

**MCM<sub>sf</sub> - Mixing-Cell Model for a Steady Flow**  
**MIG - Mixing-Cell Input Generator**

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A Short Manual for Installation and Operation of MCM<sub>sf</sub>  
Using the  
MIG - Mixing-Cell Input Generator

by  
Eilon M. Adar<sup>1</sup> and Christoph Kuells<sup>2</sup>

<sup>1</sup> Department of Environmental Hydrology & Microbiology, Zuckerberg Institute for Water Research, Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede Boqer Campus, 84990, Israel.

<sup>2</sup> Institute of Hydrology, Fahrenbergplatz, 79098 Freiburg, Germany.

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## Preface

The following MIG computer code is restricted to a steady flow and steady hydrochemical flow system. The code for a non-steady hydrological system is still heavily dependent on external optimization libraries, such as the NAG<sup>®</sup> Library. Therefore, a stand-alone "friendly" code or solver for a non-steady system has yet to be compiled. Readers looking to implement the mixing-cell approach in a non-steady hydrological flow system are encouraged to contact the authors.

In order to simplify the procedure of preparing the data and running the Mixing-Cell Model for a steady flow system ( $MCM_{sf}$ ), a special Mixing Input Generator (MIG) has been programmed. MIG is a Visual Basic Microsoft<sup>®</sup> application that runs within Excel<sup>®</sup> (5.0 or newer version) via Windows 95<sup>®</sup> or a newer environment. The program has been tested and used successfully in Windows NT<sup>®</sup>, Windows 95<sup>®</sup>, Windows 98<sup>®</sup> and Windows XP<sup>®</sup>, together with Excel 5.0, 7.0 & 2000. A stand-alone Version  $MIG_{SA}$  that runs on a Windows<sup>®</sup> system without Microsoft Excel<sup>®</sup> is also available. Section 1 provides some clarifications of terms that are used in  $MCM_{sf}$  in the MIG version, and Section 2 briefly reviews the mathematical algorithm. For elaboration of the basic assumptions and for further mathematical description, the user is referred to the explanations provided in the **Model Simplification** and to the references of scientific publications provided in this manual.

# 1 Basic Terminology

## ● Source

The term source refers to any flow component that contributes water and mass of dissolved constituents to any cell within the modeled aquifer. A source is used to represent external inputs into the flow system (for example: sources of groundwater recharge or any genuine contribution from outside the modeled aquifer or any other modeled flow system). It is considered to be a potential end-member with a constant chemical and/or isotopic composition. A source can also be used to simplify part of the modeled system, such that a complex subsystem can be introduced as a *lumped source* of inflow into the modeled area.

## ● Cell

The modeled aquifer is discretized or subdivided into homogeneous compartments within which all the considered parameters are assumed to be constant for a specific time period, such as hydraulic heads, isotopic composition and ionic concentrations. Mixing of various sources or contributors such as from upstream compartments and external sources, and dilution with water already existing in the cell, control the concentration of the characteristic chemicals and the isotopic compositions of each compartment. Therefore, every well-mixed or homogeneous aquifer section (cell or compartment) is characterized by a unique representative chemical concentration and/or isotopic composition.

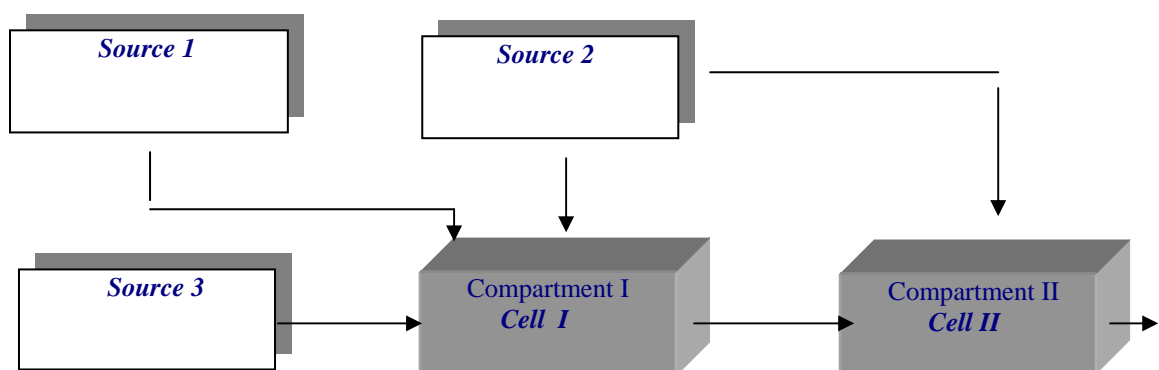


Figure 1. A schematic configuration of the cells

A cell must have input fluxes, either from output flux from an upstream cell, from a source, or from several sources. Each cell must have an output flux, either into a

downstream cell (or cells), via withdrawal of water (i.e. pumping), or via natural subsurface groundwater flow leaving the system, so that the water balance is maintained. Every cell can have a number of sources and can contribute water to several downstream cells. In the example above (Figure 1), cell 1 receives inflows from sources 1, 2 and 3 and contributes output flux to cell 2. Cell 2 receives inflow from source 2 and input flux from cell 1.

Any hydrological connection between two cells will have a unique flow direction. Fluxes into and out of cells are proposed along the downstream hydraulic head gradients. Possible hydraulic connections among cells based on groundwater head gradients are proposed prior to the optimization process, i.e., the assigned flow vector cannot change its direction during the period for which the optimization is performed. As a result of the optimization process a flow rate ( $\geq 0$ ) is attributed to each potential flow component. Some fluxes might end up with an effective rate of 0. This means that this specific component has been considered as a potential contributor, but in reality it is not active and does not contribute a substantial flux into the specific cell. In addition, in cases where a cell is assigned a potential source that has a very similar chemical concentration to another source which was also assigned to the same cell, or has a specific chemical composition that is (or close to) a linear combination of another source, the solver will combine the contribution of these two sources into one. In other words, one of these sources will be given the entire flux of the two, and the other will be assigned zero flux. The solver of this model cannot assign flux values to missing flow components that were not identified or introduced into the model.

## 2 Mathematical description

A set of balance equations for the flux of water and for the associated flux of solutes is written for each cell  $n$  over a given time period  $dt$ . For a simplified flow model of water with a constant density the mass balance for the cell  $n$  is expressed by the following equation:

$$\sum_{r=1}^R Q_{rn} + \sum_{i=1}^I q_{in} - \sum_{j=1}^J q_{nj} - W_n = S_n \frac{dh_n}{dt} \quad (1)$$

The symbol  $Q_{rn}$  denotes  $R$  different sources into cell  $n$ , and  $q_{in}$  denotes the flux from the  $i^{th}$  upstream compartment or cell into the  $n^{th}$  cell. In the above example of a schematic compartmental flow system, for cell  $I$ ,  $I = 0$  (no internal fluxes from upstream cells), and there are 3 external sources,  $r = 1, 2$  and  $3$ . In a similar way,  $q_{nj}$  stands for the outflow from the  $n^{th}$  cell into the  $j^{th}$  one.  $W_n$  accounts for withdrawal of water from cell  $n$ , i.e. a sink term or pumping rate in the  $n^{th}$  cell. The inflows and outflows are iterated over the number of inflows,  $I$ , and the number of outflows,  $J$ , into each cell.  $S_n$  represents the storage capacity within cell  $n$  and  $h_n$  denotes the hydraulic head associated with that cell.

For a steady flow system or for quasi-steady flow over a sufficiently long time interval, an average water balance expression is obtained:

$$\sum_{r=1}^R \bar{Q}_{rn} + \sum_{i=1}^I \bar{q}_{in} - \sum_{j=1}^J \bar{q}_{nj} - \bar{W}_n = \epsilon_n \quad (2)$$

The notations are the same as in Equation 1 except that each term represents the average fluxes for the specific time interval designated with top-bars. An error term,  $\epsilon_n$ , is introduced in order to account for any error associated with either measurements or assessment of the flow system and other deviations from flux balance in cell  $n$ .

For a quasi-steady state variation of the dissolved constituents, the mixing cell concept is applied, based on mass balance expressions for each tracer  $k$  ( $k = 1, 2, \dots, K$ ) in cell  $n$ :

$$\sum_{r=1}^R \overline{C_{rk} Q_{rm}} + \sum_{i=1}^I \overline{C_{ink} q_{in}} - \overline{C_{nk}} \left[ \sum_{j=1}^J \overline{q_{nj}} - \overline{W}_n \right] = \varepsilon_{nk} \quad (3)$$

$\overline{C_{rk} Q_{rm}}$  denotes the average flux of the  $k^{th}$  constituent from source  $r$  into cell  $n$ .  $\overline{q_{in}}$  represents the average flux from the  $i^{th}$  cell into the  $n^{th}$  cell, having an average concentration  $\overline{C_{ink}}$  of solute  $k$ . In equation (3)  $\overline{C_{nk}}$  denotes the concentration of the  $k^{th}$  constituent within cell  $n$  and  $\overline{q_{nj}}$  stands for the average outflow from the  $n^{th}$  cell into the  $j^{th}$  one. The average pumping from the  $n^{th}$  cell during a specific time interval is expressed by  $\overline{W}_n$ , and  $\varepsilon_{nk}$  is the error associated with the mass balance of the  $k^{th}$  constituent or the deviation from the solute balance in cell  $n$ .

Upon combining equations 2 and 3 into a matrix form for each cell  $n$ , the following is obtained:

$$\underline{\underline{C}}_n \underline{X}_n + \underline{P}_n = \underline{E}_n \quad (4)$$

where  $\underline{\underline{C}}_n$  is a matrix with known concentrations in cell  $n$ ,  $\underline{X}_n$  is a vector of the unknown fluxes through the boundaries of cell  $n$ ,  $\underline{P}_n$  is a vector containing elements with known values in cell  $n$  (such as known fluxes of pumping) and  $\underline{E}_n$  the error vector in cell  $n$ . (For further elaboration on Equations 1 to 4, the reader is referred to Adar et al. [1988<sub>a & b</sub>], Adar and Sorek [1989] and Adar [1996]).

By assembling the square error terms over all cells we obtain:

$$J = \sum_{n=1}^N (\underline{E}_n^T \underline{W} \underline{E}_n) = \sum_n (\underline{\underline{C}}_n \underline{X}_n + \underline{P}_n = \underline{E}_n)^T \underline{\underline{\Phi}} (\underline{\underline{C}}_n \underline{X}_n + \underline{P}_n = \underline{E}_n) \quad (5)$$

where  $^T$  denotes transpose and  $\underline{\underline{\Phi}}$  represents a diagonal matrix comprised of weighting values about estimated errors (independent of each other) expected for

each of the terms, which compose the mass balance for the fluid and the dissolved constituents. The weighting matrix  $\underline{W}$  also reflects the degree of confidence to which the tracers are assumed conservative and/or the degree of accuracy of the analyses.

The total flux components in the aquifer can now be estimated by minimizing the sum of square error,  $J$ .

As a result of the mathematical optimization, a flow rate is attributed to each potential flow connection. Depending on the results obtained from the mathematical optimization, the flow model might be changed by modification of the proposed flow pattern and potential sources. Repeated failures of a model optimization scheme indicate a complete disagreement between the hydrogeological and hydrochemical flow pattern versus the proposed set-up of the model. This implies the need for modification of the proposed compartmental flow pattern associated with a possible revision of the assigned set of potential contributors. In some cases, problems with model optimization even necessitate a review of the hydrogeological system analysis, i.e., the definition of compartments and possible flow and hydraulic connections among cells and suggested sources of recharge.



### 3 MIG Program installation and execution

#### 3.1 System requirements

A PC with Windows® operating system (Windows 95® or newer) is needed. **MIG** itself is an Excel® file that contains a number of "macro" routines for processing other Excel® files. Therefore, Excel 5.0® or a newer version is needed, such as Excel 2000®. The language of the system (English, German, International versions) does not seem to make any difference to the program execution. All the comments and commands of **MIG**, however, are in English.

#### 3.2 Installation of MIG

For the installation of **MIG**, the user will need Winzip (or equivalent) decompression utility software.

The installation file *MixCell\_setup.exe* contains the necessary software. The file is an archive containing compressed files. It is recommended to create a folder *c:\mixcel* in which the unzipped files can be stored. You may, however, choose any other folder. Activate (double-click) *MixCell\_setup.exe* to start the decompression. A window belonging to the decompression utility of your computer will open. If Winzip is used the caption 'WinZip Self Extractor - Mixcell\_Setup.exe' will appear (Figure 2).

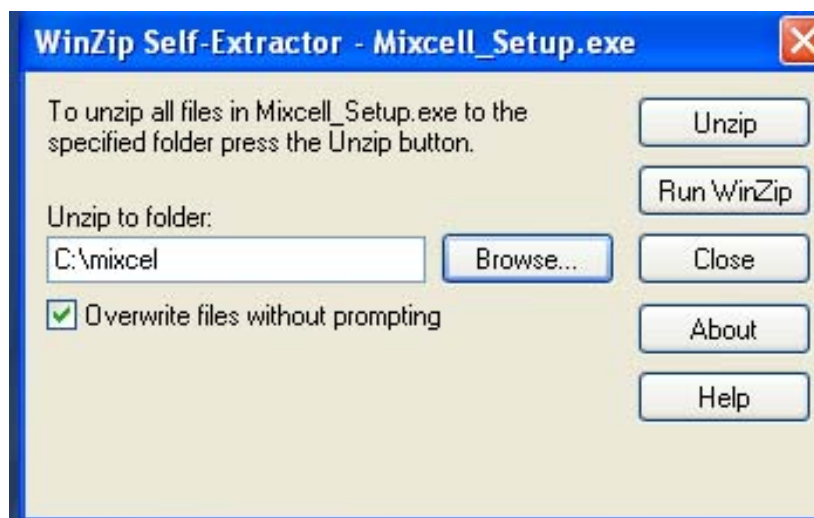


Figure 2. 'WinZip Self Extractor - Mixcell\_Setup.exe'

Please confirm or choose an alternative directory using the 'Browse' button. Clicking the 'Unzip' button will start the extraction of files to be inserted in the selected directory. After extraction of files from the archive, in this directory you will find the following files:

C:\mixcel\**Mig.xls**

C:\mixcel\**Multi.exe**

C:\mixcel\**Data\_1\_5.xls** with two ASCII files: **In15.prn** and **Out15.prn**

C:\mixcel\**Data\_4\_14.xls** with two ASCII files: **In414.prn** and **Out414.prn**

C:\mixcel\**Data\_12\_17.xls** with two ASCII files: **In1217.prn** and **Out1217.prn**

C:\mixcel\**help\_MIG.pdf**

The file **Mig.xls** is an Excel file, which contains a code in Visual Basic that assists the user to prepare the input data for the solver code. The file **Multi.exe** is the optimizer, an executable FORTRAN file that is called by the **MIG** upon the completion of the input data in the appropriate format. The file **help\_MIG.pdf** contains the documentation. Finally, the files **Data\_1\_5.xls**, **Data\_4\_14.xls** and **Data\_12\_17.xls** are example files with hydrochemical data for 1 cell with 5 sources, 4 cells with 14 sources and 12 cells with 17 sources, respectively. The ASCII files (**In15.prn** & **Out15.prn**, **In414.prn** & **Out414.prn**, **In1217.prn** & **Out1217.prn**) are examples of the input files created by **MIG** and results files from the FORTRAN module multi.exe, respectively. After extraction of the data files, **MIG** can be operated directly from the Excel-data-file (see below).

### 3.3 MIG menu structure

**MIG** is a tool for preparing the data in an appropriate format and for producing input files for the FORTRAN solver **Multi.exe**. In order to guide the user through the procedure of defining the mixing cell model, a certain procedure has been prepared as described in Figure 3.

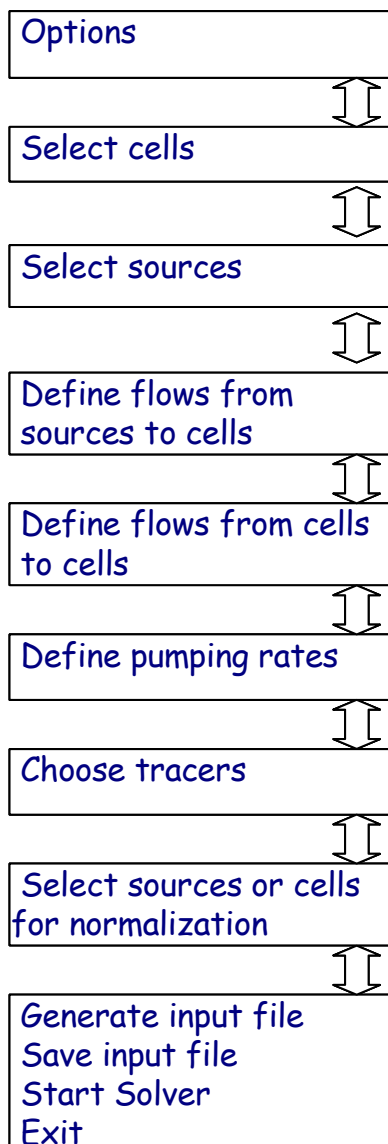


Figure 3 MIG procedure for creating an input file for the solver

After selecting some straightforward program options, first the cells and then the sources will be selected. As described in the terminology, any flow component that does not receive any inflow(s) from other components is called a *source*. Any flow component that has an input from or is receiving a flux from at least another inflow is called a *cell (compartment)*.

In the next menu, the user is asked to define the flows from sources to cells, followed by a menu where the user can define the flow direction between cells. After this menu, the user can enter or modify pumping/discharge rates from each cell - these are fluxes that are extracted from the system by pumping or natural discharge. Next, the tracers are selected and the weights (of conservancy) can be assigned or modified. Finally, the user is asked whether the data should be normalized or not. At this stage, the user can generate input files for the Solver, save them and activate the Solver directly from the **MIG** program. Detailed descriptions for each step are given below.

### 3.4 Loading and running MIG

In order to use MIG, two files are always required: Mig.xls and the appropriate Excel data file. First, you need to open and load `c:\mixcel\Mig.xls` with the Excel program. Start Excel, go to the 'File/Open' menu and open the file **Mig.xls** from the directory that you have selected during the installation (`C:\mixcel\Mig.xls`). The program is loaded and you should see the image below (Figure 4):

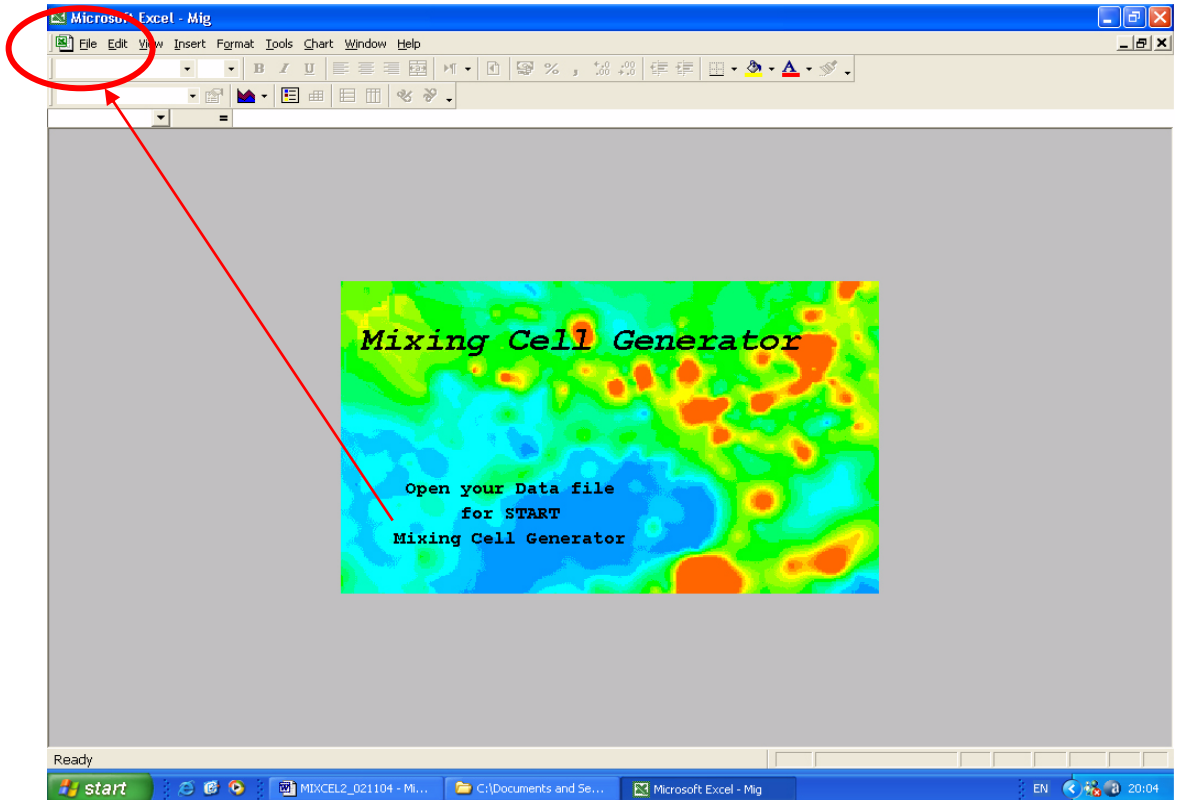


Figure 4.

**Tip:** Your system might have a warning system switched on that informs you that you are about to open a file containing *macros* - this is an additional safeguard against macro-viruses. Choose the option 'Activate Macros'. If you use MIG regularly, you can switch off this warning.

In order to activate the program, now open the data file (for example `c:\mixcel\data_4_14.xls`). As indicated by the message, the mixing cell generator is a macro file - one always needs to open a data file in order to work with MIG.

Go to 'File/Open' and select the file with hydro-chemical and/or isotope information that fits the modeled flow system. Some instructions and limitations about the format of the data file are given below.

A. The data file should be an Excel file format 5.0 (or newer version). Of course an imported dBase from other spreadsheet files may be used as well.

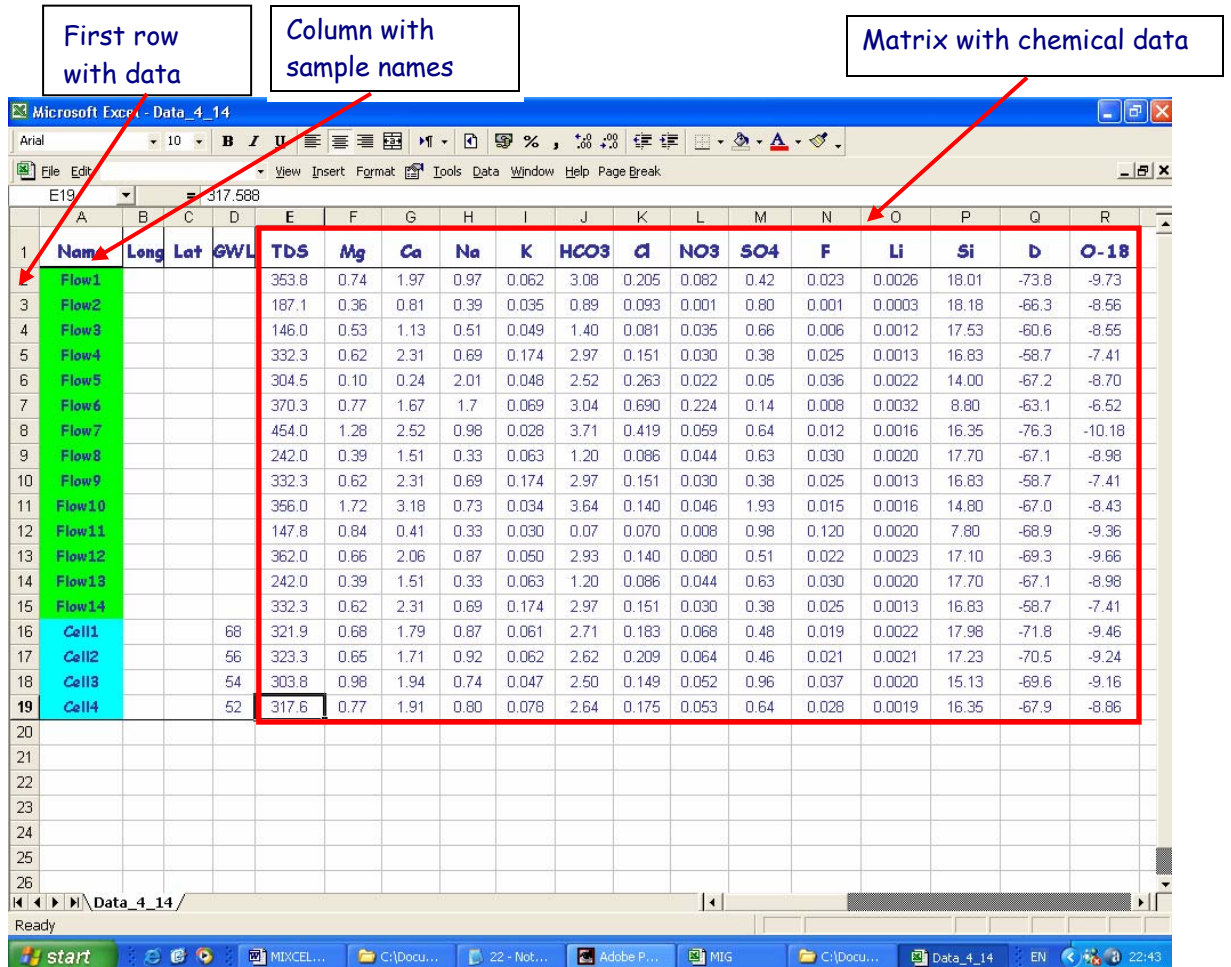


Figure 5. Data form for the MIG

B. Referring to Figure 5, the uppermost row in every data file should contain the column names. The hydrochemical and isotopic composition, which characterize each cell and/or source, should be arranged in rows. Columns represent the properties (sample name, co-ordinates (Long & Lat), heads (GWL), chemical concentrations, etc.). It does not matter which column the sample names are in or where the first column with the chemical data starts. The location of the sample name column and the location of the first column with chemical data can be specified and later introduced into the MIG data processor (see 'Program settings'). However, it is useful (set as a default) to place the column names in the first column and to have the sub-matrix with chemical data in one block (sub-matrix) that is uninterrupted by other

descriptive information not used for the modeling as demonstrated in the above example (Figure 5).

C. The data file should contain one *column with sample names*. The sample names must contain fewer than 16 characters without spaces. (This limitation is caused by a limitation of the sample name length in the FORTRAN solver: Multi.exe). If the sample names contain more than 16 characters you will be warned to shorten them during program execution.

D. The *matrix with chemical data* should be complete and should not contain null values, strings or empty cells. Remove any rows or samples that do not contain a full analysis. However, MIG also checks whether the chemical data-set is complete and only offers chemical samples for selected cells or sources that contain meaningful values: zero (real zero values) and above.

E. It can be useful to include groundwater levels, if these are available. MIG performs an automatic check of flow directions, which are consistent with water levels. The location of the column with water levels can be configured within MIG. The default column for water levels is 4.

Unless clearly specified, all the examples presented in the following manual are provided from the data file, data\_4\_14.xls, for a 4-cell flow system with 5 unknown inter-cell fluxes and 14 unknown external sources of recharge, all characterized with 14 different chemical and isotopic parameters. It is automatically installed in the MIG directory. A schematic flow system with 4 cells, 5 inter-cell fluxes and 14 external sources of recharge is presented in Chapter 4 (Examples). The data-file example given above contains only the sample names, the groundwater level for cells and the chemical data for the major elements.

After opening and selecting the data file (e.g. data\_4\_14.xls) in the menu 'File/Open' two files should already be loaded and listed in the menu 'Windows': data\_4\_14.xls and MIG.xls (see circle on Figure 6 below). MIG.xls is loaded in the background.

### 3.4.1 Adding menu items

In order to simplify the use of MIG, the program contains a macro that adds two menu elements to your Excel program. This step only needs to be executed the first time you use MIG and after any re-installation of MIG or Excel. In order to add the menu items, press **ALT+F8**, select the macro **MIG.xls!Startup** (circle) and click on the button 'Run' (rectangle).

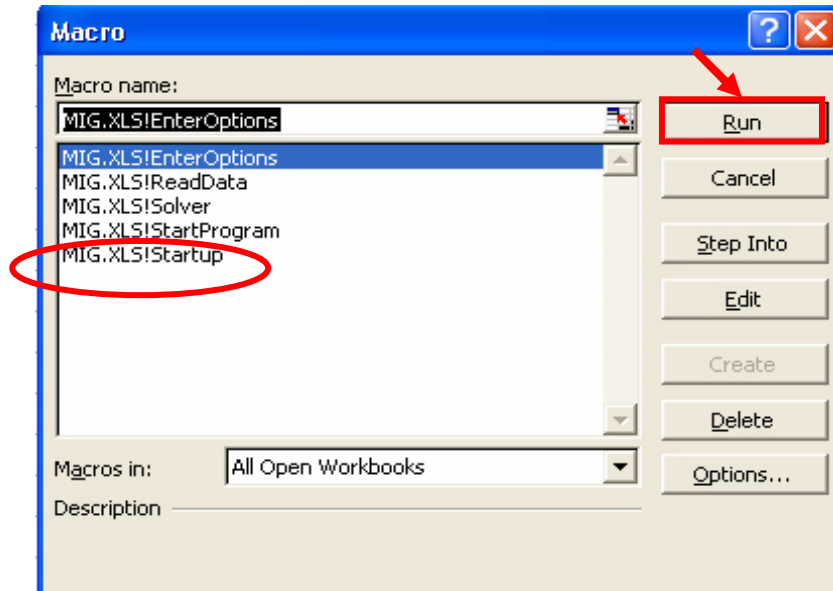


Figure 6.

The user may also reach this window by going to 'Tools/Macro/Macros', then back to the opened data file. After activating the macro, the user should see two extra menu items in the menu 'Tools'. These are 'Mixing Cell Model' and 'Start Solver' (see Figure 7 below).

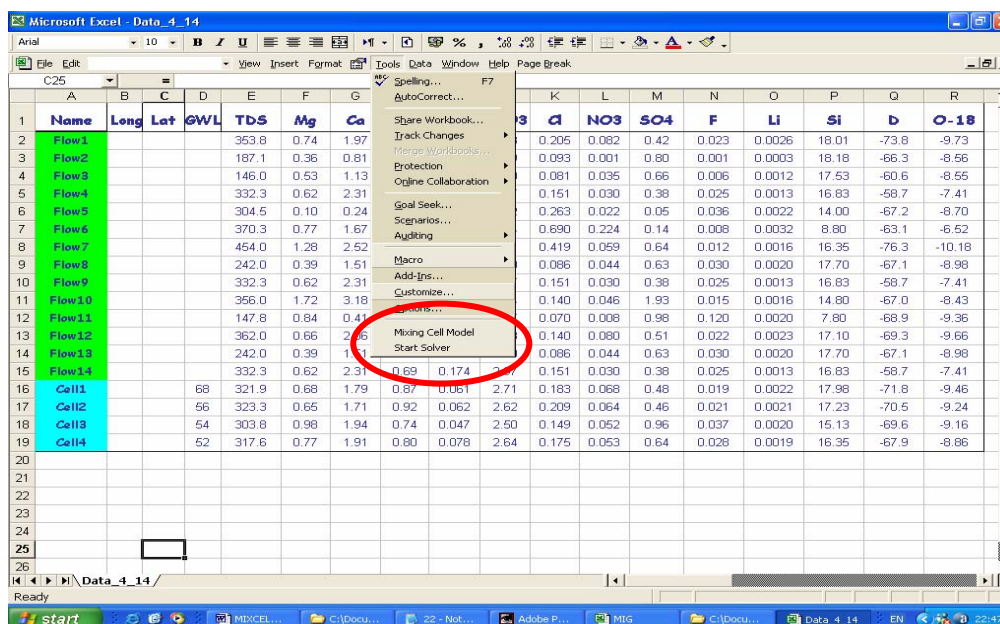


Figure 7.

**Important:** When using MIG for the very first time, please define the path to the Solver as described below in the section 'Program settings' before clicking on the button 'Start Solver'. The default path is c:\mixcel.

### 3.4.2 Starting MIG operation

Working from the Excel data file, the user starts working with MIG by clicking on 'Tools/Mixing Cell Model'. After selecting this menu element, a window should appear with the caption 'Program Settings'.

**Note:** The user may also start the 'Mixing Cell Model' by activating the Macro 'Mig.xls!StartProgram' from the Menu item /Tools/Macro/Macros... .

### 3.4.3 Program Settings (Figure 8)

The first window, 'Program Settings', allows you to configure MIG and to define default values. It contains the option sheets 'Locations', 'Dimensions' and 'Paths'.

Please note that any changes you make in the program settings only become permanent if you save MIG at the end of the session.

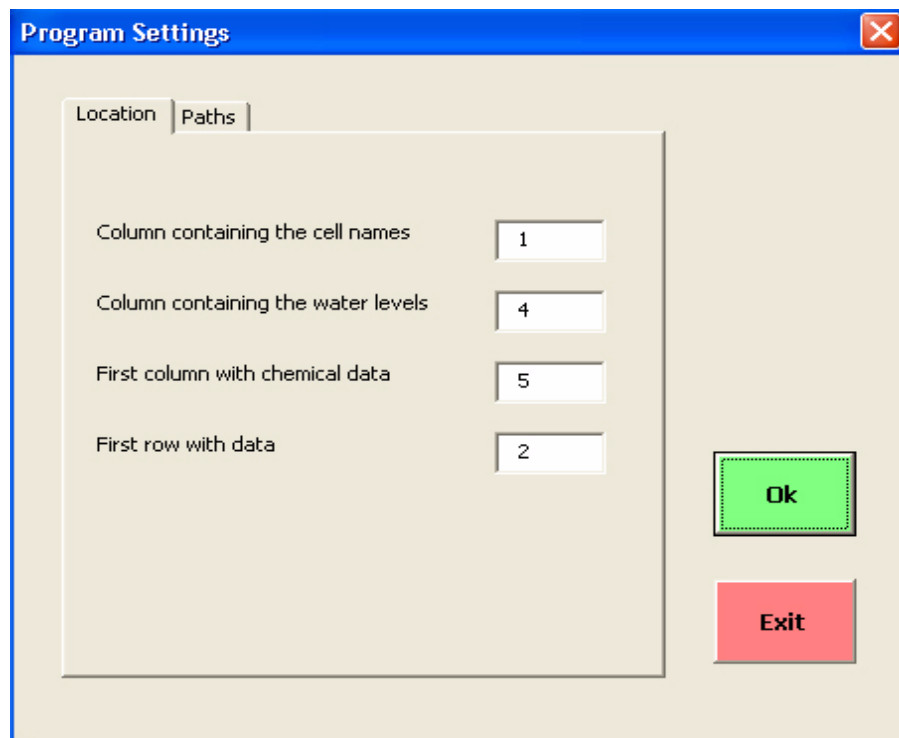


Figure 8.



### *Locations of data*

The structure of the data file is defined in the sheet 'Locations'. The '*column containing the cell names*' (default = 1) option specifies in which column the well names are listed. These names are later used to identify the samples in the configuration of the mixing cell model structure. The '*column containing the water levels*' option shows where the water levels are listed (default = 4). If this is set to a column containing real water levels, an automatic check will be made during the selection of flow pattern (cell connections) to see whether this flow connection is hydrologically feasible. If both elements have real values for water levels (not null values), flows will only be allowed for downward head gradients. If one or both of the elements do not contain water level data, this check will not be performed.

**Tip:** If you do not have water level data or if water levels are not reliable, select the number of a column that is completely empty (for example 256: Excel sheets have a maximum of 256 columns). This will not activate the water level checking routine.

The '*first column with chemical data*' indicates the column that begins the chemical data (default = 5). The '*first row with data*' is the number of the first row containing chemical data beneath the column names (default = 2).

### *Paths (Figure 9)*

This option sheet contains the path name for the locations of the FORTRAN solver **Multi.exe**. If this path is not set correctly, the solver will not be accessed successfully by MIG. Please check that this path is set correctly. The default is c:\mixcel\multi.exe.

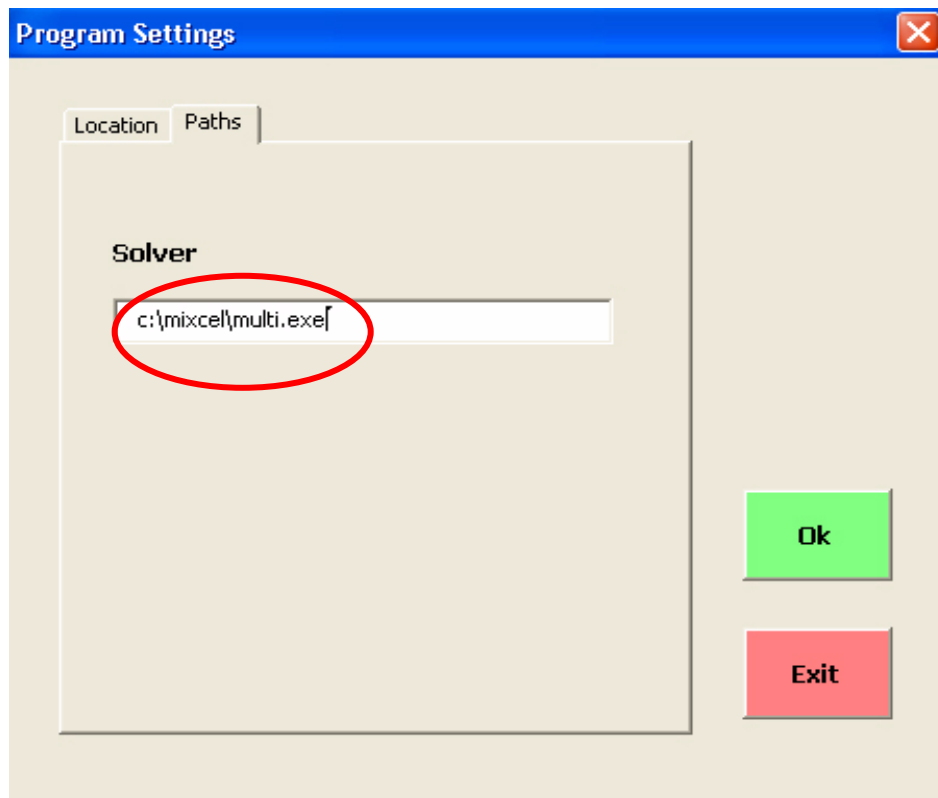


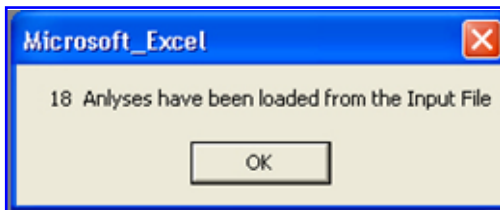
Figure 9.

### *Dimensions*

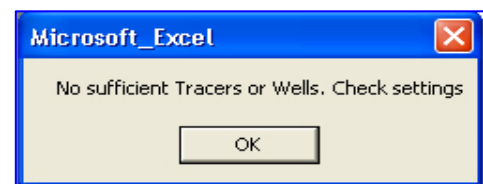
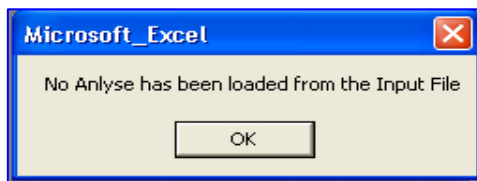
The third sheet with options in the 'Program settings' is hidden. Here, the maximum number of samples (default = 1024), tracers (default = 128), sources (default = 512) and inflows (default = 512) are selected. The default values are more than sufficient for natural and solvable problems.

After all the settings have been completed, click 'OK'. (With 'Exit' you leave MIG; to re-start, just go to 'Tools/Mixing Cell Model'.) Now, a message appears indicating the number of loaded rows with chemical and isotopes analyses. If the loading of this data file is successful, 18 analyses and 14 tracers from the example file should have been loaded. If the number of loaded analyses or loaded tracers is zero, MIG will inform the user that the number of cells and/or tracers is not sufficient and will abort. In this case, start MIG again ('Tools/Mixing Cell Model') and check the settings in 'Program settings/Location'.

If the following prompt messages appear the Program has loaded the analyses successfully.



If the following prompt messages appear the MIG program failed to load the analyses or tracers. The user is asked to check the settings in 'Program settings/Locations'.



**Possible problems:** The program stops reading data as soon as it encounters an empty row. Check the data file and delete the row with any empty (not defined) concentrations. If the loading still fails, try the standard format exactly as in the example file data.xls: column names in the first row, sample names in the first column and tracers starting from column 5. Then use the default values in the Program Settings (Figure 8):

Column containing well names	1
Column containing water levels	4
First column with chemical data	5
First row with data	2

#### 3.4.4 Selecting cells

The next form that appears is called '*Cell and index definition*'. The user selects the cells that are used for the mixing cell model. (Potential sources of recharge and other potential contributors will be selected in the next step). In Figure 10, the list in the left window contains the sample names from the sample name column that was previously defined, from which the user selects Cells or Compartments. By double clicking on these sample names in the list, the collection of cells can be completed. It is recommended to have prepared a schematic cell configuration for the flow pattern so that cells from upstream to downstream can be chosen in order, with the lowest (downstream) cell selected last. The '**Clear All**' button can be used to clear completely the list of selections. '**Re-Read Data**' allows the user to return to the Window 'Parameter Settings' and to re-read the data. '**Exit**'

terminates 'MIG'. However, **Mig.xls** is still loaded (see the list of files under 'Windows'), and MIG can easily be re-started by going back to 'Tools/Mixing Cell Model'.

In the example presented below (Figure 10), Cell 1, Cell 2, Cell 3 and Cell 4 were selected in the right window by double-clicking on their names in the left window.

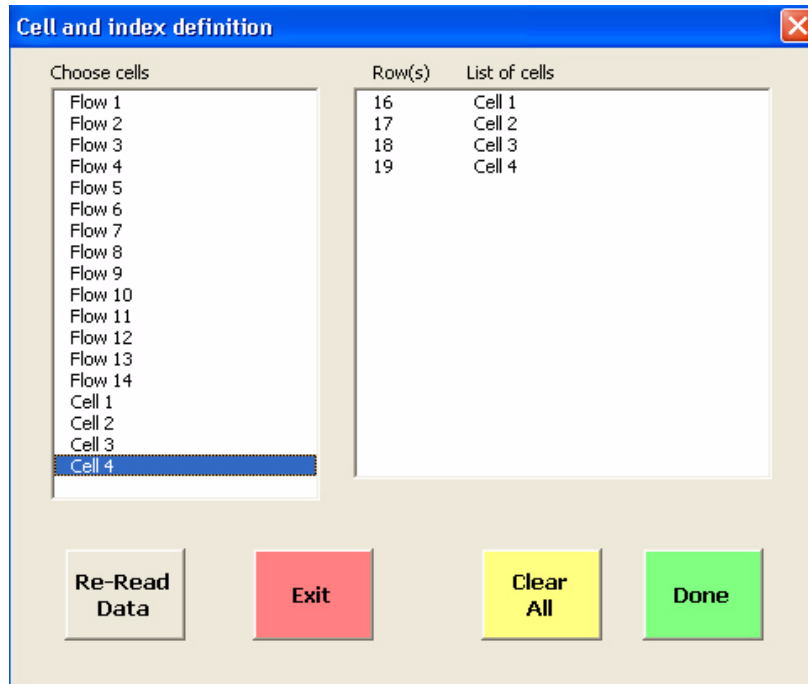


Figure 10. Cell and index definition

On the right-hand side a new list of selected cells is shown. It is composed of two columns. The first column lists the row number, the same number as the row in the data file. The second column contains the sample name. A small message appears after pressing the 'Done' button, which indicates the number of selected cells. When 'Done' is clicked, this form is closed, all the selections are saved and the next form is loaded.

### 3.4.5 Selecting potential sources

The next menu is for selecting potential sources of recharge. As defined above, sources are flow components (cluster or single boreholes) that do not receive any other potential inflow but contribute to a specific cell or cells. A source can be used as a potential contributor to more than one cell if hydrologically and hydrochemically justified. Sources can also be used to represent subsystems for a simplification of the model. In the list on the left-hand side in the window below

(Figure 11), cells that have been selected previously will not be listed again. All the sources that will be used for the definition of the mixing cell model structure must be selected from this list. Selecting more sources than cells does not pose a problem. Sources can be omitted during the succeeding definition of inflows. Again, the 'Clear All' button can be used to completely clear the list of selected sources. With '<Back' the user can return to the form 'Cell and index definition'. With 'Exit' the 'Mixing Cell Model' is terminated. With 'Done', this form is closed, all the selections are saved and the next form is loaded. A small message box indicates the number of selected sources.

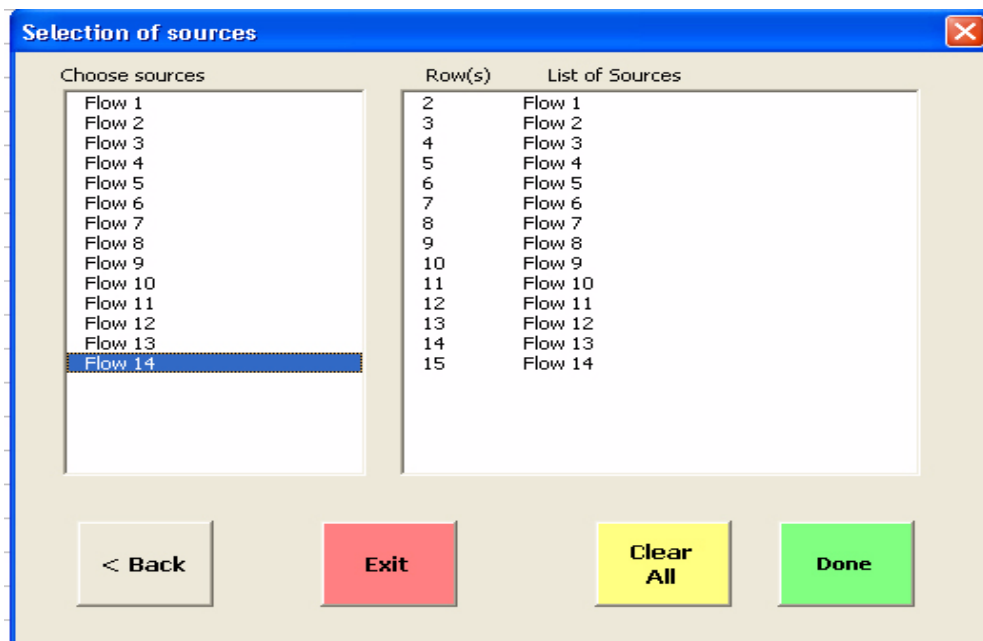


Figure 11. Selecting potential sources

### 3.4.6 Assigning inflows from potential sources to each cell

At this stage the user arrives at a form in which the sources for each cell must be defined and selected. Potential inflows are selected for each cell by first double-clicking on a certain cell in the upper left window (Figure 12). Then the user double-clicks on the source that feeds this cell in the lower left window. This flow connection will then appear in the large results window on the right.

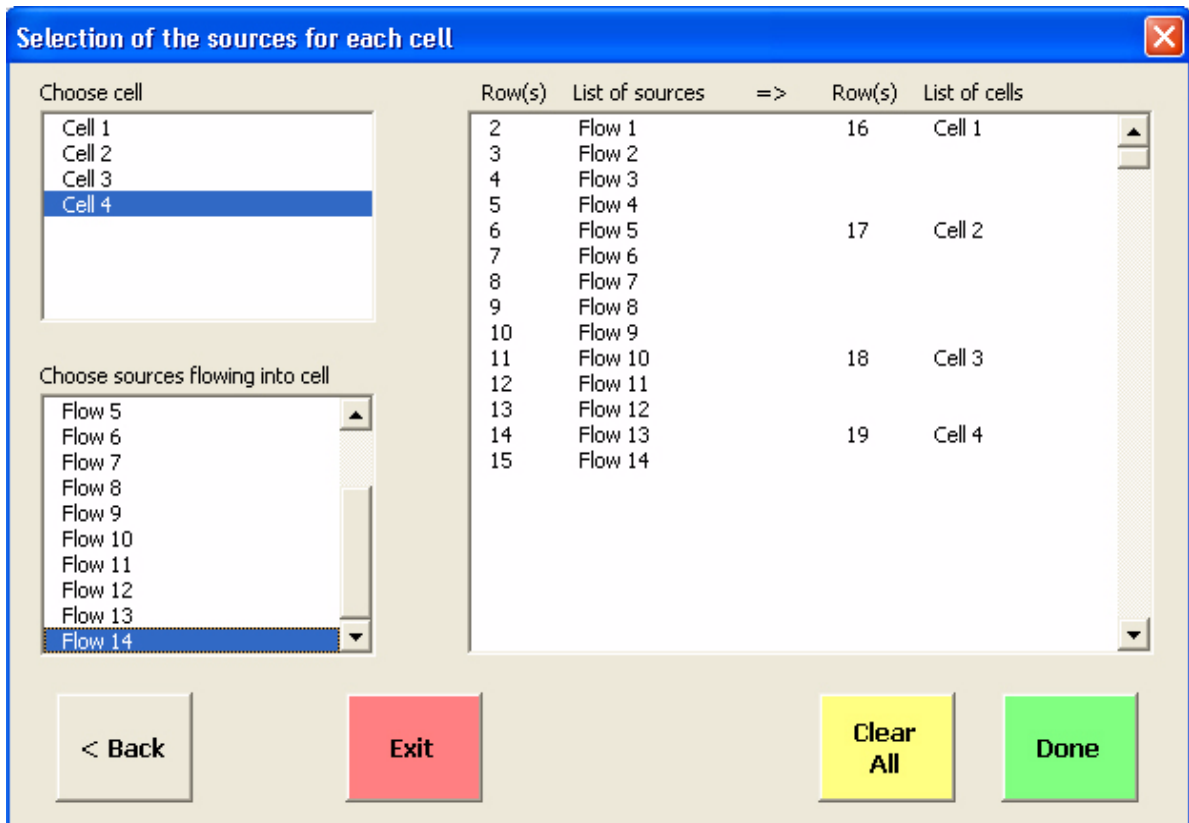


Figure 12. Assigning potential inflows for each cell

The right-hand window displays four columns, two for the sources and two for the cells. For both, the row index (from the data file) and the sample name are listed. Of course several sources can be selected for one cell. Therefore, this procedure is repeated until all the required inflows from sources for a certain cell are listed. The user now proceeds to the next cell by double-clicking on the desired cell and then selecting the respective inflows from the sources. In this example, for *Cell 4*, *Flow 13* and *Flow 14* are selected.

If a certain connection between source and cell already exists, the connection will not be accepted and a warning will appear. Also, if the user has specified a column with water levels for both sources and cells, and if these contain contradicting data, a warning will appear if this connection is hydraulically impossible. To avoid this, either go back to **'Program Settings'** and correct the specific assigned hydraulic head or specify an empty row for the column with water level data. Note however, that this constraint is very helpful for avoiding hydraulically impossible flow models!

The 'Clear All' button will completely clear the list of selected inflows. With '<Back', the user can go to the form 'Selection of sources'. Choosing 'Exit' terminates the 'Mixing cell model'. With 'Done' this form is closed, all the selections are saved and the next form is loaded. A small message box indicates the number of flows from sources into cells.

### 3.4.7 Selecting flows from cells to cells

In the next form (Figure 13), the user is asked to specify the flows between cells. In this form the flows from each cell into the nearby cell are now selected. This is done by first double-clicking on the discharging cell in the upper left window. Then double-click on the receiving cell in the lower left window. As a result, this flow connection will appear in the large results window on the right. For both cells, the row index (from the data file) and the sample name are listed. This procedure is repeated until all the required flows between cells are listed. In this example, *Cell 2* is a discharging cell to *Cell 3* and *Cell 4* (receiving cells). In order to avoid confusion, it is recommended (although not necessary for the correct solution of the problem) to select the flow connections from the highest to the lowest potential. A warning will appear:

- If a connection is re-entered when one already exists
- If an existing connection between cells is entered, but in the opposite direction
- If water level data (hydraulic heads) has been specified and an "upstream" connection is identified

Row(s)	Discharging cell	=>	Row(s)	Receiving cell
16	Cell 1		17	Cell 2
			18	Cell 3
17	Cell 2		18	Cell 3
			19	Cell 4
18	Cell 3		19	Cell 4

Figure 13. Selecting flows between cells

The '**Clear All**' button can be used to completely clear the list of selected flows. With '<Back' the user returns to the previous form. With '**Exit**', the 'Mixing cell model' is terminated. With '**Done**' this form is closed, all the selections are saved and the next form is loaded. A small message box indicates the number of flows from cells to cells. At this stage the flow connections have been defined, and the structure of the model is ready.

### 3.4.8 External out-flux from cells

In this form (Figure 14), the user may enter the rates of 'external out-flux' (water leaving the modeled domain from a specific cell). External out-flux may include extraction of water by both pumping and/or natural subsurface groundwater flow. For every cell, all types of measured or assessed out-flux must be summed in the out-flux column. For the last (most downstream) cell, the user must also specify the 'outflow', which must be greater than 0. 'Outflow' refers specifically to the external out-flux from the last cell. (The user must use the same units for rate of pumping as for the rates of out-flux and outflow.)

**Comment:** By default, the out-flux values are set to 0 for all cells except the last. The last cell has an arbitrary default outflow of 100 units (volume/time). If no values for out-flux are assigned for any cell, the fluxes calculated by the program represent a percentage of inflows relative to the total outflow.

The default external out-flux rates can be changed in this form. Click first on the cell that needs modification. Then, click on the text-field '**Change Rate**' and enter a new value. When the ENTER key is pressed, the new value will appear in the list to the left. The total sum of external out-flux/outflow is now calculated automatically. Here, as previously, the cells should be arranged according to the cascade of flows from higher to lower water levels. The outflow rate of the lowest cell corresponds to the outflow from the system. It needs to be larger than zero, otherwise the whole system has no flow and - due to a simple mass balance - all inflows will be zero as well.



CellIndex	CellName	OutFlow
16	Cell1	0.5
17	Cell2	3.5
18	Cell3	15.5
19	Cell4	0

Change Rate: 5

Outflow from the last cell: 100

Buttons: < Back, Exit, Clear All, Done

Figure 14. Assigning rates of external out-flux from each cell

With '<Back' the user returns to the previous form. 'Exit' terminates the 'Mixing cell model'. With 'Done' this form is closed, all the selections are saved and the next form is loaded.

### 3.4.9 Selecting tracers, isotopes and/or chemical compounds

Tracers that will be used as constraints of mass balance analyses in the optimization scheme are selected. The list of tracers displayed in the left window (Figure 15) contains all those found in the data matrix starting from the *'first column with chemical data'* as specified earlier (See 3.4.3; third item in Figure 8). The tracers used in the mixing cell model can be selected by double-clicking on the names (these are the same names of constituents that appear in the first row of the data set). The program automatically prevents the user from choosing the same tracer twice. In the right-hand results window, the selected tracers are shown with the index and the name of the tracer. In addition the default "weight" is shown (that is, the relative strength of impact given to each constituent, e.g. the rate of conservancy along the flow path). The default value for the weight is 1 and - in this version - cannot be changed. This list of selected tracers can be reset using the 'Clear All' function. After the selection is made, click 'Done' to call the next window. At least one tracer needs to be selected in order to proceed.

(More than one tracer, however, is needed to obtain a good solution. Note that the number of tracers plus 1 times the number of cells must be much greater than the number of unknown fluxes). A small message window indicates the number of selections.

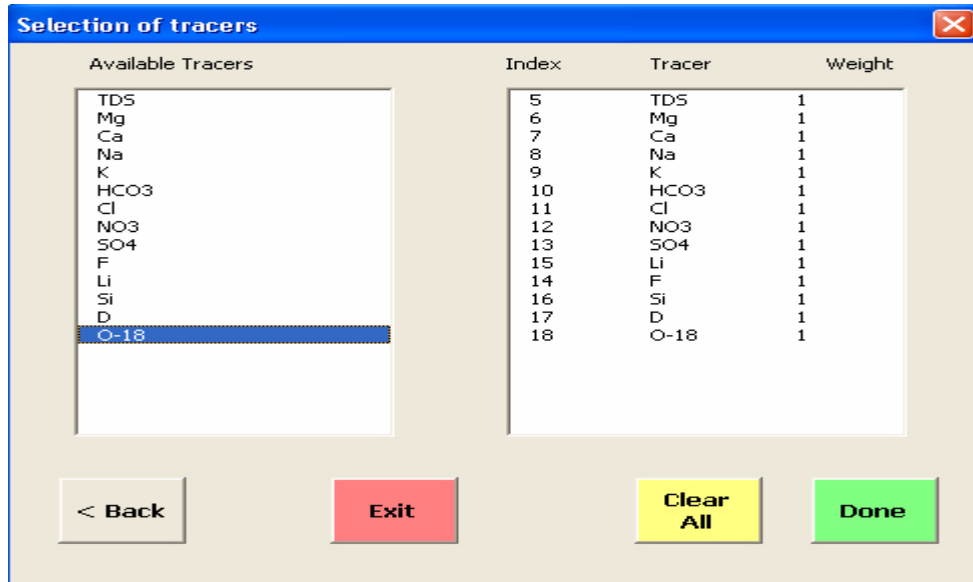


Figure 15. Selecting characteristic tracers, isotopes and chemical compounds

### 3.4.10 Selecting a reference term for normalization

In the final form (Figure 16) the "source" or a "cell" for the normalization of the chemical (or isotopic) data is selected. The program automatically checks which sources and cells are suitable for normalization and these are listed in the next window.

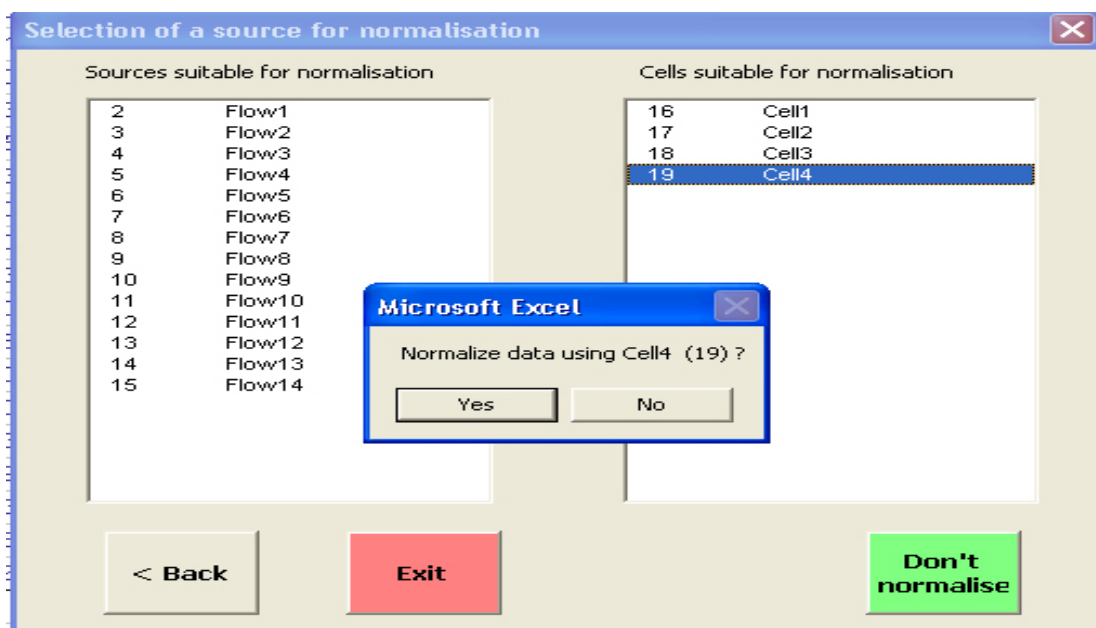


Figure 16. Assigning a reference data for normalization

To normalize, double-click on the selected source/cell. A prompt will appear asking for confirmation. If normalization is not wanted, select 'Don't normalize'.

The last toolbar before running the program has several buttons: With '<Back' the user returns to the previous form to insert changes.

### 3.4.11 Saving and running a model



Figure 17. Saving the flow configuration with data and running the model

The Wolf Algorithm is the selected optimizing solver of the MCM. The MIG uses all the above settings to prepare all necessary data input for the MCM. With 'Build Input for Wolff' (Figure 17), an input file is generated using all the settings that were created in the previous forms. Before the input data file is finalized, the user is asked to enter a descriptive name for the model. The input file is generated and formatted as an Excel table (Figure 18), later saved as "text format" (.prn). It is helpful, however, to adjust the table name according to the description of the run by double-clicking on the 'table name' tag to change the table name. Note that you only need to provide the desired descriptive name of the file without the whole path. It will automatically be saved in the MIXCELL folder (unless a different path was assigned).

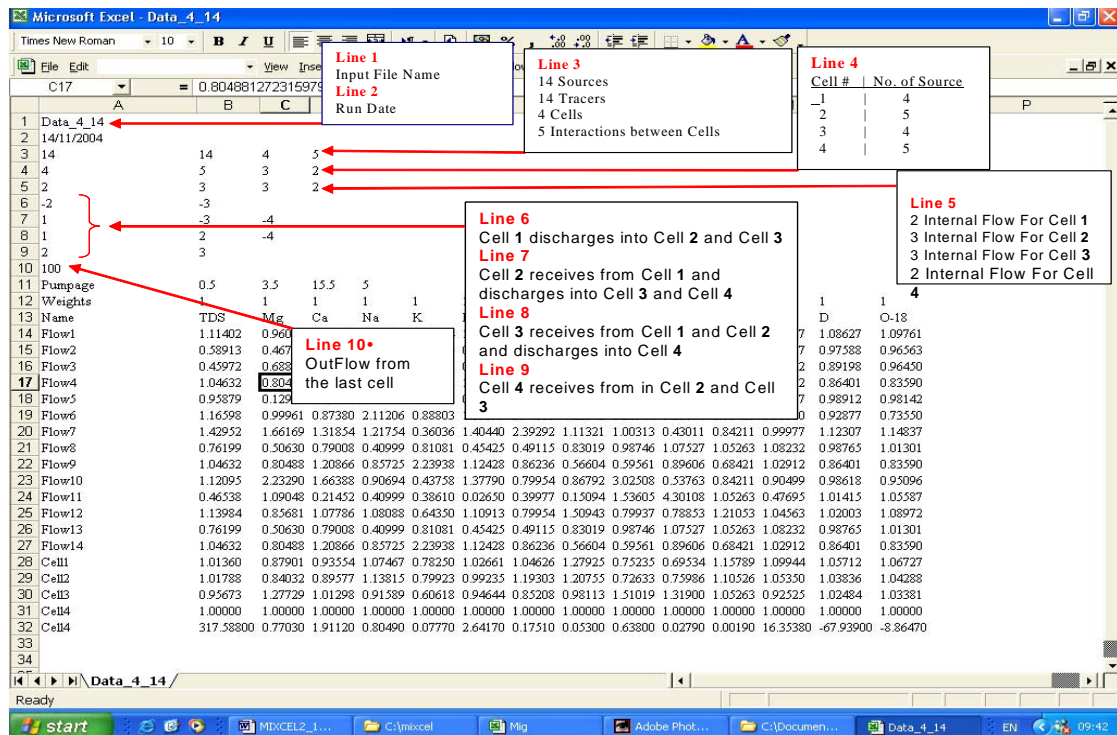


Figure 18. MIG-generated input data file for the MCM

The next step is to save this input file by choosing 'Save Input File'. You need to enter a name for this run. This operation cannot be cancelled - a name must be given. An ASCII file will be written that is used with the solver Multi.exe. If the path to the solver is set correctly, the solver can now be started by clicking on the button 'Run Wolff Algorithm'.

**Potential problem:** If program does not execute the solver, the path is probably incorrect. Identify the location of the file multi.exe. It should be contained in c:\mixcel (or in the alternative directory that the user had specified when installing the program). Restart the 'Mixing Cell Model' and adjust the path on the second sheet of 'Program settings/Path'.

The solver (the FORTRAN code) now prompts for the names of an input file and an output file (Figure 19). Type the names of the input and output files. If the set-up of the flow pattern is also supported by water and chemical balance constraints, MCM will produce a result.

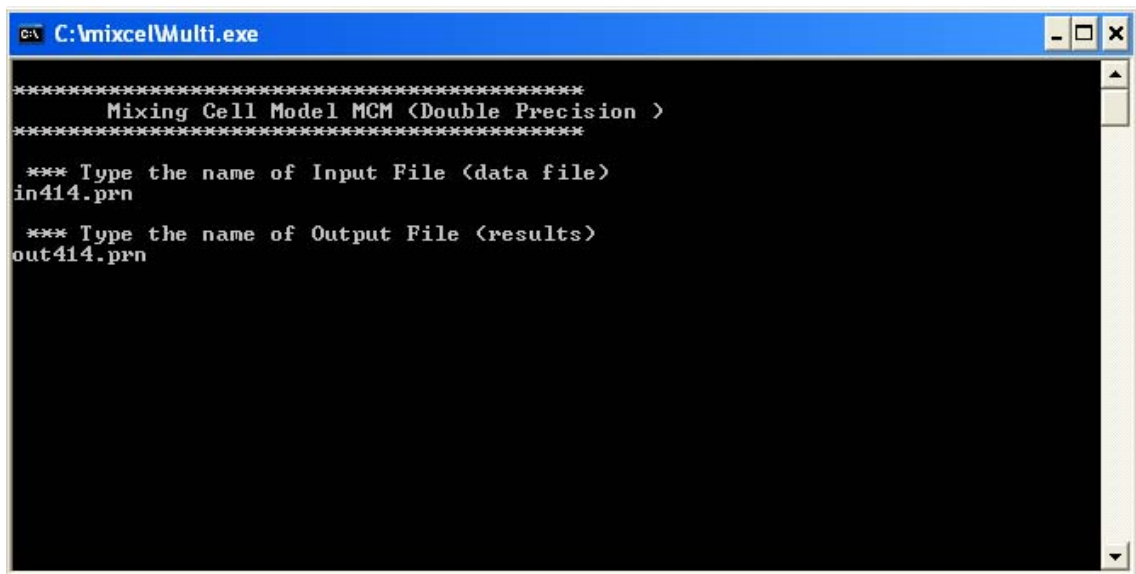


Figure 19. A prompt window asking for the input data and results (output) file names

### 3.5 Terminating MIG

Before quitting the program you are advised to save Mig.xls in case you want to save the program settings to be used in further runs and alternative flow configurations. The name of the data file needs to be reset to the original given name and the file type specified as Excel. Choose 'File/Save as...', select 'Excel file', specify a name and then save.

## 4 Examples

### 4.1 Four-cells model- data\_4\_14.xls

The first example with four cells and 14 unknown was already described in full detail throughout chapter 3. The flow configuration for this example is given in Figure 20.

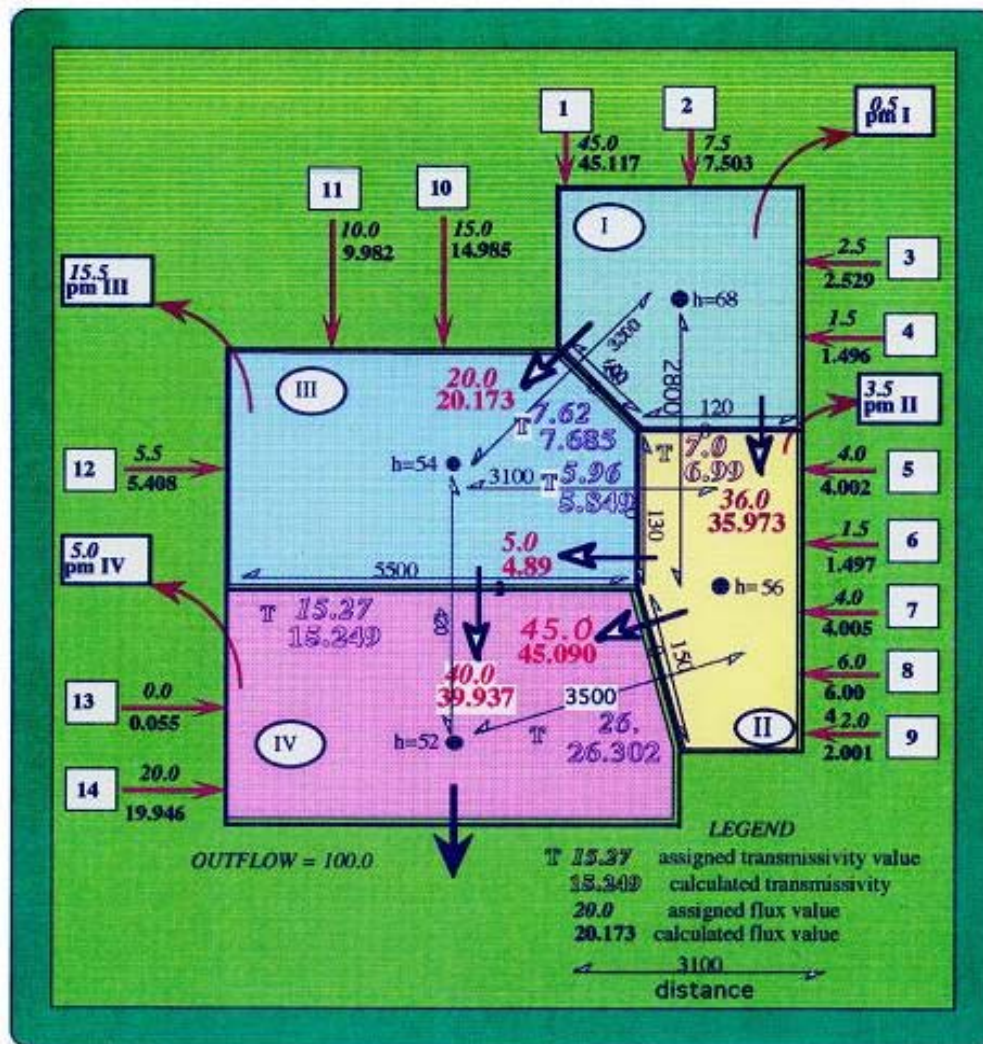


Figure 20. Flow scheme for the example of data-file 'data\_4\_14.xls'.

In the output file, Out414.prn (below), configuration of the data4\_14.xls run is described:

Output file: Out414.prn

```
*****
**              Estimation of Flow into and between Cells          **
**              Mixing Cell-MCM-Wolf Algorithm                    **
*****
Data_4_14

The date is:03:20:2005

*****
*** Input File      In414.prn
*** Output File     Output414.
*****

There are 14 potential inputs.
There are 14 tracers to be considered.
There are 4 cells in this model.
There are 5 flows between the cells.

N = 14  NN = 18  NOC = 4  NOP = 14

Number of inflows to each cell:
  Num.cell  1  2  3  4
  Inflows   4  5  3  2

Number of internal flows from and into each cell:
  Num.cell  1  2  3  4
  Interfl.  2  3  3  2

The internal flows are:
  From cell  1  1  2  2  3
  To cell    2  3  3  4  4

The outflow out of the last cell is [volume/time]:
  QOUT =      100.00

The rate of output (pumpage) and/or evapotranspiration
from each cell is [volume/time]:
  PM( 1) =      .50
  PM( 2) =     3.50
  PM( 3) =    15.50
  PM( 4) =     5.00
  Constant for Flows =      5.000
  PM( 1) =     .10
  PM( 2) =     .70
  PM( 3) =     3.10
  PM( 4) =     1.00
*****

The weighting parameters are:
  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000
  1.000  1.000

There are 60 mass balance equations.
  Number of iterations: 28

The rest of the variables are equal to zero.
```

The unknown inflows are:

	Name of inflow	Rate of inflow	Perc. of tot. inflow	Perc. of cell inflow	Flux
Cell 1	1 Flow1	= 8.95	36.0 %	79.7 %	44.74
	2 Flow2	= 1.48	6.0 %	13.2 %	7.42
	3 Flow3	= .50	2.0 %	4.5 %	2.51
	4 Flow4	= .30	1.2 %	2.6 %	1.48
Cell 2	5 Flow5	= .80	3.2 %	22.5 %	3.98
	6 Flow6	= .30	1.2 %	8.4 %	1.49
	7 Flow7	= .83	3.3 %	23.4 %	4.14
	8 Flow8	= 1.20	4.8 %	33.8 %	5.99
	9 Flow9	= .42	1.7 %	11.9 %	2.11
Cell 3	10 Flow10	= 3.00	12.1 %	49.2 %	15.01
	11 Flow11	= 2.01	8.1 %	32.9 %	10.03
	12 Flow12	= 1.09	4.4 %	17.9 %	5.45
Cell 4	13 Flow13	= .00	.0 %	.0 %	.00
	14 Flow14	= 4.01	16.1 %	100.0 %	20.05

The intermediate flows are:

From cell	To cell	Rate of flow	Real number
1	2	7.096	35.48
1	3	4.034	20.17
2	3	.981	4.91
2	4	8.973	44.86
3	4	8.012	40.06

Total:	124.41	100.00 %
QOUT + PPP =	124.50	
Absolute diff.:	.09	
Percentage diff.:	.07 %	

\*\*\*\* Ion balance over the entire basin \*\*\*\*

Id	SUMIN	SUMOUT	Abs. error:	Perc. error:
TDS	24.770	24.780	-.01	.0%
Mg	25.649	25.636	.01	.1%
Ca	24.864	24.861	.00	.0%
Na	24.714	24.743	-.03	-.1%
K	23.534	23.517	.02	.1%
HCO3	24.723	24.731	-.01	.0%
Cl	24.587	24.581	.01	.0%
NO3	24.937	25.015	-.08	-.3%
SO4	26.264	26.265	-.00	.0%
F	25.634	25.690	-.06	-.2%
Li	25.372	25.153	.22	.9%
Si	24.689	24.716	-.03	-.1%
D	24.987	25.010	-.02	-.1%
O-18	25.018	25.042	-.02	-.1%

Total salt transport:

Observed output ( MASS/TIME ):	1887.5
Estimated input ( MASS/TIME ):	1887.6

End of MCMsf Model .



The table below summarizes the results of the mixing cell model compared to the assigned flux values that were used to produce the synthetic data file.

	Name of Inflow	Rate of Inflow to cell	% of Total Inflow	% of Cell Inflow	Calculated Flux Values	Assigned Flux Values
Cell1	Flow 1	8.95	36.0	79.7	44.74	45.0
	Flow 2	1.48	6.0	13.2	7.42	7.5
	Flow 3	.50	2.0	4.5	2.51	2.5
	Flow 4	.30	1.2	2.6	1.48	1.5
Cell2	Flow 5	.80	3.2	22.5	3.98	4.0
	Flow 6	.30	1.2	8.4	1.49	1.5
	Flow 7	.83	3.3	23.4	4.14	4.4
	Flow 8	1.20	4.8	33.8	5.99	6.0
	Flow 9	.42	1.7	11.9	2.11	2.0
Cell3	Flow 10	3.0	12.1	49.2	15.01	15.0
	Flow 11	2.01	8.1	32.9	10.03	10.0
	Flow 12	1.09	4.4	17.9	5.45	5.5
	Flow 13	0.00	.0	.0	0.00	0.00
	Flow 14	4.01	16.1	100.0	20.05	20.0

## 4.2 Twelve cells model with 17 unknowns - data\_12\_17.xls

The second example is for a complex flow configuration of 12 cells with 17 unknown fluxes from external sources and 15 internal fluxes. The flow configuration for this example is given in Figure 21.

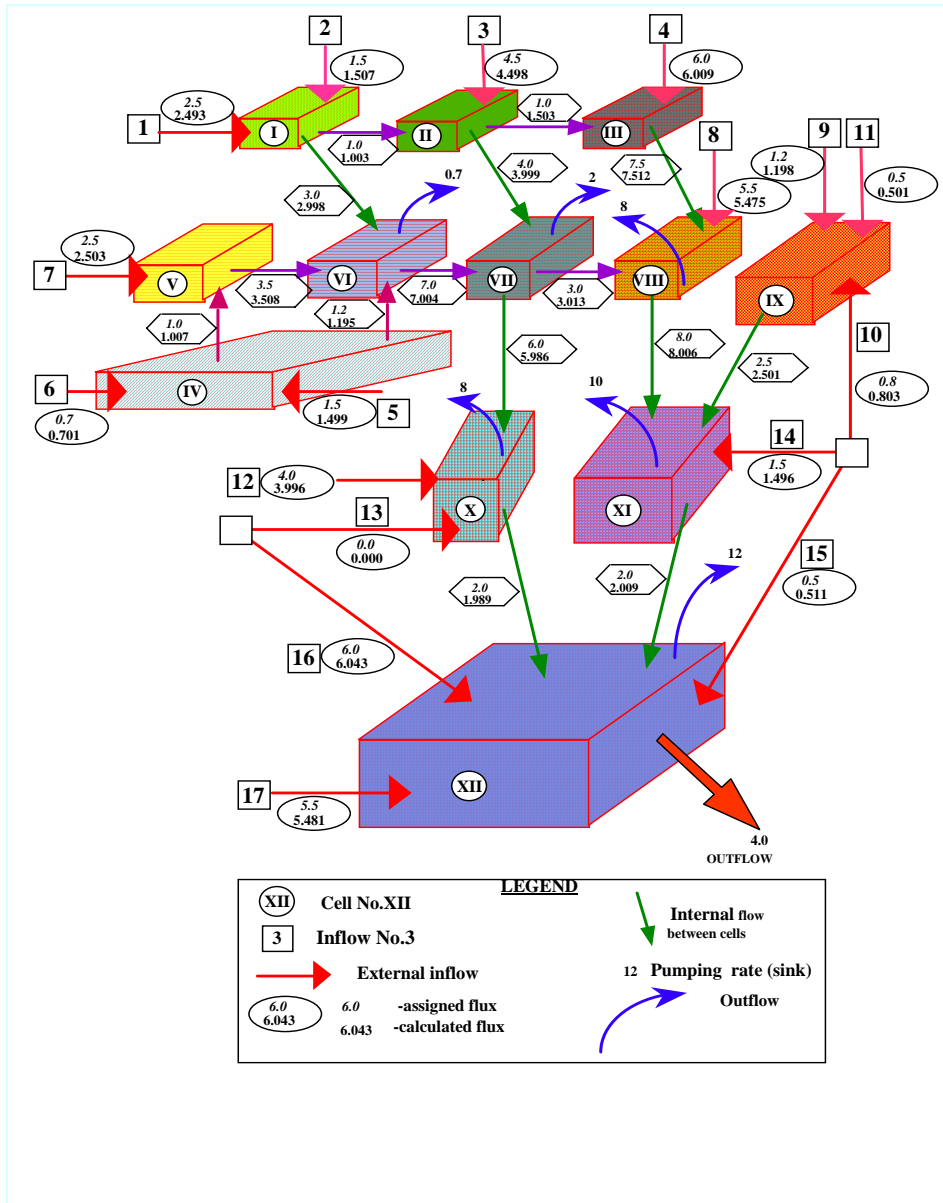


Figure 21. Flow scheme for the example of data-file 'data\_12\_17.xls'.

The input file produced by MIG is shown below.

```

In1217.prn
8/2/2005
17      14      12      15
2       1       1       2
2       3       2       2       1       0       0       1       3       2       1       3
-2      -6
1       -3      -7
2       -8
-5      -6
4       -6
1       4       5       -7
2       6       -8      -10
3       7       -11
-11
7       -12
8       9       -12
10      11
4
Pumpage
Weights 1       1       0       0       0       0       0       0.7       2       8       0       8       10       12
Name    Ec      Mg      Ca      Na      K      HCO3     Cl      NO3     SO4     F      Li      Si      D      O-18
Flow1   353.80000 0.74000 1.97000 0.97000 0.06200 3.08000 0.20500 0.08200 0.42000 0.02300 0.00260 18.01000 -73.80000 -9.73000
Flow2   187.10000 0.38000 0.81000 0.39000 0.03500 0.89000 0.09300 0.00100 0.80000 0.00100 0.00030 18.18000 -66.30000 -8.58000
Flow3   146.00000 0.53000 1.13000 0.51000 0.04900 1.40000 0.08100 0.03500 0.68000 0.00600 0.00120 17.53000 -60.60000 -8.55000
Flow4   332.30000 0.62000 2.31000 0.69000 0.17400 2.97000 0.15100 0.03000 0.38000 0.02500 0.00130 16.83000 -58.70000 -7.41000
Flow5   304.50000 0.10000 0.24000 2.01000 0.04800 2.52000 0.26500 0.02200 0.05000 0.03600 0.00220 14.00000 -67.20000 -8.70000
Flow6   370.30000 0.77000 1.67000 1.70000 0.06900 3.04000 0.69000 0.22400 0.14000 0.00800 0.00320 8.80000 -63.10000 -6.52000
Flow7   454.00000 1.28000 2.52000 0.98000 0.02800 3.71000 0.41900 0.05900 0.64000 0.01200 0.00160 16.35000 -76.30000 -10.18000
Flow8   242.00000 0.39000 1.51000 0.33000 0.06300 1.20000 0.08600 0.04400 0.63000 0.03000 0.00200 17.70000 -67.10000 -8.98000
Flow9   356.00000 1.72000 3.18000 0.73000 0.03400 3.64000 0.14000 0.04600 1.93000 0.01500 0.00160 14.80000 -67.00000 -8.43000
Flow10  147.80000 0.84000 0.41000 0.33000 0.03000 0.07000 0.07000 0.00800 0.98000 0.12000 0.00200 7.80000 -68.90000 -9.36000
Flow11  362.00000 0.68000 2.08000 0.87000 0.05000 2.93000 0.14000 0.08000 0.51000 0.02200 0.00230 17.10000 -69.30000 -9.68000
Flow12  355.50000 0.70000 2.10000 0.89000 0.05000 2.90000 0.17500 0.14200 0.56000 0.02400 0.00230 18.55000 -72.30000 -9.68000
Flow13  302.80000 0.05000 0.30000 2.89000 0.02000 2.52000 0.32000 0.02100 0.19000 0.08000 0.00370 14.25000 -74.80000 -9.44000
Flow14  147.80000 0.84000 0.41000 0.33000 0.03000 0.07000 0.07000 0.00800 0.98000 0.12000 0.00200 7.80000 -68.90000 -9.36000
Flow15  147.80000 0.84000 0.41000 0.33000 0.03000 0.07000 0.07000 0.00800 0.98000 0.12000 0.00200 7.80000 -68.90000 -9.36000
Flow16  302.80000 0.05000 0.30000 2.89000 0.02000 2.52000 0.32000 0.02100 0.19000 0.08000 0.00370 14.25000 -74.80000 -9.44000
Flow17  444.20000 1.15000 3.21000 0.78000 0.02900 3.39000 0.27500 0.02700 1.36000 0.05200 0.00160 14.58000 -68.60000 -9.56000
Cell1   291.28750 0.59750 1.53500 0.75250 0.05190 2.25870 0.16300 0.05160 0.56250 0.01470 0.00170 18.07370 -70.98750 -9.29120
Cell2   172.41590 0.54230 1.20360 0.55410 0.04950 1.55610 0.09590 0.03800 0.64230 0.00760 0.00130 17.62890 -62.48960 -8.68480
Cell3   300.32320 0.60450 2.08870 0.66280 0.14910 2.68720 0.14000 0.03160 0.43250 0.02150 0.00130 16.98980 -59.45770 -7.66500
Cell4   325.43640 0.31320 0.69500 1.91140 0.05470 2.68550 0.39890 0.08630 0.07860 0.02710 0.00250 12.34550 -65.89550 -8.00640
Cell5   417.26750 1.00380 1.99860 1.24610 0.03560 3.41730 0.41320 0.06680 0.47960 0.01630 0.00190 15.20580 -73.32730 -9.55900
Cell6   353.87310 0.73790 1.61480 1.15750 0.04490 2.85190 0.31350 0.06390 0.44940 0.01740 0.00190 15.87740 -71.25750 -9.21270
Cell7   287.88860 0.66670 1.46530 0.93810 0.04660 2.38070 0.23440 0.05450 0.51950 0.01380 0.00170 16.51450 -68.06880 -9.02070
Cell8   277.94310 0.54240 1.77290 0.60000 0.10030 2.11850 0.13910 0.04020 0.51670 0.02300 0.00160 17.14480 -63.69930 -8.37120
Cell9   290.57600 1.22640 2.06960 0.63000 0.03590 2.35560 0.11780 0.04060 1.34200 0.05000 0.00190 13.02000 -68.06800 -8.97360
Cell10  314.93320 0.68000 1.71920 0.91880 0.04800 2.58840 0.21080 0.08950 0.53570 0.01790 0.00190 17.32860 -69.76130 -9.28440
Cell11  264.30710 0.72210 1.66430 0.57250 0.07810 1.91180 0.12600 0.03620 0.74650 0.04070 0.00170 15.11730 -65.25960 -8.62030
Cell12  343.26750 0.61560 1.65170 1.54170 0.03420 2.67500 0.25880 0.03310 0.72970 0.05900 0.00250 14.65510 -70.66200 -9.35680
NORMAL

```

The results of the optimization with the Wolf algorithm (Multi.exe) are given in the following output list.

```

*****
**              Estimation of Flow into and between Cells              **
**              Mixing-Cell-Model MCMsf-Wolf Algorithm                  **
*****

The date is:08:02:2005

*****
*** Input File      Inl217.prm
*** Output File     Outl217.prm
*****

There are 17 potential inputs.
There are 14 tracers to be considered.
There are 12 cells in this model.
There are 15 flows between the cells.

N = 17  NN = 29  NOC = 12  NOP = 14

Number of inflows to each cell:
Num.cell  1  2  3  4  5  6  7  8  9 10 11 12
Inflows   2  1  1  2  1  0  0  1  3  2  1  3

Number of internal flows from and into each cell:
Num.cell  1  2  3  4  5  6  7  8  9 10 11 12
Interfl.  2  3  2  2  2  4  4  3  1  2  3  2

The internal flows are:
From cell  1  1  2  2  3  4  4  5  6  7  7  8  9 10 11
To cell    2  6  3  7  8  5  6  6  7  8 10 11 11 12 12

The outflow out of the last cell is [volume/time]:
QOUT =      4.00

The rate of output (pumpage) and/or evapotranspiration
from each cell is [m3/time]:
PM( 1) =      .00
PM( 2) =      .00
PM( 3) =      .00
PM( 4) =      .00
PM( 5) =      .00
PM( 6) =      .70
PM( 7) =      2.00
PM( 8) =      8.00
PM( 9) =      .00
PM(10) =      8.00
PM(11) =     10.00
PM(12) =     12.00
Constant for Flows =      12.000
PM( 1) =      .00
PM( 2) =      .00
PM( 3) =      .00
PM( 4) =      .00
PM( 5) =      .00
PM( 6) =      .06
PM( 7) =      .17
PM( 8) =      .67
PM( 9) =      .00
PM(10) =      .67
PM(11) =      .83
PM(12) =      1.00
*****

The weighting parameters are:
1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000
1.000  1.000

There are 180 mass balance equations.
Number of iterations: 40

```

The unknown inflows are:

	Name of inflow	Rate of inflow	Perc. of tot. inflow	Perc. of cell inflow	Fluxes
Cell 1	1 Flow1	= .21	5.6 %	62.3 %	2.49
	2 Flow2	= .13	3.4 %	37.7 %	1.51
Cell 2	3 Flow3	= .37	10.1 %	100.0 %	4.50
Cell 3	4 Flow4	= .50	13.4 %	100.0 %	6.01
Cell 4	5 Flow5	= .12	3.4 %	68.2 %	1.50
	6 Flow6	= .06	1.6 %	31.8 %	.70
Cell 5	7 Flow7	= .21	5.6 %	100.0 %	2.50
Cell 6					
Cell 7					
Cell 8	8 Flow8	= .46	12.2 %	100.0 %	5.48
Cell 9	9 Flow9	= .10	2.7 %	47.9 %	1.20
	10 Flow10	= .07	1.8 %	32.1 %	.80
	11 Flow11	= .04	1.1 %	20.0 %	.50
Cell110	12 Flow12	= .33	8.9 %	100.0 %	4.00
	13 Flow13	= .00	.0 %	.0 %	.00
Cell111	14 Flow14	= .12	3.3 %	100.0 %	1.50
Cell112	15 Flow15	= .04	1.1 %	4.2 %	.51
	16 Flow16	= .50	13.5 %	50.2 %	6.04
	17 Flow17	= .46	12.3 %	45.5 %	5.48

The intermediate flows are:

From cell	To cell	Rate of flow	Real number
1	2	.084	1.00
1	6	.250	3.00
2	3	.125	1.50
2	7	.333	4.00
3	8	.626	7.51
4	5	.084	1.01
4	6	.100	1.19
5	6	.292	3.51
6	7	.584	7.00
7	8	.251	3.01
7	10	.499	5.99
8	11	.667	8.01
9	11	.208	2.50
10	12	.166	1.99
11	12	.167	2.01

Total:	44.72	100.00 %
QOUT + PPP =	44.70	
Absolute diff.:	.02	
Percentage diff.:	.04 %	

\*\*\*\* Ion balance over the entire basin \*\*\*\*

Id	SUMIN	SUMOUT	Abs. error:	Perc. error:
Ec	1142.052	1141.821	.23	.0%
Mg	2.390	2.392	.00	-.1%
Ca	6.250	6.256	-.01	-.1%
Na	3.778	3.769	.01	.2%
K	.220	.220	.00	.0%
HCO3	8.864	8.861	.00	.0%
Cl	.741	.741	.00	.1%
NO3	.174	.174	.00	.0%
SO4	2.408	2.409	.00	-.1%
F	.143	.143	.00	.2%
Li	.007	.007	.00	-.1%
Si	58.810	58.799	.01	.0%
D	-253.202	-253.074	-.13	.1%
O-18	-33.485	-33.471	-.01	.0%

Total salt transport:

Observed output ( MASS/TIME ): 5068.0  
 Estimated input ( MASS/TIME ): 5068.6

End of MCM Model .

### 4.3 Single Cell Model- data\_1\_5.xls

Executing the *Mixing Cell Model* for a single cell configuration is suggested for analyzing complex flow configurations. Any complex system can be broken down into a series of single-cells. The possible sources entering each single cell can now be confirmed with the *Single Cell Model*. After testing and verification, the cells can be regrouped into a cluster representing the entire, complex flow system.

An example file in Excel (file: data\_1\_5.xls) with chemical data for a meso-scale application of *MIG* is in the installed folder. This file contains chemical data for sources and cells and can be used for testing the *MIG* program and training.

As has been outlined before, a hydro-geological conceptual model needs to be developed before starting the calculations. Based on the conceptual scheme of possible flow connections in the groundwater system, the flow rates are determined by optimization.

The most common case is the quantification of flow rates from different sources into one cell. In general, single-cell and multi-source models are used as a preliminary assessment before a more complex multi-cell flow configuration is analyzed. This case is thus shown here. The idea behind using the *Multi-Cell* code to solve a *Single-Cell* problem is to create two cells with identical chemical and isotopic compositions. The first cell represents the chemical composition of the modeled cell and the second is a fictitious cell, which corresponds to its outflow. The program mig.xls needs to be started as described in section 3.4. The data file data\_1\_5.xls must be opened and loaded (See sections 3.4.1-3.4.2).

● In the menu '**Program Settings**' (3.4.3), the cell names are in column 1, water levels are listed in column 4, the first column with chemical data is 5 and the first row with data is 2. Upon confirmation of these default settings messages indicating the download of 25 analyses with 9 tracers are displayed and need to be confirmed.

● In the next menu '**Cell and index definition**' (3.4.4), select the lines 'cell4' and 'o-cell4' by double-clicking. Please note that both cells are

identical and carry the same chemical composition (See 'cell and index definition' window below). After clicking the button 'Done' in the 'cell and index definition' menu the message '2 cell(s) selected' should appear.

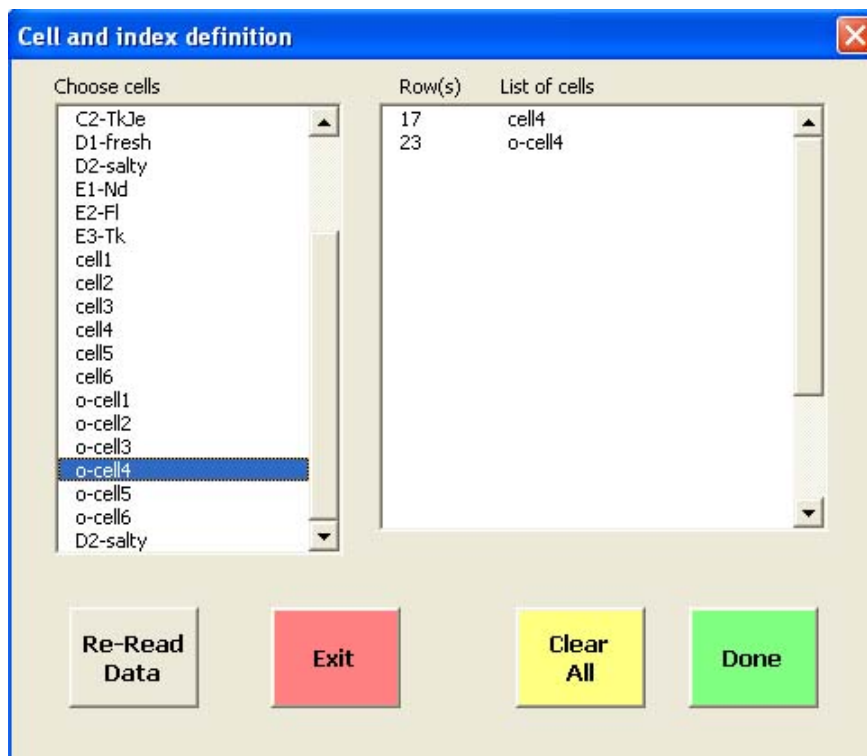


Figure 22. Definition of cells

● In the next menu for '**Selection of sources**' (3.4.5), the user will notice that the list in the menu does not contain, and therefore does not allow, the selection of 'cell4' and 'o-cell4' as sources. The list contains all the potential sources and cells except the ones that have already been selected as cells in the previous menu.

Select 'B-Nta', 'Flood', 'D1-fresh', 'D1-salty' and 'E2-FI' as sources (the order is not important). These sources will be stored as a sub-set of sources from which the user can attribute sources to individual cells in the following menu. After pressing the button 'Done' the message '5 Sources selected' should appear.



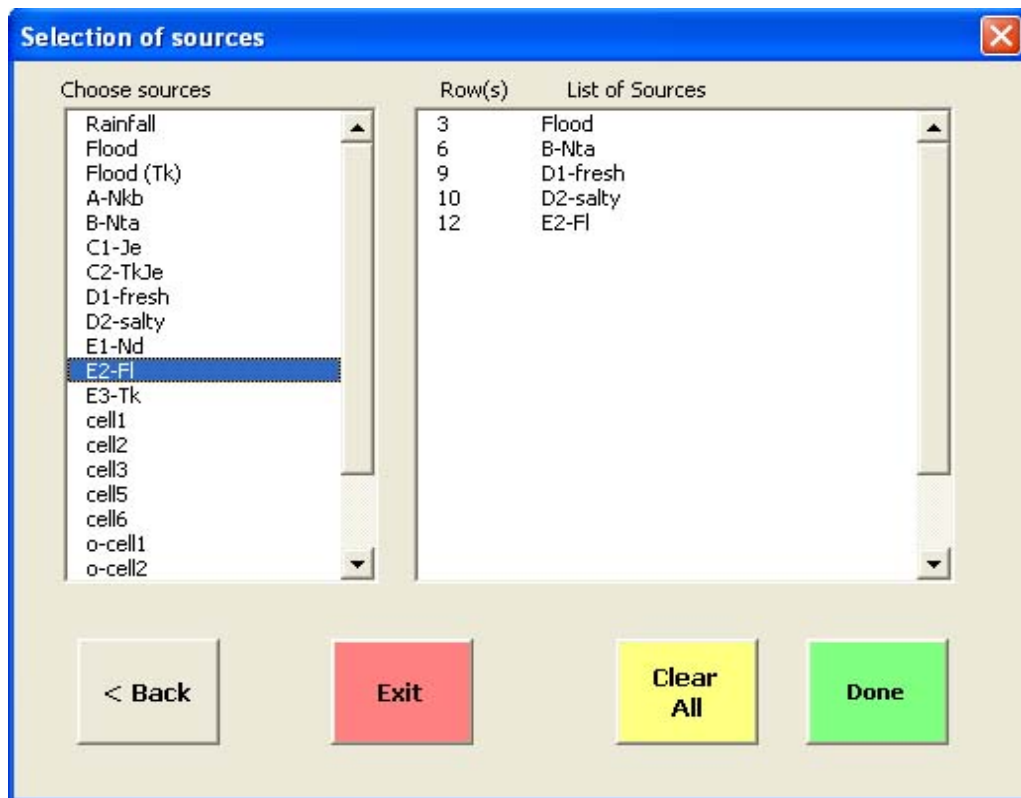


Figure 23. Selection of sources

- The menu '**Selection of sources for each cell**' will be shown next (3.4.6). For this example 'cell4' should be selected first by double-clicking on the corresponding item in the list of cells; then the corresponding sources 'B-Nta', 'Flood', 'D1-fresh', 'D1-salty' and 'E2-FI' should be selected.

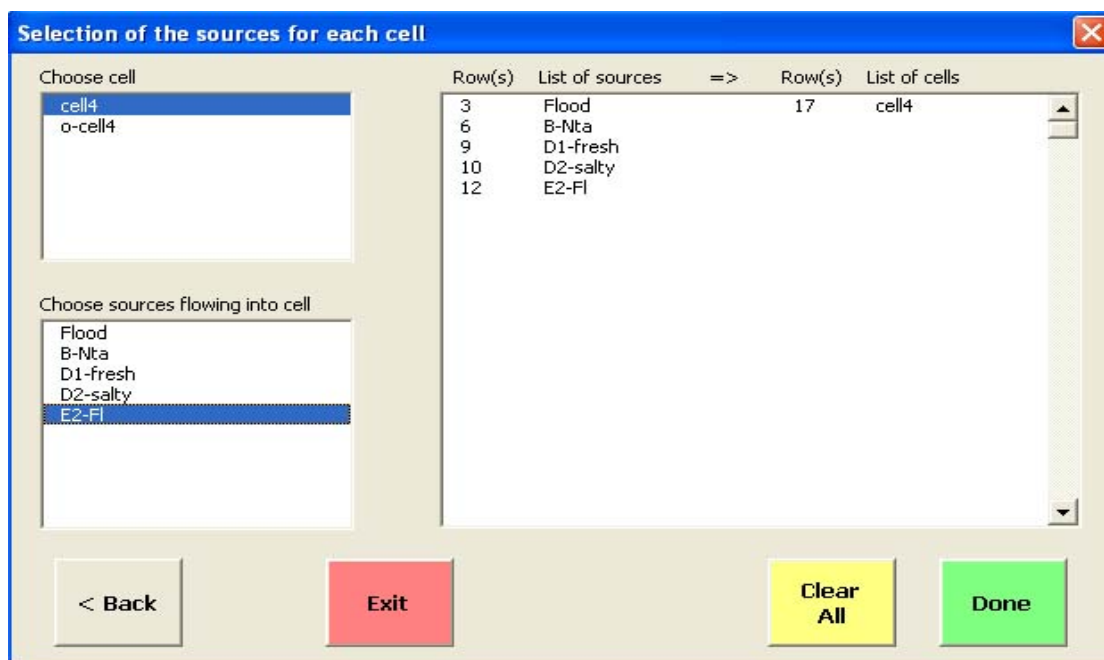


Figure 24. Assigning the sources to the cell

● The result of the configuration will appear in the window on the right. When all 5 sources are listed as sources to 'cell4' the 'Done' button can be pressed invoking the message '5 flows from sources into cells have been defined'. Note that no potential sources are allocated to 'o-cell4' as this cell is in fact fictitious, accounting only for the outflow.

● The configuration of the flow system will now be finalized by defining the flow from the modeled cell into the receiving cell: '**Definition of flows between cells**' (3.4.7). Double click on 'cell4' in the window above, and then on 'o-cell4' in the window below. A line with the discharging and receiving cells and their corresponding row numbers will appear on the right-hand side. A message confirms that one flow has been defined.

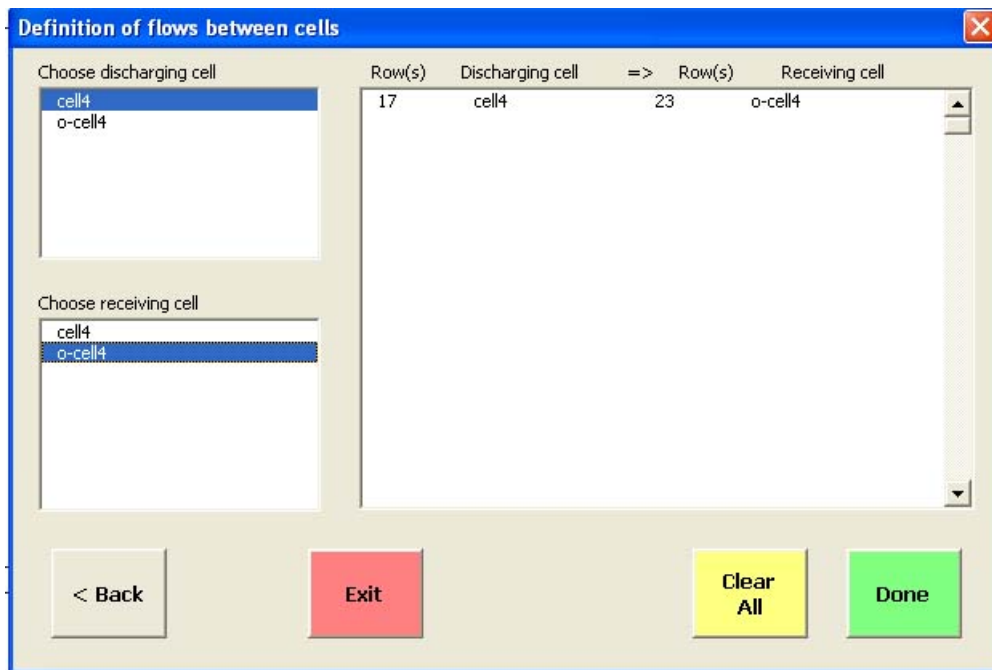


Figure 25. Definition of flows between cells

● The menu with '**rates of external out-flux and outflows**' does not require any changes in this case (3.4.8). The out-flux for 'cell4' is set to zero as no additional pumping or losses are accounted for. The outflow from the last cell - in this case 'o-cell4' - is set to 100.

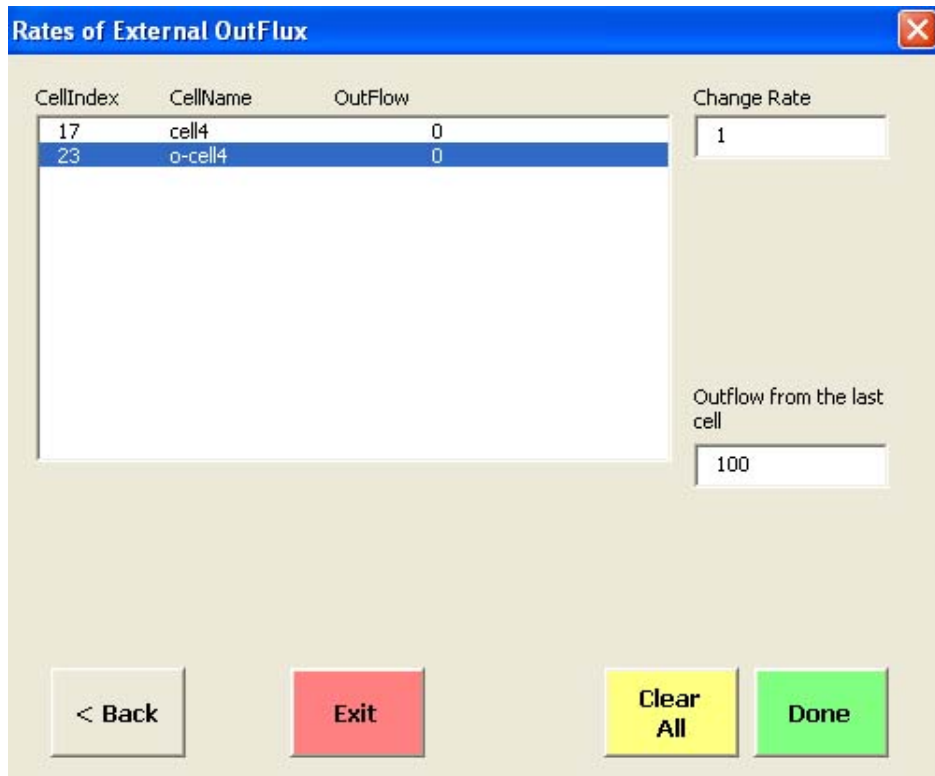


Figure 26. Assigning the output flux (pumping rates and natural subsurface flow)

- By clicking 'Done', the menu for the selection of tracers will be opened (see 'Selection of tracers' [3.4.9]). In this example 'Mg', 'Na' and 'Cl' were selected as tracers as they are more or less conservative in the corresponding hydro-geological system.

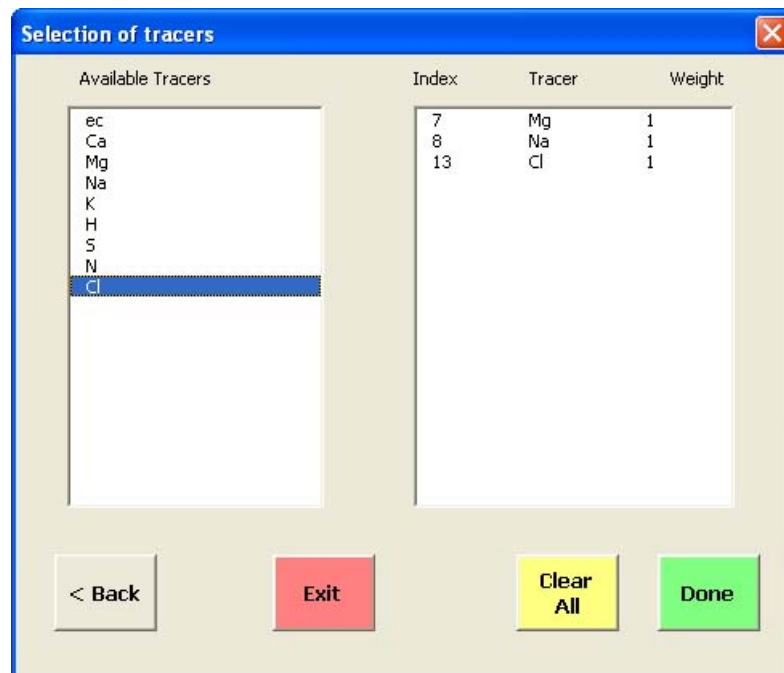


Figure 27. Selection of tracers

The tracers are selected by double-clicking on the corresponding items in the list. In the right window the list of selected tracers is shown. The message box ('3 tracers have been selected') indicates the number of tracers. In the actual version modification of the tracer weight (column 3, default = 1) can only be made in the file produced by MIG.

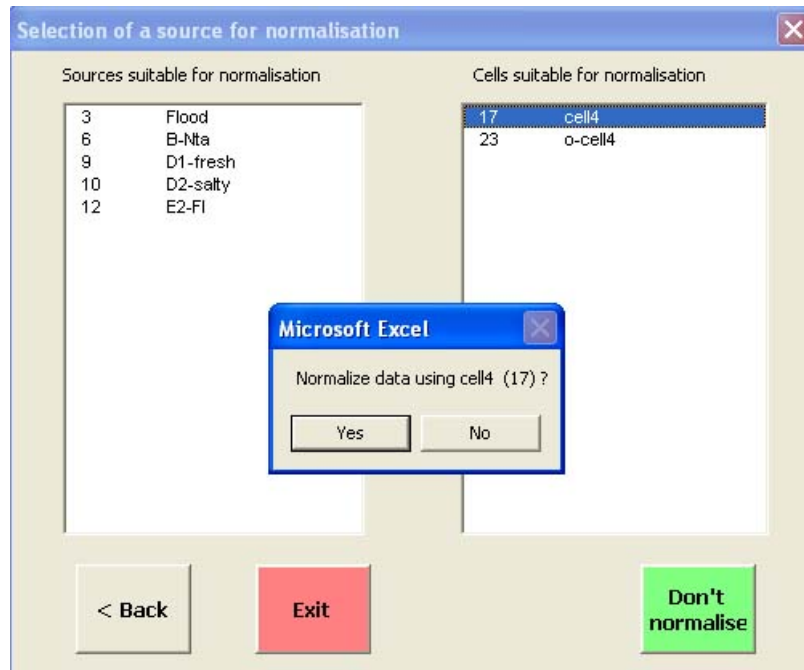


Figure 28. Choice of the cell used for normalization of the hydrochemical/isotope data

● The last menu offers a list of all sources and cells that have been used in the flow model and that can be used for normalization of the data matrix (3.4.10). By default all sources or cells containing a zero element are eliminated from the list of potential candidates to be used for normalization. Normalization improves the optimization process if the absolute differences between tracer concentrations are significant. In this case the chemical data of 'cell4' was chosen for normalization by double-clicking on the item 'cell4'. A message box will pop up indicating the name of the cell to be used for normalization. The final stage of the configuration has now been reached.

● By pressing on the button '**Build input for Wolff**' an Excel table will be written that contains the configuration in a conceptualized format. Type a descriptive name for this specific data to be executed by the MIG model.

In the background a format table will appear summarizing the chemical data and the information on the number of sources, cells and their respective connections.



Figure 29. Menu bar for building and saving the input file, running the Multi.exe and exiting MIG

This table must be saved as an ASCII file before it can be processed by the optimizer. Pressing 'Save Input File' performs this. Type a name for the ASCII file (in this case: 'In15.prn'). In the final step, pressing '**Run Wolff algorithm**' starts the optimizer. This program processes the ASCII file that has been produced in the previous step. It works automatically on the directory in which the configuration will be saved. Re-type the same name for the ASCII data file that was used for the input file. Then type any name for the output file (for example, 'Output15.prn').

The optimizer now asks the user whether the concentration data should be printed: Type '1' for yes. Finally, the number of iterations for the Wolff optimization needs to be specified. In general a number between 100 and 500 will be sufficient. In some rare cases the user needs to increase the number of iterations, up to 5000. The result in the specified Results File can now be checked with any text editor in the working directory. MIG can be terminated by pressing '**Exit**', or other runs can be generated by going backwards in the menu structure.

The results of this run are listed in Output15.prn file.

The contribution from B-Nta amounts to 94%; about 6% (5.7%) is derived from floods. A minor contribution of less than 1% comes from the saline end-member 'E2-FI'.

The unknown inflows are:

	Name of Inflow	Rate of Inflow	% of Total Inflow	% of Cell Inflow	Calculated Flux Values
Cell4	B-Nta	1.78	94.0	94.0	1.78
	Flood	.11	5.7	5.7	.11
	D1-Fresh	.00	.0	.0	.00
	D2-salty	.00	.0	.0	.00
	E2-FI	.01	.3	.3	.01
0-Cell4					

Id	SUMIN	SUMOUT	Abs. Error	% Error
Mg	2.06	2.00	.06	3.0%
Na	2.07	2.00	.07	3.5%
Cl	.95	2.00	-.05	-2.3%

The output file (Output15.prn) also indicates the mass balance errors for water (5.26%) and for each single tracer. If the corresponding errors exceed 15 to 25%, the model configuration is probably inadequate and needs to be improved.

In this example all the major elements that have been used are relevant for multi-cell modeling. The only difference is that the steps for the selection of sources (3.4.5) for different cells are iterated for each cell and that the definition of flows from cell to cell is extended to more than one flow (as above).

For further questions and assistance users may contact the authors:

Eilon Adar

[eilon@bgumail.bgu.ac.il](mailto:eilon@bgumail.bgu.ac.il)

Fax: ++972 8 659 6909

Christoph Kuells

[christoph.kuells@hydrology.uni-freiburg.de](mailto:christoph.kuells@hydrology.uni-freiburg.de) Fax: ++49 761 203 3594

## 5 References

- Adar, E., S. P. Neuman and D. A. Woolhiser (1988). "Estimation of spatial recharge distribution using environmental isotopes and hydrochemical data: I. Mathematical model and application to synthetic data." *Journal of Hydrology*, Vol. 97, pp. 251-277.
- Adar, E. and S. P. Neuman (1988). "Estimation of spatial recharge distribution using environmental isotopes and hydrochemical data: II. Application to Aravaipa Valley in Southern Arizona." *Journal of Hydrology*, Vol. 97, pp. 279-302.
- Adar, E. and S. Sorek (1989). "Multi-compartmental modelling for aquifer parameter estimation using natural tracers in non-steady flow." *Advances in Water Resources*, Vol. 12, pp 84-89.
- Adar, E., E. Rosenthal, A.S. Issar and O. Batelaan (1992). "Quantitative assessment of flow pattern in the southern Arava Valley (Israel) by environmental tracers in a mixing cell model." *Journal of Hydrology*, Vol. 136, pp 333-354.
- Adar, M. E. (1995). "Assessment of groundwater fluxes and transmissivities by environmental tracers - summary of theory, application and sensitivity analysis." In: *Mathematical Methods for Quantitative Evaluation of Isotope Data in Hydrology*. IAEA -TECDOC, Y. Yurtsever, Ed. International Atomic Energy Agency (IAEA), Vienna, Austria, pp. 93-122.
- Adar, M.E. (1996). "Quantitative evaluation of flow systems, groundwater recharge, and transmissivities using environmental tracers". In: *Manual on Mathematical Models in Isotope Hydrology*". IAEA - TECDOC-910, Y. Yurtsever, Ed. International Atomic Energy Agency (IAEA), Vienna, Austria, pp 113-154.