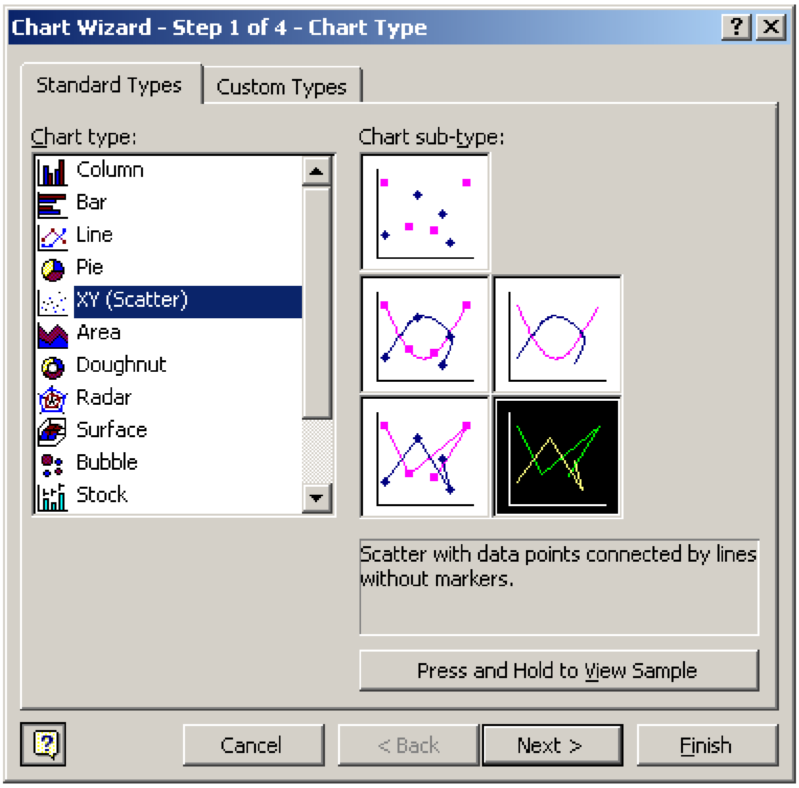


Figure 22 Selection of XY (Scatter) plot used to plot depletion rates

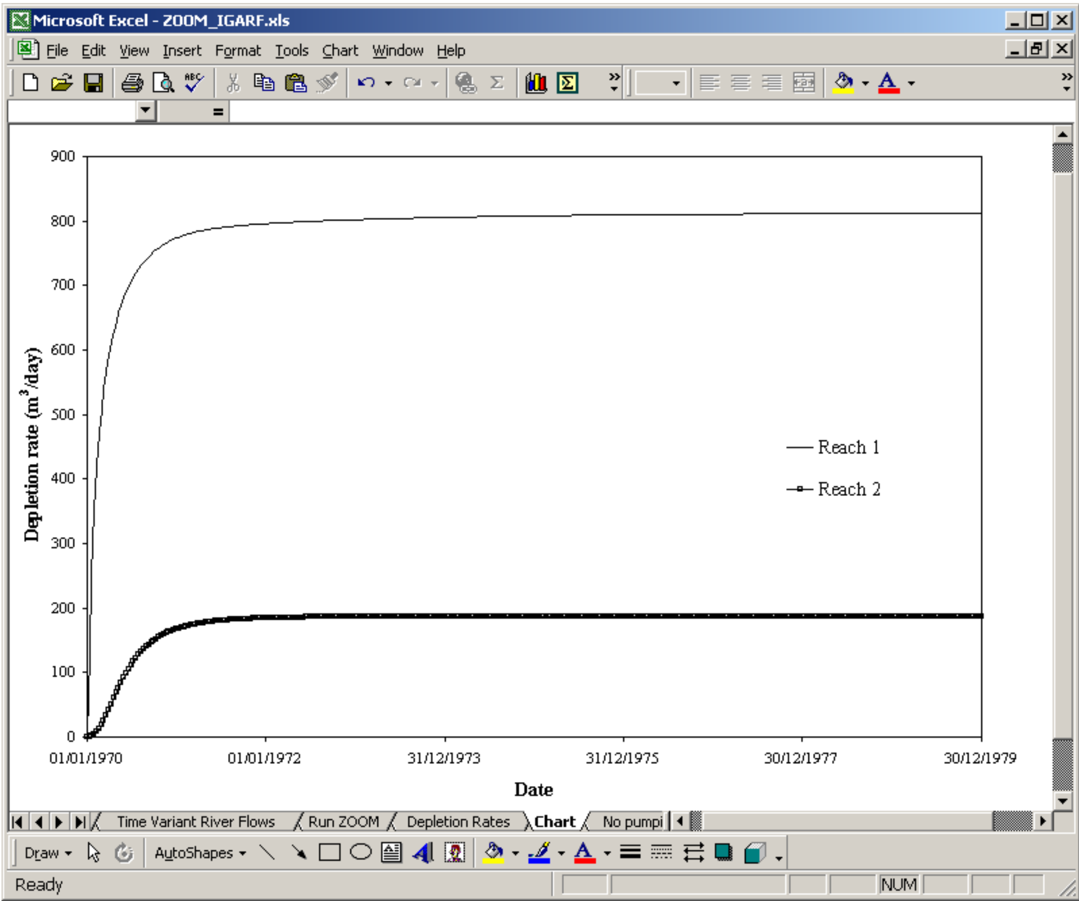


Figure 23 Example plot of depletion rates along two reaches

4 Using ArcView to add complex rivers

4.1 BACKGROUND

After the user has entered data into the "Rivers" worksheet (Figure 24) the button "Run ZETUP" must be pressed. This runs the program, which constructs the model mesh and the model rivers. On pressing this button the user is presented with a Console Application Window (DOS Box) similar to that shown in Figure 24. The user must answer 'y' (yes) or 'n' (no) to the question "Add a river? (y or n)". If the user answers 'y', the name of the file containing the point information for one of the rivers in the model must be entered. These text files are referred to as "spline" files. When straight line rivers are created using the Excel worksheet as shown in Figure 24, these files are created automatically and given the name "River##_SplinePts.dat" where ## represents the two digit ID number of the river (01 to 99). If the user needs to create more complicated, for example dendritic, rivers these text files must be created manually. To simplify this process a routine has been developed using ArcView and a bespoke Windows application that assists the user in performing this task.

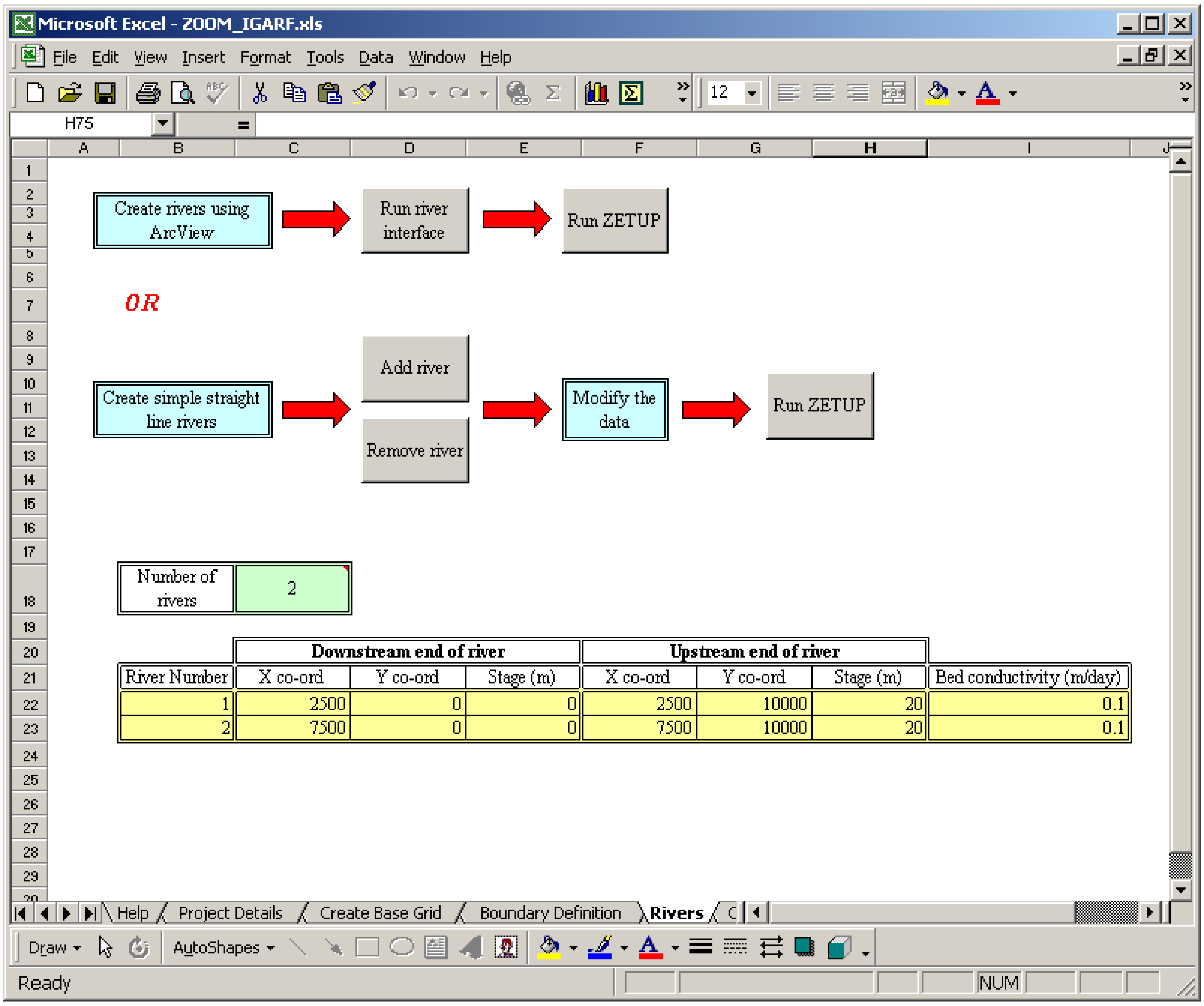


Figure 24 The "Rivers" worksheet

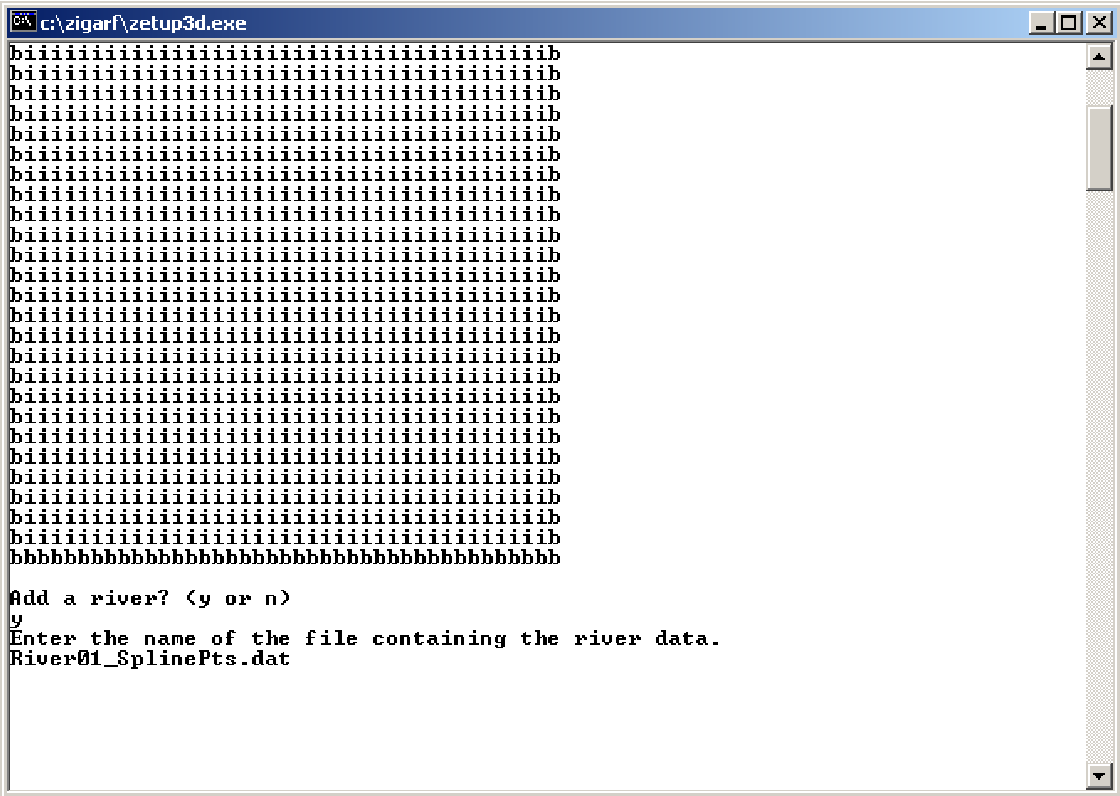


Figure 25 Entry of river spline file name to ZETUP during execution

A technique is implemented in ZETUP and ZOOMQ3D that differentiates between *model* rivers and the structures (objects) that describe their real geometry and characteristics. Information is defined in ZETUP to represent the real structure of rivers. This data is read into the program using the text *spline* files, which the user must create for non-straight line rivers. The objects describing the shape and connectivity of the river channels are termed 'maps' of the basin. When the mesh is created, the river maps examine the grid structure and use it to construct the numerical model's rivers on the finite difference grid. This process is described briefly in this section. First the representation of rivers as 'maps' is described.

4.1.1 Approximating reality: rivers and splines

This sub-section illustrates how rivers are represented in ZETUP, how they are translated into the form required by ZOOMQ3D. Rivers are represented within ZETUP by structures that aim to represent their real geometry closely. Three types of structures (or objects) are defined to represent real rivers. These are termed *catchment maps*, *river maps* and *river branches.* Catchment maps store and manage a number of river maps, which are composed of one or more river branches. The hierarchy is shown in Figure 26. The objects are described as follows:

Catchment map: A catchment map is a collection of river maps.

River map: A river map is composed of a series of polylines (or splines) that describe the geometry of the channels within a dendritic river basin i.e. the main river channel and all its tributaries. In addition to describing the geometry of the basin, river maps store data relating to the physical and hydraulic characteristics of the channels at specific points along their length. **A river map cannot represent two separate river basins i.e. all the channels within a river map must be connected**. River maps are referenced using a unique integer number.

River branch: Either the main channel of a river basin or one of its tributaries. A numbering scheme must be adopted in which the upstream branches have a higher value. The main channel is assigned number 1. A river branch is one of the polylines forming the river map.

River parameter information is specified at user-defined points along each river branch. This data has to be entered into the text spline files that the program ZETUP reads. ZETUP reads this point information and creates the numerical representation of the rivers on the finite difference mesh. For example Figure 27a shows a dendritic river system, each branch of which is defined by a series of points. ZETUP draws a smooth curve, or *spline*, through the points and then uses this curve to create the model rivers, which for this case are shown in Figure 27b. **Reiterating, it is these text files containing the point information along the rivers that the user has to create. The Excel spreadsheet, "ZOOM_IGARF.xls" performs this task for the user for straight-line rivers, however, for more complex rivers ArcView and the utility CREATE_RIVER_SPLINES must be used.**

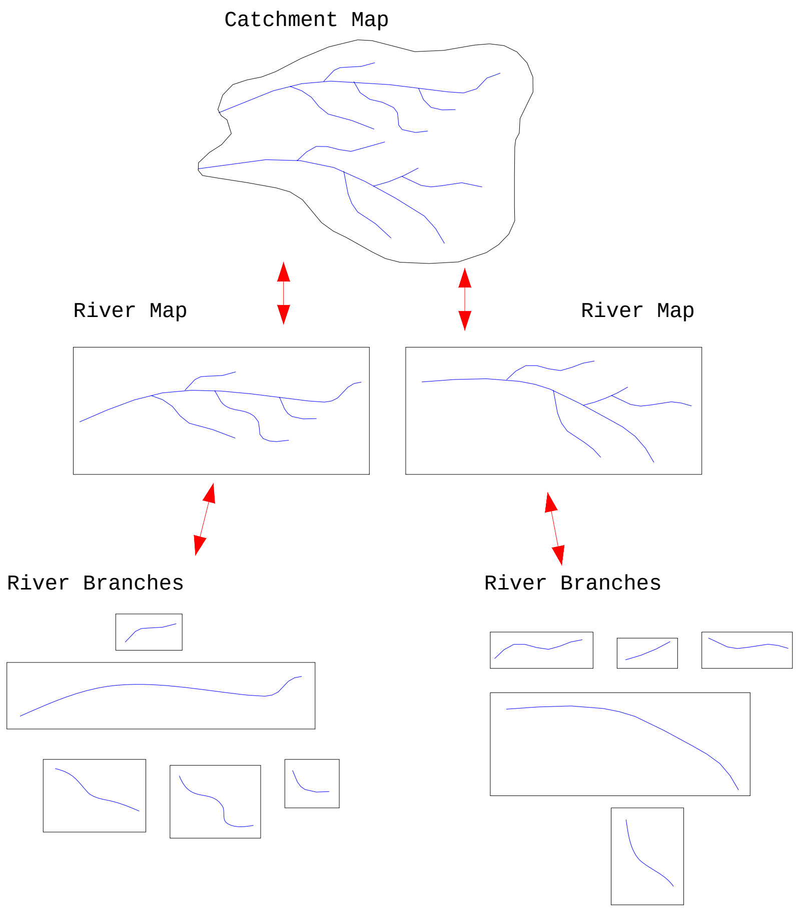


Figure 26 Representation of real rivers as catchment map, river map and river branch objects

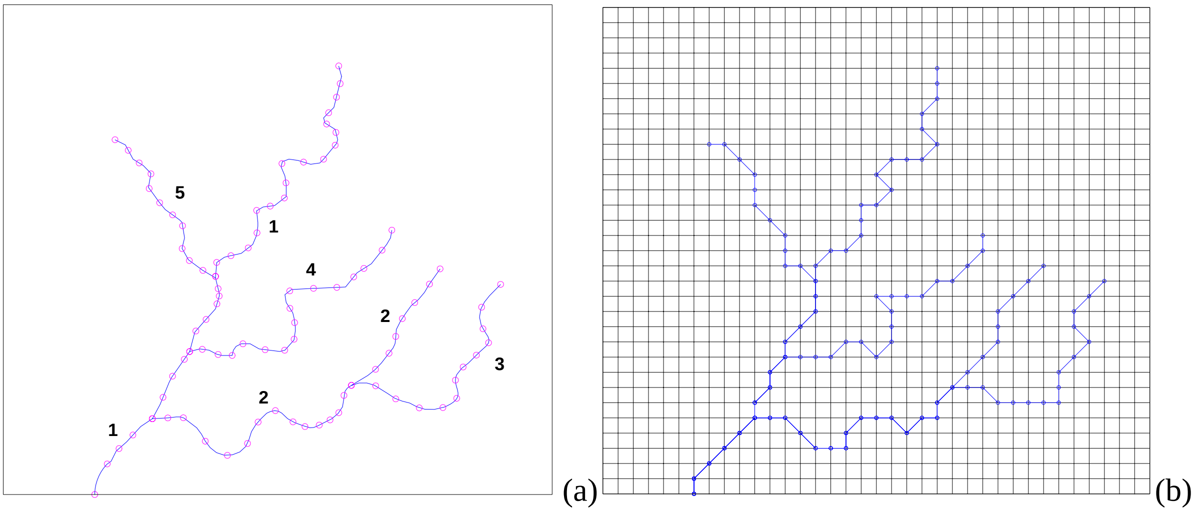


Figure 27 (a) Definition of spline points along a river and branch numbers and (b) model rivers after construction on finite difference mesh

Each river branch is defined by its associated spline points and the data at these locations. In Figure 27a there are five river branches, numbered as shown. Branch 1 is the main river channel. **A numbering scheme must be adopted in which the upstream branches have a higher value. Similarly, for each branch, spline points are numbered from downstream to upstream. Spline points must be defined at the ends of the branches and at the confluence of two or more channels. A spline point at a confluence exists on all the tributaries flowing to this point (and has to be defined on each branch within the river map input file).**

4.2 TRANSLATING ZETUP'S RIVER MAPS INTO ZOOMQ3D RIVERS

After the river maps have been created and the real rivers approximated by splines, the maps are used to generate the rivers required by the *simulation* model, ZOOMQ3D.

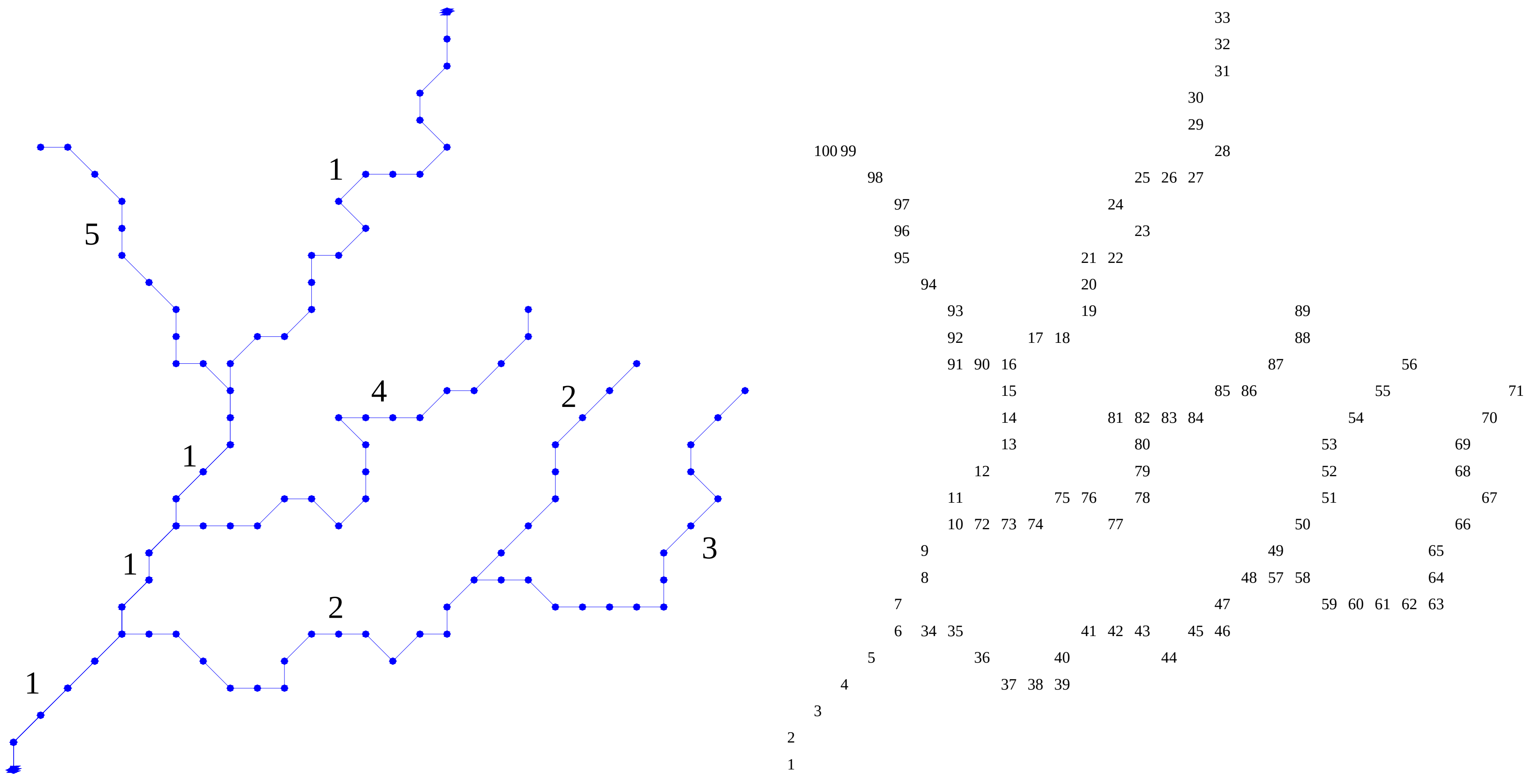
ZOOMQ3D can simulate the baseflow within dendritic river basins. Both the baseflow along the river and the interaction between the river and the aquifer are modelled. The structure of the numerical model rivers within ZOOMQ3D is described using three terms: rivers, branches and river nodes, which have the following definition:

> *Rivers*: a river is composed of both an interconnected series of river branches and a interconnected series of river nodes. **A river cannot be composed of two sets of interconnected river nodes that are not themselves connected, i.e. a river cannot represent multiple separate catchments**. ZOOMQ3D rivers represent the translation of a ZETUP river map onto the finite difference grid.
>
> *Branch*: a branch represents the main channel in a catchment or a tributary within the river (catchment). Only dendritic river catchments can be modelled and consequently, each branch has one node at its upstream end and one node at its downstream end.
>
> *River node*: a river node represents a point on the river that coincides with a horizontal point of the finite difference mesh. The characteristics of the river are defined at each river node. A river node can have up to five upstream connections to river nodes but only one downstream connection.

Branches and river nodes are organised in a specific order described by a numbering scheme. **For river branches a numbering scheme is implemented in which the upstream branches have a higher integer value (Figure 28a)**. This numbering scheme is defined by the river map file containing the spline point data. **River node numbers also increase upstream and from low branch numbers to high branch numbers (Figure 28b)**. The river node at the bottom of the catchment is number 1.

As stated above, model rivers are represented by a series of linked river nodes, which are also connected with upper most active aquifer node as illustrated in Figure 29. Each river node is located at the centre of the reach that it represents. The limits of a reach are the mid-points between the central river node and its adjacent river nodes. River nodes are characterised by the following set of parameters:

- Location specified by x and y co-ordinates.
- Channel width (m). This is set to 1 when "ZOOM_IGARF.xls" and its associated utilities are used.
- Reach length (m). Equivalent to the half the straight-line distance between the adjacent two river nodes.
- River stage (m).
- River-bed elevation (m). This is set equal to the river stage when using "ZOOM_IGARF.xls" and it associated utilities.
- River-bed thickness (m). This is set equal to 1 m when using "ZOOM_IGARF.xls" and it associated utilities.
- Vertical hydraulic permeability (m day^{-1}). Different values for hydraulic conductivity can be specified for influent and effluent river conditions in ZOOMQ3D, however, these are set equal when "ZOOM_IGARF.xls" and its associated utilities are used.



(a) (b)

Figure 28 Numbering schemes in ZOOMQ3D for (a) river branches and (b) river nodes for an example model river

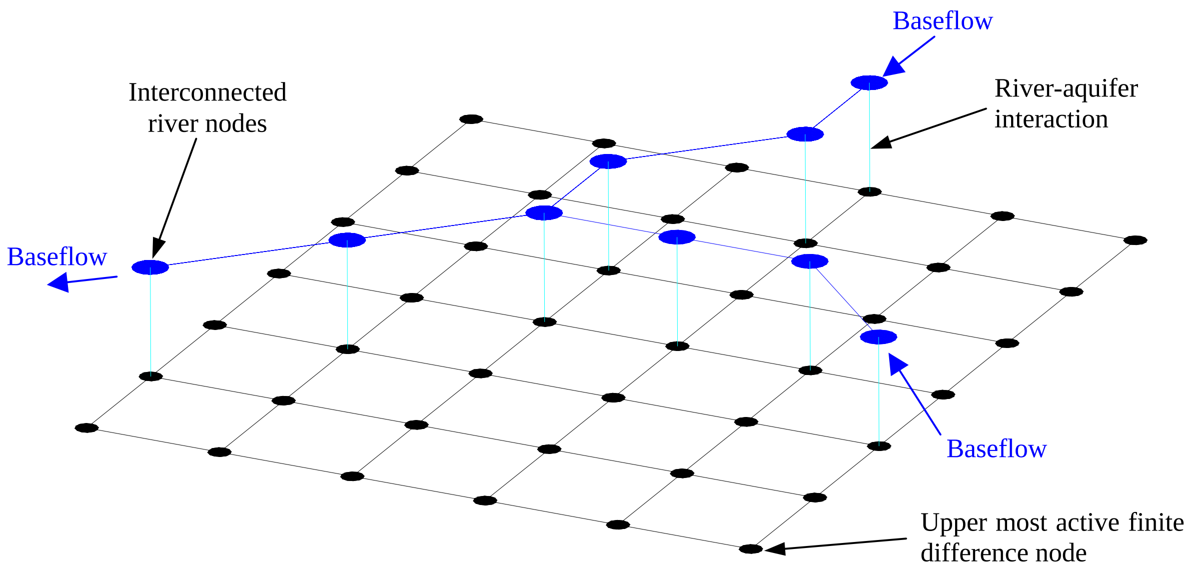


Figure 29 Schematic representation of connections between river nodes and grid nodes

4.3 USING ARCVIEW AND THE CREATE_RIVER_SPLINES APPLICATION

A Window application "CREATE_RIVER_SPLINES" is used in conjunction with ArcView to create the text files containing the river information required by ZETUP. The Windows application is used to number the rivers and branches, to link the nodes along each branch, to link the branches of each river and to produce the text files required by ZETUP. These files are then processed by ZETUP to translate the rivers onto the finite difference mesh.

4.3.1 Using ArcView to generate river data

There are four steps required to produce the spline files.

- Use ArcView to create polylines representing the shapes of the rivers.
- Use the ArcView extension "poly2pts" to convert the polylines to a series of points.
- Use the CREATE_RIVER_SPLINES Windows application to number and connect the points along the branches of the rivers.
- Export the spline files.

4.3.1.1 Using ArcView to create rivers

Set up a simple project that includes:

- A polyline shape file of the rivers
- A shape file of the model boundary
- A DTM (gridded theme)

Ensure that the following extensions are installed:

- Cad Reader
- Geoprocessing
- Graticules and measured grids
- Grid analyst

- Spatial analyst
- poly2pts. This is not a standard extension. If it has not been provided it can be downloaded from the ESRI web site. It converts polylines into series of points.

Start a new ArcView project:

- Add the river, boundary and DTM themes to your project using View->Add Theme.
- If the DTM information is available as ASCII data, import it into the project as follows:
    - File->Import data source
    - Select ASCII Raster
    - Select data file
- Use the Clip feature in the Geoprocessing Wizard in ArcView to produce a shape file in which all river polylines fall within the model boundary.
    - From View->GeoProcessing Wizard select "Clip one theme based on another"
    - Press "Next" and select the river shape file as the input theme and the model boundary as the polygon overlay theme
- Select the new tidied up river theme.
- Select "Theme-> Convert to points" to create a new shapefile containing only points along the rivers (N.B. the poly2pts extension must have been added).
    - Select an interval for the laying out points e.g. 250 m.
    - Select a file name for the new shape file
- The newly created point theme can be edited and tidied where it appears too complicated, however, this can also be performed at a later stage.
- Next extract the elevation of these points from the DTM. Select the new point theme and choose "Grid Analyst->Extract X, Y and Z values for Point theme from Grid theme".
- Open the table associated with the river point theme and export the data "File->Export data source". Modify the exported data file using Excel and a text editor to produce a space separated file containing the three columns X, Y and Z for each point in the river point theme. Z is the elevation of the DTM at the x, y point.
- Save the new file as a "tab delimited" text file and call it "GISRivers.dat"

4.3.2 Using the Windows application to create the river input files for ZETUP

The CREATE_RIVER_SPLINES Windows application is composed of three main parts: the display window, a menu bar and a toolbar (Figure 30). The display window is used to number and connect the river points. The menu bar allows the selection of the functions used to manipulate the points in the display window. The tool bar provides the user with some specific functions that can be selected quickly.

When the Windows application is launched from the Excel worksheet, the text file "GISRivers.dat" is read and the points produced by ArcView displayed as illustrated in Figure 30. The menu bar is used to define the rivers and branches, to link the nodes and to connect the branches. Three steps are required to complete any of these operations. These are: "Select number", "Start associating nodes", "Stop associating nodes" (Figure 30). The Windows application can be used to zoom to a window, zoom to all, to draw individual or all the rivers, and to delete river nodes or their connections. These functions can also be accessed from the toolbar.

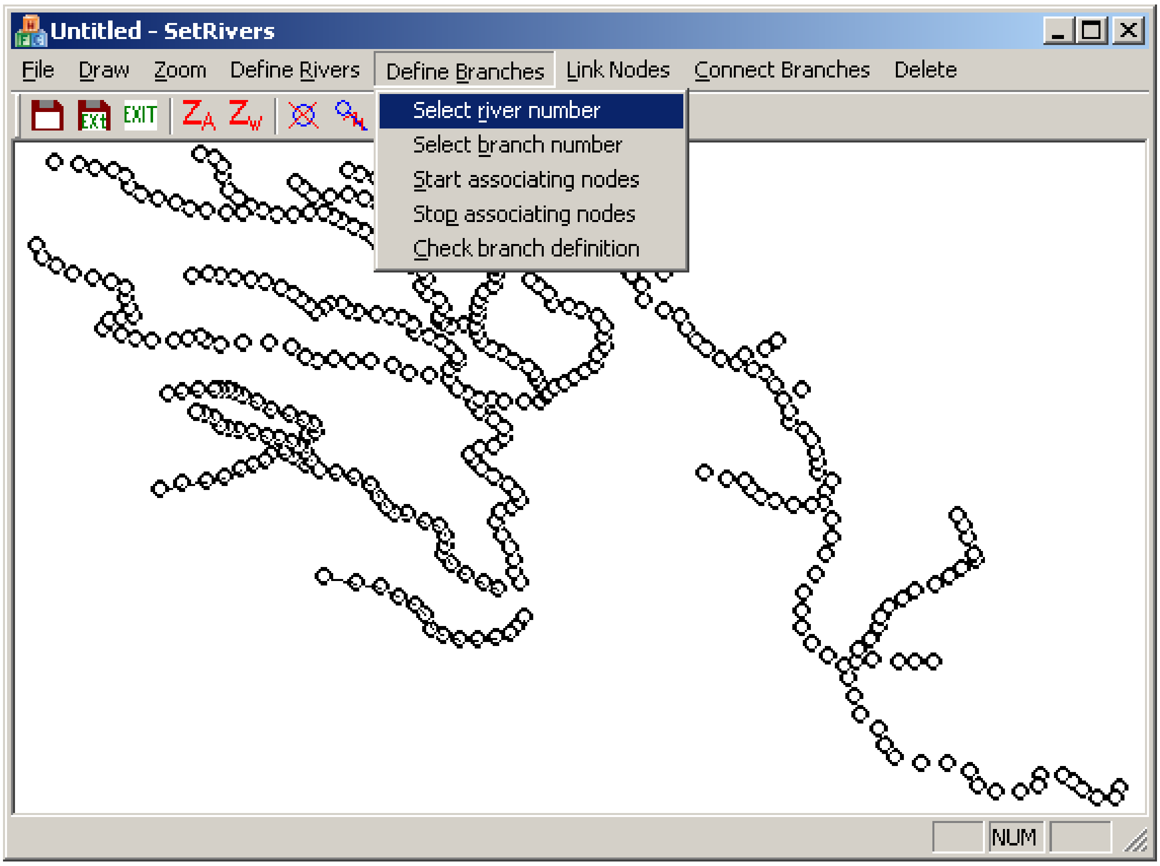


Figure 30 Display of the spline points before numbering and linking

To define a ID number of a river select “Define Rivers” from the menu then:

- Select “Select river number” and enter the river number.
- Select “Start associating nodes”. Draw (click and drag) a box around the nodes to be included in the river.
- Select “Stop associating nodes” when finished.
- Repeat for each river (connected set of points).
- You can check that all the nodes have been assigned to a river by selecting “Check river definition”.

The perimeter of the circles representing the river nodes change colour according to the river number they belong to. The circle is filled with a colour that indicates the branch number the river node belongs to (Figure 31). To define the branch numbers of a river select “Define Branches” from the menu then:

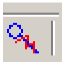
- Select “Select river number”. Enter the river number. Only the selected river is displayed.
- Select “Select branch number”. Enter the branch number.
- Select “Start associating nodes”. Draw (click and drag) a window around the nodes to be included in the selected branch.
- Repeat for each river branch in the selected river

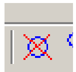
- Select “Stop associating nodes” when finished.

You can check that all the nodes have been assigned a branch number by selecting “Check branch definition”.

To link the nodes of a river branch select “Link Nodes” from the menu then:

- Select “Select river and branch”. Enter the river number and the branch number. Only the selected branch is displayed.
- Select “Start linking nodes”.
- A popup dialog box will appear asking the user to double click on the downstream node of the branch.
- Start linking the nodes by drawing a box (click and drag) around the nodes to be linked:
    - The box should include the downstream node or one node that is linked to its downstream node.
    - The window cannot include more than one node that has already been linked.
- Select “Stop linking nodes” when finished.

It is possible to unlink all the nodes in a branch by selecting “Clear node links of branch” under the “Link Nodes” menu option. Separate links can be deleted by pressing the button  on the toolbar or by selecting “Delete connection” from “Delete” and then double clicking on the node whose downstream link is to be deleted.

It is also possible to delete nodes if required. This can be done by pressing the button  on the toolbar or by selecting “Delete node” from “Delete” and then double clicking on the node to be deleted.

After completing the river and branch definition and linking process, the spline files can be produced. Select “Write spline file” from the “File” menu option. This will create a separate spline file for each river defined in the Windows application named “River##_SplinePts.dat” where ## represents the river ID number.

The toolbar allows the following operations:

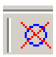
 Save work as you progress.

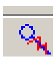
Save work and exit the Windows application.

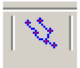
Exit the Windows application without saving.

Zoom all. The display is enlarged to include all the rivers though not all the rivers are necessarily plotted.

Zoom to a selected window.

 Delete a node. Press this button then double click the node to delete.

 Delete a connection. Press this button and double click the node whose downstream link is to be deleted.



Draw all rivers. All the rivers within the current display are plotted.

Gives the river and branch number at a node

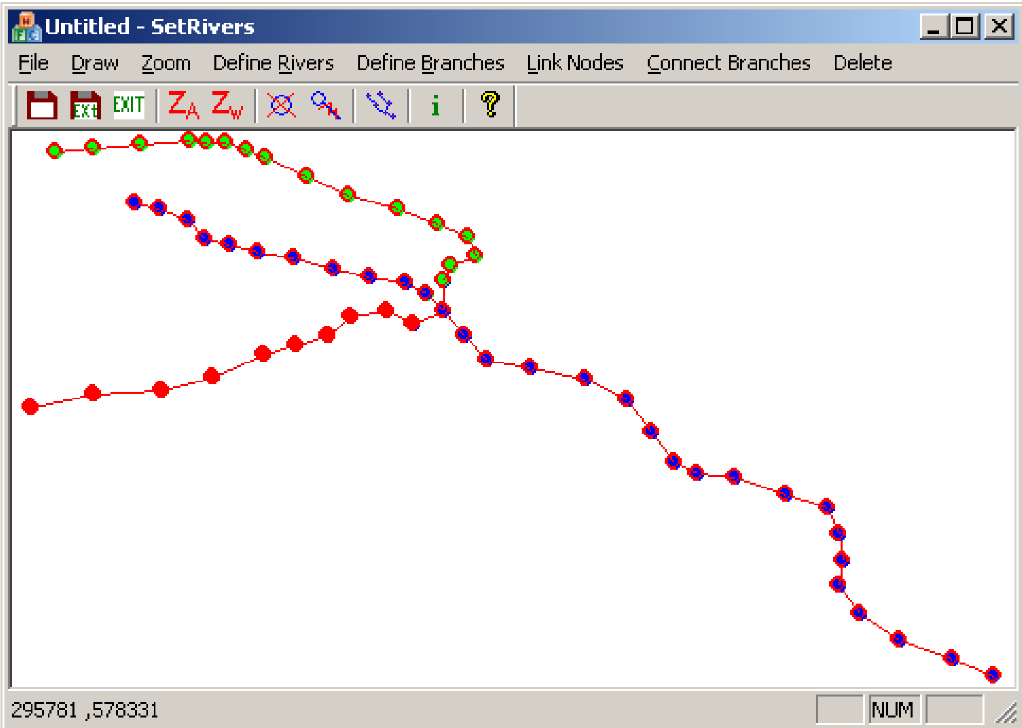


Figure 31 Display of one river after numbering the rivers and numbering and linking the branches

5 Modifying model river parameters

The river spline text files, produced using the "CREATE_RIVER_SPLINES" Windows application, are processed by "ZETUP" to produce the model rivers that are linked to the finite difference mesh. ZETUP produces the file text file "rivers.dat", which contains all the model river information. The hydraulic parameters of the model river nodes are set to the default values listed in Table 2. For simplicity only the river bed hydraulic conductivity and river stage can be modified without manually editing the text file. The bed permeability and river stage at each river node can be modified using the Windows application MODIFY_MODEL_RIVERS, which is run from the worksheet "Run ZOOM" in the Excel tool "ZOOM_IGARF.xls". This program modifies the ZOOMQ3D input file "rivers.dat".

Table 2 Model river node parameters

River node parameter	**Value**
Channel width (m)	Set to 1 m
Reach length (m)	Determined by the mesh spacing
River stage(m)	Set by the user
River bed elevation (m)	Set equal to the river stage
River bed thickness (m)	Set to 1 m
River bed hydraulic conductivity (m day^{-1})	Set by the user.

This application has a display window and a menu bar with one function only. This is to save the work and to exit. When the application is launched, the data file "rivers.dat" produced by "ZETUP" is read and the river networks are drawn in the display window (Figure 32). The values of the parameters at the nodes can then be modified. To adjust the parameter values at one node double click on it. A dialog box will then popup showing the co-ordinates of the node and the values of the river stage and the bed conductivity (Figure 33a). The river stage and bed conductivity can then be edited in this dialog box.

To adjust the parameter values of a set of nodes the user must draw (click and drag) a box around the relevant nodes. A dialog box will popup and show the number of nodes selected and values of zero for the bed conductance and the river stage (Figure 33b). Care should be taken at this stage because pressing "OK" will set the parameter values to zero at the selected nodes. If the selection is not correct "Cancel" should be used. Enter the new parameter values in the dialog box and press "OK".

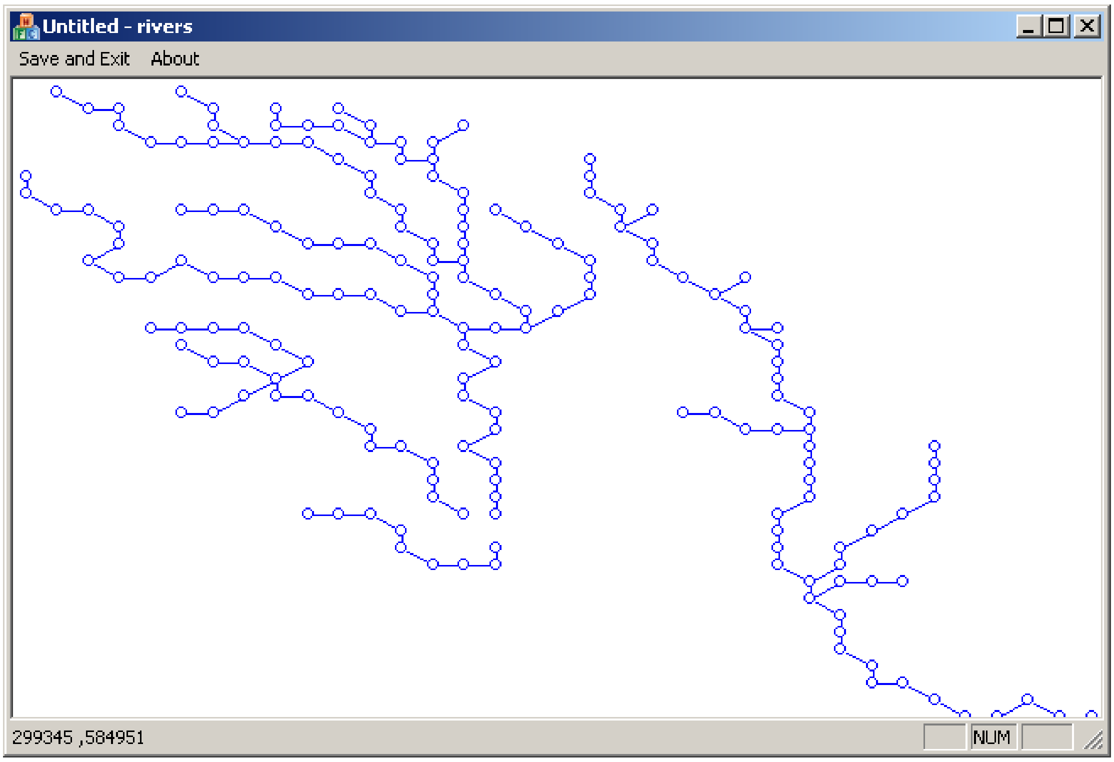
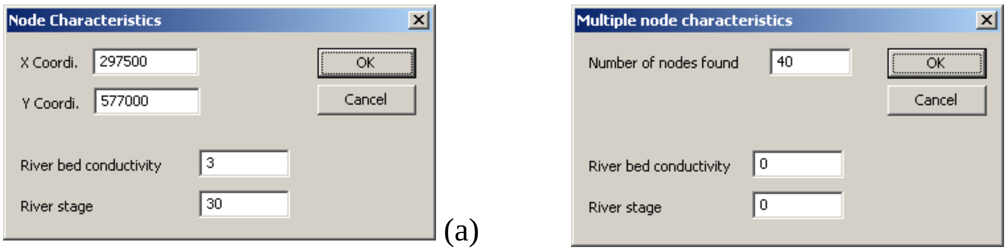


Figure 32 Display of the river network produced by "ZETUP"



(a) (b)

Figure 33 Dialog box for changing the characteristics of (a) one node and (b) multiple nodes

6 References

GOLDEN SOFTWARE INC (1994). Surfer for Windows. User's Guide. Golden Software Inc, Colorado.

Appendix A Summary of ZOOM text output files

A1 THE PHILOSOPHY OF MODEL OUTPUT

The philosophy behind the structure of ZOOMQ3D model output is to separate different types of data between files. That is, each file contains one specific type of information only. This simplifies the post-processing of model output and means that standard software packages can be used to interpret and visualise results. All the output files are ASCII text files with a very simple format. They are easily examined using a text editor or processed using spreadsheet software.

The list of output files produced by ZOOMQ3D is presented in Table 3, though not all of these are always produced. For example, if no rivers are included the model, three fewer files are created. Each of the ZOOMQ3D output files is described in the following section.

Table 3 List of all ZOOMQ3D output files

Model feature	Relevant file names
Groundwater heads	
1. Over time	obswells.out
2. For restarting model	finalh.out
3. For contouring	contour.txt
Rivers	gauging_stations.out, accretion.out*, riverflow.out*
Water balances	
1. Global water balances	global.out, global_tv.out
2. Nodal flow balances	flowbal.out*
De-watering and re-wetting	dewatering.out
Progress of solution	zoomq3d.out, transcycle.out

N.B. Files appended with an asterisk (*) are tab delimited

A2 PROCESSING MODEL OUTPUT

Model output is readily processed and visualised using spreadsheet software, Surfer (Golden Software Inc., 1994) and a text editor. Because each model file contains only one type of data, the user is not required to extract information from many different locations within a single file. All text files are space delimited except for three that are tab delimited. These three files are identified in Table 3.

A3 DESCRIPTION OF OUTPUT FILE FORMATS

The format of each of the files listed in Table 3 is described in detail in the following sub-sections.

A3.1 Observation well data

The nodes at which groundwater head is monitored over time are specified in the input file named in the file 'zoomq3d.dat', for example 'obswells.dat'. The time versus groundwater head record at these nodes is output to the file also named in 'zoomq3d.dat', for example 'obswells.out'. This output file contains one line of data for each time-step of the simulation with the following format

`day stress_period block time_elapsed` h_1 h_2 h_3 h_4 … h_n

where

`day` is the end of the day when the flow was recorded, `stress period` is the stress period number,

`block` is the time block number of the flow measurement,

`time_elapsed` is the time simulated since the beginning of the model run,

h_1 is the head (m) in the first observation well defined in ‘obswells.dat’,

h_2 is the head (m) in the second observation well defined in ‘obswells.dat’,

h_n is the head (m) in the nth observation well defined in ‘obswell.dat’.

The output file is space delimited and is easily opened using spreadsheet software, which can be used to produce groundwater head hydrographs.

A3.2 Contouring groundwater heads

The computed groundwater heads are written to an output file in a format suitable for contouring. The name of the output file is specified in the input file ‘zoomq3d.dat’. This output file, for example ‘contour.txt’ contains groundwater head data for a single time-step only and is over-written periodically during the simulation. The frequency with which the file is produced is defined in the input file ‘clock.dat’. Each time it is written, the previous data set is lost. However, groundwater head data, in this format, can be saved by specifying the times of interest in the input file ‘contour_times.dat’.

The format of this output file is simple and is suitable for contouring using Surfer (Golden Software Inc., 1994). The groundwater head at each horizontal location is written on a separate line. The file has the following format

$$x \quad y \quad h_1 \quad h_2 \quad h_3 \quad \ldots \quad h_n$$

where

x is the x co-ordinate of the grid point,

y is the y co-ordinate of the grid point,

h_i is the groundwater head in the ith layer.

If a node is dry the groundwater head value is replaced by –999.

ZETUP produces a Surfer (Golden Software Inc., 1994) blanking file, which can be used to blank the data around the boundary of the model when contouring. This file is called ‘boundary.bln’.

A3.3 Groundwater heads in format to re-start a simulation

Groundwater heads are written to an output file in a format that enables a model run to be re-started from conditions modelled during the current simulation. The name of this output file, for example ‘finalh.out’, is specified in the input file ‘zoomq3d.dat’. It contains the groundwater head at each node of the model at the end of a single time-step and is over-written periodically during the simulation. The frequency with which the file is produced is defined in ‘clock.dat’. Each time it is written, the previous data set is lost.

In order to use this output file to re-start a simulation it is necessary to rename it ‘initialh.dat’ and change the character flag on the following line in the input file ‘clock.dat’ to a ‘t’ for true:

```
Rerunning t(true) of f(false)
t
```

A3.4 River flow gauging

The river nodes at which the baseflow is monitored over time are specified in the input file named in the file 'zoomq3d.dat', for example 'gauging_stations.dat'. The time-discharge record at these nodes is output to the file also named in 'zoomq3d.dat', for example 'gauging_stations.out'. This output file contains one line of data for each time-step of the simulation with the following format

`day  month  year time_elapsed` Q_1 Q_2 Q_3 Q_4 … Q_n

where

`day` is the end of the day when the flow was recorded,

`month` is the month number,

`year` is the year number of the flow measurement,

`time_elapsed` is the time simulated since the beginning of the model run,

Q_1 is the flow (m^3 day^{-1}) in the first river node defined in 'gauging_stations.dat',

Q_2 is the flow (m^3 day^{-1}) in the second river node defined in 'gauging_stations.dat',

Q_n is the flow (m^3 day^{-1}) in the n^{th} river node defined in 'gauging_stations.dat'.

The river nodes are listed in the same order as they are defined in the input file. The output file is space delimited and is easily opened using spreadsheet software, which can be used to produce river baseflow hydrographs.

A3.5 River baseflow accretion profiles

River baseflow (not total flow) accretion data is written to the output file named in 'zoomq3d.dat', for example 'accretion.out'. The data is in a form suitable for the rapid production of accretion profiles using spreadsheet software. This output file contains flow data for a single time-step only and is over-written periodically during the simulation. The frequency with which the file is produced is defined in the input file 'clock.dat'. Each time it is written, the previous data set is lost. Accretion profiles at different times can be saved by specifying each node along the river section of interest as a gauging station in the relevant input file.

The output file is tab delimited and has a simple format. An example output file is shown in Figure 34. The number of rivers in the model is written on the first line. A block of data then follows for each river. Eleven columns of data are defined within each block, which are separated by comment lines composed of a series of dashes. Each row represents one node of the river. The eleven columns contain the following data:

1. River branch number.
2. River node number.
3. x co-ordinate of river node (m).
4. y co-ordinate of river node (m).
5. Distance downstream from uppermost node in branch (m).
6. Baseflow ($m^3 day^{-1}$).
7. Groundwater head (m).
8. River stage (m).

9. River bed elevation (m).

10. River bed vertical hydraulic conductivity under effluent conditions (m day^{-1}).

11. River bed vertical hydraulic conductivity under influent conditions (m day^{-1}).

A3.6 River baseflows in a format to re-start a simulation

River baseflows are written to an output file in a format that enables a model run to be re-started from conditions modelled during the current simulation. The name of this output file, for example ‘riverflow.out’, is specified in the input file ‘zoomq3d.dat’. It contains the river baseflow at each node each river in the model at the end of a single time-step and is over-written periodically during the simulation. The frequency with which the file is produced is defined in ‘clock.dat’. Each time it is written, the previous data set is lost.

The file has exactly the same format as the input file ‘riverflow.dat’, which is used to define initial river baseflow conditions. Consequently, in order to use this output file to re-start a simulation it is only necessary to rename it ‘riverflow.dat’.

```
2
----------------------
River 1
Branch   Node   X        Y        Dist.downstream   Flow      Head    Stage   Bed Elevation   Kz Effluent   Kz Influent
1        9      294500   572500   0                 5765.87   7.80    7.5     6.5             1             1
1        8      295000   572500   500               5931.98   7.53    7.5     6.5             1             1
1        7      295500   572500   1000              7050.44   7.68    7.5     6.5             1             1
1        6      296000   572000   1707.11           7362.65   7.54    7.49    6.49            1             1
1        5      296000   571500   2207.11           8172.72   7.35    7.21    6.21            1             1
         etc for each node in each branch of river 1
----------------------
River 2
Branch   Node   X        Y        Dist.downstream   Flow      Head    Stage   Bed Elevation   Kz Effluent   Kz Influent
1        14     292500   575500   0                 12500     32.69   68      67              1             1
1        13     293000   575500   500               17239.4   16.42   16.03   15.03           1             1
1        12     293500   576000   1207.11           21484.3   8.85    8.55    7.55            1             1
1        11     294000   576500   1914.21           31937.7   7.09    7       6               1             1
1        10     294000   576000   2414.21           32773.8   8.08    8       7               1             1
1        9      294500   576000   2914.21           36011.6   6.36    6.09    5.09            1             1
         etc for each node in branch 1 of river 1
2        20     292000   578000   0                 2000      22.12   37      36              1             1
2        19     292500   578000   500               0         21.7    36      35              1             1
2        18     293000   578000   1000              0         17.13   33.53   32.53           1             1
         etc for each node in branch 2 of river 1
```

Figure 34 Example output file containing river baseflow accretion data

A3.7 De-watering and re-wetting

At the end of each time-step information is written to the file ‘dewatering.out’ informing the user of which nodes have de-watered and which have re-wetted. The layer number and co-ordinate of each of these nodes is written to the file.

A3.8 Nodal flow balances

Nodal flow balance information for every node in the model is written to the file, ‘flowbal.out’, for example, named in the input file ‘zoomq3d.dat’. This output file contains flow balance data for a single time-step only and is over-written periodically during the simulation. The frequency with which the file is produced is defined in the input file ‘clock.dat’. It is always re-written at the end of the simulation. The first line of the file is a text string that specifies the time at which information is output. The second line contains the headings for the following columns of data. Each subsequent line represents one node in the model. A description of each column is given in Table 4.

Table 4 Data contained in nodal flow balance output file

Column of file	**Description of data** (Rates of flow are for the last time-step only)
1	Layer of the node
2	x co-ordinate of the node
3	y co-ordinate of the node
4	Area of the node (m^2)
5	Flow imbalance at the node (m^3 day^{-1})
6	Inflow to the node in the x-direction from the left (m^3 day^{-1})
7	Outflow from the node in the x-direction to the right (m^3 day^{-1})
8	Inflow to the node in the y-direction from below (m^3 day^{-1})
9	Outflow from the node in the y-direction to above (m^3 day^{-1})
10	Inflow to the node in the z-direction through the base (m^3 day^{-1})
11	Outflow from the node in the z-direction through the top (m^3 day^{-1})
12	Specified inflow at the boundary (if a boundary node) (m^3 day^{-1})
13	Rate of change of storage at node (m^3 day^{-1}). Positive values are increases in storage.
14	Recharge applied at the node (m^3 day^{-1})
15	Rate of leakage between the aquifer and the river (m^3 day^{-1}) Positive values represent influent river nodes
16	Rate of leakage to a leakage node (m^3 day^{-1}) Positive values represent an outflow from the aquifer
17	Rate of abstraction at the node (m^3 day^{-1}) Abstraction is represented by negative values
18	Spring flow (m^3 day^{-1}) Positive values represent flow of the aquifer (negative values not possible)

A3.8 Global flow balances

Global flow balance information for the model is written to the file 'global.out'. This output file contains flow balance data for a single time-step only and is over-written periodically during the simulation. The frequency with which the file is produced is defined in the input file 'clock.dat'. It is always re-written at the end of the simulation. This file gives a water balance for the whole model over a time-step. An example file is shown in Figure 35. Information includes the total recharge to the model, the total flow across its boundary, the total abstraction, the total downstream flow and anthropogenic input to each river, the total outflow to leakage nodes and fixed heads, the total change in storage over the last time-step and the total spring flow. These flow rates are summed to give a global flow imbalance figure, which is written on the last line of the file.

```
GLOBAL FLOW BALANCE AT END OF 4/12/1974 (TS/SP/BLOCK)
---------------------------------
Total recharge: 192554 m3/d
Total boundary inflow: 0 m3/d
Total abstraction: 32900 m3/d
River 1
 Downstream flow: 8213.6 m3/d
 Anthropogenic input: 5000 m3/d
River 2
 Downstream flow: 48155.2 m3/d
 Anthropogenic input: 32000 m3/d
River 3
 Downstream flow: 1.31088e+006 m3/d
 Anthropogenic input: 1.217e+006 m3/d
River 4
 Downstream flow: 41388 m3/d
 Anthropogenic input: 24000 m3/d
Total leakage out of aquifer: 27884.4 m3/d
Total outflow to fixed heads: 0 m3/d
Total increase in aquifer storage: 19.3241 m3/d
Total spring flow: 1111.31 m3/d

GLOBAL FLOW IMBALANCE: 0.61335 m3/d
```

Figure 35 Example global flow balance output file

A3.9 Time-variant global flow balances

Global flow balance information for every time-step of a simulation is written to the file, 'global_tv.out'. The file contains the columns of data listed in Table 5. One line of data is written to the file per time-step. The file is space delimited and is readily opened using spreadsheet software for manipulation.

Table 5 Data contained in 'global_tv.out'

Column	Description of data
1	Time within stress period (days)
2	Stress period number
3	Block number
4	Time since start of simulation (days)
5	Total recharge (m^3 day^{-1})
6	Total inflow at model boundary (m^3 day^{-1})
7	Total abstraction (m^3 day^{-1})
8	Total outflow from rivers (m^3 day^{-1})
9	Total discharge/inflow to rivers (m^3 day^{-1})
10	Total flow through leakage nodes (m^3 day^{-1}). Positive out of aquifer.
11	Total outflow to fixed head nodes (m^3 day^{-1})
12	Total storage increase (m^3 day^{-1}). Positive values are increases in storage
13	Total spring flow (m^3 day^{-1})
14	Global flow imbalance (m^3 day^{-1})

A3.10 Convergence of solution

Information describing the progress of the solution during each time-step is written to the output file 'zoomq3d.out'. At the end of each user defined number of iterations (the last number entered in 'sor.dat') of the successive over-relaxation solution process the following information is output

- the sum of the absolute values of the flow imbalance (residual) at each model node (m^3 day^{-1}).
- the location of the node with the greatest nodal flow imbalance (residual) and the value of this flow imbalance (m^3 day^{-1}).
- the location of the node where the greatest change in groundwater head occurred during the last iteration.

When the numerical solver converges to the solution for a time-step the global flow imbalance is also written to the output file.

A3.11 Variation in transmissivity

Unconfined conditions are simulated by repeating the solution for a time-step in a cyclical process. At the beginning of each cycle, transmissivity is calculated by integrating the hydraulic conductivity over the saturated thickness of the finite difference nodes. The cyclical process ceases when either the change in transmissivity between cycles is below a user-defined value or after the maximum number of cycles has been performed. The variation in transmissivity (m^2 day^{-1}) over a cycle is written to the output file 'transcycle.out' to that the user can examine the progress of the process. An example 'transcycle.out' file is shown in Figure 36.

```
---- Change in transmissivity for each cycle ----
Time:4  Month:1  Year:1970
 Cycle: 1   Max T Change: 1.25901
 Cycle: 2   Max T Change: 0.502317
---- Change in transmissivity for each cycle ----
Time:10  Month:1  Year:1970
 Cycle: 1   Max T Change: 2.11305
 Cycle: 2   Max T Change: 1.04613
 Cycle: 3   Max T Change: 0.518062
      etc for each time-step
```

Figure 36 Example ‘transcycle.out’ output file