triwaco

groundwater modelling software

5 Execution of Groundwater Flow Simulations: FLAIRS and MODFLOW

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Chapter 5: Execution of groundwater flow simulations

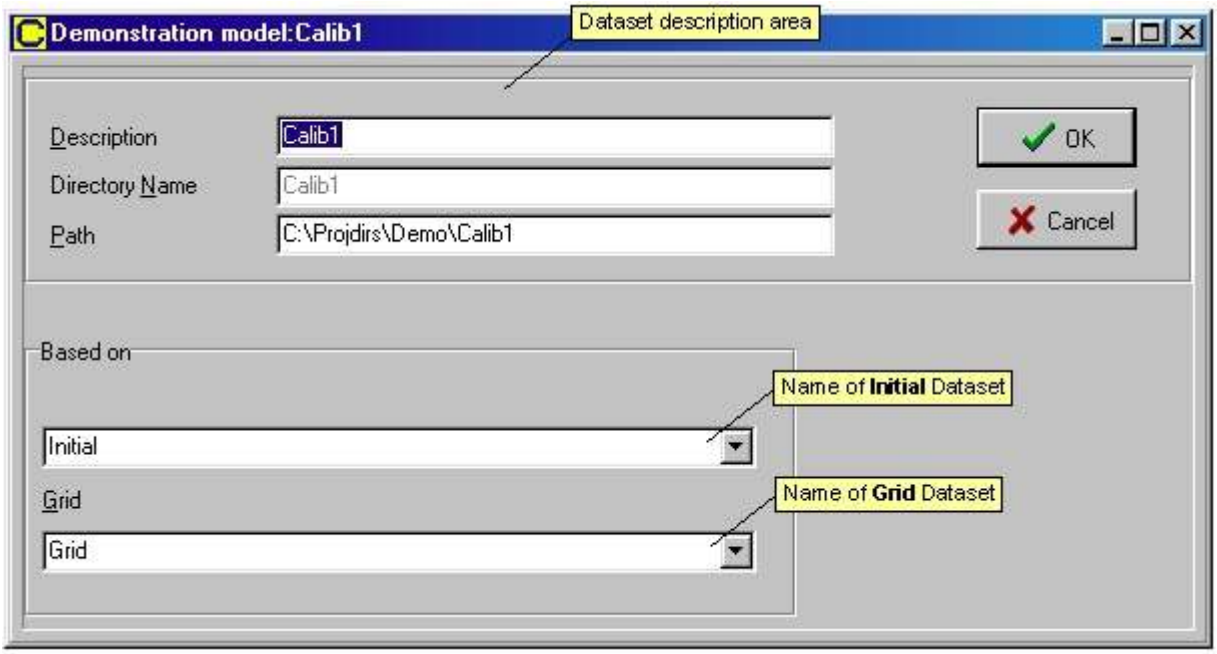
5.1 Creating a Calibration data set

5.1.1 Introduction

So far the model parameters are defined in the '***Initial data set***' by their ***map*** and ***par files*** only and no link to grid exists. Therefore, this link will be established by creating a so-called '***Calibration data set***'.

5.1.2 Opening a Calibration data set

Selecting 'data set' 'Add' from the pull down menu and 'Calibration' from the ***'create new data set'*** dialog window displays the ***'calibration data info window'***.



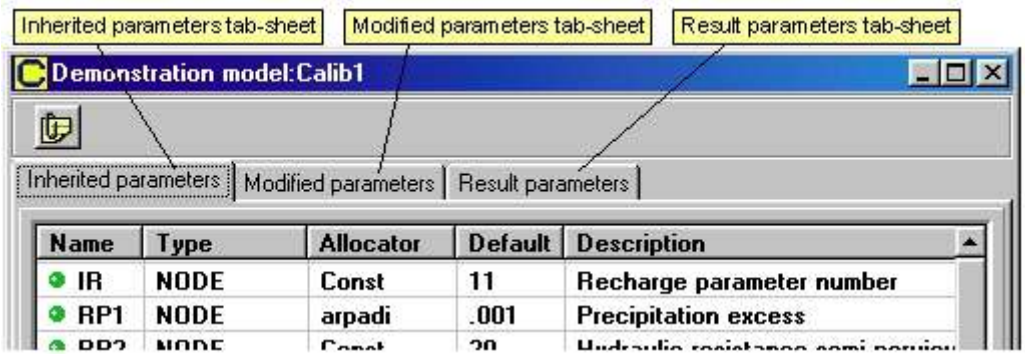
The user has to provide the following information:

A. A descriptive name of the data set and the data set's directory name where the files needed for the groundwater model calculations are located.
B. The name of the data sets the calibration set is based on; e.g. an '***Initial data set***' and a '***Grid data set***'.

Confirming the selection with the 

-button causes the program to open the ***'Calibration data set window'***, displaying all model parameters defined. The ***'Calibration data set window'*** consists of three tab-sheets:

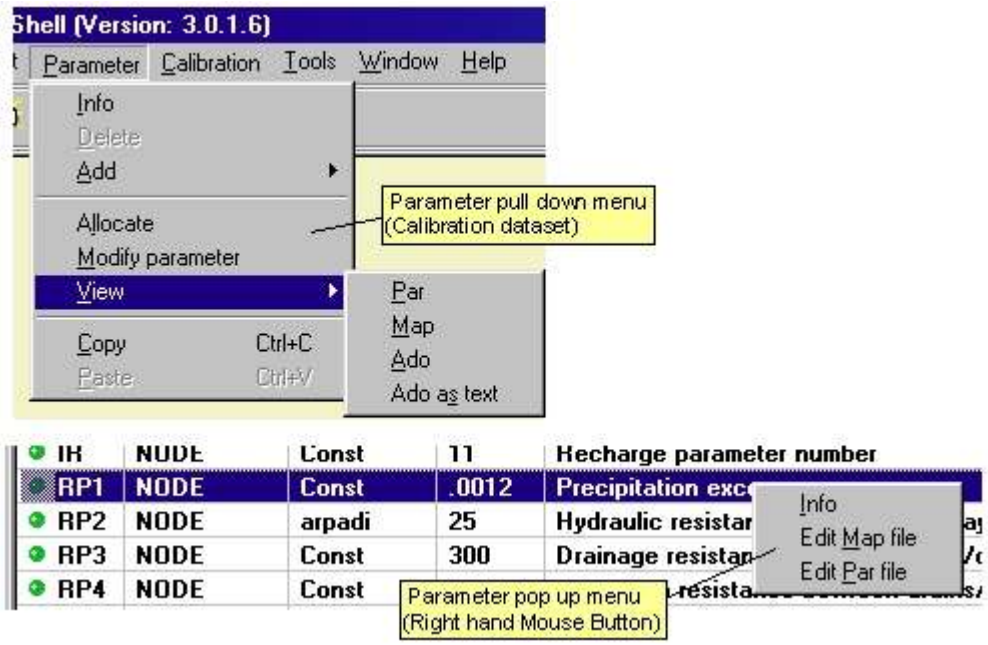
Inherited parameters	This sheet displays all model parameters defined in the (initial) data set the calibration set is based on
Modified parameters	This sheet displays all parameters created or modified in the (actual) calibration data set
Result parameters	This sheet displays all parameters that result from the model calculations. It is displayed only after model calculations have been carried out.



Double clicking on one of the parameters starts the graphical editor DigEdit. For each of the parameters the user can create a new ***map*** and ***par file*** or modify the existing ***map*** and ***par file***. These changes take place in the directory of the Initial data set the Calibration set is based on!

Pressing the right hand mouse button displays the parameter pop-up menu. This menu allows the user to retrieve 'Info', to 'View' or edit the ***map*** or ***par file***, to 'View' the ***Ado*** file (the file containing the parameter values assigned to the nodes of the grid), to 'Allocate' the parameter selected or to 'Modify' the parameter.

Choosing the Parameter pull down menu from the menu bar displays a slightly different selection of possibilities: 'Info', 'Delete', 'Add', 'Allocate', 'View' ('Map', 'Par', 'Adore' and 'Adore as text'), 'Copy' and 'Paste'.



Selecting 'Modify parameter' moves the selected parameters from the ***'Inherited parameters'*** Tab-sheet to the ***'Modified parameters'*** Tab-sheet. The parameter's original par and map files (in the Initial data set's directory) remain unaffected and a new set of par and map files may be created. These files will be located in the Calibration data set's directory.

To add or delete a parameter the ***'Modified parameters'*** Tab-sheet should be active (visible). Only here a parameter (other than the Inherited parameters) can be added. Adding a parameter displays the '***parameter info window***'. This window can also be accessed from the 'Info' command in the pull down and pop-up windows. Deleting a (modified) parameter from the ***'Modified parameters'*** Tab-sheet restores the original settings for this parameter. The parameter reappears in the ***'Inherited parameters'*** Tab-sheet.

5.1.3 Allocating model parameters

Selecting 'Allocate' from the parameter pull down or pop-up menu starts the selected allocator and an ***Ado*** or ***Adore*** file will be generated. After allocation the status of the parameter will change from ✗ to ● .

The ***Ado*** file contains an array with parameter values, interpolated at the locations of the nodes of the grid. This array is preceded by the name of the parameter, a code indicating whether the array contains one (constant) value or as many values as there are nodes and the number and format of values that follow. The array is concluded with the text ENDSET. Such an array with parameter values is called an ***Adore*** set. The number of values in the array depends on the type of parameter and equals the total number of nodes, the number of river nodes, the number of source nodes or the number of boundary nodes. (see appendix B for a complete overview and the lay out of the map, parameter and corresponding ado files, appendix C gives an overview of currently available allocator types).

5.1.4 Viewing the allocated parameters

Selecting 'View Ado file' from the parameter pull down or pop-up menu starts the graphical presentation program TriPlot, loads the grid information and a spatially visualisation of the selected parameter. In this GIS like environment the parameters can easily be checked, compared with other parameters on a spatial scale but also for individual cells/nodes.

5.1.5 Definition of initial head parameters

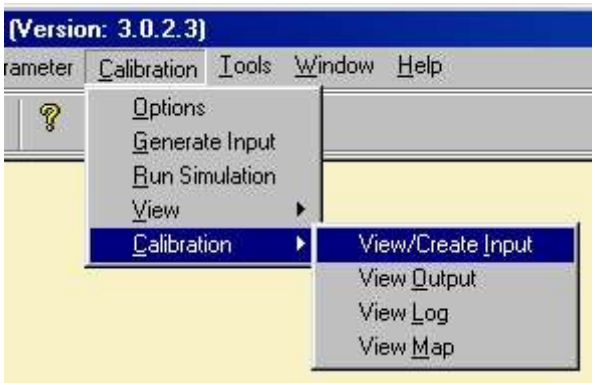
The initial head for each aquifer is defined by HH***i***. The initial head for the topsystem is defined by HT. Defining the initial head may be required for some cases. It is, however, more often used to speed up the simulation run of Flairs in the calibration process or as initial heads for scenario calculations. The initial head is then defined by the output of the former simulation result.

Triwaco computes groundwater heads/flow by iteration, starting from groundwater heads equal to 0.0. A quicker calculation process may be obtained if initial headvalues are used which are closer to the heads to be calculated. The initial head is often defined by the output of the former simulation result.

The initial head for each aquifer is defined by HH***i***. The initial head for the topsystem is defined by HT. These parameters can be defined under the Modified-tab by choosing Parameter | Add | Internal. The groundwaterhead from a former simulation result is defined by using an expression: PH***i*** (where ***i*** is the aquifer number, HT is defined as PHIT).

5.1.6 Definition of a calibration file (calib.chi)

If a **calibration file** (**calib.chi**) is present, **Triwaco** automatically compares calculated hydraulic heads, fluxes with the data from observation wells. After comparison **Triwaco** will calculate the average deviation, the average absolute deviation, the squared average deviation, the minimum deviation and the maximum deviation. To view or edit the calibration file select 'Calibration'|'Calibration'|'View/Create Input' from the pull down menu. The input file has a fixed format described in chapter 10. The output of the calibration can be viewed as table ('Calibration'|'Calibration'|'View Output') or as a background map in **Triplot** ('Calibration'|'Calibration'|View Map'). A comprehensive description on the usage of the calibration (calib.chi) file is given in chapter 10.



5.2 Executing model simulations with FLAIRS

5.2.1 Introduction

Triwaco can handle two types of grids, Finite Element Grids and Finite Difference Grids. Once one of these is selected in the 'Grid definition'- window **Triwaco** will use the corresponding simulation package. The choice between the two is depending on the type of problem, possibilities and/or limitations of the simulation package. The default grid has finite elements with the corresponding simulation package **Flairs**. **Flairs** is a three-dimensional saturated groundwater flow simulation program. The program uses triangular elements with linear shape functions. The numerical calculations are based on Galerkin's method.

For Finite Difference Grid **Triwaco** uses ModFlow-96 provided by the USGS. ModFlow also is a three-dimensional saturated groundwater flow simulation program. Executing model calculations with ModFlow is explained in chapter 5.4.

5.2.2 Simulation Package FLAIRS

Flairs uses a Finite Element grid created by the program **Tesnet** and parameter files in **Adore** format (generated by various **allocators** and with the extension ***.ado**). With the aid of the program **TriPlot** or other Windows programs the results can be visualized as contour maps or hydrographs. The results can directly be used for post-processing and auxiliary programs.

Flairs calculates the groundwater heads and fluxes in a groundwater domain that is divided into aquifers and aquitards. Important features in **Flairs** are the **rivers** (line-source/sinks) and (point)-**sources**, which are active within aquifers, and the large selection of different **top systems** that control the flux from the surface or confining layer to the first aquifer. Hydrogeological parameters are given at the nodes of a Finite Element Grid. These input parameters have to be available in **Adore** format.

The program is capable of handling a variety of problems, such as:

- steady-state and transient flow;
- anisotropy and inhomogeneities (K_{xx}, K_{xy}, K_{yx}, K_{yy}, K_{zz});
- Dirichlet, Neuman and mixed boundary conditions;
- phreatic conditions possible for parts of the model area;
- multi-layered systems containing many aquifers and aquitards;
- flow in a vertical cross section;
- transient recharge imported from **Fluzo**, the **Triwaco** program for the calculation of flow in the unsaturated zone;
- (non)linear recharge relations for sources and sinks, rivers, boundaries and top-systems,
- groundwater flow under variable density conditions,
- clustering of rivers (line-sinks) or sources to simulate drains or multi-screen wells with given abstraction rate.

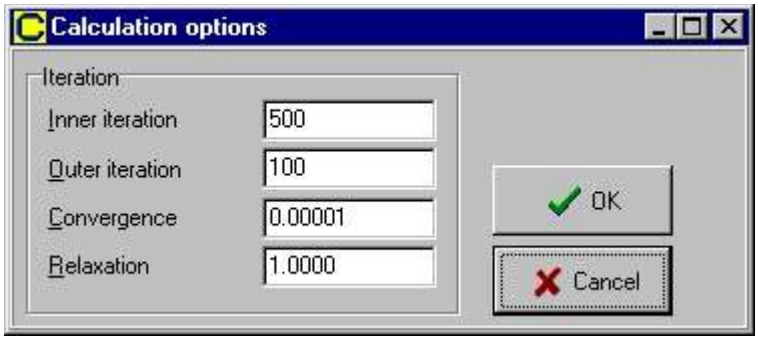
The mathematical background of the simulation package is given in paragraph 5.3.

The program requires a number of readable (standard ASCII) input files and generates various output files. When used in combination with the **TriShell** default file names are assumed for all input and output files.

5.2.3 Simulation options

After allocation of the values for all model parameters one may start the groundwater flow calculations. First, selecting 'Calibration' 'Options' from the menu bar, the ***'Calculation options'*** dialog box is opened.
In this dialog box the user specifies parameters related to the iteration process:

Description	Function
Inner iteration	Sets the maximum number of inner iterations
Outer iteration	Sets the maximum number of outer iterations
Convergence	Sets the criterion for convergence ε
Relaxation	Sets the relaxation factor $(\zeta \leq 1)$



During calculations **Flairs** will pause and display a warning if the maximum number of linear or ***inner iterations*** is exceeded. If the user decides to continue calculations **Flairs** automatically doubles the number of inner iterations. For each ***outer iteration***, the number of inner iterations will be checked.

Calculations will proceed until the number of inner iterations during a single outer iteration equals 2 or less or until the maximum number of outer iterations is reached. Apart from the maximum number of iterations, the user has to specify a ***criterion for convergence***. The program checks whether or not differences are less than the criterion specified. The initial conditions for each outer iteration depend on the head change between (outer) iterations. In case of badly converging systems a ***relaxation factor*** may be defined. In that case the head change between (outer) iterations is multiplied with the relaxation factor. This causes a more stable iteration process but also results in smaller head changes, thus requiring more iterations to reach a solution.

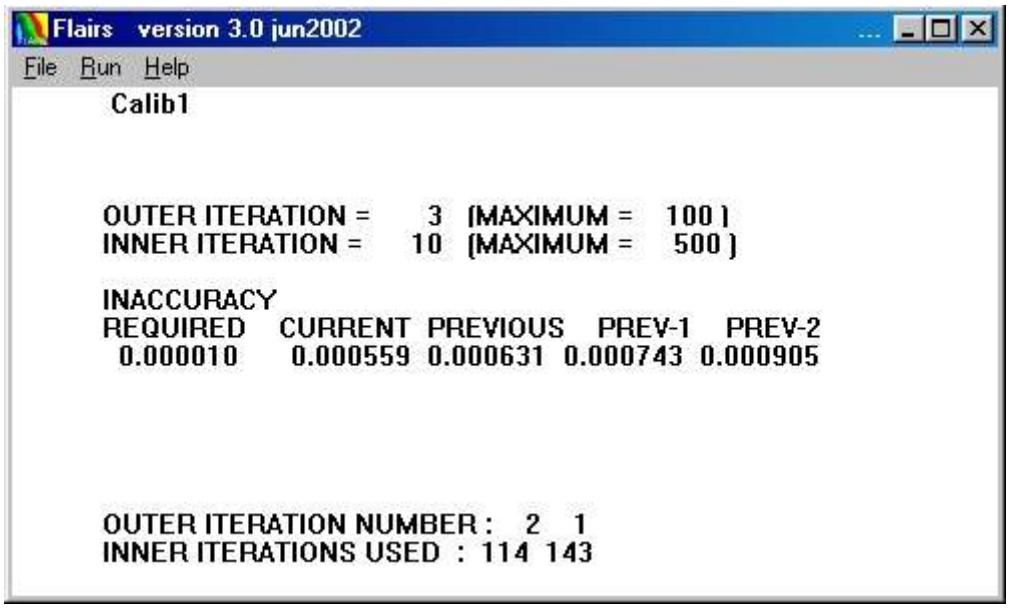
5.2.4 Executing the model simulation

For starting the model calculations one first selects 'Generate input' from the Calibration pull down menu bar. This will generate the input file needed (***flairs.fli***). This input file may be viewed or edited selecting 'View' 'Input' from the pull down menu. The input file contains all parameters needed for the calculations. A description of the input file ***flairs.fli*** is given in paragraph 5.2.6.

Selecting 'Run Simulation' from the Calibration pull down menu starts model simulations.

A window, showing the calculation process will be displayed and the program will be added to the tasks window. Once the calculation has stopped the ***'Result parameters'*** Tab-sheet will be updated. After the first run this Tab-sheet will be added to the ***'Calibration data set'***. If a '***calibration file***' has been defined, the program automatically compares the calculation results with the observed heads/fluxes.

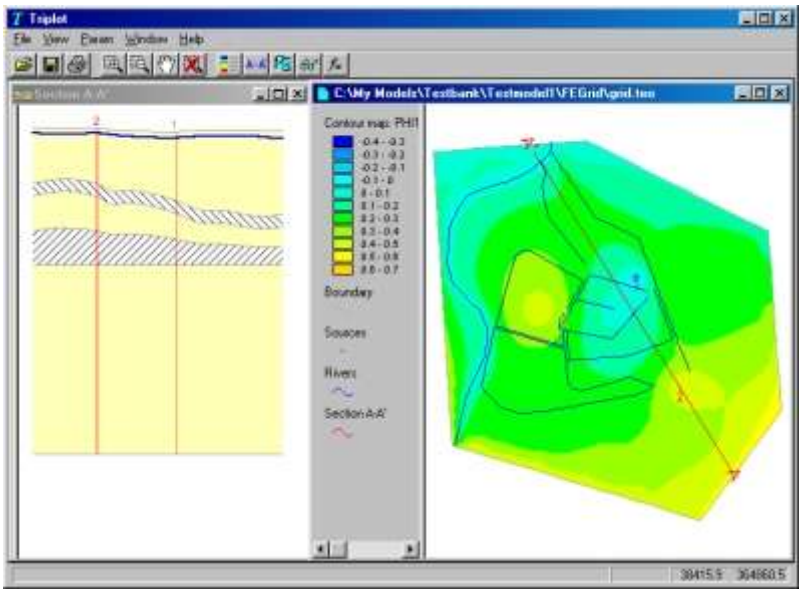
The simulation program produces different types of output files. Some of these files contain information on the calculation process, errors encountered, (***flairs.flg***) others contain the calculation results using various formats (***flairs.flp***, ***flairs.flo***).



Triwaco computes groundwater heads/flow by iteration, starting from groundwater heads equal to 0.0. A quicker calculation process may be obtained if initial headvalues are used which are closer to the heads to be calculated. The initial head is often defined by the output of the former simulation result. Definition of the initial head is described in par. 5.1.5.

5.2.5 Viewing output results (maps)

Selecting 'View' 'Results' from the Calibration pull down menu starts the graphical presentation program **TriPlot**, loads the grid information and displays the layout of the model area. Now the user can contour or classify the result parameters and view the results in plane view or can select a cross-section of the model area.



Alternatively, the user can select one of the parameters from the 'result parameters' sheet and viewing the parameter separately selecting 'View' 'Adore' from the Parameter pull down menu or 'View Adore file' from the pop-up menu (right hand mouse button). Adding other parameters (selecting 'Param' 'Load' from the **TriPlot** menu bar) gives the user the opportunity to compare result parameters with model input parameters.

5.2.6 Input data description

The input file (***flairs.fli***) for the groundwater simulation program contains the definition of the hydrogeological system, including references to all input parameter files, boundary conditions, output options and so on. The input file may be generated automatically from the **TriShell** or edited manually.

The input required in the ***flairs.fli*** consists of the following sets:

Set 1:

HEAD	· identification of project or grid	Format A40

HEAD is an alphanumerical string for identification of the project's grid

Set 2:

Naq, Iffr, Ifss, Ifsf, Iftr, Nsar, Rrlax	· number of aquifers · flag for confined / phreatic calculations · flag for steady-state / transient calculations · flag for variable density or salt / fresh water interface · dummy flag (used only in previous versions of Flairs) · number of sub-areas for water balance calculation · relaxation factor for non-linear iterations	Format 6(I5), F10.4

Naq	the number of aquifers
Iffr	a flag for (semi) confined (=0) or phreatic (=1) calculations
Ifss	a flag for steady state (=0) or transient (=1) computations; also used for the definition of the Surface water option (**FLAIRSSF**).

Ifsf	a flag for absence (=0), presence (=1) of a salt/fresh water interface, variable density (FLAIRSVD)(=2)
Iftr	a dummy-flag (in former versions for preparing Trace output)
Nsar	the number of sub-areas a water balance will be calculated for
Rrlax	the relaxation factor for the non-linear iterations.

Set 3a:

NB	· number of boundary points for water balance sub-areas	Format I5

NB the number of boundary points defining the sub-area for water balance calculations (NB $\leq$ 20)

Set 3b:

XB, YB	· coordinates of boundary points for water balance sub-areas	Format 2(F10.4)

XB,YB the X and Y coordinates of the boundary points. The coordinates of the last boundary point are not necessarily equal to the coordinates of the first boundary point.
Set 3b will be repeated (NBP-1) times.

Sets 3a and 3b should be repeated Nsar times, for each of the water balance sub-areas, and omitted if Nsar = 0.

Set 4a:

HCU, NCriv, NCsrc	· name of collection unit · number of rivers in collection unit · number of sources in collection unit	Format A20, 2(I5)

HCU	identification string for the collection unit. A collection unit is a combination of rivers and sources for which the total recharge is computed and written tot the print output file ***flairs.flp***
NCriv	number of rivers belonging to the collection unit
NCsrc	number of sources belonging to the collection unit

Set 4b:

ICriv, Iaq, Iriv	· sequential number of collection unit's river · aquifer number of river · river number / river ID	Format 3(I5)

ICriv	sequential number of the river, ICriv = (1,,NCriv)
Iaq	sequential number of the aquifer the river or source is active in
Iriv	identification number of the river involved

Set 4b will be repeated NCriv times.

Set 4c:

ICsrc, Iaq, Isrc	· sequential number of collection unit's source · aquifer number of source · source number / source ID	Format 3(I5)

ICsrc	sequential number of the source, ICriv = (1,,NCsrc)
Iaq	sequential number of the aquifer the river or source is active in
Isrc	identification number of the source involved

Set 4c will be repeated NCsrc times.

Set 4 should be repeated for each collection unit and omitted if no collection units are defined. The maximum number of collection units equals 50.

Set 5:

End of sum input	· literal text string

This string should always be present, it indicates the end of the section

Set 6:

Isrc, Iaq, Ist, Qsrc, Hsrc	· source ID · active aquifer number · type of source · discharge or recharge rate · groundwater head	Format 3(I5), 2(E10.4)

Isrc	the source **ID** as defined in the ***grid.teo*** file
Iaq	the number of the aquifer the source is active in
Ist	a flag for identifying the type of sources
If Ist =0	the source is defined by a given rate Qsrc
If Ist =1	the source is defined by a given head Hsrc
Qsrc	abstraction or infiltration rate (Qsrc<0: abstraction)
Hsrc	fixed groundwater head

Set 6 should be repeated as many times as required.

In stead of using **Set 6**, sources are generally defined using the source parameter sets **IS*i***, **SH*i*** and **SQ*i*** (***i***=1,,N). Moreover, using the source parameters, the user may also specify 'clustered' sources (**IS*i***=2).

The use of source parameter sets overrides the values defined by **Set 6**.

If no source parameter sets are defined, sources that are not defined by **Set 6** will have a default abstraction rate of Qsrc=0 (with source type Ist=0).

Set 7:

End of sources input	· literal text string

This string should always be present, it indicates the end of the section

Set 8:

Ibnd, Iaq, Ibt, Hbnd	· boundary point number · active aquifer number · type of boundary · groundwater head	Format 3(I5), E10.4

Ibnd	the boundary point number as defined in the ***grid.teo*** file
Iaq	the number of the aquifer the boundary condition is given for
Ibt	a flag for identifying the type of boundary condition
. If Ibt =0	the boundary is defined by a given head Hsrc
. If Ibt =1	the boundary is defined by a head dependent flux
Hbnd	fixed groundwater head (for Ist =0)

or

Ibnd, Iaq, Ibt, BA, BB	· boundary point number · active aquifer number · type of boundary · head dependent flux parameter · head dependent flux parameter	Format 3(I5), 2(E10.4)

BA, BB	head dependent flux parameters (for Ist =1)

Set 8 should be repeated as many times as required.
In stead of using **Set 8**, boundary conditions are generally defined using the boundary parameter sets **IB*i***, **BH*i***, **BA*i*** and **BB*i*** (***i***=1,,N). Parameters **BA*i*** and **BB*i*** define the head dependent boundary flux (**IB*i***=1).

The use of boundary parameter sets overrides the values defined by **Set 8**. If no boundary parameter sets are defined, boundaries that are not defined by **Set 8** will have a default boundary head of Hbnd=0 (with boundary type Ibt=0).

Set 9:

End of boundary input	· literal text string

This string should always be present, it indicates the end of the section

Set 10:

Iriv, Iaq, Irt, Hriv	· river ID · active aquifer number · type of river · river water level	Format 3(I5), E10.4

Iriv the river **ID** as defined in the ***grid.teo*** file
Iaq the number of the aquifer the river is active in
Irt a flag for identifying the type of boundary condition
. If Irt =0 the river is defined by a given water level Hriv
. If Irt =1 the river is defined by a given flux Qriv
Hriv the river water level (for Irt =0)

or

Iriv, Iaq, Irt, Qriv, Nclus	· river ID · active aquifer number · type of river · river discharge or recharge · river cluster number	Format 3(I5), E10.4, I5

Qriv the recharge or discharge rate (for Irt =1)
Nclus the river cluster number (for Irt =1); clustered rivers will have the same head.

Set 10 should be repeated as many times as required.

In stead of using **Set 10**, the rivers are generally defined using the river parameter sets **RA*i***, **HR*i***, and **RQ*i*** (***i***=1,,N). The value for **RA*i*** equals (Irt+1). For clustered rivers the parameter **RC*i*** should be defined also.

The use of river parameter sets overrides the values defined by **Set 10**. If no river parameter sets are defined, rivers that are not defined by **Set 10** will not be active (equivalent to **RA*i***=0).

Set 11:

End of river input	· literal text string

This string should always be present, it indicates the end of the section

In stead of using **Sets 6, 8 and 10** the user is advised to define the parameters in question by the appropriate parameter sets (***Adore*** -files). The text strings defined in **Sets 7, 9 and 11**, however, should never be omitted.

In the next section all model parameters are being defined. The boundary, river and source parameters mentioned above should be defined here too, unless the user has specified **Sets 6, 8 and 10**.

Set 12: consists of three records

Pname	· Triwaco parameter name	Format A4
Fname	· parameter file name	Format A60
FPname	· user defined parameter name	Format A20

Pname is the pre-defined **Triwaco** parameter name
Fname the name of the file containing the parameter, including the full path
FPname a user defined name describing the parameter; this name may be different from the predefined parameter name.

Set 12 should be repeated as many times as required. If Pname is not one of the pre-defined **Triwaco** parameter names, Set 12 will be ignored. Parameters that are not defined by **Set 12** will obtain a default value equal to 0, except for the anisotropy parameters **PY*i*** and **TY*i***, which will be assigned the value of the corresponding **PX*i*** and **TX*i***.

Set 13:

End	· literal text string

This string should always be present, it indicates the end of the section

In the next section the calculation parameters are being defined. One can discriminate between parameters needed for steady-state calculations and those needed for the transient calculations only. Of course the latter only need to be present if transient calculations are required and Ifss=1 (see **Set 2**).

Set 14:

IImax, IOmax, EPS	· maximum number Inner Iterations · maximum number Outer Iterations · convergence criterion	Format 2(I5), E10.4

IImax the maximum number of iterations allowed for the linearized equations
IOmax the maximum number of iterations allowed for the non-linear equations
EPS the criterion for convergence for the linearized equations

For steady-state calculations continue with **Set 17**.

Set 15a:

Ngrf	· number of nodes for time series	Format I5

Ngrf the number of nodes for which time-series output will be generated

Set 15b:

I1, I2, …, INgrf	· node number for time series	Format 16(I5)

I***i*** (***i***=1,,Ngrf) the numbers of the FE-nodes for which time-series output is required. The node numbers correspond with the numbers from the FE-grid file ***grid.teo***

Set 15b should be repeated Ngrf/16 times and omitted if Ngrf=0.

The time-series output for the Ngrf nodes defined by the node numbers of **Set 15b** are written to the output file ***graphnode.out***.

Set 16:

Tend, DHmx, DT	· stress input time · maximum allowable head change per time step · initial time-step size	Format 3(E10.4)

Tend the stress-input time or time at which a new time-step starts and new input data may be defined (end time of calculation period)
DHmx the maximum allowable change in groundwater head per time-step for the time period considered
DT the size of the initial time-step for the time period considered

Set 17:

Iprn, Irst, Iphit, Iqrch, (Iphi***n***, Iqkw***n***)***n***=1,,Naq (Iqri***n***, Iqsc***n***)***n***=1,,Naq	· print and output flags	Format (4+4***n***)I5

Iprn code for printing (=1) or not printing (=0) calculation results to the print output file ***flairs.flp*** (default value 0, no print output)
. If Iprn=0 calculation results not to the print output file
. If Iprn=1 calculation results to the print output file (default)
. If Iprn=2 calculation results to the print output file and top-system fluxes will be written to file ***Top4Q.out*** (only if top-system 4 is selected) and ***flairs.flo***
Irst code for generating restart record
. If Irst=0 no restart record (default)
. If Irst=1 a restart record will be written at time T_{END} (transient calculations only)
Iphit code for writing (=1) or not writing (=0) calculation results for the parameter **PHIT** to the output files ***flairs.flo*** (default value 1)
Iqrch code for writing (=1) or not writing (=0) calculation results for the parameter **QRCH** to the output files ***flairs.flo*** (default value 1)

Iphi***n***	code for writing (=1) or not writing (=0) calculation results for the parameter **PHI*n*** (***n*** ranges from 1 to **Naq**, see **Set 2**) to the output files ***flairs.flo*** (default value 1)
Iqkw***n***	code for writing (=1) or not writing (=0) calculation results for the parameter **QKW*n*** (***n*** ranges from 1 to **Naq**, see **Set 2**) to the output files ***flairs.flo*** (default value 1)
Iqri***n***	code for writing (=1) or not writing (=0) calculation results for the parameter **QRI*n*** (***n*** ranges from 1 to **Naq**, see **Set 2**) to the output files ***flairs.flo*** (default value 1)
Iqsc***n***	code for writing (=1) or not writing (=0) calculation results for the parameter **QSC*n*** and **QBO*n*** (***n*** ranges from 1 to **Naq**, see **Set 2**) to the output files ***flairs.flo*** (default value 1)

The flags Iphit, Iqrch and following are only required in case of transient calculations. Selecting a value 0 (not writing to output) diminishes the size of the output file considerably. However, calculation results for those parameters will be lost. Note that the last flag for QKWn (n=Naq) is a dummy, because the parameter does not exist.

Set 17 is the last input set for steady state calculations.

For transient calculations a number of input sets have to be repeated to define new input at successive stress-input times or to redefine the calculation parameters and print output options if desired.

Set 18 to 25 redefine the input parameters by repeating **Sets 6 to 13**.
Starting at stress-input time T_{END} (the end of the previous calculation period, see **Set 16**) new parameter values may be defined. If a parameter is not redefined the values from the previous calculation period are assumed to remain valid.
At least the **Sets 7, 9, 11 and 13** should be repeated.

Set 26 and 27 are similar to **Set 16 and 17** and redefine the transient calculation parameters and the print output options. A new stress-input time T_{END} will be defined, and new values for the initial time-step or maximum allowable head change may be given.

Sets 18 to 27 should be repeated for every new stress-input time, thus producing **Sets 28+*n**10** to **37+*n**10**.

The transient calculation stops if the value of T_{END}, defined in one of the **Sets 26** or **36+*n**10**, is smaller than the previous value of the parameter Tend.

Example Flairs input file *Flairs.fli*

Set	Example text
1	MATRIX Transient calculation
2	3 1 1 0 0 2 1.0000
3a	5
3b	142811 471333
3b	142654 471117
3b	142890.11 470345.87
3b	143169 470972
3b	142884 471332
3a	4
3b	142338.13 470137.27
3b	142968.77 470229.18
3b	142578.13 470333.86
3b	142324.09 470356.84
5	end of sum input
7	end of sources input
9	end of boundary input
11	end of river input
12	IR
	..\Calib\IR.ado
	IR
12	RP2
	..\Calib\RP2.ado
	RP2
12	RP3
	..\Calib\RP3.ado
	RP3
	… …
12	HT
	HT.ado
	HT

12	HH1
	HH1.ado
	HH1
12	SC1
	SC1.ado
	Storage Coeff Aqf 1
	… …
12	RP1
	RP1.ado
	RP1,TIME= 0.00
13	end
15a	100 100.00001000
15b	0
16	10.0000 1.0000 0.2500
17	1 0 1 1 1 1 1 1 1 1 1 1 1 1 1
7	end of sources input
9	end of boundary input
11	end of river input
12	RP1
	RP1.ado
	RP1,TIME= 10.00
13	end
16	20.0000 1.0000 0.2500
17	1 0 1 1 1 1 1 1 1 1 1 1 1 1 1
7	end of sources input
9	end of boundary input
11	end of river input
12	RP1
	RP1.ado
	RP1,TIME= 152.00
13	end
16	162.0000 1.0000 0.2500
17	1 0 1 1 1 1 1 1 1 1 1 1 1 1 1
7	end of sources input
9	end of boundary input
11	end of river input
12	RP1
	RP1.ado
	RP1,TIME= 345.00
13	end
16	345.0000 1.0000 0.2500
17	1 0 1 1 1 1 1 1 1 1 1 1 1 1 1
7	end of sources input
9	end of boundary input
11	end of river input
13	end
16	0.0000 1.0000 0.2500
	File ends with an empty line

END OF FILE

5.2.7 Output data description

The simulation program produces different types of output files. Some of these files contain information on the calculation process (***flairs.flg***) others contain the calculation results using various formats (***flairs.flp***, ***flairs.flo***), and the time-series output file ***graphnode.out***).

Print output file (flairs.flp)

Selecting 'View' 'Print' from the Calibration pull down menu displays the print output file (***flairs.flp***). This file contains information on the water balances of the various aquifers, including the error in the water balance for each aquifer. These errors should be within reasonable limits, e.g. less than a few percent at a maximum. Furthermore, the discharges towards the rivers, sources and boundaries are summarized.

The print output file ***flairs.flp*** is always generated and contains:

- A water balance for every aquifer. For transient calculations this water balance is given for every time step together with a cumulative water balance.
- A water balance for the ***sub-areas*** defined in the input file (usage described together with flairs.fli).
- The total recharge or discharge for each ***collection unit*** defined in the input.
- The recharge from or the discharge towards all river nodes.
- The recharge from or the discharge towards all point sources and sinks.

- The boundary heads and boundary fluxes for all boundary nodes.

Optionally the following output may be added to the print file, provided the corresponding print-flags are enabled in the ***flairs.fli***-input file:

- The groundwater heads for each aquifer and for every node.
- The location of the salt-fresh water interface for every node.
- The recharge from the top-system and the leakage through the aquitards for every node.

In case of transient calculations this output is given at the end of every calculation period for which the user enabled print output by setting the appropriate flag. If all print-flags are enabled the print file may become very large. Therefore, by default these print-flags are disabled and the print file only contains the water balances and an overview of the river, source and boundary fluxes.

Simulation log file (flairs.flg)
Selecting 'View' 'Log' displays the execution log file (***flairs.flg***). This file contains information on the progress of the calculation process. Any error during the simulation are written to this file. The following information is written to this file:

- General information regarding the used grid, the number of aquifers, the type of the top aquifer and the computation of a salt-fresh water interface.
- Information concerning the input parameters and the parameter files used. Warnings and Error messages are included.
- Information concerning the iteration process. The convergence criterion, the maximum number of iterations and the number of iterations used are reported.

Consultation of the execution-log file is advised whenever an error message is generated. Even if the calculation seems to have finished without problems, a quick check of the log file may confirm whether or not the program has terminated correctly.

Simulation result file (flairs.flo)
Finally, all calculation results are stored in the result file ***flairs.flo***, which contains the output parameters in ***Adore*** format. These parameters provide the result of the calculation.

For ***steady-state*** calculations the output file contains the following variables:

- average groundwater heads for the top-system,
- groundwater heads for each aquifer,
- piezometric head at the salt-fresh water interface,
- recharge to the top-system,
- (sum of drainage/infiltration in topsystem)
- leakage through the separating layers,
- discharge or recharge of rivers for each aquifer,
- discharge or recharge of sources for each aquifer,
- boundary fluxes for each aquifer.

Similarly, for ***transient*** calculations the output file contains the following variables:

- average groundwater heads for the top-system at the end of each period,
- groundwater heads for each aquifer at the end of each period,
- recharge to the top-system at the end of each period,
- leakage through the separating layers at the end of each period,
- discharge of rivers for each aquifer at the end of each period,
- discharge of sources for each aquifer at the end of each period,
- boundary fluxes for each aquifer at the end of each period.

The parameter sets in the file ***flairs.flo*** have the following names:

steady-state calculations	transient calculations
Phreatic and piezometric heads	
PHIT, STEADY-STATE==	PHIT,TIME:nnnnnnnnnn
PHI***x***, STEADY-STATE==	PHI***x***,TIME:nnnnnnnnnn
(***x*** = number of aquifer)	
Variable density correction fluxes	
V10***nn***, STEADY-STATE==	V10***nn***, STEADY-STATE==
V20***nn***, STEADY-STATE==	V20***nn***, STEADY-STATE==
V30***nn***, STEADY-STATE==	V30***nn***, STEADY-STATE==
Top system fluxes and leakage	
QS***xx***, STEADY-STATE==	QS***xx***,TIME:nnnnnnnnnn
QRCH, STEADY-STATE==	QRCH,TIME:nnnnnnnnnn
(QDR1, STEADY-STATE==)	(QDR1, TIME:nnnnnnnnnn)
QKW***x***, STEADY-STATE==	QKW***x***,TIME:nnnnnnnnnn
(***x*** indicates leakage from aquifer ***x + 1*** to aquifer ***x***)	
Recharge and discharge to rivers	
QRI***x***, STEADY-STATE==	QRI***x***,TIME:nnnnnnnnnn
Recharge and discharge to sources	
QSC***x***, STEADY-STATE==	QSC***x***,TIME:nnnnnnnnnn
Boundary fluxes	
QBO***x***, STEADY-STATE==	QSC***x***,TIME:nnnnnnnnnn
(***x*** = number of aquifer)	

The string '**nnnnnnnnnn**' stands for one of the output times defined by the user; the format used for the output times is (F10.4). The length of the output parameter name is in all cases twenty characters, including spaces or blanks.

Drainage result file (top4q.out)
If applicable for topsystem 4 (see input description) then the drainage/infiltration fluxes are written to ***top4q.out***. Is same as Qs***xx,..*** in the ***flairs.flo*** file.

steady-state calculations	transient calculations
Drainage /infiltration fluxes	
TOP1 AT TIMESTEP 1	TOP1 AT TIMESTEP nnn
TOP2 AT TIMESTEP 1	TOP2 AT TIMESTEP nnn
TOP3 AT TIMESTEP 1	TOP3 AT TIMESTEP nnn
TOP4 AT TIMESTEP 1	TOP4 AT TIMESTEP nnn

Where the result of :
- TOP1 is governed by the topsystem parameters RP4 (drainage resistance),RP7 (infiltration resistance) and RP10 (base elevation of system)
- TOP2 is governed by the topsystem parameters RP5 (drainage resistance),RP8 (infiltration resistance) and RP11 (base elevation of system)
- TOP3 is governed by the topsystem parameters RP6 (drainage resistance),RP9 (infiltration resistance) and RP12 (base elevation of system)
- TOP4 is governed by the topsystem parameters RP13 (surface level)

Graphnode (graphnode.out)
The output file ***graphnode.out*** contains time-series output for ***transient*** calculations. For a number of nodes, defined by the user in the input file for transient calculations, groundwater heads and the interface can be written as a function of time. The time and parameter values are exported to the time-series output file (***graphnode.out***). The time-series data is listed in columns. The first of these columns contains the time value, the other columns contain values for the various parameters, successively for each of the grid nodes specified. The heading of the file specifies for which nodes parameters have been exported to the time-series output file. The information from the time-series output file can easily be imported in a spreadsheet.

5.2.8 Command line calls

Program for the calculation of groundwater flow; program name: ***Flawin95, FlawinVD, FlawinVDEXT***.

Normally if a calibration file (***calib.chi***) exists a comparison between calculated and observed heads will be carried out.

A standard input file (***flairs.fli***) must be generated from the **TriShell**. Also, a standard grid file (grid.teo) is required. Output will be written to files: ***flairs.flo, flairs.flp*** and ***flairs.log***. If no arguments are given the program opens in Windows mode. The appropriate input files (***grid.teo, flairs.fli*** and ***calib.chi)*** can be selected and the program may be run using the pull-down menus.

Command line call:

```
Flawin95.exe  [set-dir  grid-dir  flairs.fli  calib.chi  [options]]
```

One may choose from the following options:

-c **no** calibration file checking
-f **no** Flairs computation

Example:

```
Flawin95  C:\model\cal  C:\model\grid  flairs.fli  calib.chi
Flawin95  C:\model\cal  C:\model\grid  flairs.fli  calib.chi  -f
```

5.3 Mathematical background of FLAIRS

5.3.1 Introduction

In this documentation, a description will be given of the governing differential equations and the Finite Element formulation of these equations. Furthermore a description will be given of the way recharges and fluxes are treated in the program. Special options, such as anisotropy and phreatic transmissivity are discussed and the way the Finite Element equations are solved will be described.

5.3.2 Partial differential equation

The partial differential equation that is solved (by approximation) in the program ***Flairs***, follows from Darcy's law and the equation of continuity. In the derivation of the equations the Dupuit-Forchheimer assumption is used, so that the partial differential equation can be written in terms of the potential '***h***' (or groundwater head) as:

$$\frac{\partial}{\partial x}\left[T_{xx}\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial x}\left[T_{xy}\frac{\partial h}{\partial y}\right]+\frac{\partial}{\partial y}\left[T_{yx}\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial y}\left[T_{yy}\frac{\partial h}{\partial y}\right]+q=S\frac{\partial h}{\partial t} \qquad [1]$$

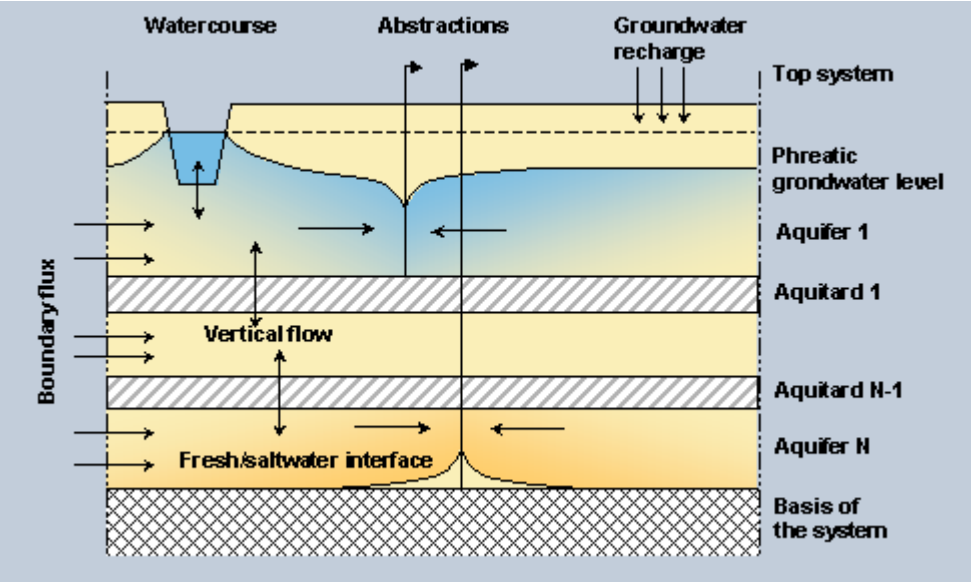
There are no restrictions on the ***transmissivity*** tensor '$\underline{T}$'. Therefore, the transmissivity can be anisotropic, while the principal directions do not coincide with the coordinate axes.

For a multi-aquifer system, the equation [1] holds for each aquifer. The aquifers are coupled through the recharge term '***q***'.

The top aquifer may be phreatic. In that case, transmissivity is a function of the groundwater head and the permeability of the aquifer, while ***storativity*** changes if the aquifer changes from confined to phreatic conditions.

In the lower most aquifer a salt-fresh water interface may be present. The salt water is assumed to be at rest, and the interface can be obtained from the 'Badon-Ghijben / Herzberg' equation. In that case, transmissivity is again a function of the groundwater head and the aquifer permeability. Also storativity changes when the aquifer changes from completely fresh to partly fresh. (**Note** that ***Flairs*** should **not** be used for transient calculations with a salt fresh water interface, due to the assumption of a stagnant salt-water body). Phreatic conditions and a salt-fresh water interface may be defined in one and the same aquifer in case of single aquifer systems.

In case of transient calculations, or if salt water is present in more than one aquifer the variable density module of FLAIRS (FLAIRSVD) should be used. The use of this module requires additional input and some minor changes in the standard Flairs input file which is carried out in the **TriShell** automatically when the corresponding Program Group is choosen in the Grid data set.



The recharge term '***q***' comprises a number of different effects. In the program ***Flairs***, '***q***' is divided into four distinctive components, depending on the origin of the water:

recharge from a top-system at the top of the uppermost aquifer due to e.g. precipitation, infiltration etc.;
- leakage through the separating aquitards between aquifers;
- discharge to point sources or recharge from point sinks;
- discharge to rivers and drains and recharge from line-sinks.

A multi-aquifer system with several recharge terms is shown below. ***Note****, that the numbering of aquifers and aquitards in* ***Triwaco*** *is always top down, and the number of aquifers is one greater than the number of aquitards. The layer covering the uppermost aquifer is also referred to as aquifer number 0, and is part of the* ***top-system****.*

5.3.3 Finite element equations

The Finite Element equations are derived from the partial differential equation given in equation [1]. Subdividing the recharge term '***q***' in four distinctive components, this equation is written as:

$$\frac{\partial}{\partial x}\left[T_{xx}\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial x}\left[T_{xy}\frac{\partial h}{\partial y}\right]+\frac{\partial}{\partial y}\left[T_{yx}\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial y}\left[T_{yy}\frac{\partial h}{\partial y}\right]+q_a+q_l+q_r+q_s=S\frac{\partial h}{\partial t} \quad \textbf{[2]}$$

The components of the recharge term are:

q_a	Recharge from the top-system (the shallow drainage system)
q_l	Recharge due to leakage
q_r	Recharge from rivers, canals and drains
q_s	Recharge from sources or sinks

For the sake of simplicity the first four terms of the equation [2] will be combined:

$$\nabla_{xy}\cdot\left[\underline{T}\,\nabla_{xy}\,h\right] \quad \textbf{[3]}$$

with '***T***' representing the transmissivity tensor.

The ***Finite Element*** equations are derived using Galerkin's method. The following simplifying assumptions are made:

- The spatially distributed recharge terms 'q_a' (recharge) and 'q_l' (leakage) can be approximated by an infiltration or abstraction in the nodal points of the grid. If the value 'q_a' in point '***i***' is given by '$q_{a,i}$', the strength at that point is given by:

$$q_{a,i}\cdot A_i\cdot\delta\left(x-x_i\,,y-y_i\right) \quad \textbf{[4]}$$

where 'A_i' represents the area of influence of nodal point '***i***'.

- The recharge due to rivers, canals and drains can be approximated by a series of point sources or sinks situated in a series of nodal points (the river nodes).

- The transmissivities and storage coefficients are constant within an element and are equal to the average of the values at the nodal points.

This so-called lumped parameter approach has the advantage that these terms are easily incorporated and the system of equations will be symmetric.
We will now define an 'a priori' solution for the given differential equation:

$$\tilde{h} = \sum_{i=1}^{n} h_i(t) \cdot \Phi_i(x,y) \quad \textbf{[5]}$$

with:

h_i	the unknown coefficient
Φ_i	a known shape function

The shape functions are defined piecewise linear, such that:

$\Phi_i = 1,$	in nodal point '***i***'
$\Phi_i = 0,$	in all other nodal points.

Hence, 'h_i' will have the value of '$\tilde{h}$' in nodal point '***i***'.

Substitution of '$\tilde{h}$' in the partial differential equation results in the following equation:

$$R = \nabla_{xy}\left[T \nabla_{xy}\right] + q_a + q_l + q_r + q_s - S\frac{\partial \tilde{h}}{\partial t} \neq 0 \quad \textbf{[6]}$$

The coefficients 'h_i' have to be determined such, that '***R***' is minimized over the model area. The value of '***R***' is minimized by making it orthogonal with the shape functions 'Φ_i':

$$\iint_G R \cdot \Phi_i \, dG = 0 \qquad i = 1, N \quad \textbf{[7]}$$

and integrating over the model area '***G***'.
The integration can be performed by using Greens theorem:

$$\iint \left[T \nabla_{xy} \tilde{h}\right] \Phi_i \, dG = -\iint T\left(\nabla_{xy} \tilde{h}\right) \cdot \left(\nabla_{xy} \Phi_i\right) dG + \int_\Gamma \left(T \nabla_{xy} \tilde{h}\right) n \, \Phi_i \, d\Gamma \quad \textbf{[8]}$$

with:

Γ	the boundary of the model area
n	the normal on the boundary directed outward.

Using Darcy's law one obtains:

$$\int_\Gamma \left(T \nabla_{xy} \tilde{h}\right) n \, \Phi_i \, d\Gamma = \int q_b \Phi_i \, d\Gamma \quad \textbf{[9]}$$

with:

q_b	the flux across the boundary into the model area.

Through substitution of the approximate solution and approximation of the boundary flux by a series of point sources or sinks, we obtain the following Finite Element equation:

$$-\sum_{j=1}^{n}\left(\iint T\left(\nabla_{xy}\Phi_j\right)\cdot\left(\nabla_{xy}\Phi_i\right)dG\right)+q_{q_i}A_i+q_{l_i}A_i+q_{r_i}R_i+Q_{s_i}+q_{b_i}L_{b_i}+$$

[10]

$$-\sum_{j=1}^{N}\left\{\left(h_j-h_i^0\right)\iint_{i=1,N}\frac{S}{\nabla_t}\Phi_j\Phi_i\,dG\right\}=0$$

The time derivative has been given by a completely implicit finite difference equation. The integrations in the equations can be easily performed, due to the simple form of the shape function.

***Note** that, due to the definition of the different recharge terms, the Finite Element equations can be nonlinear. This implies that both nonlinear and linear iterations have to be carried out to solve the equations.*

The linear iterations, used to determine the solution of a linearized system of equations, are referred to as ***inner iterations***.

The nonlinear iterations are referred to as ***outer iterations***. These are used to update the linearization of the equations in order to obtain an accurate solution to the nonlinear problem.

5.3.4 Solution technique

The resulting Finite Element equations will generally form a system of nonlinear equations, mainly due to the nonlinear character of the recharge term '***q***'. Moreover, the fact that both the transmissivity and the storativity of the top or bottom aquifer may change with the groundwater head, also results in non-linearity of the equations. This is the case whenever phreatic conditions or a salt-fresh water interface are present.

The Finite Element equations are given in an implicit way. So, they contain parameters related to the (unknown) groundwater head at the new time level; for instance the recharge '***q***'. Hence, the recharge '***q***' will be unknown too.

The recharge '***q***' is approximated in the following way:

$$q^n=q^0+\frac{\partial q}{\partial h}\left(h^n-h^0\right) \qquad \textbf{[11]}$$

In case of phreatic conditions both the transmissivity and the storativity are calculated for the known values of the groundwater head. The resulting linear equations are solved by the ***conjugate gradient method***. When a solution is found, the process may be repeated using the new values of the groundwater head.

Thus, two types of iterations are performed:

- ***inner iterations*** or linear iterations;
- ***outer iterations*** or nonlinear iterations.

For both types of iterations, the user defines the maximum number of iterations allowed. A maximum for the number of linear or inner iterations is, as a rule of thumb, equal to the total number of unknowns, which will be sufficient in most cases. The number of outer iterations required is strongly dependent on the non-linearity of the different terms. For a completely linear system, one single outer iteration is sufficient. The number of iterations for more complex situations may increase strongly with complexity. Default the program sets the maximum number of outer iterations to 100, a number that is hardly ever reached, and the maximum number of inner iterations to 500. If the number of inner iterations appears not to be sufficient, the program asks the user whether or not to continue the calculations. If the user agrees to continue the program doubles the number of inner iterations allowed.

The program will stop if the maximum number of outer iterations is exceeded. For each outer iteration, the number of inner iterations will be checked. For transient calculations the program will proceed with a new time step if the maximum number of outer iterations has been reached, or if the number of inner iterations during an outer iteration equals 2 or less.

Apart from the maximum number of inner iterations, the user has to specify a criterion for convergence 'ε'. The program checks whether or not the norm of the right-hand side vector and the residual vector differ less than the criterion given.
Hence, if the system of equations to be solved is given in matrix notation:

$$\underline{A} \cdot \underline{h} = \underline{b} \qquad \textbf{[12]}$$

the residual vector becomes, for an approximate solution:

$$\underline{A} \cdot \underline{\tilde{h}} - \underline{b} = \underline{r} \neq \underline{0} \qquad \textbf{[13]}$$

and we accept '$\underline{\tilde{h}}$' as the correct solution if

$$\frac{\|\underline{r}\|}{\|\underline{b}\|} < \varepsilon \qquad \textbf{[14]}$$

where:

$$\|\underline{r}\| = \sqrt{\left(r_1^2 + r_2^2 + \cdots + r_{n-1}^2 + r_n^2\right)} \qquad \textbf{[15]}$$

For a description of the ***conjugate gradient method***, the user is referred to the handbooks on numerical methods.

When transient calculations are carried out, the user also has to provide the maximum change in groundwater head that is allowed during each time step. The program will now compute the size of the time step to be used. This time step depends on the maximum change in groundwater head during the previous time step and the maximum allowable change defined by the user. If the calculated change '***dh***' is smaller than the allowable change '$dh_{\max}$', the new time step will become:

$$\Delta t^n = \frac{2\, dh_{\max} - dh}{dh_{\max}} \Delta t^0 \qquad \textbf{[16]}$$

If the change in groundwater head ('***dh***') during a time step is greater than the maximum change '$dh_{\max}$', the calculation will be repeated once with a time step:

$$\Delta t^n = \frac{dh_{\max}}{dh} \Delta t^0 \qquad \text{for} \qquad \frac{dh_{\max}}{dh} > 0.5$$

$$\Delta t^n = 0.5\, \Delta t^0 \qquad \text{for} \qquad \frac{dh_{\max}}{dh} < 0.5 \qquad \textbf{[17]}$$

Hence, the multiplication factor between two successive time-steps varies between a minimum value of 0.5 and a maximum of 2.0.

5.3.5 Recharge terms and Boundary fluxes

As discussed in the previous section, vertical recharge into an aquifer can be divided into four parts, depending on the origin of the water (see equation [2]):

- recharge from or discharge towards a so-called top-system;
- recharge or discharge due to leakage through a separating layer;
- recharge from or discharge towards rivers, canals and drains;
- recharge from sinks or discharge towards sources.

Horizontal recharge is given by the boundary fluxes. In this section all recharge terms are treated in more detail. In all cases a relation between the recharging (or discharging) flux and the piezometric head in the aquifer can be defined. These relations vary from simple to very complicated as can be seen from the description of the various recharge terms in the following sections. First the boundary fluxes are treated and next the vertical recharge terms, in order of increasing complexity.

Boundary fluxes

Boundary fluxes can be considered to result from a line source or line sink in the two-dimensional model area. In the Finite Element program, these line sources are approximated by a series of point sources located at the boundary nodes. The boundary flux is defined positive flowing into the model area.

There are two ways in which the boundary fluxes can be calculated:

- The groundwater head at the boundary may be given and the flux will be calculated as function of the gradient of the groundwater head at the model's boundary.

$$Q_b = \underline{T} \nabla_{xy} h_b \qquad \textbf{[18]}$$

- The groundwater flux across the boundary is given as function of the groundwater head at the boundary.

$$q_b = B_a h + B_b \qquad \textbf{[19]}$$

Here 'B_a' (m^3/d per m^2 = m/d) and 'B_b' (m^3/d per m^1 = m^2/d) are the boundary flux parameters.

A given (constant) flux, independent of the groundwater head, may be obtained by setting the value for 'B_a' to zero. Setting the value for 'B_b' also to zero, a 'natural' or no-flow boundary is created.

Both types of boundary conditions can be used simultaneously for parts of the boundary. The type of boundary condition that will be used is determined by the ***boundary type parameter***, to be defined by the user. By default the program assumes the boundary condition to be defined by a given head.

Leakage

The leakage term ('q_l' in the equations) defines the flow of groundwater between two adjacent aquifers. The leakage is defined assuming the following simplifications:

- The flow in the aquitards is vertical.
- The storage in aquitards can be neglected.

Taking these two assumptions into account, the leakage term is given by the next equation:

$$q_l = \frac{h' - h}{c} \qquad \textbf{[20]}$$

with:

h	the groundwater head in the aquifer under consideration,
h'	the groundwater head in the adjacent aquifer
c	the hydraulic resistance of the aquitard

Sources
In the program ***Flairs*** the terms 'sources' and 'sinks' are reserved for groundwater abstractions or infiltrations defined in nodal points. These nodal points have to be defined as such in the Finite Element Grid. The abstraction or infiltration rate of a point source or sink can be defined in two ways in the program:

- An abstraction or infiltration can be defined by a given rate. The amount of water to be abstracted or infiltrated is given by the user and the program computes the hydraulic head at the sources' location. For multi-screen wells the sources may be clustered over successive aquifers; the separate abstraction rates are totaled and the hydraulic heads is assumed to be equal for all aquifers considered. Similarly, wells in the same aquifer that are connected by a suction-pipe are treated in the same way.

- The head at the abstraction or infiltration well is given and the program will calculate the rate.

Both cases are easily treated in the Finite Element equations. The type of source or sink that will be used is determined by a ***source type parameter***, to be defined by the user. By default the program assumes the source to be defined by a given rate.

Note *that due to the definition in the partial differential equations, an infiltration rate must be given by positive values whereas abstraction rates have negative values.*

Rivers
Rivers and drains are line sources or line sinks, usually defined in the top aquifer. In the program ***Flairs*** these line sources are approximated by a series of point sources situated in the so-called river points, nodes that together define the river's course. Similarly to the point sources the discharge from or recharge towards these rivers may be defined in two ways:

- The head at the river or the piezometric head in the drain is given. The program will calculate the discharge rate.
- A discharge or recharge rate is given; either for one single river or drain or for a number of connected (clustered) rivers or drains. In that case the amount of water to be abstracted or infiltrated is given and the program computes the head. The program assumes that the head over the whole river is constant and the same for all rivers belonging to the cluster.

At each river point the abstraction or infiltration rate is computed by:

$$Q_r = A_r \frac{(h_r - h)}{C_r} \qquad \textbf{[21]}$$

with:

Q_r	abstraction or infiltration rate
A_r	the area of the river or drain in the given point. This area is computed from the length of the river assigned to the point and the hydraulic radius (R_w) of the river or drain at that point.
h	the groundwater head in the aquifer
h_r	the water level in the river or the piezometric head in the drain.
C_r	the resistance to flow towards a line sink or from a line source. This river resistance usually has different values for infiltration ($h_r > h$) and for drainage ($h_r < h$). The program offers the possibility to define a different resistance for drainage and for infiltration.

For fully penetrating rivers, the hydraulic resistance will have a value of zero. In that case, the infiltration rate can not be calculated from the given relation. Still, the rate 'Q_r' will be treated as the unknown, but the groundwater head is given the same value as the river level.

For clustered rivers with a given infiltration or abstraction rate the head will de treated as the unknown while the rate 'Q_r' of the cluster of rivers is given. The type of river or drain that will be used is determined by a ***river type parameter***, defined by the user. By default the program assumes that the river is defined by a given water level.

Top-systems

The discharge or recharge of groundwater at the top of the first aquifer can be characterized by the so-called ***top-systems***. A top-system describes the interaction between the groundwater system and a drainage/infiltration system consisting of generally small surface waters and drains. A short description of the topsystems is listed below. A more detailed description is given in Appendix A.

1. Precipitation; Top-system number 1, defined by 1 parameter; groundwater recharge is equal to the precipitation excess.
2. Polder with fixed water level; Top-system number 2, defined by 3 parameters; groundwater recharge and discharge depend on a fixed water level and the (total) resistance of the drainage/infiltration system.
3. Phreatic drainage; Top-system number 3, defined by 3 parameters; groundwater discharge depends on the head in the top aquifer, the resistance and the base of the drainage system.
4. Three-level drainage system; Top-system number 4, defined by 13 parameters; groundwater recharge or discharge depends on the precipitation excess and the resistance and levels of a primary, secondary and tertiary drainage/infiltration system.
5. Pipe drainage and irrigation or precipitation; Top-system number 5 (drainage only) and Top-system number 6 (both drainage and infiltration), defined by 8 parameters; groundwater discharge depends on the precipitation or irrigation excess, the head in the top aquifer and the drainage resistance.
6. Polder with a fixed water level and precipitation; Top-system number 7, defined by 4 parameters; groundwater recharge or discharge depends on a fixed water level, the (total) resistance of the drainage system and the precipitation excess.
7. Phreatic drainage with precipitation; Top-system number 10, defined by 4 parameters; groundwater discharge depends on the head in the top aquifer, the resistance and the base of the drainage system and on the precipitation excess.
8. Polder with a fixed water level and single drainage system; Top-system number 11, defined by 5 parameters; groundwater recharge or discharge depends on the precipitation excess and the resistance and level of a single drainage system.
9. Predefined recharge or discharge characteristic; Top-system number 12, defined by 5 parameters; groundwater recharge or discharge depends on meteorological quantities and soil parameters. The soil parameters are obtained by curve fitting of the Van Genuchten relations.

IR	RP1	RP2	RP3	RP4	RP5	RP6	RP7	RP8	RP9	RP10	RP11	RP12	RP13
1	P												
2	H_P	C_0	W										
3	H_S	W	BD										
4	P	C_0	H_P	$W_{d,1}$	$W_{d,2}$	$W_{d,3}$	$W_{i,1}$	$W_{i,2}$	$W_{i,3}$	BD_1	BD_2	BD_3	H_S
5	P	H_S	H_d	H_T	K_v	K_h	L	R					
6	P	H_S	H_d	H_T	K_v	K_h	L	R					
7	P	C_0	W	H_P									
8	not in use												
9	not in use												
10	P	W	BD	H_S									
11	P	C_0	W_d	W_i	H_p								
12	P	ET_{mx}	a	b	H_S								

As can be noticed from this table the top system parameters **RP*xx*** for different top systems do not necessarily represent the same physical parameter. For example, parameter RP1 may represent precipitation (*P*), the surface level elevation (*Hs*) or the controlled water level (*Hp*). Moreover, different top systems require a different number of parameters, ranging from only one (for top system type 1) to as much as thirteen (top system type 4).

The physical parameters associated with the top system parameters are listed in the following table. One can distinguish parameters related to the meteorological condition (precipitation and evapotranspiration), soil parameters, surface and surface water levels and parameters with respect to the geometry and resistances of the drainage system.

Name	Definition of parameter
P	Precipitation excess or irrigation excess
ET_{mx}	Maximum Evapotranspiration
A	soil parameter obtained by curve fitting
B	soil parameter obtained by curve fitting (b > 1)
C_0	Hydraulic resistance of semi-pervious top layer
H_d	Drain level of system of (pipe)—drains
H_P	Polder water level or controlled water level
H_S	Surface level (with respect to the ordnance level)
H_T	Level of base of semi-pervious top layer
K_h	Horizontal permeability of semi-pervious top layer
K_v	Vertical permeability of semi-pervious top layer
L	Horizontal distance between drains
R	Wetted perimeter of (pipe)—drains
BD	Drainage base or bottom level of the (open) drains
BD_1	Drainage base or bottom level of the primary drainage system
BD_2	Drainage base or bottom level of the secondary drainage system
BD_3	Drainage base or bottom level of the tertiary drainage system
W	Drainage or infiltration resistance between ditches or drains
W_d	Drainage resistance between ditches or drains
$W_{d,1}$	Drainage resistance of the primary drainage system
$W_{d,2}$	Drainage resistance of the secondary drainage system
$W_{d,3}$	Drainage resistance of the tertiary drainage system
W_I	Infiltration resistance between ditches or drains
$W_{i,1}$	Infiltration resistance of the primary drainage system
$W_{i,2}$	Infiltration resistance of the secondary drainage system
$W_{i,3}$	Infiltration resistance of the tertiary drainage system

5.3.6 Special options

Regarding the transmissivity or permeability of the aquifers **Triwaco** offers a number of special options. The options available are:

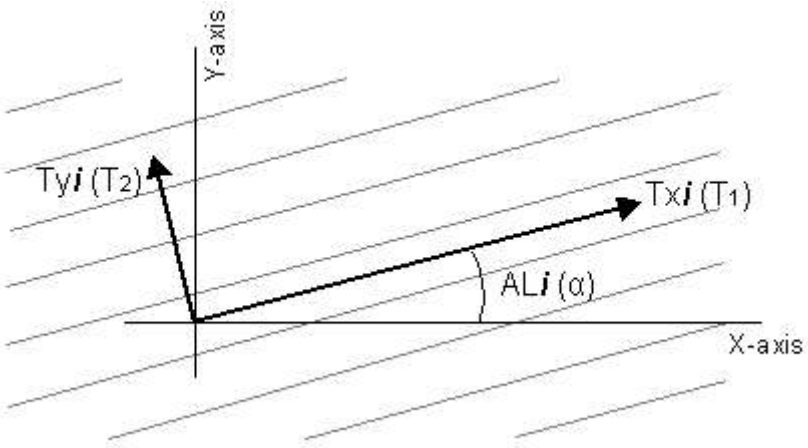
- aquifer anisotropy,
- computation of a phreatic surface in the top aquifer and
- computation of a sharp salt-fresh water interface in the lowermost aquifer.

Anisotropy
Although **Triwaco** assumes that transmissivities and permeabilities of all aquifers are by default isotropic, the user can define an anisotropic transmissivity (or permeability). The transmissivity (or permeability) tensor may vary through the model area, which implies that the principal axes of the tensor can have different orientations in different points of the model's domain.

The values in the direction of the principal axes of the transmissivity tensor are given by 'T_1' and 'T_2'. The angle between the direction of 'T_1' and the positive X-axis is given by 'α'. Now the values of the transmissivity components in the Cartesian coordinate system ('T_{xx}', 'T_{xy}', 'T_{yx}' and 'T_{yy}') are given by Mohr's circle and may be written as:

$$\begin{aligned} T_{xx} &= T_1 \cdot \cos^2 \alpha + T_2 \cdot \sin^2 \alpha \\ T_{xy} &= T_{yx} = (T_1 - T_2) \cdot \cos \alpha \cdot \sin \alpha \\ T_{yy} &= T_1 \cdot \sin^2 \alpha + T_2 \cdot \cos^2 \alpha \end{aligned} \qquad \textbf{[21]}$$

For each element of the Finite Element Grid the values of 'T_1', 'T_2' and 'α' are calculated from the values in the nodes that constitute the corner points of the element. The transformation (equations [21]) is carried out using the average values of 'T_1', 'T_2' and 'α'.



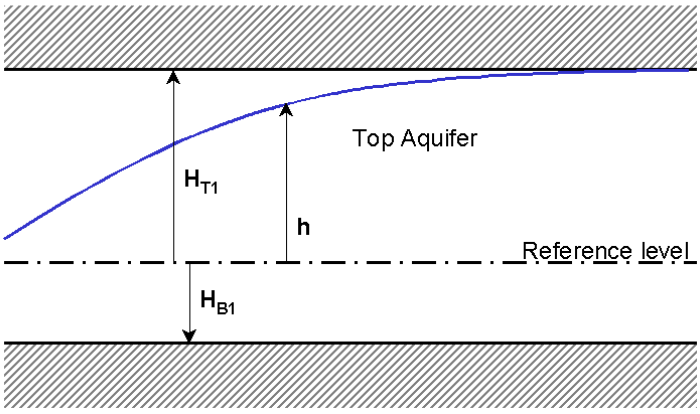
Phreatic conditions
Whenever the groundwater table falls below the top of the upper aquifer the aquifer is phreatic. This implies that aquifer transmissivity becomes a function of the piezometric head '*h*'.

The phreatic transmissivity is calculated by the program ***Flairs*** using the following parameters, which have to be specified by the user:

- permeability tensor, which may be anisotropic '$\underline{K}$' ('K_1', 'K_2' and 'α');
- the elevation of the base of the upper aquifer ('H_{B1}');
- the elevation of the top of upper aquifer ('H_{T1}').

The elevation of the top and the base of the upper aquifer are measured with respect to the same reference level that is used for the piezometric heads.

Definition scheme Phreatic conditions



The aquifer's transmissivity is computed with the following assumptions:

- When the piezometric head is below the base of the aquifer, the aquifer is dry, hence:

$$T = 0 \qquad \text{for} \qquad \left(h \le H_{B1}\right) \qquad \textbf{[22a]}$$

- When the piezometric head is between the base and the top of the aquifer the aquifer is phreatic, hence:

$$T = K \cdot \left(h - H_{B1}\right) \qquad \text{for} \qquad \left(H_{B1} < h < H_{T1}\right) \qquad \textbf{[22b]}$$

- When the piezometric head is above the top of the aquifer the aquifer is confined, hence:

$$T = K \cdot \left(H_{T1} - H_{B1}\right) \qquad \text{for} \qquad \left(h \ge H_{T1}\right) \qquad \textbf{[22c]}$$

It is assumed that the phreatic surface will not fall below the base of the aquifer and reach the underlying aquifer.

Thus, aquifer conditions may vary depending on the value of the piezometric head. The value of the piezometric head differs for each node of the Finite Element Grid. Hence, the upper aquifer can be partly dry, partly phreatic and partly confined at the same time. Moreover, when transient calculations are carried out, aquifer conditions at a given location may also vary in time.

The aquifer conditions will also influence the value of the storage coefficient to be used. For a confined aquifer the storage coefficient is defined by the elastic storativity ('***S***'), whereas for phreatic conditions the storage coefficient is given by the effective porosity '***n***'.

Interface conditions
The groundwater in the lowermost aquifer can be flowing over a body of a heavier, but supposedly stagnant, fluid. For example: in coastal areas the fresh water is separated by a (relatively) sharp interface from (relatively) stagnant salt water.

The elevation of the interface (H_i) is given according to the 'Badon-Ghyben / Herzberg' equation:

$$H_i = \frac{\left(\beta + 1\right)}{\beta} h_s - \frac{1}{\beta} h \qquad \left(H_{B,n} \le H_i \le H_{T,n}\right) \qquad \textbf{[23]}$$

The variables 'h_s' and 'h' represent the salt-water head in the stagnant salt-water body and the piezometric head in the fresh water respectively. The parameter 'β' is a measure for the density differences between the

fresh and the salt water and is defined by:

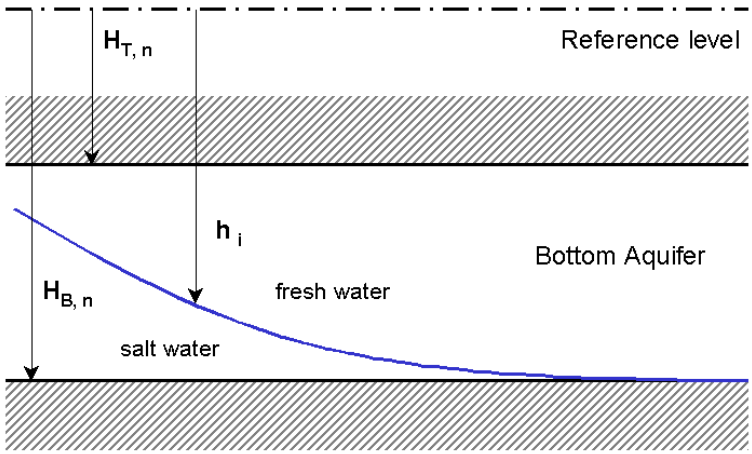
$$\beta = \frac{\rho_s - \rho}{\rho} \qquad \textbf{[24]}$$

with:

ρ	the fluid density for the fresh-water body
ρ_s	the fluid density for the salt-water body.

For each element of the Finite Element Grid the values of 'h_s', '$H_{B,n}$' and '$H_{T,n}$' are calculated from the values in the nodes belonging to the element.

Definition scheme Interface conditions



Similarly to a phreatic aquifer one can distinguish the following situations:

- The aquifer is completely fresh; the interface is below the base of the aquifer, hence:

$$T = K \cdot \left(H_{T,n} - H_{B,n}\right) \qquad \text{for} \qquad \left(h_i \le H_{B,n}\right) \qquad \textbf{[25a]}$$

- The aquifer is partly fresh; the interface is between the top and the base of the aquifer, hence:

$$T = K \cdot \left(H_{T,n} - h_i\right) \qquad \text{for} \qquad \left(H_{B,n} < h_i < H_{T,n}\right) \qquad \textbf{[25b]}$$

- The aquifer is completely salt; the interface is above the top of the aquifer, hence:

$$T = 0 \qquad \text{for} \qquad \left(h \ge H_{T,n}\right) \qquad \textbf{[25c]}$$

It is assumed that the interface will not pass the top of the aquifer and reach the overlying aquifer.

Thus aquifer conditions may vary depending on the value of the piezometric head. The value of the piezometric head differs for each node of the Finite Element Grid. Consequently, the lowermost aquifer can be completely fresh, partly fresh and partly salt or completely salt at the same time.

The aquifer conditions will also influence the value of the storage coefficient to be used. For a completely fresh aquifer the storage coefficient is defined by the elastic storativity ('**S**'). For interface conditions, with a partly fresh aquifer, the storage coefficient is defined by 'n/β' with '**n**' representing the effective porosity.

In case of a single aquifer model, both a phreatic surface and a salt-fresh water interface may appear in the same (top) aquifer.

***Note** that the program **Flairs** should not be used for transient calculations with a salt-fresh interface, because the salt-water body is assumed to be stagnant. In that case or if the interface passes the top of the lower-most aquifer one should use the variable density module FLAIRSVD.*

5.4 Executing model simulations with MODFLOW

5.4.1 Introduction

Groundwater flow calculations can be carried out in a way similar to the calculations with the standard **Triwaco** programs. In stead of running the program ***Flairs*** the program ***runMFfli*** will be called. This program reads the standard input file ***flairs.fli***, translates the input into ModFlow input files, runs ModFlow with these files and writes and converts the standard ModFlow output back into standard **Triwaco** output format (default file name ***flairs.flo***). All ModFlow files remain present, so the user can not only check the regular log, print and output files but also the ModFlow output **flairs.out.** The ModFlow input files all have standard file names, which differ only by their extension, e.g. FLAIRS.BAS, .BCF, .DRN, .RIV, .GHB, .RCH, .PCG et cetera.

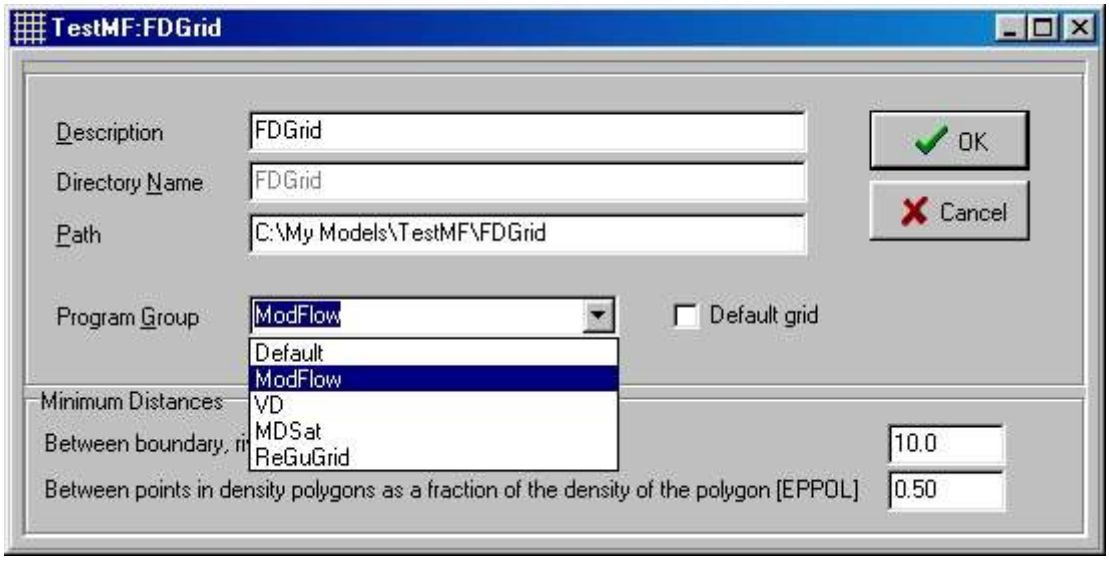
There are however some restrictions in using **ModFlow**. The program ***runMFfli*** does not support at this time all top systems, boundary conditions and river or source types which can be defined for ***Flairs***. The program however does support the following:

- Steady state calculations for multi-layered aquifer systems, both semi and fully 3D.
- Top system type 1, 2, 4 and 11, defined by the RCH, GHB and DRN packages.
- Rivers of type 1 (RA***x***=1), defined by the GHB and DRN packages.
- Rivers to be defined by the RIV and DRN packages (special type RA***x***=3).
- Constant head boundaries (IB***x***=0), defined by constant head cells.
- Given rate abstraction wells (IS***x***=0), defined by the WEL package.

For transient calculations and implementation of other boundary conditions the user should modify the ModFlow input files or contact the Triwaco Help Desk assistant.

5.4.2 Using the Simulation Package MODFLOW

Groundwater flow calculations can be carried out in a way similar to the calculations with the standard **Triwaco** programs. One only has to define ModFlow as the simulation package in the Grid data set info window by selecting ModFlow in the Progam Group pull down menu. **Triwaco** will then use **Monet** for generating the finite difference grid and ModFlow-96 to calculate grondwaterflow.



Monet is used as two-dimensional mesh generator for **Triwaco** when the simulation is carried out with ModFlow. Monet produces a Tesnet compatible output file with a number of additional sets that facilitate the generation of Modflow datafiles.

1. Mesh refinement around sources in the input file is ignored.
2. Density polygons may be digitised clockwise or counter clockwise and do not have to appear in a particular order in the input file

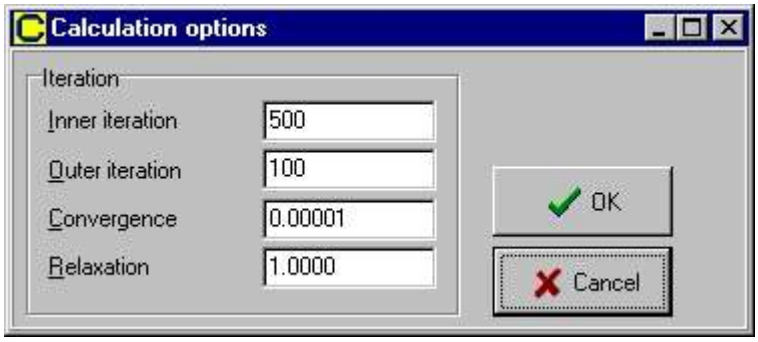
3. The density of the polygon with the largest area is used as the default area constraint for the entire model
4. Rivers that cross the boundary more than once will be split into separate rivers with the same river id.

Monet first reads the boundary, river and source input and snaps all input points that are closer to each other than EPFIX. Set EPFIX to 0 if you don't want nodes to be snapped. The intersection points with the rivers and the boundary are calculated and the rivers and sources are clipped to the boundary polygon. Next, the density polygons are read and sorted on de-creasing area. After reading all input, the smallest rectangle enclosing the boundary polygon is calculated and rectangular grid cells are created within the enclosing rectangle. The distance between the gridlines is determined by the node distance of the density polygons. Finally, the centers of the grid cells are calculated and used to generate a triangular mesh.

5.4.3 Simulation options

After allocation of the values for all model parameters one may start the groundwater flow calculations. First, selecting 'Calibration' 'Options' from the menu bar, the ***'Calculation options'*** dialog box is opened.
In this dialog box the user specifies parameters related to the iteration process:

Description	Function
Inner iteration	Sets the maximum number of inner iterations
Outer iteration	Sets the maximum number of outer iterations
Convergence	Sets the criterion for confergence ε
Relaxation	Sets the relaxation factor $(\zeta \leq 1)$



Apart from the maximum number of iterations, the user has to specify a ***criterion for convergence***. The program checks whether or not differences are less than the criterion specified. The initial conditions for each outer iteration depend on the head change between (outer) iterations. In case of badly converging systems a ***relaxation factor*** may be defined. In that case the head change between (outer) iterations is multiplied with the relaxation factor. This causes a more stable iteration process but also results in smaller head changes, thus requiring more iterations to reach a solution.

ModFlow calulation settings

The program ***runMFfli*** assumes that Version 2 of the Preconditioned Conjugate Gradient solver is used (PCG2) in the ModFlow calculations. The parameters for this solver are partly fixed and partly read from the *flairs.fli* input file. The parameters read from the input file are the maximum number of inner and outer iterations (II_{max} and IO_{max}, set 14 of the input file), the relaxation factor (R_{rlax}, set 2 of the input file) and the criterion of convergence (EPS, set 14 of the input file)

Note that the parameter EPS specified in the calculation options window has a quite different meaning within **Triwaco** than the criterion for convergence within ModFlow. The parameter EPS is now used to define the (physical) closure limits, which depend on the system units. The head change criterion HCLOSE has the dimension of [Length] and the residual criterion of convergence RCLOSE the dimension of [Length^3/Time]. Where ModFlow generally uses the system units **meters** and **seconds** most **Triwaco** users employ the system units **meters** for length and **days** for time. Therefore the recommended value of 0.01 or 0.001 for the head change criterion HCLOSE can be adopted. However, because the residual criterion for convergence RCLOSE depends on the time unit, the recommended value (equal to HCLOSE) should be multiplied by 86400 (the number of seconds per day).

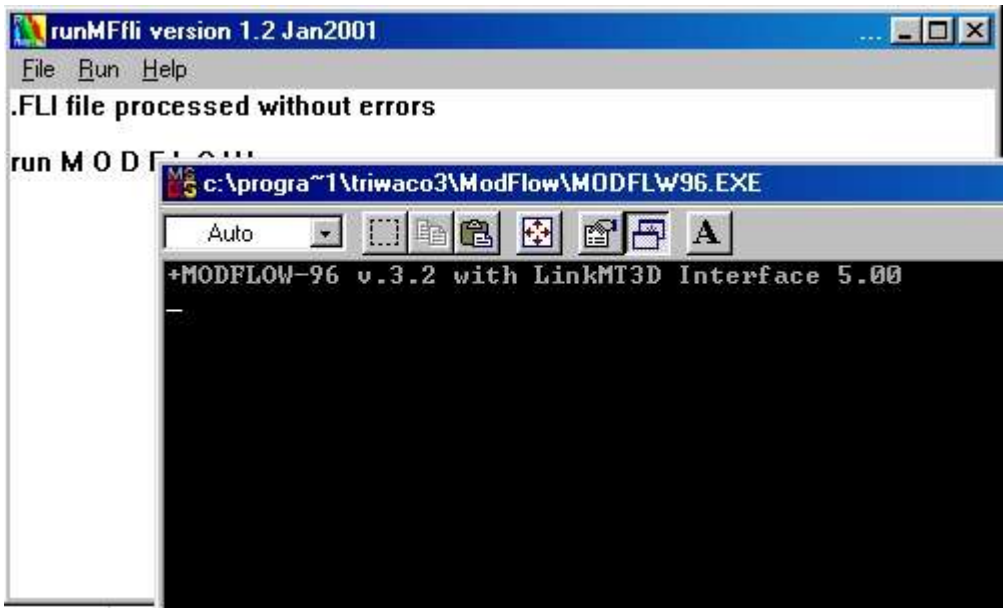
The program ***runMFfli*** reads the value for HCLOSE from the input file and computes the value for RCLOSE afterwards.

ModFlow PCG2 parameter	Description and source
MXITER	Maximum number of outer iterations per time step. Taken from .FLI file (II_{max} usually less than 100 will be enough).
ITER1	Maximum number of inner iterations per time step. Taken from .FLI file (IO_{max}, usually <=30 for linear problems, and 3 à 10 for non-linear problems).
NPCOND	Type of preconditioning to be used. Fixed at 1 (Modified, Incomplete Cholesky method)
HCLOSE	Head change criterion for convergence. Taken from .FLI file (EPS; Usually 0.01 or 0.001)
RCLOSE	Residual criterion for convergence. Computed from HCLOSE: RCLOSE = 86400 * HCLOSE
RELAX	Relaxation parameter. Taken from .FLI file (R_{rlax}, Usually set to 1; however, a value of 0.97 to 0.99 may prevent zero divide and non-diagonally dominant matrix errors in case rewetting is active).
NBPOL	Not used for NPCOND=2. Fixed dummy value
IPRPCG	Printout interval. Fixed to 1
MUTPCG	Print type. Fixed to -1 (number of iterations, head changes and residuals are printed).
IPCGCD	Recalculation Cholesky decomposition. Fixed at 0 (recalculated each outer iteration)

5.4.4 Executing the model simulation

For starting the model calculations one first selects 'Generate input' from the Calibration pull down menu bar. This will generate the input file needed (***flairs.fli***). This input file may be viewed or edited selecting 'View' 'Input' from the pull down menu. The input file contains all parameters needed for the calculations.

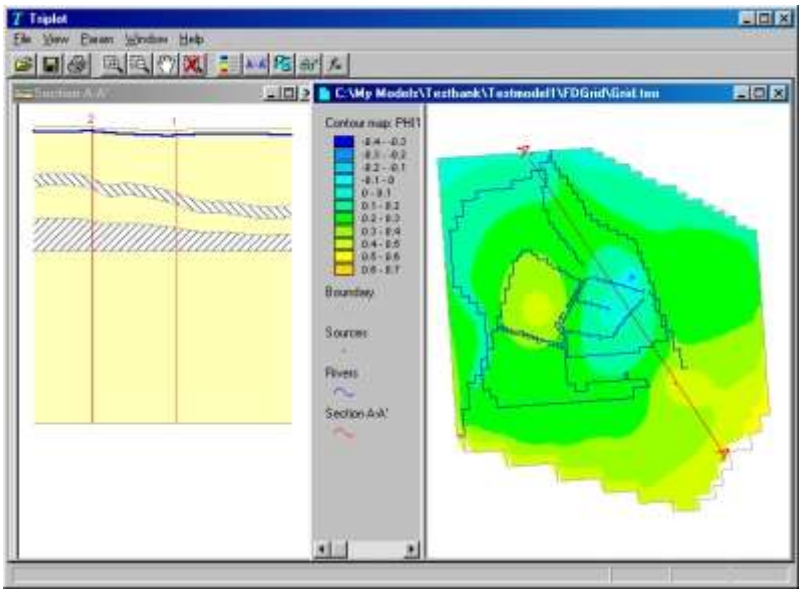
Selecting 'Run Simulation' from the Calibration pull down menu starts model simulations. A window, showing the calculation process (***RunMFli*** and a dosbox with ModFlow) will be displayed and the program will be added to the tasks window. Once the calculation has stopped the ***'Result parameters'*** Tab-sheet will be updated. After the first run this Tab-sheet will be added to the ***'Calibration data set'***. If a '***calibration file***' has been defined, the program automatically compares the calculation results with the observed heads/fluxes.



The simulation program produces different types of output files. ***RunMFli*** writes and converts the standard ModFlow output back into standard **Triwaco** output format (default file name ***flairs.flo***). All ModFlow files remain present. Some of these files contain information on the calculation process, errors encountered, (***flairs.flg***) others contain the calculation results using various formats (***flairs.flp***, ***flairs.flo***).

5.4.5 Viewing output results (maps)

Selecting 'View' 'Results' from the Calibration pull down menu starts the graphical presentation program **TriPlot**, loads the grid information and displays the layout of the model area. Now the user can contour or classify the result parameters and view the results in plane view or can select a cross-section of the model area.



Alternatively, the user can select one of the parameters from the 'result parameters' sheet and viewing the parameter separately selecting 'View' 'Adore' from the Parameter pull down menu or 'View Adore file' from the pop-up menu (right hand mouse button). Adding other parameters (selecting 'Param' 'Load' from the **TriPlot** menu bar) gives the user the opportunity to compare result parameters with model input parameters.

5.4.6 Output data description

The output description of **Triwaco** files is described in section 5.2.7. The simualtion results are saved in bot **Triwaco** standard output files (***flairs.flo***, ***flairs.flg*** and ***flairs.flp***) but also in the standard ModFlow output file format (***flairs.out***). The output of ModFlow files is described in the standard ModFlow manual provided by the USGS.

5.4.7 MODFLOW parameter handling by TRIWACO

The standard input file, with the default model parameters, may be used without any modifications. In that case the program will generate ModFlow input files that are compatible with the **Triwaco** stratification of aquifers with horizontal groundwater flow and aquitards with vertical flow. The prevailing parameters are the aquifer transmissivity and the hydraulic resistance of the intermediate confining layers. The depths and thickness of the various layers are not taken into account other than by their hydrogeological properties.

Fully 3D

For combined groundwater flow and transport modeling, however, it is usually preferred to create a fully 3-dimensional model, taking all layer boundaries into consideration. The program ***runMFfli*** will translate the input file to a fully 3-D ModFlow model if the following **Triwaco** parameters are used, in stead of the transmissivity **TX***x*:

- the aquifer's permeability **PX*x***,
- the aquifer's top elevation **RL*x*** and
- the aquifer's base elevation **TH*x***.

The parameters representing the aquitards don't need any modification. The input file can be generated as usual selecting 'Generate input' from the 'Calibration' pull down menu. It is recommended to check the input file and to remove the lines defining the parameter **TX*x***, which may appear in the input file if both **TX*x*** and **PX*x*** are defined in the same data set.

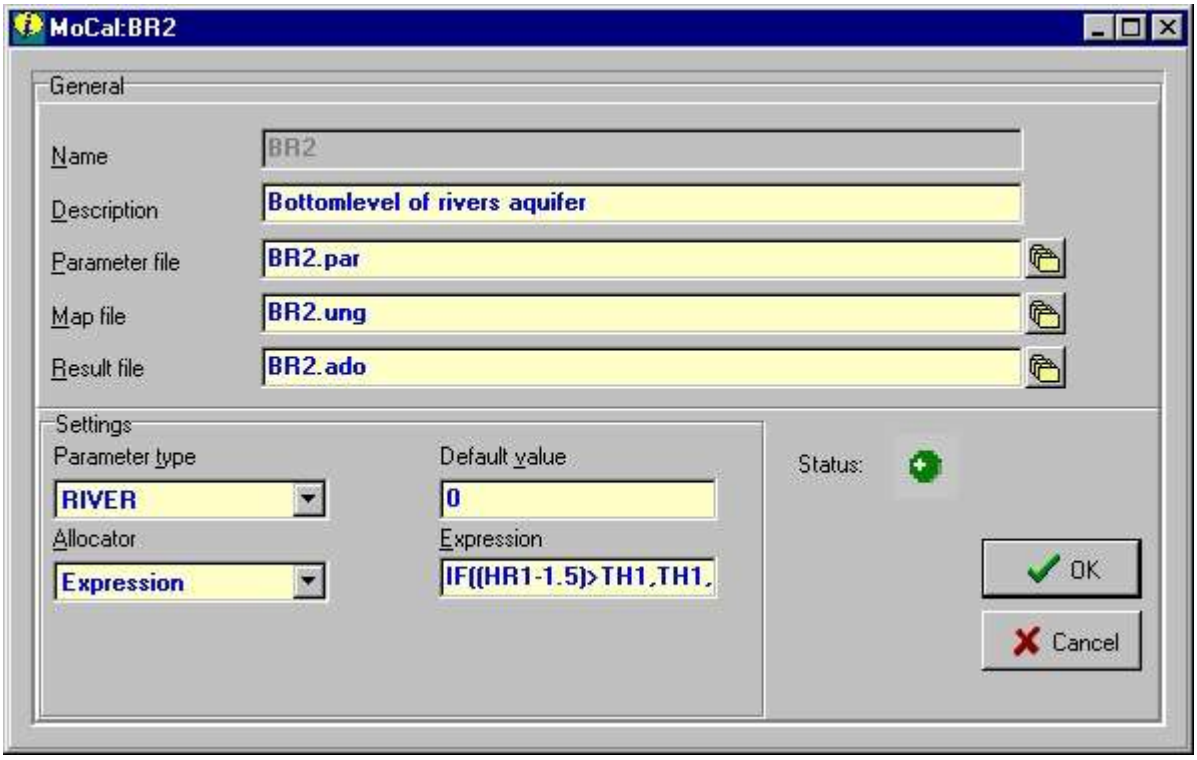
Recharge and rewetting
The recharge is computed for each cell from the corresponding **Triwaco** parameter (generally top system parameter RP1). By default recharge is supposed to take place in the uppermost active cell (NRCHOP = 3 in the RCH1 package).

Unlike **Triwaco** ModFlow allows cells to go dry if the water table falls below the base of the aquifer (in **Triwaco** only the uppermost layer may become dry, resulting in a zero value for this aquifer's transmissivity). For cells that become dry the value of 1.0 E+32 is assumed, signifying the cell is inactive and does not participate in the groundwater flow.

However, whenever the water table rises above the aquifer's base elevation the cell should participate in the groundwater flow again. This process is called 'rewetting' and is supposed to be active. Values for the rewetting threshold and the frequency of updating are fixed.

Rivers
Streams and rivers are usually defined by line elements and will be converted to a combination of ModFlow's DRAIN- and GHB-package, thus accounting for differences in drainage and infiltration resistances. Generally this approach will be permitted as long as the groundwater head does not fall below the bottom level of the river. However, in cases very low groundwater heads may be expected the linear relation between the head difference and the infiltration flux is not valid any more. In that case the RIV-package should be used in stead of the GHB-package.

The user can specify which line elements are to be defined by the RIV-package by adding the parameter **BR*x*** and modifying **Ra*x***.



For those rivers that should be converted to the RIV-package, the river activity parameter **RA*x*** should be set to **3**. In addition the parameter **BR*x*** is added, representing the river's bottom elevation. This parameter can be added selecting 'Add' 'User Defined' from the 'Parameter' pull down menu and filling in the parameter definition window. After having allocated all parameters the input file can be generated as usual.

Translation of model parameters

For the definition of the upper boundary condition **Triwaco** uses the so-called ***top systems*** together with line elements or ***rivers***. The top system parameters are distributed parameters, defined in each node of the grid and represent the node's influence area. The river parameters, representing line elements, are defined in each river-node and are valid for an area equal to the length of the river stretch multiplied by the river width, which is generally considerably smaller than the river-node's influence area.

In ModFlow the upper boundary condition is defined for cells belonging to the uppermost layer, regardless of the fact whether the boundary condition represent a distributed parameter or a line element. The area represented is accounted for in the ***conductance*** parameter (Cond).

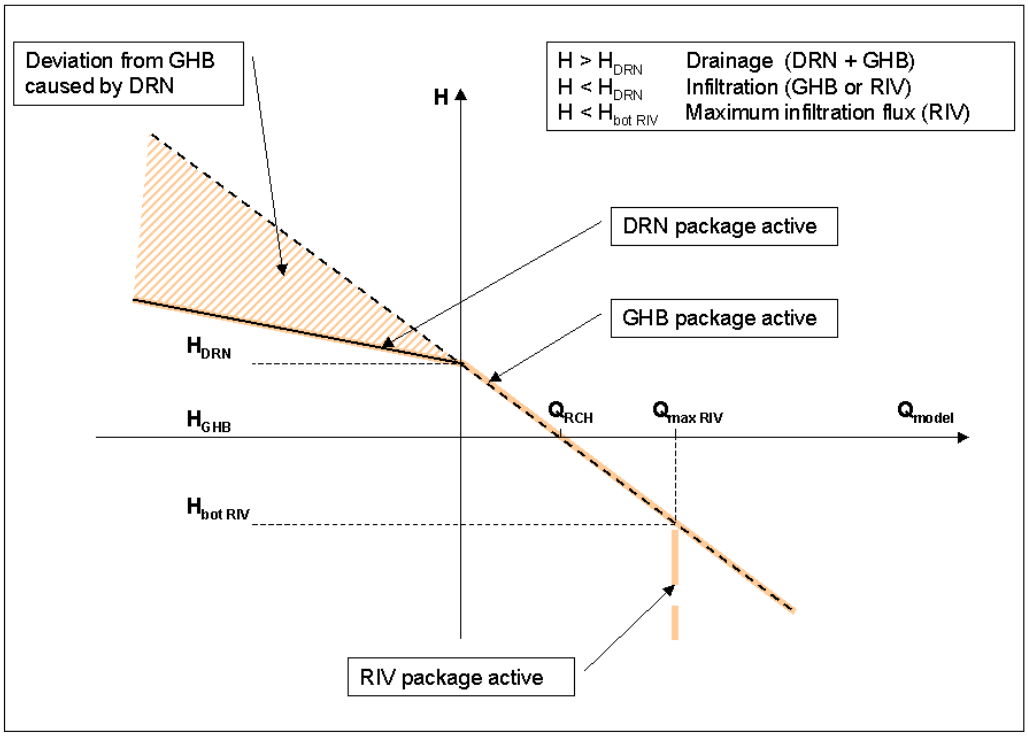
The following ModFlow packages are used to define the upper boundary condition:

Code	Package	Input parameter	dimension
RCH	Recharge package:	RECH	[L/T]
GHB	General Head Boundary	Cond	[L^2/T]
		H_{BND}	[L]
	Q = Cond * (H_{BND} - H_{CELL})		[L^3/T]
DRN	Drain package	H_{DRAIN}	[L]
		Cond	[L^2/T]
	Q = Cond * (H_{BND} - H_{CELL}) Q = 0	{H_{CELL} > H_{BND}} {H_{CELL} $\leq$ H_{BND}}	[L^3/T]
RIV	River Package	R_{BOT}	[L]
		H_{RIV}	[L]
		Cond	[L^2/T]
	Q = Cond * (H_{RIV} - H_{CELL}) Q = Cond * (H_{RIV} - R_{BOT})	{H_{CELL} > R_{BOT}} {H_{CELL} $\leq$ R_{BOT}}	[L^3/T]

Where in **Triwaco** a distinction can be made between an infiltration and a drainage situation, the GHB, DRN and RIV package do not differentiate between these two situations. The conductance is supposed to be a constant, regardless of the prevailing condition. Therefore, the upper boundary condition in **Triwaco**, be it a top system or a river, is translated into a combination of the ModFlow boundary packages mentioned. The precipitation excess or groundwater recharge is simulated using the RCH package.

The conductance of the GHB or RIV package is based on the infiltration resistance of top system or river, whereas the conductance of the DRN package is based on the drainage resistance. Thus, the program ***runMFfli*** will interpret the top system and river information and generate the corresponding ModFlow packages:

Triwaco Top system			ModFlow packages
IR = 1	Precipitation excess	RP1	RCH
IR = 2	Controlled water level Hydraulic resistance Drainage resistance	RP1 RP2 RP3	GHB
IR = 4	Not yet fully functional	RP1 - RP13	
IR =11	Precipitation excess Hydraulic resistance Drainage resistance Infiltration resistance Controlled water level	RP1 RP2 RP3 RP4 RP5	GHB and DRN
River	River water level River width Drainage resistance Infiltration resistance	HRx RWx CDx CIx	GHB and DRN ***or*** RIV and DRN


Deviation from GHB caused by DRN
H > H DRN Drainage (DRN + GHB)
H < H DRN Infiltration (GHB or RIV)
H < H bot RIV Maximum infiltration flux (RIV)
H
DRN package active
GHB package active
H DRN
H GHB
H bot RIV
Q RCH
Q max RIV
Q model
RIV package active

5.4.8 Command line calls

RUNMFli
Program for the generation of ModFlow model input files and for carrying out groundwater flow calculations with ModFlow. Calculation results are converted to a **Triwaco** output file (***flairs.flo***).

The command call is similar to that for the standard **Triwaco** groundwater flow module **FLAIRS**.
A standard input file (***flairs.fli***) must be generated from the **TriShell**. Also, a standard grid file (grid.teo) is required. Output will be written to files: ***flairs.flo, flairs.flp*** and ***flairs.log***. If no arguments are given the program opens in Windows mode. The appropriate input files (***grid.teo, flairs.fli*** and ***calib.chi)*** can be selected and the program may be run using the pull-down menus.

Command line call:
RunMFfli.exe set-dir grid-dir flairs.fli [calib.chi]

No options are available.

Example:
RunMFfli C:\Projdirs\Modflow C:\Projdirs\Monet flairs.fli

MFU2FLO
Program for the conversion of ModFlow output to a standard **Triwaco** output file (***flairs.flo***). The existence of a MODFLOW compatible grid file is required.

The program searches the working directory (set-dir) for a MODFLOW output file with the same name as the input file mentioned on the command line.

Command line call:
MFu2Flo.exe set-dir grid-dir flairs.fli [calib.chi]

No options are available

Example:
MFu2Flo C:\Projdirs\Modflow C:\Projdirs\Monet flairs.fli