

FREEWAT

Free and Open Source Software Tools for Water Resource Management

EU HORIZON 2020 Project

FREE and Open Source Software Tools for WATer Resource Management

FREEWAT User Manual

Volume 1

Groundwater modeling using MODFLOW-OWHM (One Water Hydrologic Flow Model)

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This version is confidential, only for FREEWAT Project Partners



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FOREWORD

FREEWAT is an HORIZON 2020 project financed by the EU Commission under the call WATER INNOVATION: BOOSTING ITS VALUE FOR EUROPE. FREEWAT main result is an open source and public domain GIS-integrated modeling environment for the simulation of water quantity and quality in surface water and groundwater with an integrated water management and planning module. Specific objectives of the FREEWAT project are: to coordinate previous EU and national funded research to integrate existing software modules for water management in a single environment into the GIS-based FREEWAT platform and to support the FREEWAT application in an innovative participatory approach, gathering technical staff and relevant stakeholders in designing scenarios for the proper application of water policies.
The open source characteristics of the platform allow to consider this an initiative "ad includendum", as further research institutions, private developers etc. may contribute to the platform development. Capabilities integrated in FREEWAT are:

- a dedicated module for water management and planning;
- a whole module for calibration, uncertainty and sensitivity analysis;
- a module for solute transport in the unsaturated zone;
- a module for crop growth and rural water management;
- a module dedicated to time-series processing to support advanced model calibration;
- tools for dealing with groundwater quality issues;
- tools for the analysis, interpretation and visualization of hydrogeological data.

FREEWAT Development has received funding from the following projects:

1. Hydrological part has been developed starting from a former project, named SID&GRID, funded by Regione Toscana through EU POR-FSE 2007-2013 (sidgrid.isti.cnr.it).
2. Porting of SID&GRID under QGIS has been performed through funds provided by Regione Toscana to Scuola Superiore S.Anna - Project Evoluzione del sistema open source SID&GRID di elaborazione dei dati geografici vettoriali e raster per il porting negli ambienti QGIS e Spatialite in uso presso la Regione Toscana (CIG: ZA50E4058A)
3. Saturated zone solute transport simulation capability has been developed within the EU FP7-ENV-2013-WATER-INNO-DEMO MARSOL. MARSOL project receives funding from the European Union's Seventh Framework Programme for Research, Technological Development and Demonstration under grant agreement n. 619120 (www.marsol.eu)
4. The previous codes have been integrated into FREEWAT under development within EU H2020 project FREEWAT - Free and Open Source Software Tools for Water Resource Management. FREEWAT project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement n. 642224 (www.freewat.eu)
This User Manual provides guidelines to properly install and use the FREEWAT plugin.

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Capabilities of the FREEWAT platform were tested either by the developers group and by Project Partners. However, future applications of the platform may reveal errors and drawbacks not detected to date. Users are kindly requested to notify any error in both platform and User Manual. Please send this info to: rudy.rossetto@sssup.it

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Abstract

The FREEWAT platform includes a hydrologic model integrated in the QGIS GIS interface, where data are managed through a Spatialite Data Base Management System (DBMS), enabling the assessment of water balances and the availability of water resources in space and time, in order to support the planning process.

The hydrologic model implemented in FREEWAT allows to simulate the whole water cycle (including surface- and ground-water relationships) or subsets of it, based on climate, hydrologic, hydrodynamics and land use data.

In *FREEWAT*, the simulation of the water cycle is performed through the application of two versions of the *MODFLOW*family code, a physically-based, spatially distributed code, which simulates the groundwater flow dynamics using a 3D block-centered *finite-difference* approach, in which the spatial domain is discretized in rectangular cells. Flow associated with external stresses, such as wells, areal recharge, evapotranspiration, drains, and rivers, can be simulated as well.

The two versions of the *MODFLOW* code integrated into the FREEWAT platform are: *MODFLOW-2005* (Harbaugh, 2005) and the latest version *MODFLOW-OWHM* (Hanson et al., 2014).

MODFLOW-OWHM is a free code developed by the U.S. Geological Survey aimed at simulating the whole hydrological cycle. It is the latest and most complete version, to date, of the *MODFLOW* family of hydrological simulators and it is an evolution of the previous version. The need to properly manage the conjunctive use of ground- and surface-water required extending *MODFLOW-2005* to a fully-coupled, integrated hydrological model that can simulate the complete dynamics and use of water across the land surface and within the surface water and groundwater systems. In *MODFLOW-OWHM*, this is attempted by integrating the Farm Process within *MODFLOW-2005*. Farm Process module is described in the FREEWAT User Manual Volume 3 (Water management and crop-growth modeling).

This Volume describes the steps to install and to activate the FREEWAT plugin (Chapter 1) and contains instructions to set up and run a hydrologic model.

Chapter 2 presents the hydrological model and its capabilities. The workflow to be followed to create and set up a new hydrologic model is described. Possible limitations and default options are reported. Starting from Chapter 3, the procedure needed to create a new hydrologic model and the related geodatabase is shown. In Chapter 4, the definition of spatial and temporal discretization of the model is detailed, by creating the finite difference grid and defining Stress Periods.

Chapter 5 reports a description of tools for parameterization of model layers; the User may perform classical GIS operations (i.e., selection and editing) using QGIS tools and use new capabilities integrated in FREEWAT to manage data contained in vector and raster layers.

The implementation and setting-up of each *MODFLOW* Package for definition of boundary conditions and source/sink terms (*CHD*, *WEL*, *MNW*, *RCH*, *RIV*, *DRN*, *GHB*, *EVT*, *SFR*, *LAK*) is then described in Chapter 6, including also the simulation of vertical flow through the unsaturated zone with the *UZF* Package. Among the new groundwater flow simulation capabilities embedded in *MODFLOW* and implemented within the *FREEWAT* platform, it is worth mentioning the inclusion of the latest version of the Multi-Node Well Package (MNW2; Konikow et al., 2009), used also to simulate farm wells in Farm Process (refer to Volume 3), and the Lake Package for the simulation of lake-aquifer interaction (Merrit and Konikow, 2000).

Finally, the steps for running simulations and visualization of results are described in Chapters 7 and 8.

CHAPTER 1

FREEWAT Installation & Requirements

QGIS

The first step in order to use *FREEWAT* is to install **QGIS**.

It is strongly recommended to download the last stable and Long Term Release (LTR) version of QGIS, that is at present version 2.14 *Essen*.

FREEWAT has been tested with version 2.8 *Wien*, 2.10 *Pisa*, 2.12 *Lyon* and 2.14 *Essen* of QGIS, but it is also compatible with other **stable** releases (2.16, 2.18).

In order to install QGIS on the different OS, please refer to the official documentation available at the QGIS web site.

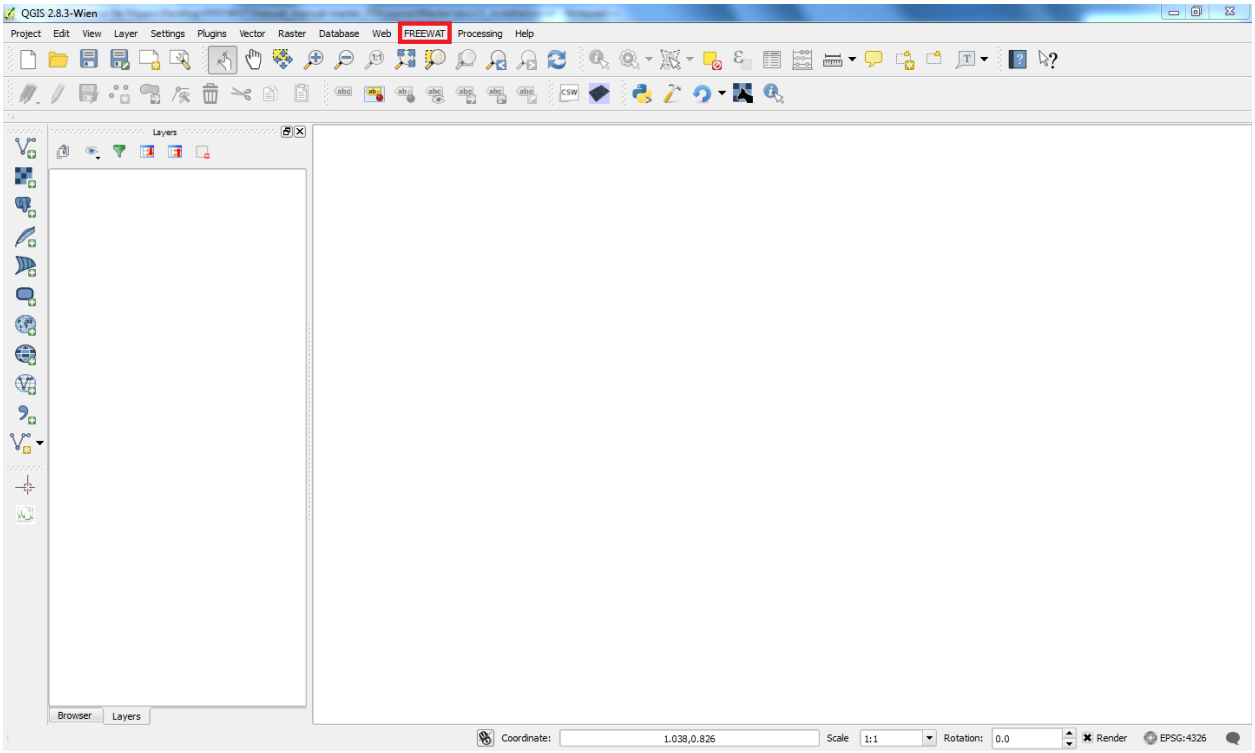
FREEWAT plugin

In all OS, once QGIS is executed, the `.qgis2` folder is created.

On *Windows* machines you can find this folder under *C:Usersyour_name.qgis2*, while on *Linux* machines it is located in your home folder (*/home/user/.qgis2*).

In order to use the *FREEWAT* plugin you have to extract the **entire folder provided** (the folder name is `freewat`) in the `C:\User\your_name\.qgis2\python\plugins` folder.

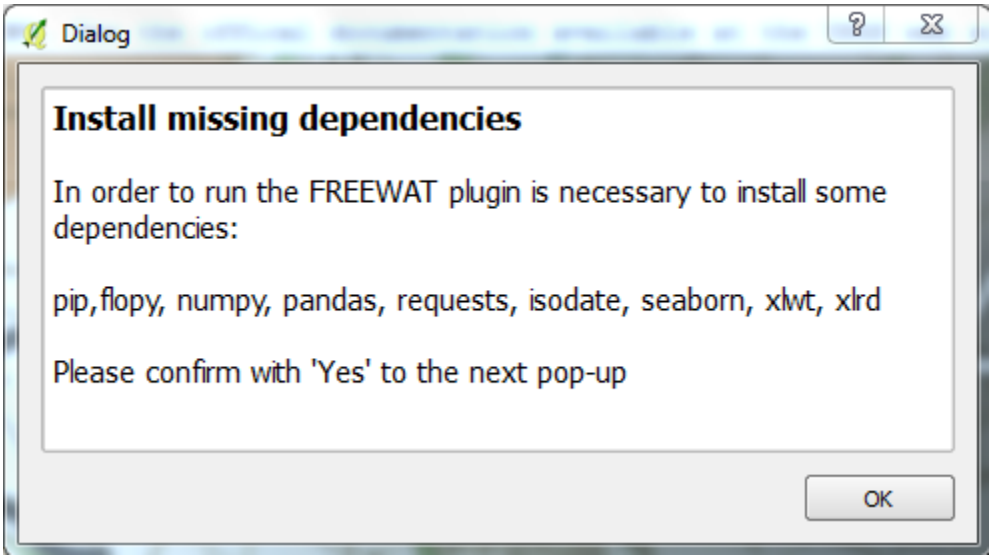
Sometimes the `plugins` folder does not exist, so you can just create it.



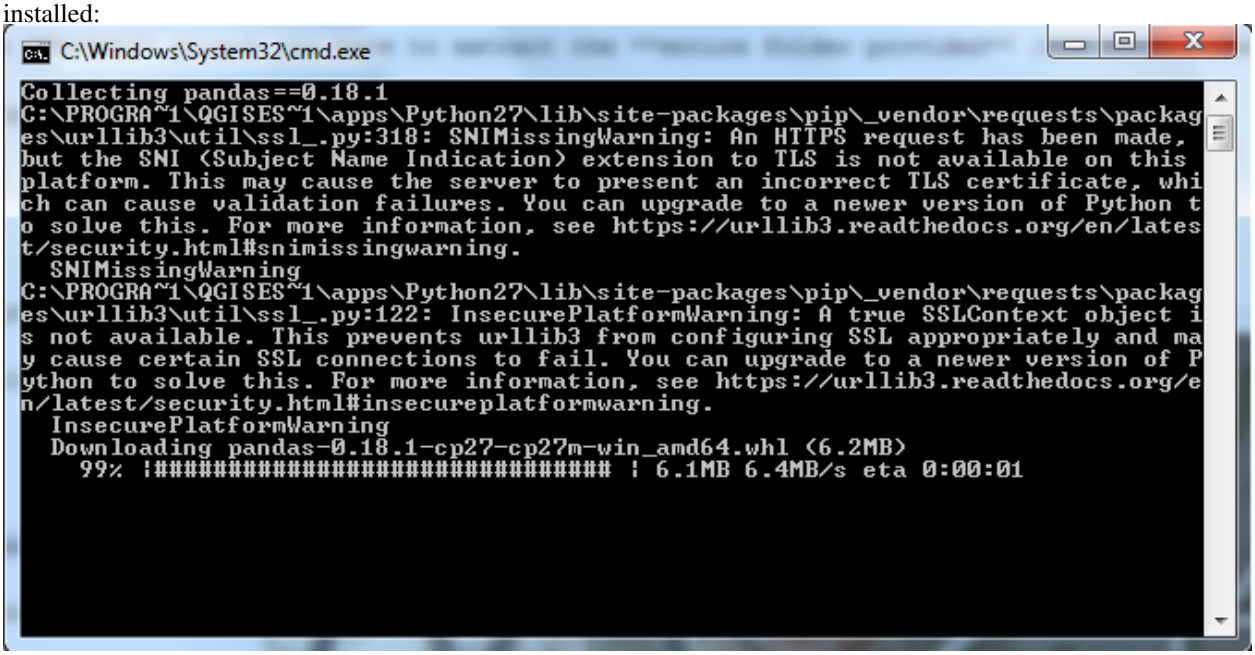
Once QGIS has been installed and the `freewat` folder has been extracted in the `C:\User\your_name\.qgis2\python\plugins` folder, run QGIS.

A **Dialog** window appears, reporting that the follwing dependencies are needed:

- *pip*;
- *flopy*;
- *numpy*;
- *pandas*;
- *requests*;
- *isodate*;
- *seaborn*;
- *xlwt*;
- *xlrd*.



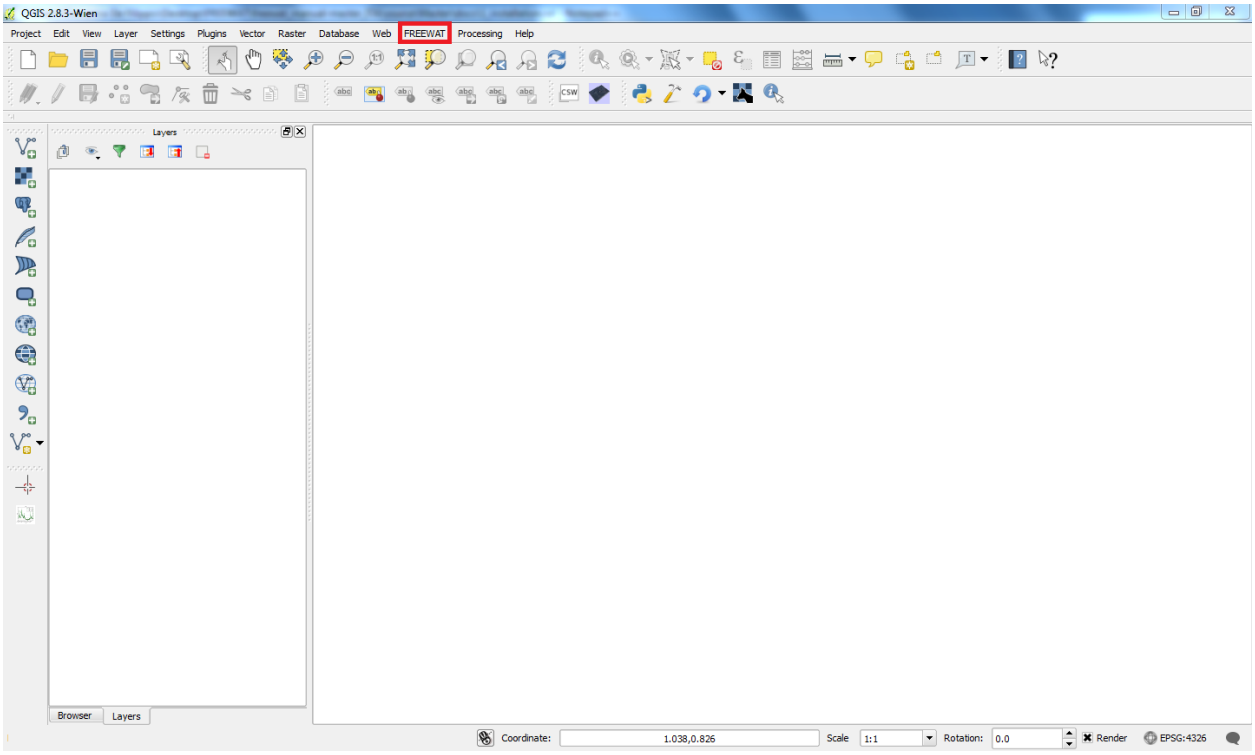
Once you click *OK*, several pop-up windows will appear and all the missing dependencies will be automatically installed:

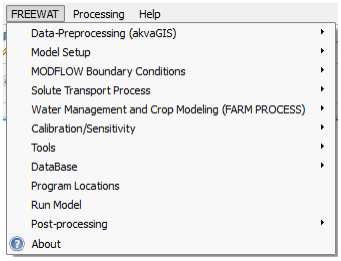


Note: Installing each missing dependency requires authorization, so you will be asked to enter a password so that each pop-up window is run as administrator.

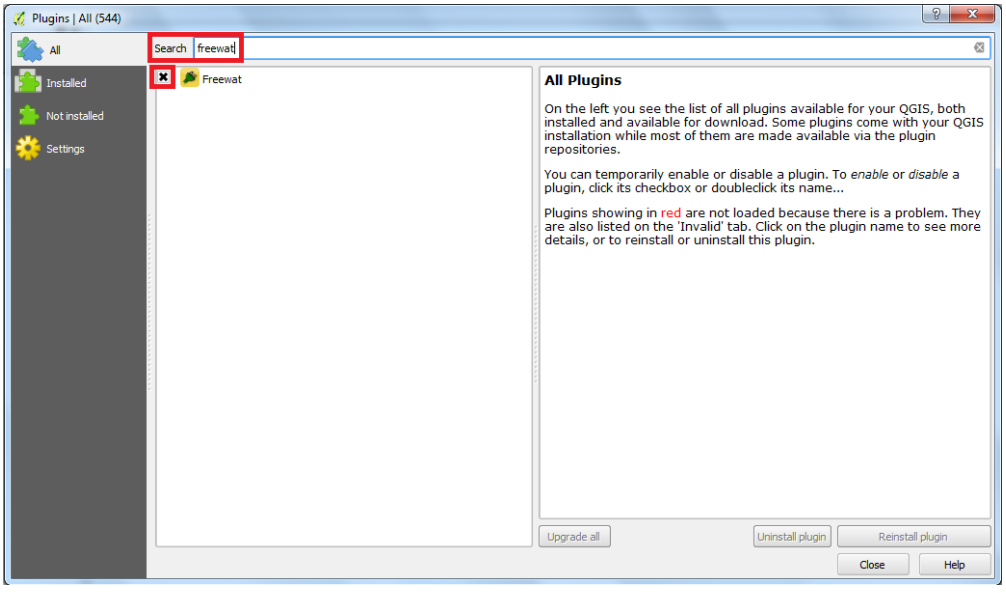
Start FREEWAT

After *QGIS* and all the needed dependencies have been correctly installed, *FREEWAT* will appear as a dropdown menu in the toolbar of the *QGIS* GUI:



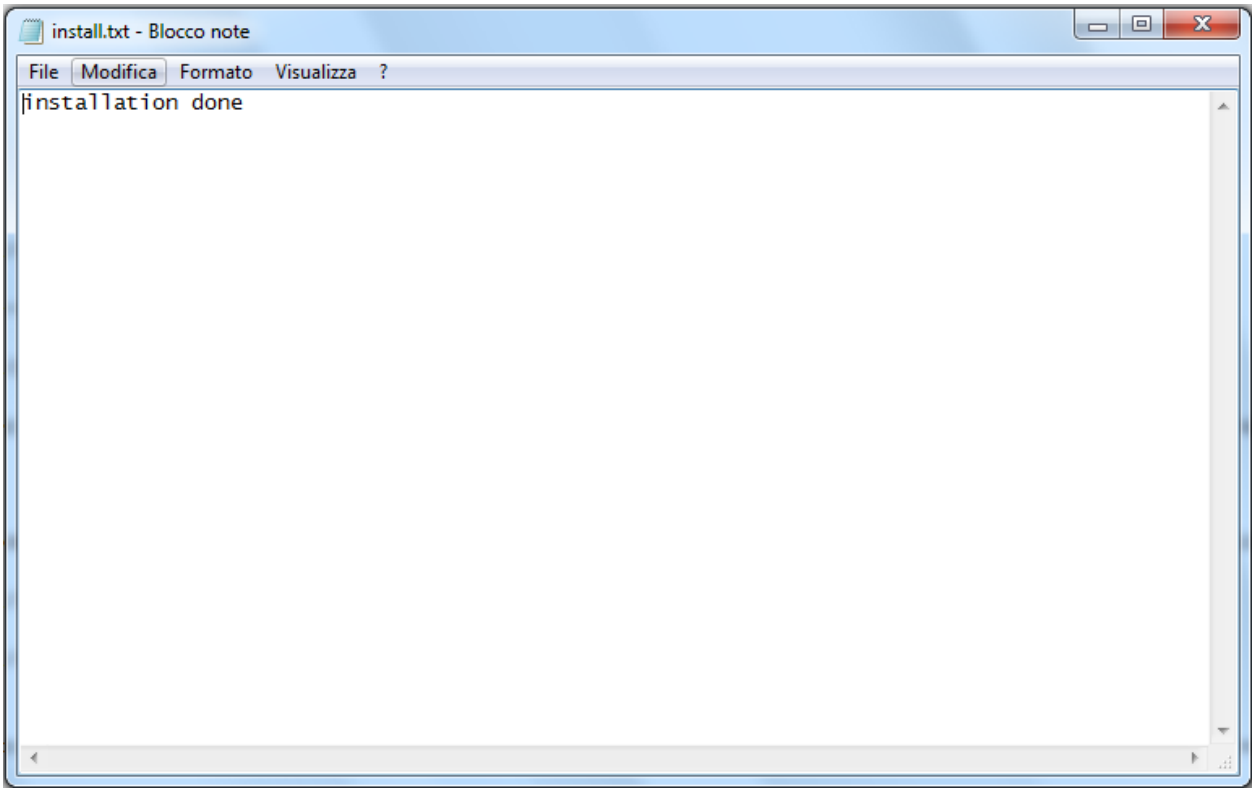


If not, just go in *Plugins* -> *Manange and Install Plugin..*, search *FREEWAT* and click on the checkbox to activate the plugin, as shown in the picture below.



The *FREEWAT* platform can now be used by following the logical workflow presented in the following Chapters.

Note: It can happen that, even if all the needed dependencies have been correctly installed (and *FREEWAT* appears in the toolbar of the *QGIS* GUI), installation procedure starts each time you re-run *QGIS*. If this happens, a txt file named `install.txt` must be created manually in the `C:\User\your_name\.qgis2\python\plugins\freewat\install` folder. This txt file must contain only the sentence `installation done`.



CHAPTER 2

FREEWAT Hydrological Model

The hydrological model implemented in *FREEWAT* allows to simulate the entire hydrological cycle, provided that climate data, like rainfall and temperature, are available. Anyway, it is also possible to focus only on selected parts of the model.

The simulated processes described in this Volume are:

1. groundwater flow in the saturated zone, including interaction with surface water features (e.g., rivers, lakes, drains);
2. vertical flow through the unsaturated zone and beneath surface water streams.

The processes described in this Volume can be simulated either with *MODFLOW-2005* (Harbaugh, 2005) and *MODFLOW-OWHM* (*One-Water Hydrologic Flow Model*; Hanson et al., 2014).

Specific capabilities for rural water management are described in Volume 3.

Simulated processes

MODFLOW has a wide range of different Packages that allow to simulate several processes. The current *FREEWAT* plugin includes only some of these Packages which, however, are useful for the simulation of the main hydrological and hydrogeological processes.

Hereinafter, a list of the *MODFLOW* Packages (Harbaugh, 2005), grouped in categories, is provided:

- **Basic Packages**:
  - Basic (BAS)
  - Discretization (DIS)
  - Layer Property Flow (LPF)
- **Hydrogeological processes**:
  - specified-head boundaries
    - Time-Variant Specified Head (CHD)
  - specified-flux boundaries
    - Recharge (RCH)
    - Well (WEL)
  - head-dependent flux
    - Unsaturated Zone Flow (UZF)

        * River (RIV)
        * Lake (LAK)
        * Drain (DRN)
        * General-Head Boundary (GHB)
        * Evapotranspiration (EVT)
        * Multi-Node Well (MNW)
        * Stream Flow Routing (SFR)
- **Numerical solvers**:
    - Preconditioned Conjugate-Gradiente (PCG)
- **Output handling**:
    - Output Control Option (OC)

Workflow of the FREEWAT plugin

The modeler can use the *FREEWAT* plugin in order to implement the model, execute simulations and view and process results within *QGIS*.

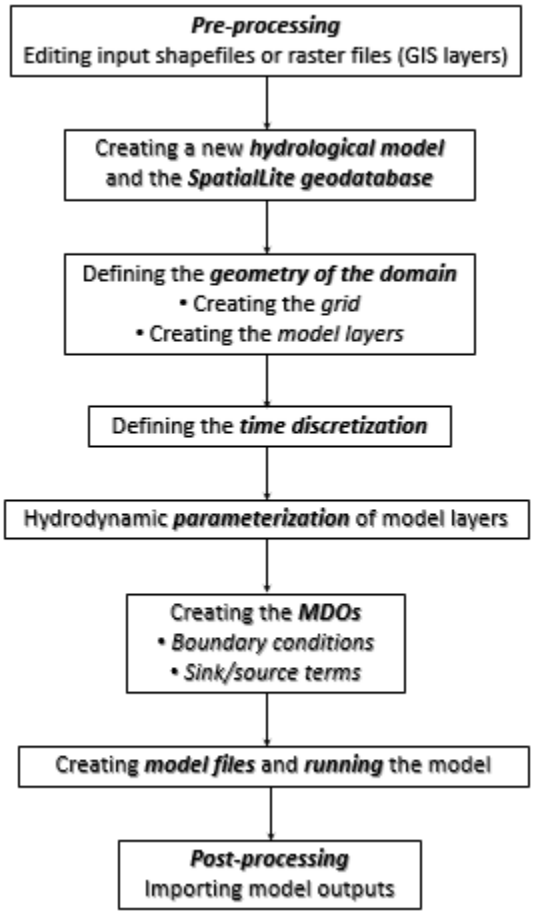
Each process is based on a well encoded procedure: from a generic *GIS layer*, to a *model layer/Model Data Object* and finally to a text file required by the numerical solver.

The *FREEWAT* terminology is the following:

- *GIS layer* - it indicates a generic geographic informative layer, not still processed for the modelling scenario;
- *model layer* - the discrete domain is divided in n layers (model layers) corresponding to the hydrostratigraphic units identified in the conceptual model;
- *Model Data Object (MDO)* - it is the GIS layer processed according to the model properties and containing at least the information on both spatial (row and column) and temporal (Stress Period - SP) discretization;
- *model file* - is a text file generated from an MDO and required to run the simulation.

The user has to organize all the GIS data (vector and raster) referring to the study area. This means importing or creating each layer in *QGIS* in a proper Coordinate Reference System (CRS), eventually clipping it according to the extent of the study area.

Once this first step is completed, the user is ready to start building the model. Firstly, a new hydrological model and the related geodatabase must be created (Chapter 3). Then, the spatial and time discretizations will be defined, including the parameterization of the hydrodynamic properties of each model layer (Chapters 4 and 5). Boundary conditions and sink/source terms will be defined as well, defining proper MDOs from the available GIS layers (Chapter 6). Finally, once selected all the Packages which have to be activated for the aims of the simulation, all the model layers and MDOs are translated in *MODFLOW* input files and the model can be run (Chapter 7). Visualization and post-processing of results (e.g., the simulated hydraulic head) and zone budgets are described in Chapter 8.



Limitations

During the building of the input files for the *MODFLOW* Packages, *FREEWAT* has some limitations regarding some flags and options. This means that some parameters have default values which the user cannot change. The aim is to make the model implementation easier.

Limitations about implementation of *MODFLOW* Packages will be described in detail in Chapter 6. The following limitations, instead, concern mandatory *MODFLOW* input files:

- the flag *LAYCBD* in the Discretization (DIS) file is set to *0*: this means that confining beds cannot be simulated;
- the default options set for the Output Control Option (OC) file are:
  - hydraulic head, drawdown and cell-by-cell flow are stored at the end of each Time Step (TS) within external binary files;
  - model balance is printed in the Listing (LST) file at the end of each TS, while the simulated hydraulic head values are not stored here to avoid creating an oversized file.

Anyway, these limitations concern **only** the graphical user interface. The advanced user can eventually edit the *MODFLOW* input files created and set there flags and parameters as needed.

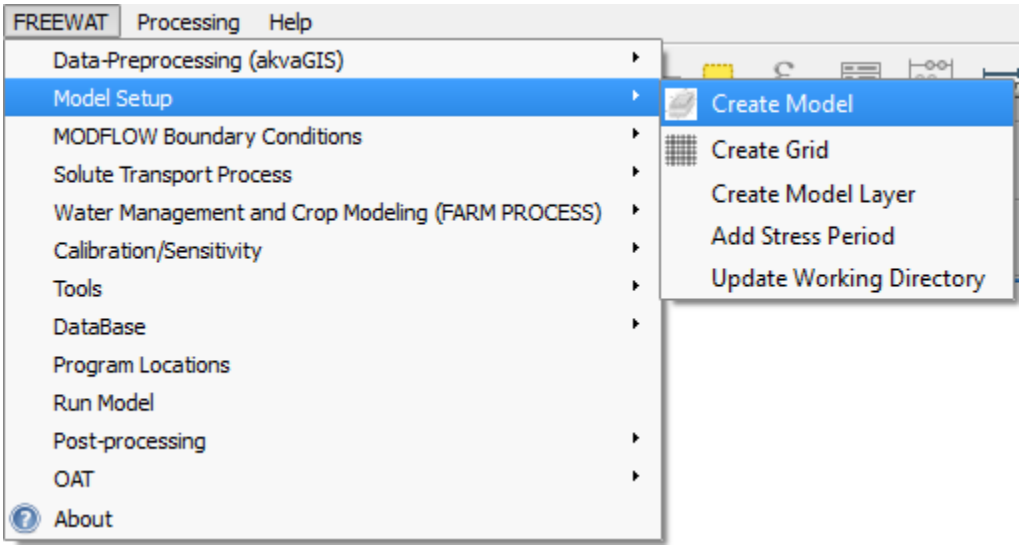
CHAPTER 3

Creating a new hydrological model and geodatabase

The simulation of a new scenario requires creating a new hydrological model and a model DataBase (DB).

To create a new hydrological model, the following menu must be used:

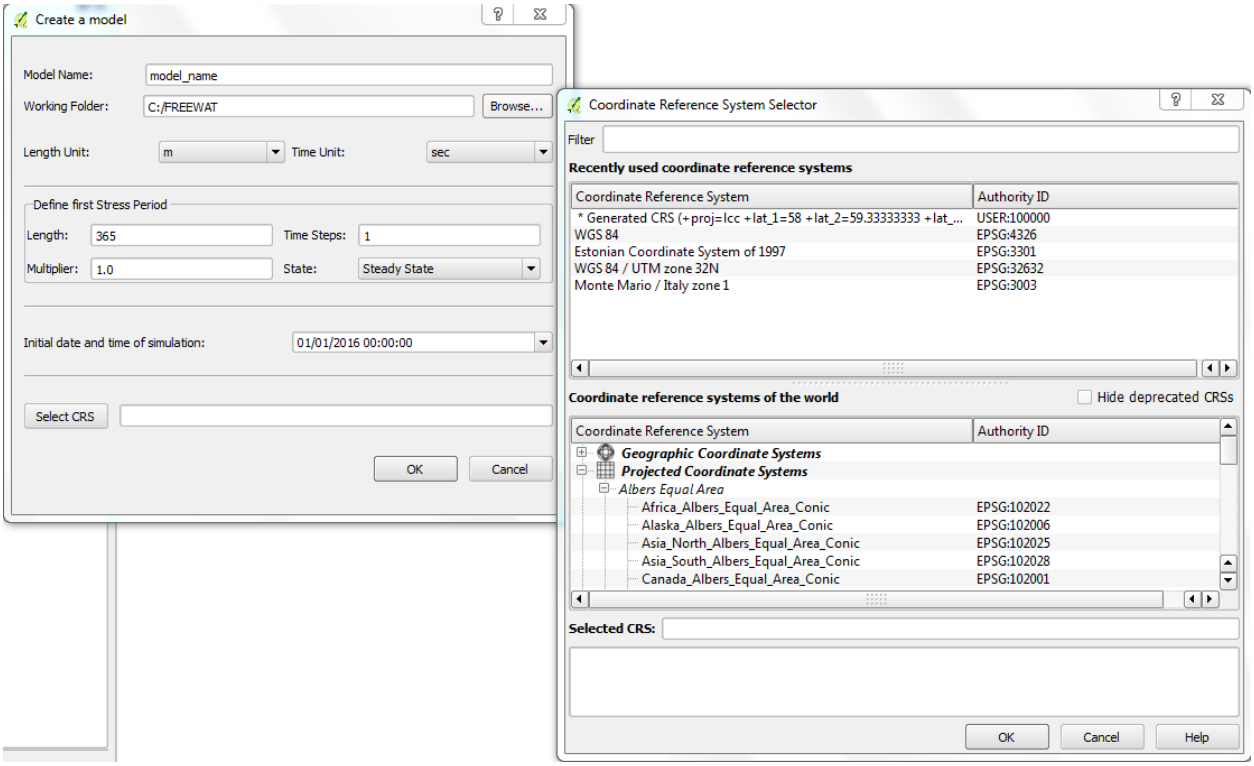
FREEWAT -> Model Setup -> Create Model



In the **Create a model** window, the following data are required:

- *Model Name*: name of the new hydrological model;
- *Working Folder*: folder within which the geodatabase, the *MODFLOW* input files and the output files will be stored;
- *Length Unit*: four options are available (*m*, *cm*, *ft*, *undefined*);
- *Time Unit*: seven options are available (*sec*, *min*, *hour*, *day*, *month*, *year*, *undefined*);
- in the *Define first Stress Period* section:
  - *Length*: length of the first SP in time units;
  - *Time Steps*: number of TS within the first SP;
  - *Multiplier*: multiplier to calculate the length of TS within the first SP;
  - *State*: two options are available, *Steady State* and *Transient*;

- *Initial date and time of simulation*: starting date and time of the simulation, using formats gg/mm/yy and hh:mm:ss, respectively (it is also possible to choose the starting date from a drop-down calendar);
- by clicking on *Select CRS*, it is possible to select the Coordinate Reference System (CRS) to be assigned to the model through the *Coordinate Reference System Selector*.



Note: Once defined *Length Unit* and *Time Unit*, pay attention to be coherent when assigning values to model parameters (e.g., hydrodynamic properties and geometry of model layers), even if the option *undefined* is selected.

Note: There shouldn't be spaces and/or special characters in the path of the *Working Folder*.

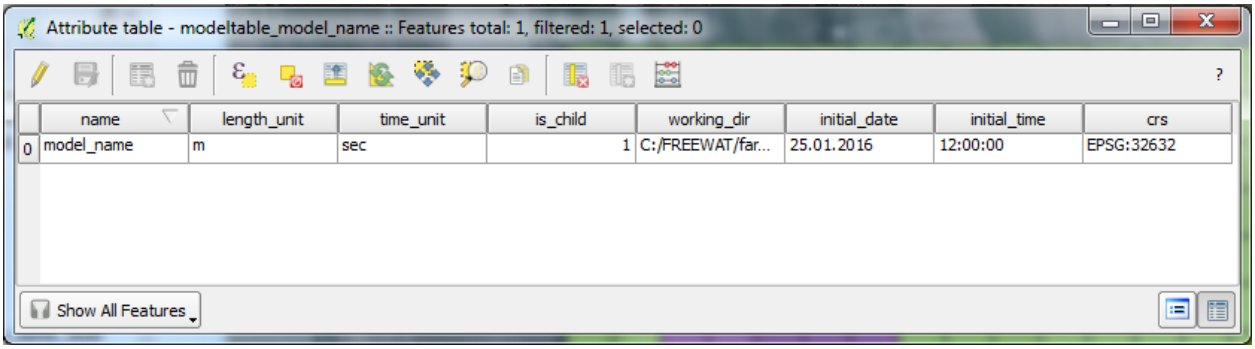
Once the new model is created, the corresponding model DB is created and stored in the *Working Folder* as *model_name.sqlite*. This model DB can be consulted by using *QGIS* tools. For example, with the *DB Manager* plugin each MDO stored within the model DB can be simply renamed, deleted or added to the Map Canvas as needed.

Three tables named *modeltable_model_name*, *timetable_model_name* and *prg_locations_model_name* are loaded in the Layers Panel and stored within the model DB.

The model table contains the following fields:

- *name*: name of the hydrological model created;
- *length_unit*: indication of the *Length Unit* defined when creating the model (*m*, *cm*, *ft* or *undefined*);
- *time_unit*: indication of the *Time Unit* defined when creating the model (*sec*, *min*, *hour*, *day*, *month*, *year* or *undefined*);
- *is_child*: this field is not relevant for the current version, as the LGR (Local Grid Refinement) method (Mehl and Hill, 2005; Mehl and Hill, 2007; Mehl and Hill, 2013) is not yet implemented;
- *working_dir*: indication of the path for the *Working Folder* defined when creating the model;

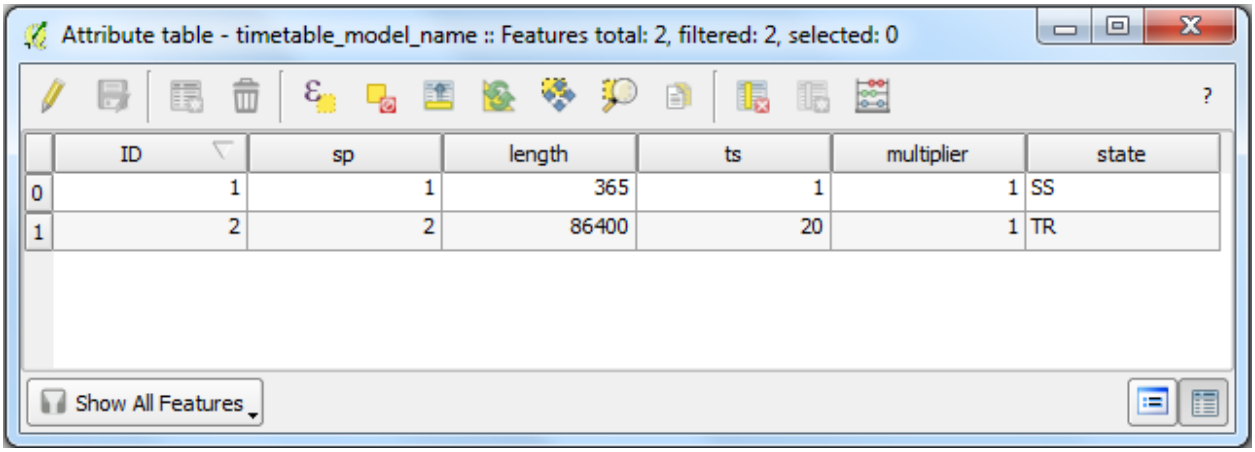
- *crs*: CRS set when creating the model.



The time table contains the following fields:

- *ID*: database primary key (it must not be modified);
- *sp*: progressive ID of each SP;
- *length*: length of each SP in time units;
- *ts*: number of TS within each SP;
- *multiplier*: multiplier used to calculate the length of each TS within each SP;
- *state* with indication of the *State* defined when creating the model (*SS* for *Steady State*, *TR* for *Transient*).

Note: If more SPs are defined later, the time table is automatically updated.



The table of program locations is needed to load the executables of the codes which have to be used to simulate specific processes. It contains the following fields:

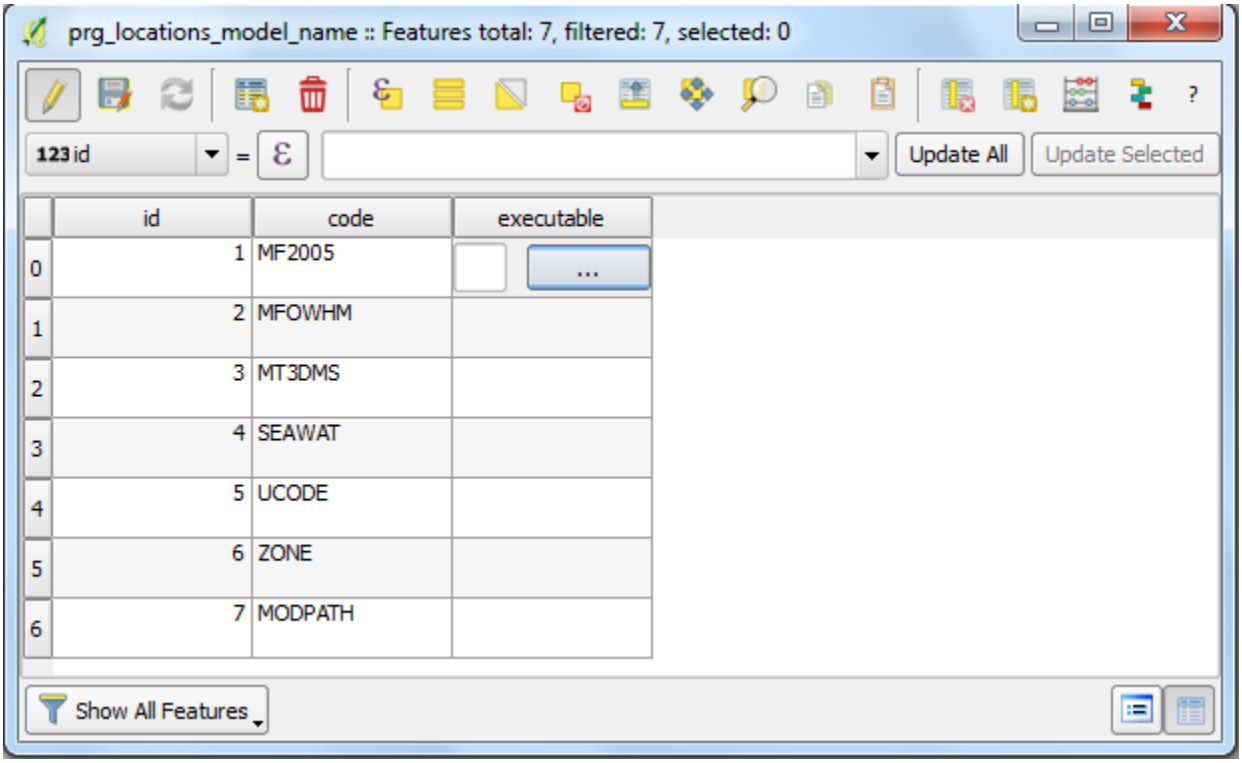
- *id*: progressive ID of each executable;
- *code*: name of the software;
- *executable*: path defined for each executable.

This table can be done editing the corresponding fields (a browse button is present).

The following executables are needed, according to the processes to be simulated:

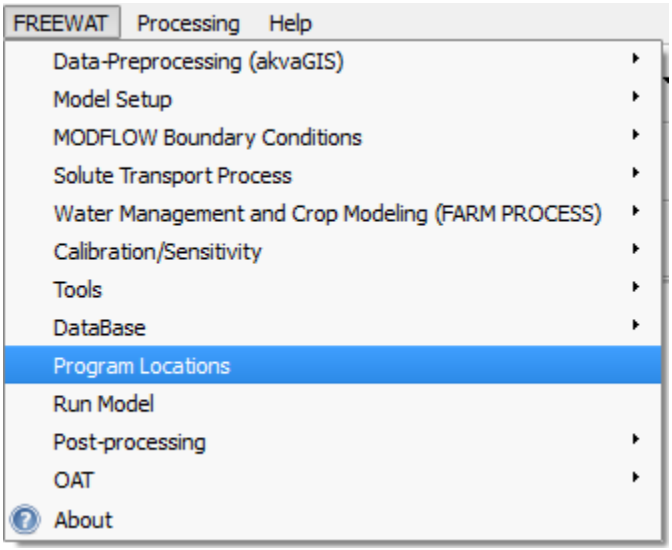
- *MF2005* for groundwater flow modeling with *MODFLOW-2005*;
- *MFOWHM* for groundwater flow modeling and water management with *MODFLOW-OWHM*;

- *MT3DMS* for transport modeling in the saturated zone with *MT3DMS*;
- *SEAWAT* for coupled flow and transport modeling in the saturated zone with *SEAWAT*;
- *UCODE* for sensitivity analysis and parameter estimation with *UCODE*;
- *ZONE* to explicit the water budget for different zones of the active domain with *ZONE BUDGET*;
- *MODPATH* for particle-tracking post-processing model with *MODPATH*.

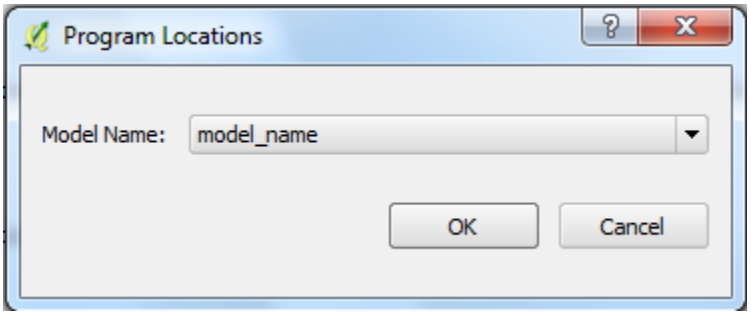


If the table *prg_locations_model_name* is accidentally deleted both from the Layers Panel and from the model DB, it is possible to create it again through the following menu:

FREEWAT -> Program Locations.



In the **Program Locations** window, the *Model Name* (i.e., the name of the hydrological model) is required:



Importing a DB

Importing an existing DB requires having the *.sqlite* file in a folder which will be the User's *Working Directory*.

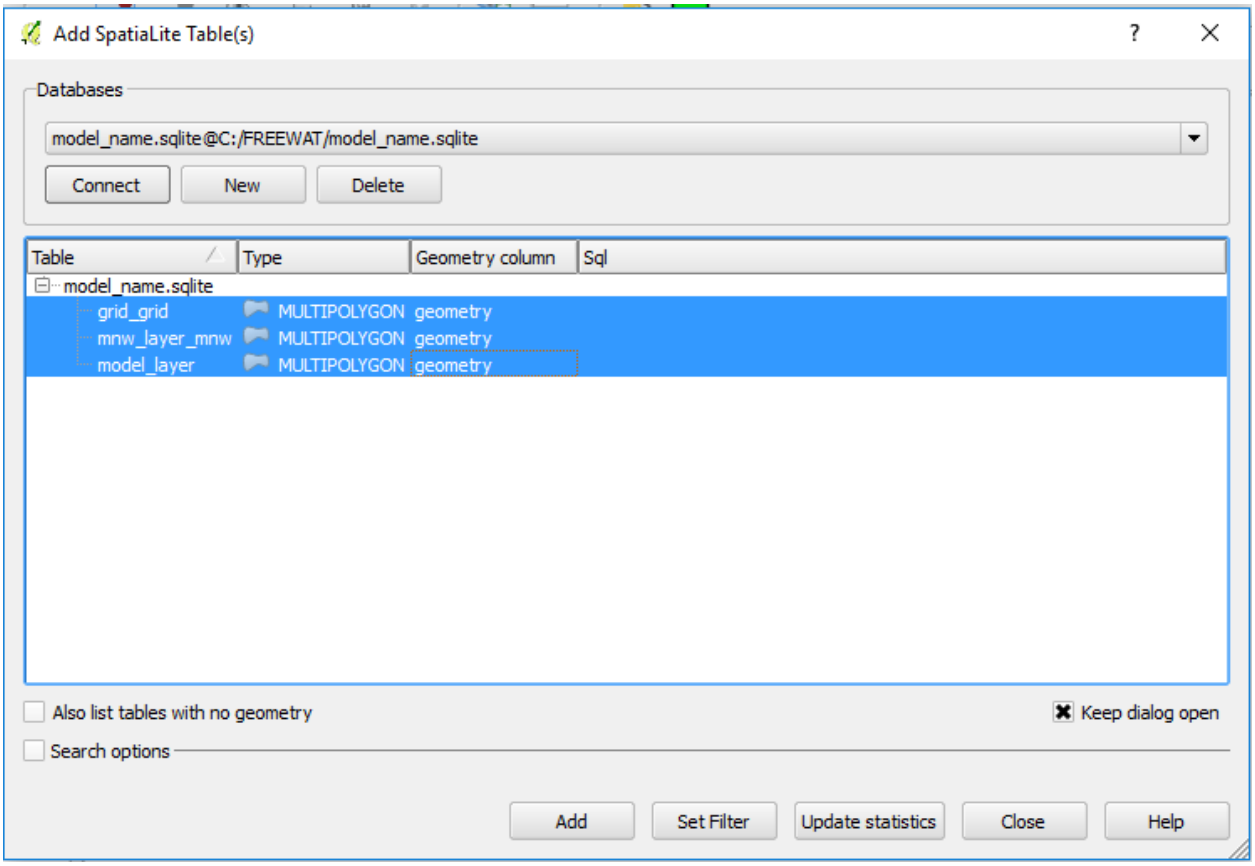
Note: Pay attention not to have spaces and/or special characters in the path of the *Working Directory*.

Once *QGIS* has been run, the User must use the button *Add SpatiaLite Layer*, click on *New*, browse until the *Working Directory* to load the *.sqlite* file and click on *Connect*.

Note: If an *.sqlite* file with the same name has been already loaded in advance, the User must previously delete the old one.

Before to proceed with the next steps, the User should check the *Keep dialog open* checkbox.

Once the DB is connected, some layers with *MULTIPLOLYGON geometry* type should be displayed, corresponding to the MDO stored within the DB itself. The User must select all these MDOs and click on *Add* to add them to the Layers Panel.

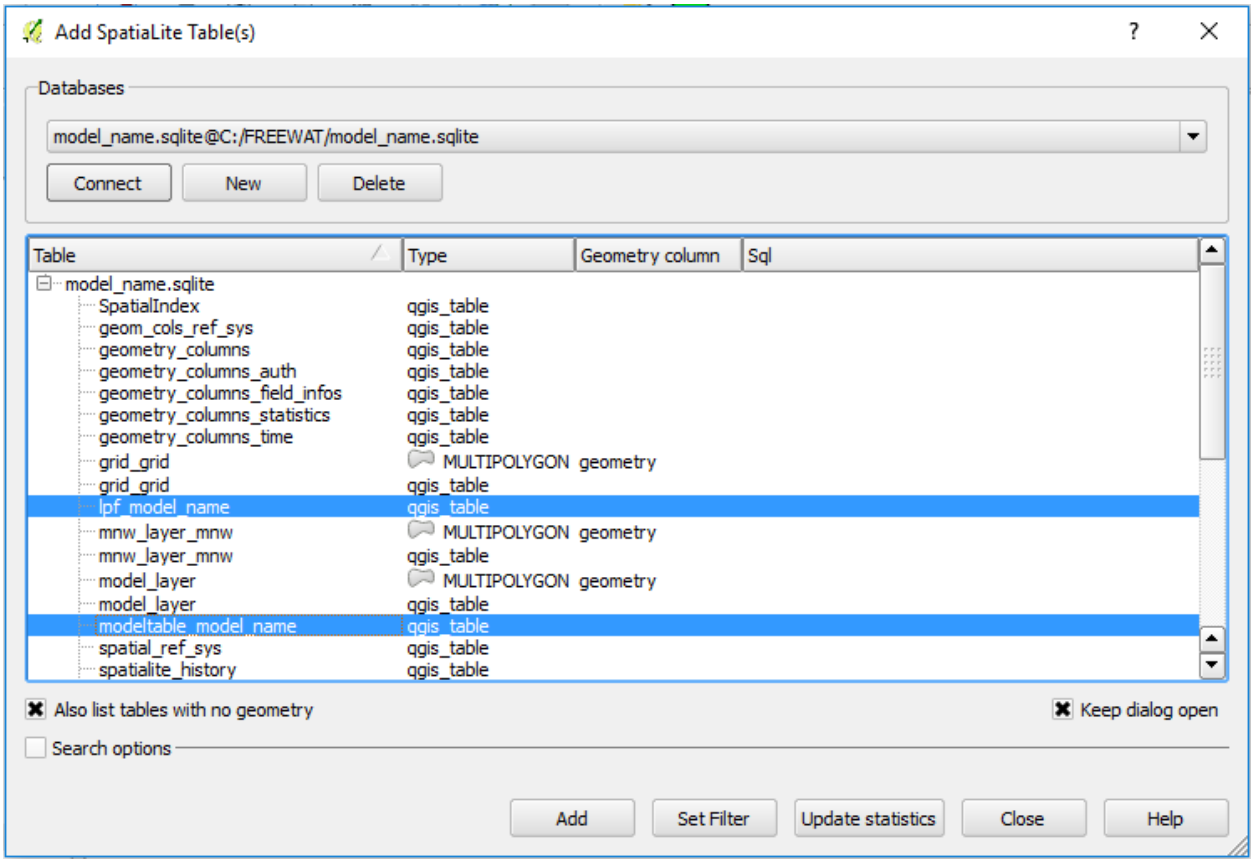


As some tables are also needed, the User must check the *Also list tables with no geometry* checkbox, select the tables needed and click on *Add* to add them to the Layers Panel.

The following tables are mandatory:

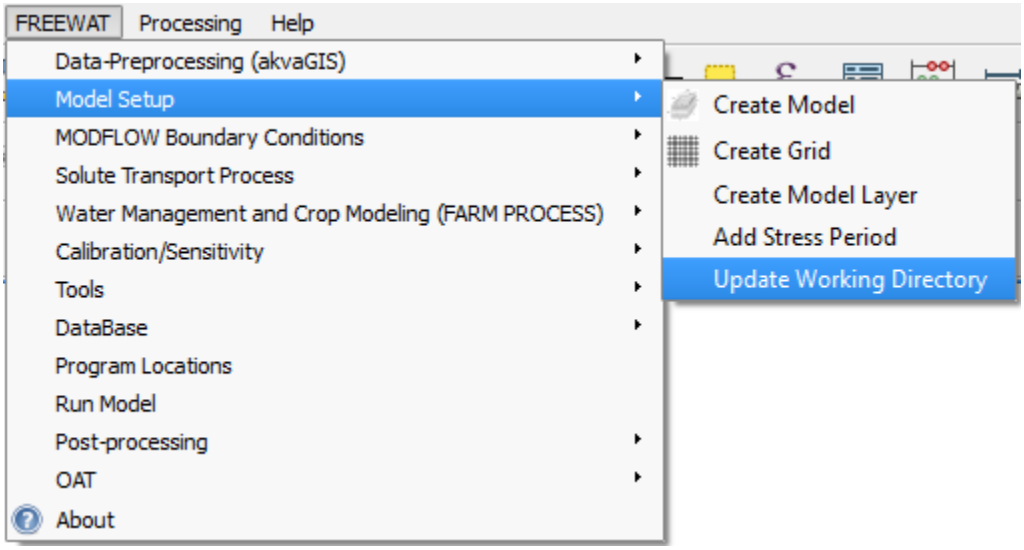
- *model table*;
- *time table*;
- *lpf table*;
- *program locations*.

Furthermore, if the SFR Package is implemented, the related table must be loaded (further details will be provided in Chapter 6).



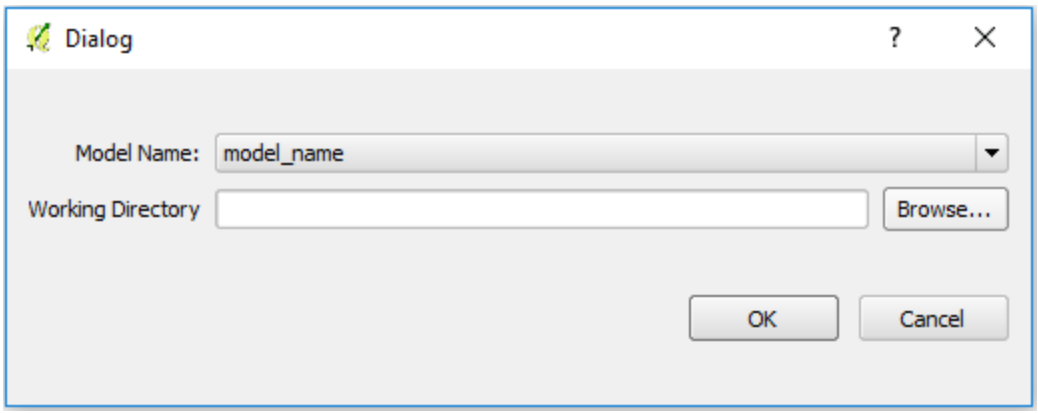
Once all the needed MDOs and tables are loaded in the Layers Panel, the path of the *Working Directory* in the model table must be updated through the following menu:

FREEWAT -> Model Setup -> Update Working Directory



The following data are required:

- *Model Name*: name of the new hydrological model;
- *Working Directory*: folder within which the *.sqlite* file has been saved and where the *MODFLOW* input files and the output files will be stored (it must be selected through the *Browse* button).



The path for all the needed executables must be updated as well editing the fields *executable* in the table of program locations

CHAPTER 4

Spatial and time discretization

Once the input geographical files are ready and the conceptual model defined, it is necessary to set up the 3D geometry of the aquifer system (i.e., the finite-difference horizontal grid and the vertical discretization) and the time discretization of the simulation. It is so required defining:

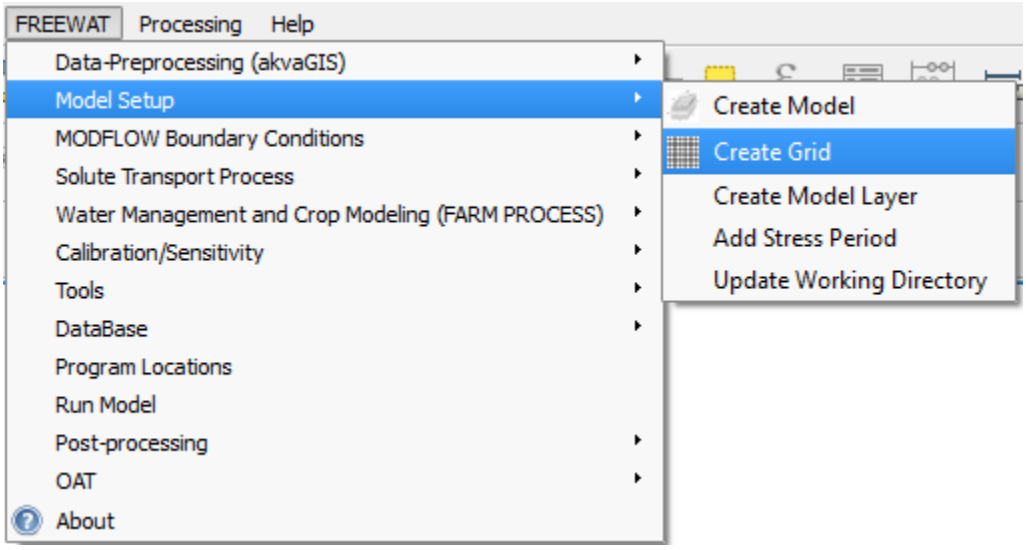
- the cell size;
- the number of SPs to be simulated.

Creating the finite-difference grid

To create the computational grid, the boundaries of the study area must be known. For this purpose, a polygon shapefile may be edited, defining a polygon which limits the study area and within which the grid will be created. We suggest to edit such polygon so that each border size (both along the x and y directions) is a multiple of the cell size (e.g., if the cell size is 100 m, each border can extend for 1000 m, but not for 1025 m). Alternatively, a background map cut to the study area extent can be used.

To create the grid, use the menu:

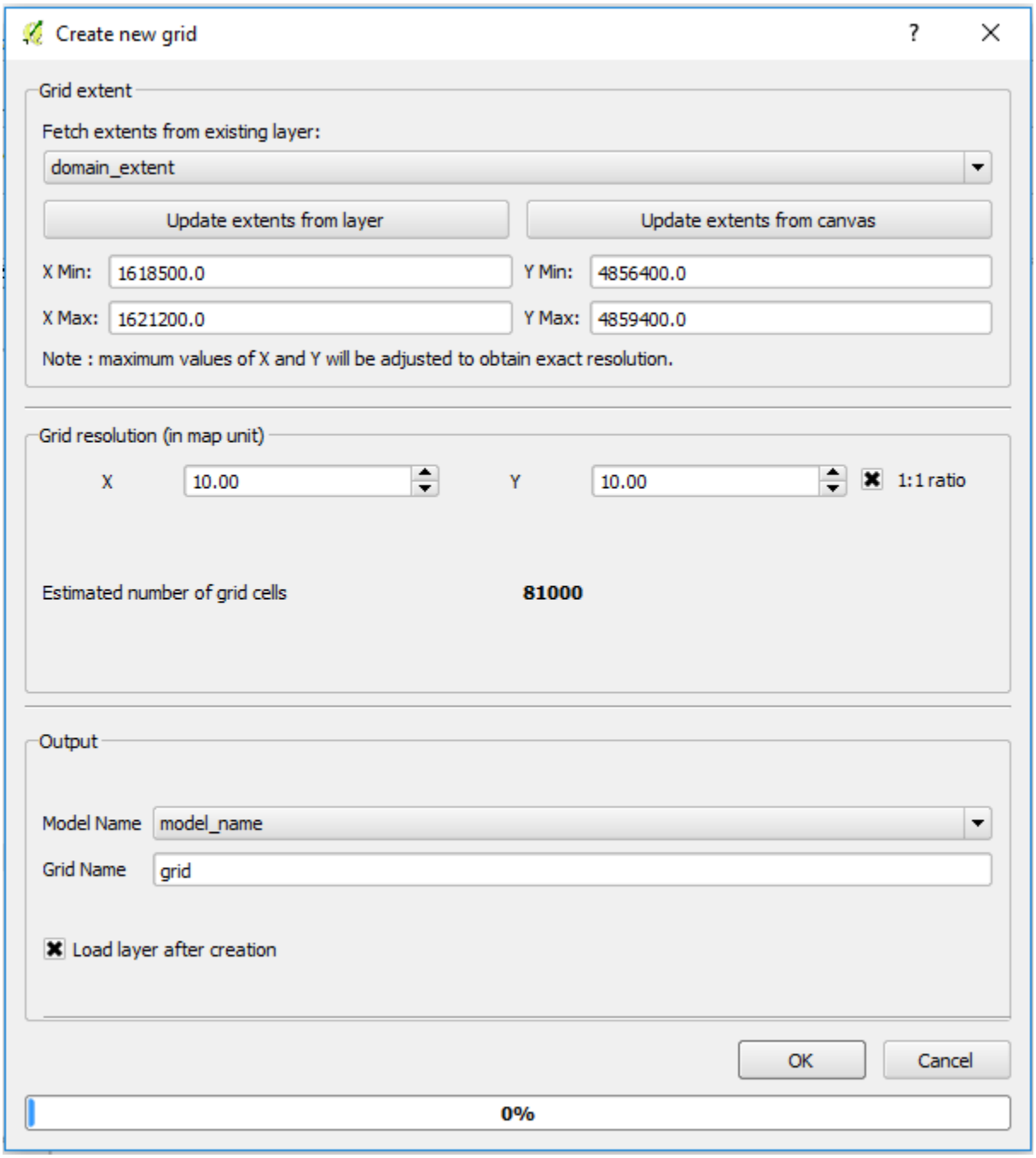
FREEWAT -> Model Setup -> Create Grid.



The generated grid will be used to create further MDOs (e.g., the model layers or the areally distributed recharge) and to assign properties (e.g., top and bottom surfaces and hydrodynamic properties of model layers) at each cell of the grid itself.

The following data are required in the **Create new grid** window:

- the polygon shapefile previously created (if any), containing the extent of the domain, or a background map cut to the study area extent: it must be selected under *Fetch extents from existing layer* in the *Grid extent* section;
- *X Min*, *X Max*, *Y Min* and *Y Max* are the spatial coordinates of the vertices of the polygon. There are three options to specify them:
  - they can be loaded from the polygon shapefile (*Update extents from layer*);
  - they ca be loaded from the background map (*Update extents from canvas*);
  - they can be entered by the User;
- the *Grid resolution (in map unit)* along *X* and *Y* directions: if the box *1:1 ratio* is checked, square grid cells will be generated;
- in the *Output* section:
  - *Model Name*: name of the hydrological model;
  - *Grid Name*: name to be assigned to the grid MDO; if the box *Load layer after creation* is checked, the grid MDO will be loaded in the Layers Panel after creation.



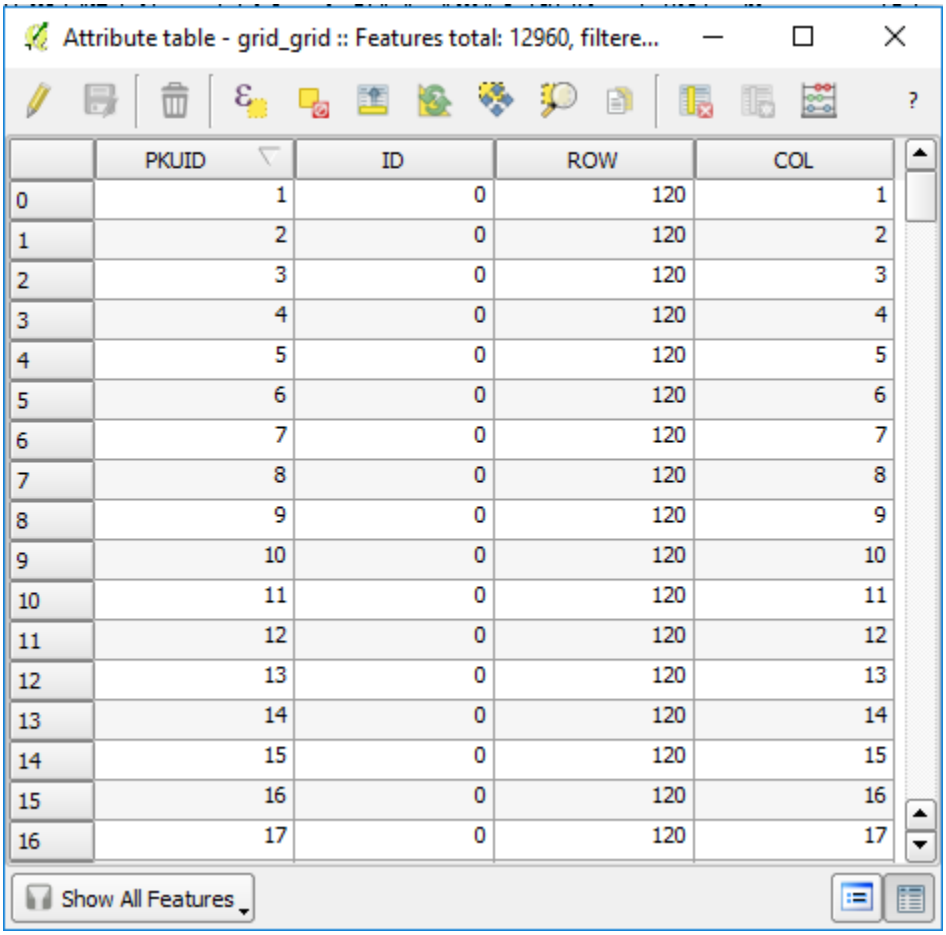
Note: According to the domain extent and to the grid resolution, the total number of grid cells is calculated (*Estimated number of grid cells*).

Once the grid MDO is created, it is stored within the model DB with the name *grid_grid* and eventually loaded in the Layers Panel.

Note: The extension *_grid* must not be changed in the LP and neither in the DB, as the grid MDO will be filtered in each dialog according to such extension.

The Attribute Table of such MDO may contain several records, according to the number of grid cells, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell.



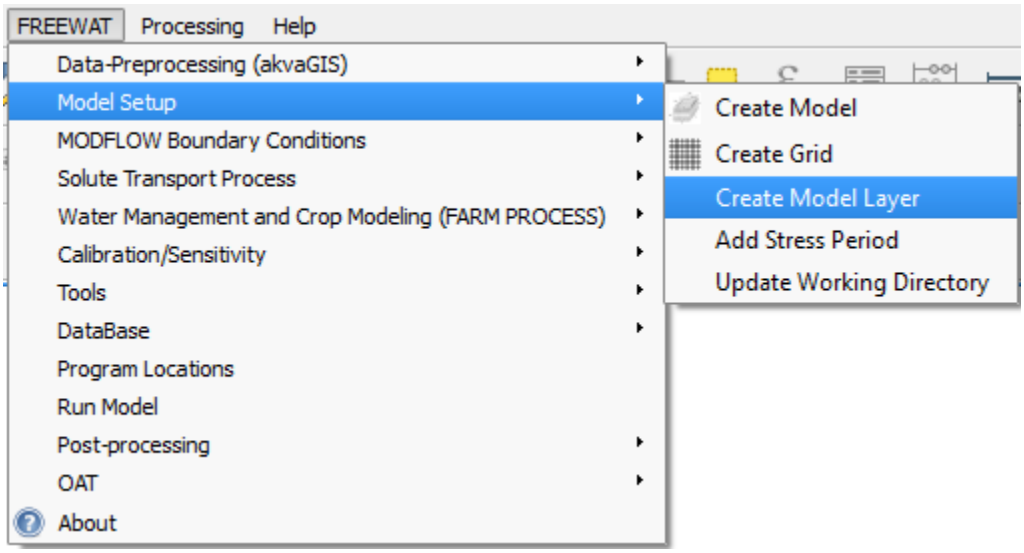
	PKUID	ID	ROW	COL
0	1	0	120	1
1	2	0	120	2
2	3	0	120	3
3	4	0	120	4
4	5	0	120	5
5	6	0	120	6
6	7	0	120	7
7	8	0	120	8
8	9	0	120	9
9	10	0	120	10
10	11	0	120	11
11	12	0	120	12
12	13	0	120	13
13	14	0	120	14
14	15	0	120	15
15	16	0	120	16
16	17	0	120	17

Defining model layers

Once defined the model grid, the user can create the model layers corresponding to the hydrostratigraphic units identified in the conceptual model. Each model layer will be stored within the model DB as an MDO grid-related, meaning that its properties (specifically geometry and hydrodynamic parameters) are assigned at each grid cell.

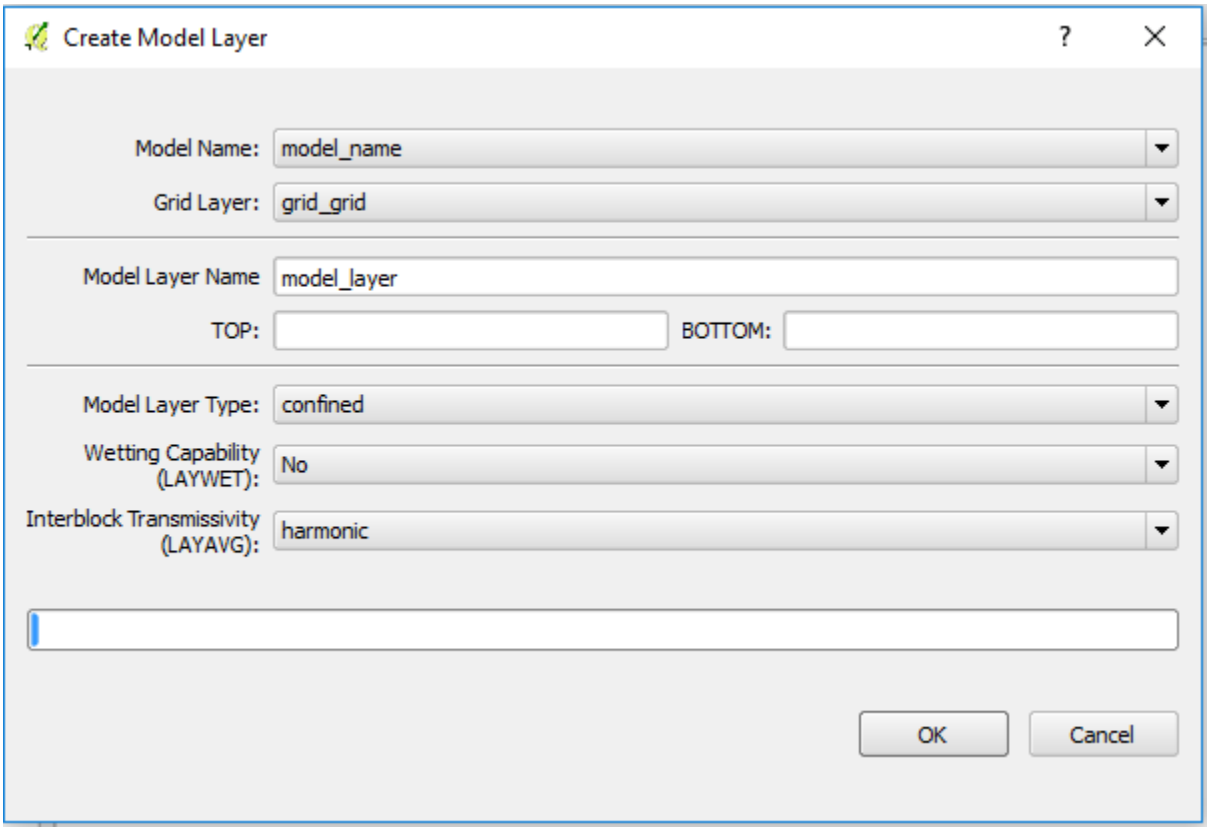
To create each model layer, use the menu:

FREEWAT -> Model Setup -> Create Model Layer.



The following data are required in the **Create Model Layer** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: name of the grid MDO;
- *Model Layer Name*: name to be assigned to the current model layer;
- *TOP*: top surface of the model layer [L];
- *BOTTOM*: bottom surface of the model layer [L];
- *Model Layer Type*: two options are available, *confined* if the conductance terms for cell-to-cell flow are computed at the beginning of the simulation and remain constant, *convertible* if the conductance terms are updated at each iteration based on saturated thickness of each cell (for details refer to Harbaugh, 2005);
- *Wetting Capability (LAYWET)* (just for convertible model layers): two options are available, *Yes* if cells which become dry during the simulation can be rewetted, *No* otherwise (for details refer to Harbaugh, 2005);
- *Interblock Transmissivity (LAYAVG)*: method used to calculate the horizontal interblock transmissivity (three options are available, *harmonic*, *logarithmic* and *arithmetic-mean*; for details refer to Harbaugh, 2005).



Note: Since constant values are assigned to *TOP* and *BOTTOM*, at this stage the corresponding model layer MDOs are limited by flat horizontal sufaces. These fields can be edited later.

Once each model layer is created, the corresponding MDOs are stored within the model DB with the names assigned, and loaded in the Layers Panel.

The Attribute Tables of such MDOs contain several records, according to the number of grid cells, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *BORDER*: integer value which allows to distinguish between a border cell (i.e., a cell along the border of the domain - *BORDER=1*) and an internal one (*BORDER=0*);
- *ACTIVE*: integer value corresponding to the *IBOUND* flag in *MODFLOW* (Harbaugh, 2005), which allows to distinguish among active variable-head cells (i.e., where the hydraulic head will be calculated at each iteration - *ACTIVE=1*), non-active cells (i.e., where the groundwater flow equation is not solved - *ACTIVE=0*) and active specified-head cells (i.e., where the hydraulic head is specified and will not vary throughout the simulation - *ACTIVE=-1*);
- *TOP*: height of the top surface of the model layer at each cell [L];
- *BOTTOM*: height of the bottom surface of the model layer at each cell [L];
- *THICKNESS*: thickness of the model layer, calculated as *TOP* minus *BOTTOM* at each cell [L];

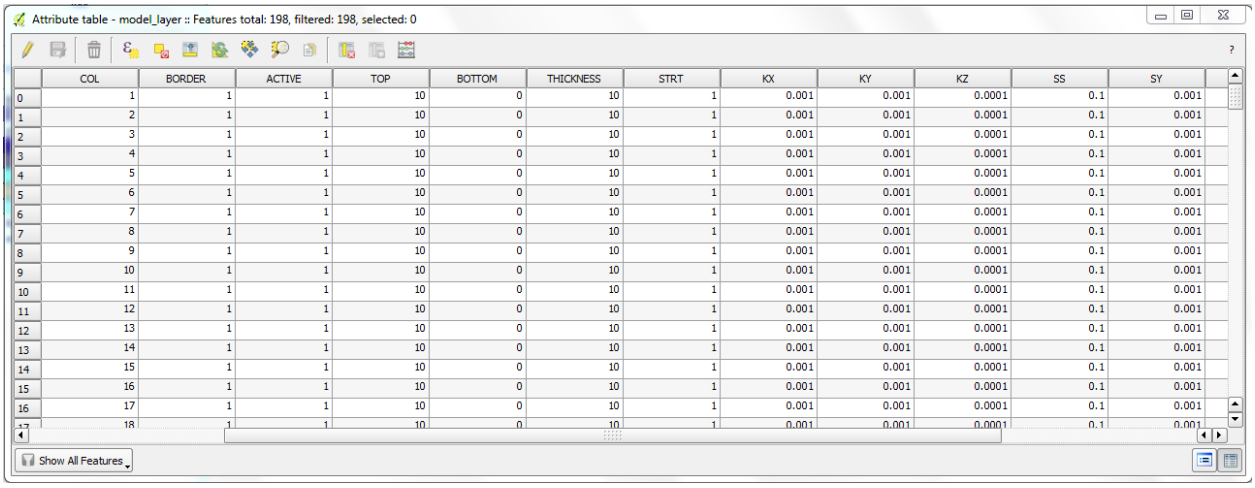
- *STRT*: hydraulic head assigned at each cell at the beginning of the simulation (initial condition) [L];
- *KX*: hydraulic conductivity along the x direction [L/T];
- *KY*: hydraulic conductivity along the y direction [L/T];
- *KZ*: hydraulic conductivity along the z direction [L/T];
- *SS*: specific storage [L^{-1}];
- *SY*: specific yield;
- *NT*: total porosity;
- *NE*: effective porosity;
- *WETDRY*: flag indicating if the cell can be re-wetted thanks to water exchange with the cell below it (*WETDRY<0*), or with the cell below it and the four horizontally adjacent cells (*WETDRY>0*). *WETDRY* is *0* if the cell cannot be re-wetted.

Note: All the dimension quantities must be expressed in model units and elevations are referred to a reference datum.

Note: *STRT* should be at least above the *BOTTOM* surface of the model layer to avoid that cells are dry at the beginning of the simulation.

Note: *NT* and *NE* are not used in groundwater flow simulations, but will be used in solute transport simulations (Volume 2).

The fields *ACTIVE*, *TOP*, *BOTTOM*, *STRT*, *KX*, *KY*, *KZ*, *SS*, *SY*, *NT*, *NE* and *WETDRY* are filled with default values or according to what defined during the creation of the corresponding MDO. They can be edited using standard *QGIS* tools and procedures described in Chapter 5.



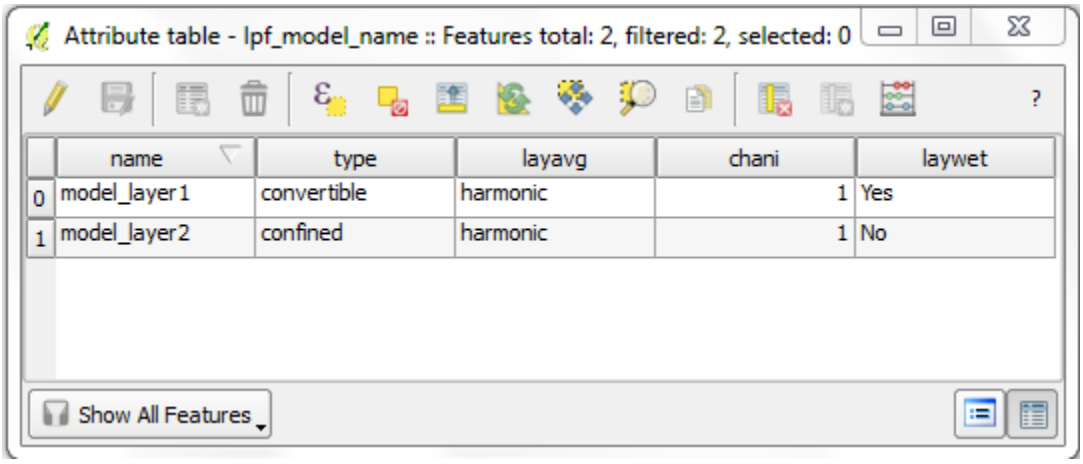
	COL	BORDER	ACTIVE	TOP	BOTTOM	THICKNESS	STRT	KX	KY	KZ	SS	SY
0	1	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
1	2	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
2	3	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
3	4	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
4	5	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
5	6	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
6	7	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
7	8	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
8	9	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
9	10	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
10	11	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
11	12	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
12	13	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
13	14	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
14	15	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
15	16	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
16	17	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001
17	18	1	1	10	0	10	1	0.001	0.001	0.0001	0.1	0.001

After the first model layer MDO is created, a table named *lpf_model_name* is created, stored within the model DB and loaded in the Layers Panel. It updates as soon as a new model layer MDO is created. Such table may contain several records, according to the number of model layer MDOs created, and the following fields:

- *name*: name of each model layer MDO;
- *type*: *Layer Type* (*confined* or *convertible*) defined during the creation of the corresponding MDO;

- *layavg*: method used to calculate the horizontal *Interblock Transmissivity (LAYAVG)* (*harmonic*, *logarithmic* or *arithmetic-mean*), defined during the creation of the corresponding MDO;
- *chani*: integer value grater than 0, which defines the horizontal anisotropy for the corresponding model layer;
- *laywet*: flag indicating if the *Wetting Capability (LAYWET)* is active (*Yes*) or not (*No*), according to what defined during the creation of the corresponding MDO.

All these fields are filled with default values or according to what defined during the creation of each model layer MDO, but they can be edited if needed.



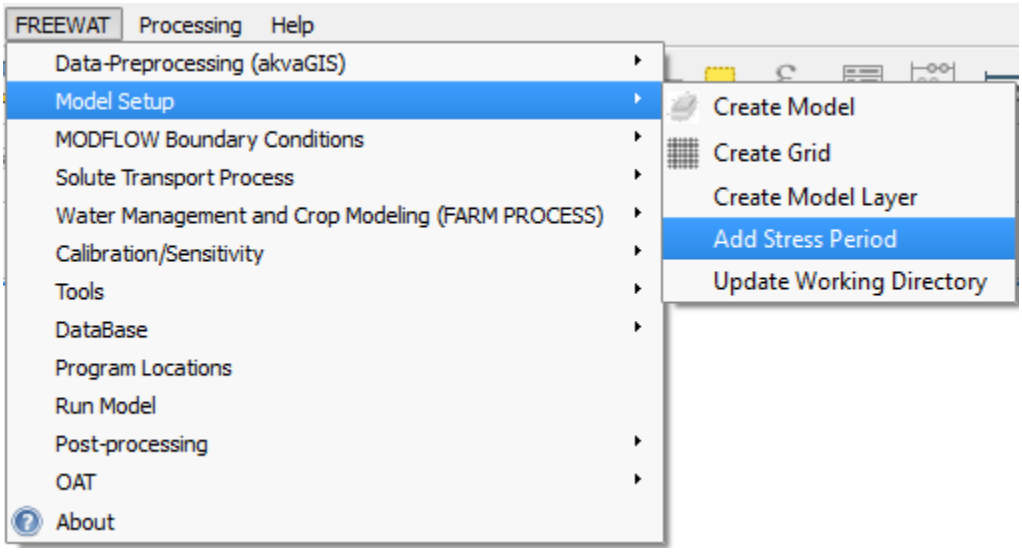
Time discretization

Time discretization in *MODFLOW* is based on *Stress Periods* (*SP*), namely time intervals during which boundary conditions and sink/source terms are constant. Each SP can be further subdivided into n *Time Steps* (*TS*), during which the solution is calculated within each cell of the domain.

The first SP of the simulation is defined when the model is created (see Chapter 3).

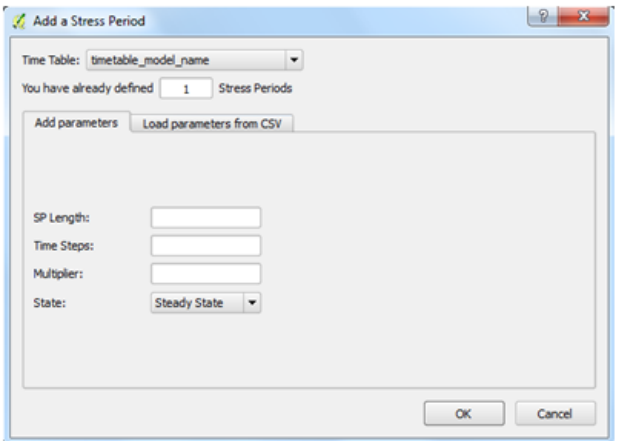
To add a SP, use the menu:

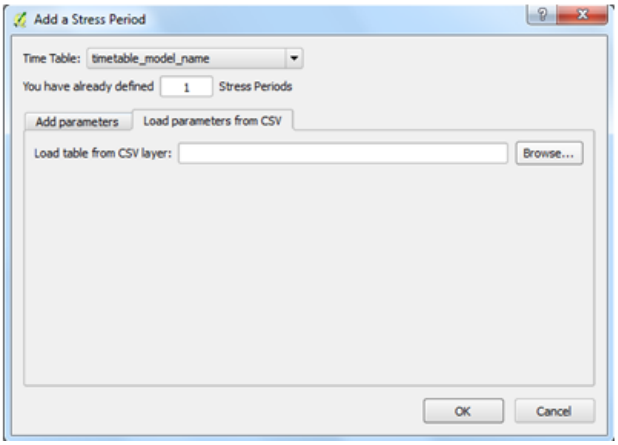
FREEWAT -> Model Setup -> Add Stress Period.



The following data are required in the **Add a Stress Period** window:

- *Time Table*: name of the time table created (see Chapter 3);
- in the *Add parameters* section:
  - *SP Length*: length of the current SP;
  - *Time Steps*: number of TS within the current SP;
  - *Multiplier*: multiplier to calculate the length of TS within the current SP;
  - *State*: two options are available for the current SP, *Steady State* or *Transient*;
- in the *Load parameters from CSV* section the path of a CSV file containing parameters for the SPs to be defined must be entered in the *Load table from a CSV layer* bar.





Note: The length of each SP must be expressed in model units.

Note: If *n* SPs have been already defined, such information is reported when adding a new SP (*You have already defined n Stress Periods*).

Note: In the CSV file required to load SPs parameters, the User must specify:

- *length*: length of each SP;
- *time_steps*: number of TS within each SP;
- *multiplier*: multiplier to calculate the length of TS within each SP;
- *state*: two options are available for each SP, *SS* for *Steady State* or *TR* for *Transient*.

The CSV file must have the following scheme:

add_sp.csv

```
1  length,time_steps,multiplier,state
2  10,1,1.0,SS
3  60,15,1.3,TR
4  180,15,1.3,TR
```

The User can also edit any SP within the time table if needed.

CHAPTER 5

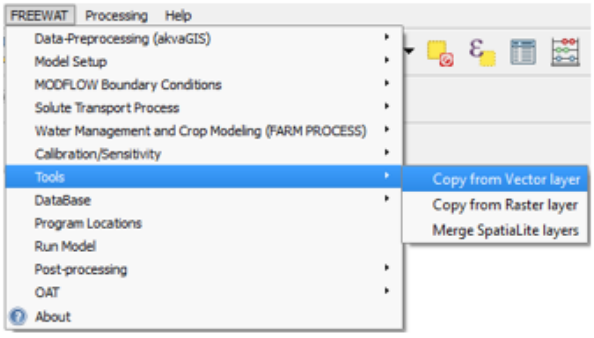
Tools for model layers parameterization

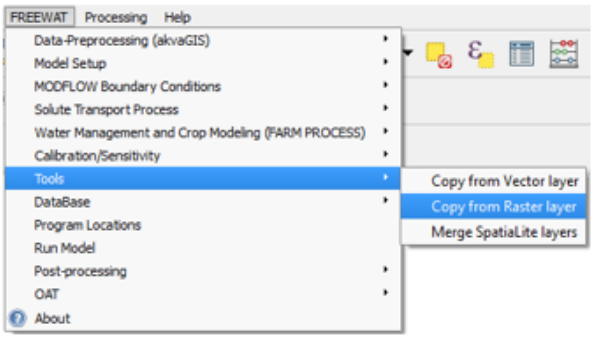
Once the model layer MDOs are created, the following data are required for each of them: the height of their top and bottom surfaces (usually corresponding to those of a hydrostratigraphic units), the *ACTIVE* flag to distinguish between active, inactive and specified-head cells, its hydrodynamic properties, the *WETDRY* flag for active cells to define if the rewetting option is active or not.

The *FREEWAT* platform allows to edit the Attribute Table of the model layer MDOs either manually and/or with the *QGIS* selection tools, or with two specific assignment methodologies. The latter can be activated by using one of the menus:

FREEWAT -> Tools -> Copy from Vector layer

FREEWAT -> Tools -> Copy from Raster layer.





Manual editing with selection tools

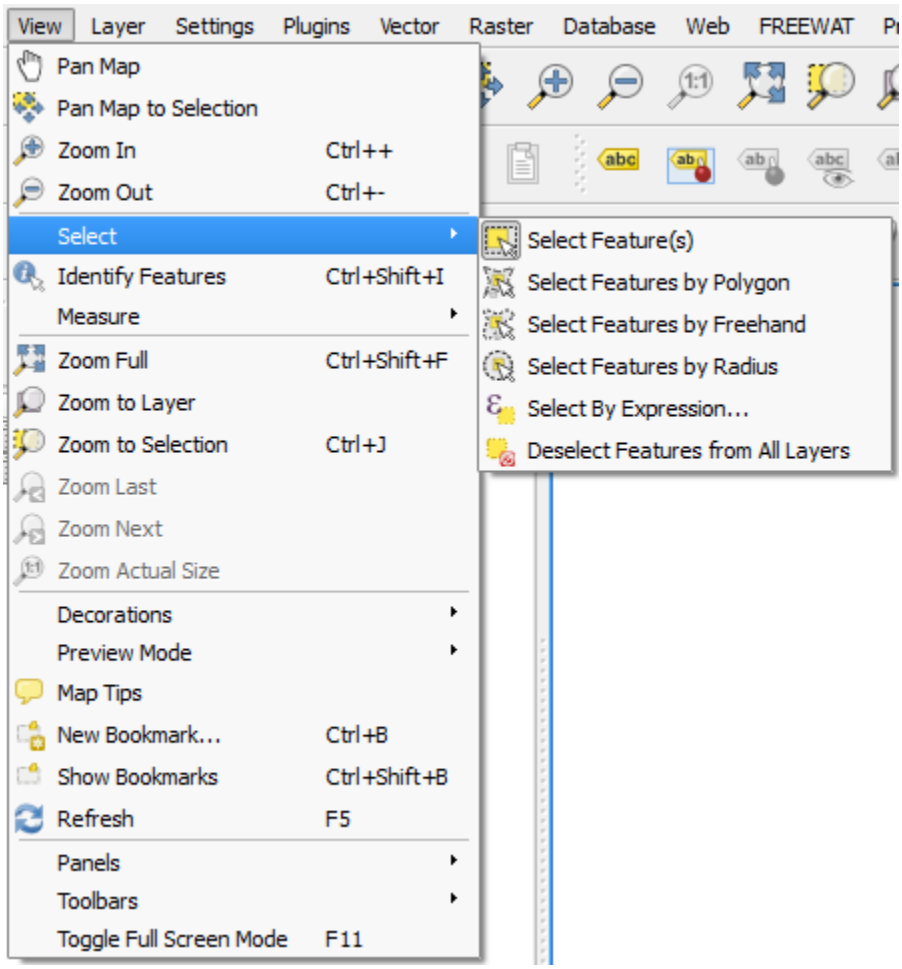
This editing methodology may use the *QGIS* tools to select data by acting on the spatial component (i.e., points, lines or polygons) or on the alphanumeric values stored within the Attribute Table of a model layer MDO. Such procedure can be applied to any parameter defined in the Attribute Table of the model layer MDO. Hereinafter, we describe how to edit the *ACTIVE* field to distinguish between active, inactive and specified-head cells.

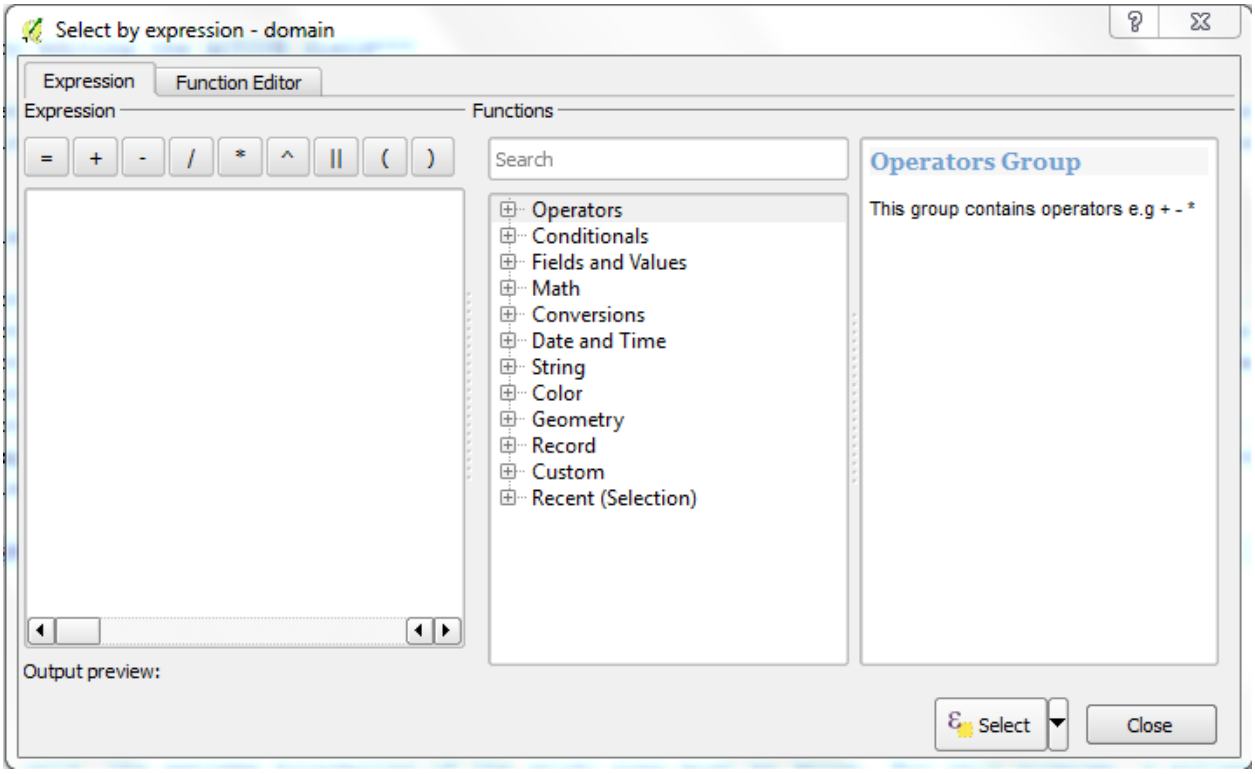
Once created the model layer MDO, *1* is assigned at each cell as a default value for the *ACTIVE* field. This means that all cells of the model grid are active. To edit such value, so defining inactive cells (*ACTIVE=0*) or specified-head cells (*ACTIVE=-1*), several *QGIS* selection tools are available using the following menu:

View -> Select.

- The *Select Feature(s)* tool allows to select cells one by one, eventually using the *Ctrl* button of the keyboard;
- the *Select Features by Polygon* tool allows to select cells intersected by a polygon, whose border is a polyline;

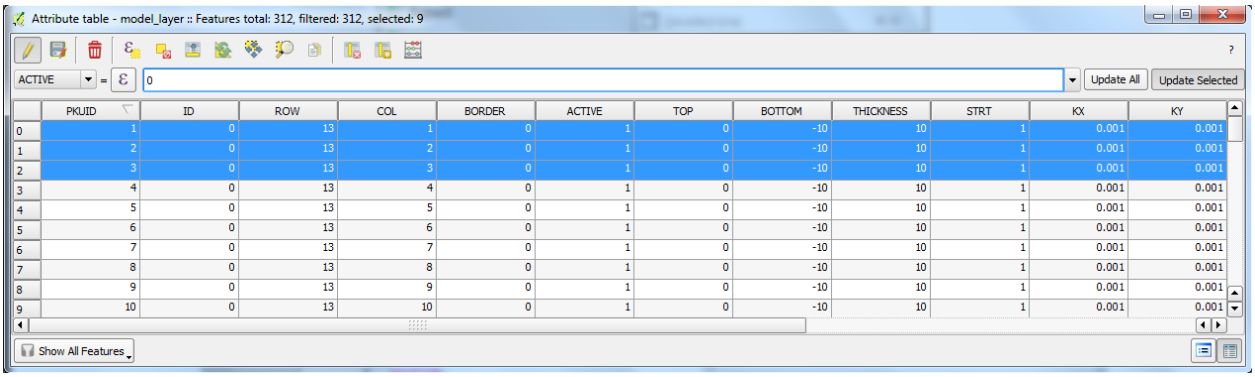
- the *Select Features by Freehand* tool allows to select cells intersected by a polygon, whose border is a curved line;
- the *Select Features by Radius* tool allows to select cells intersected by a circle;
- the *Select Features By Expression...* tool allows to select cells for which particular conditions occur: a condition is described by an expression typed in the *Expression* bar by using mathematical, logical, conditional operators and/or values from other fields within the Attribute Table of the MDO involved in the selection.



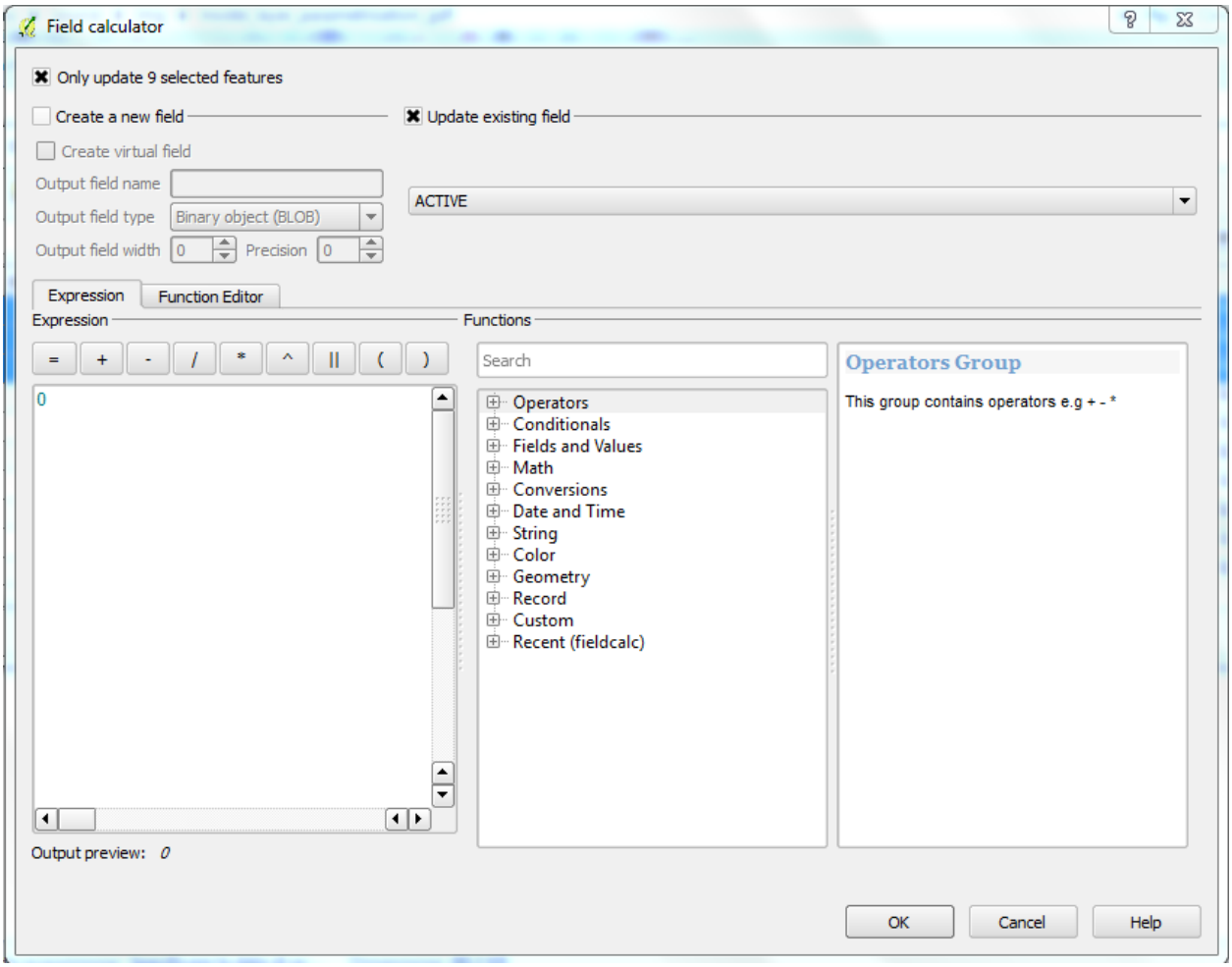


Note: To use one of the available selection tools, it is necessary to select, in the Layers Panel, the model layer MDO which is the object of the selection.

Once the cells to be edited have been selected in the Map Canvas, the corresponding records in the Attribute Table of the model layer MDO are highlighted (blue records) and the *ACTIVE* values of such cells can be edited, by activating the *Toggle editing mode* and using the expression bar or the *Field calculator*.

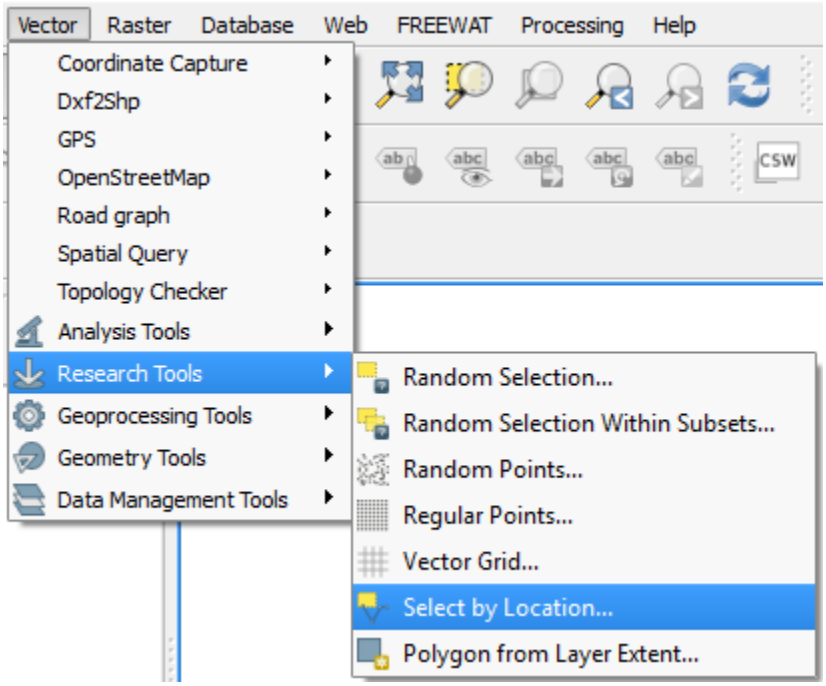


	PKUID	ID	ROW	COL	BORDER	ACTIVE	TOP	BOTTOM	THICKNESS	STRT	KX	KY
0	1	0	13	1	0	1	0	-10	10	1	0.001	0.001
1	2	0	13	2	0	1	0	-10	10	1	0.001	0.001
2	3	0	13	3	0	1	0	-10	10	1	0.001	0.001
3	4	0	13	4	0	1	0	-10	10	1	0.001	0.001
4	5	0	13	5	0	1	0	-10	10	1	0.001	0.001
5	6	0	13	6	0	1	0	-10	10	1	0.001	0.001
6	7	0	13	7	0	1	0	-10	10	1	0.001	0.001
7	8	0	13	8	0	1	0	-10	10	1	0.001	0.001
8	9	0	13	9	0	1	0	-10	10	1	0.001	0.001
9	10	0	13	10	0	1	0	-10	10	1	0.001	0.001



Among the *QGIS* selection tools, it is worth mentioning also the *Select by location* tool. It can be activated using the following menu:

Vector -> Research Tools -> Select by Location....

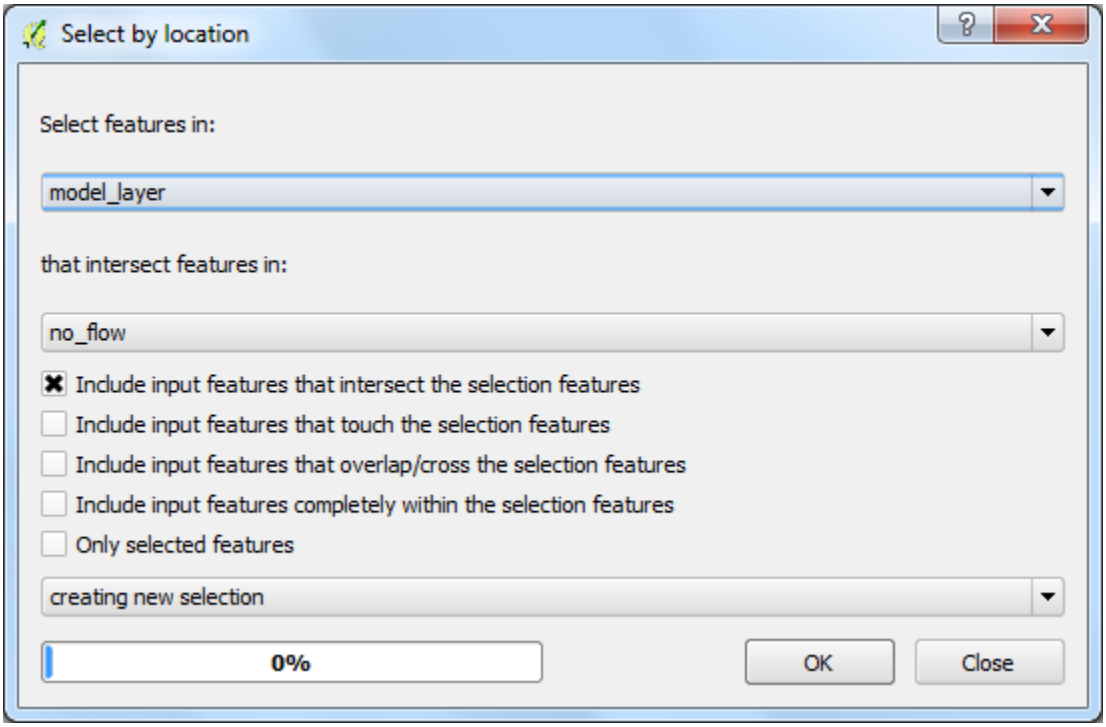


As an example, if a polygon shapefile with the extent of the inactive domain is available, it would be useful to select all grid cells of a model layer which are intersected by this polygon, in order to edit their *ACTIVE* values. In this case, the target of selection (*Select features in*) is the involved model layer and its grid cells will be selected according to the extent of the available polygon shapefile (*that intersect features in*). Several options are available to perform such selection:

- *Include input features that intersect the selection features*;
- *Include input features that touch the selection features*;
- *Include input features that overlap/cross the selection features*;
- *Include input features completely within the selection features*;
- *Only selected features*.

The drop-down menu at the bottom allows to:

- create a new selection (*creating new selection*);
- add a new selection to the current one (*adding to current selection*);
- remove a selection from the current one (*removing from current selection*).



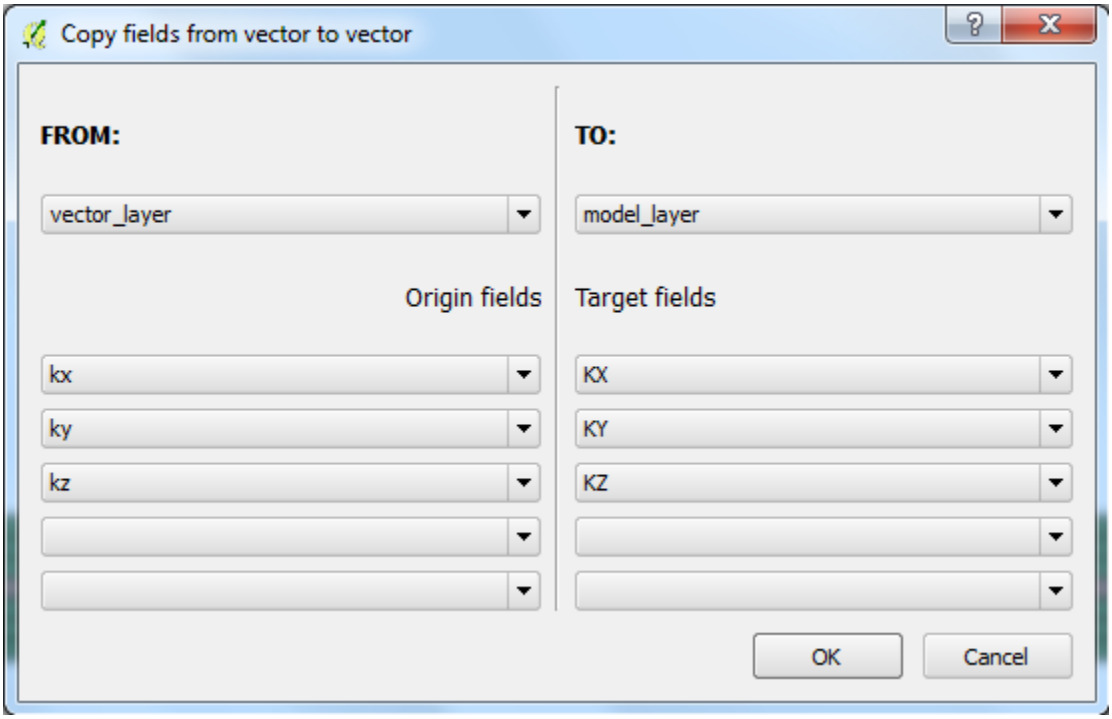
Note: Further details about the selection tools and the use of the *Toggle editing mode* can be found in the QGIS training manual.

Note: Once editing is done, remember to use *Deselect Features from All Layers*.

Copy from vector layer

If a polygon shapefile containing, e.g., the values of the hydraulic conductivity along each Cartesian direction is available, such values can be used to assign *KX*, *KY* and *KZ* at each cell of the model layer MDO. The algorithm checks for a correspondence between each node of the grid cells and the polygons defined within the shapefile: if a node is inside a certain polygon, hydraulic conductivity values along x, y and z directions of that polygon are assigned to *KX*, *KY* and *KZ* within the corresponding cell. The interface requires selecting the origin and target vector layers and the fields involved in the copy procedure. Furthermore, it is possible to copy a maximum of five parameters at once.

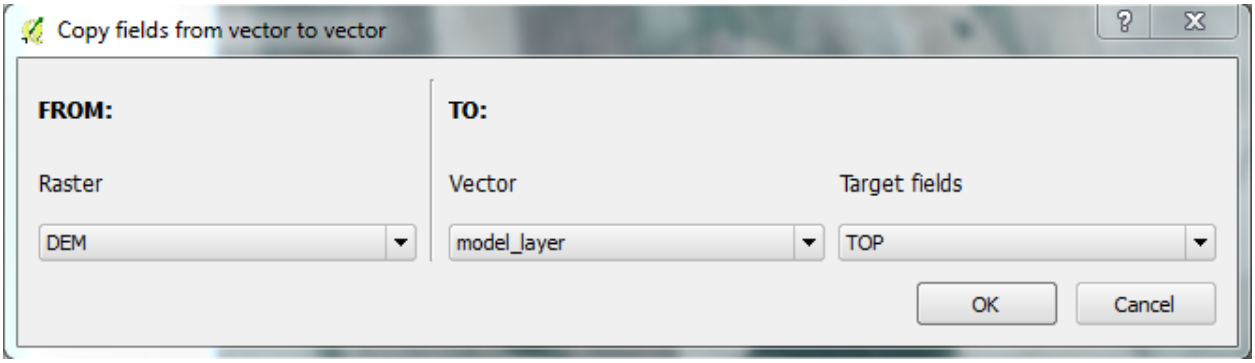
Hereinafter, an example about how to assign values to *KX*, *KY* and *KZ*, by using the *Copy from Vector layer* tool, is provided.



Copy from raster layer

If a raster file, e.g., the Digital Elevation Model (DEM) is available, it can be used to assign *TOP* values at each cell of the model layer MDO. The interface requires selecting the origin raster file, the target vector layer and the field to be updated.

Hereinafter, an example about how to assign values to *TOP* surface, by using the *Copy from Raster layer* tool, is provided.



Note: The origin raster layer must have at least the same extension as the model domain, in order to assign features at each node of the grid. Furthermore, if the origin raster layer has a finer spatial discretization than the model grid, the average value, calculated involving raster cells matching a single grid cell, is assigned at each node of the coarse scale grid. On the other hand, if the model grid has a finer spatial discretization than the origin raster layer, the same value will be assigned at grid cells matching a single raster cell.

CHAPTER 6

Implementing processes to be simulated: boundary conditions and source/sink terms

Once defined the geometry of the domain and the hydrodynamic parameterization of each model layer, boundary conditions and source/sink terms must be set, according to the conceptual model. This means expressing, with proper mathematical formalism, processes involved in the hydrological cycle. For the conceptualization of most of these processes, the reader can refer to the MODFLOW online guide, section *Ground-Water Flow Processes -> Boundary Condition Packages*.

In *FREEWAT*, the following kinds of boundary conditions can be defined: time-variant specified head, specified-flux, head-dependent flux.

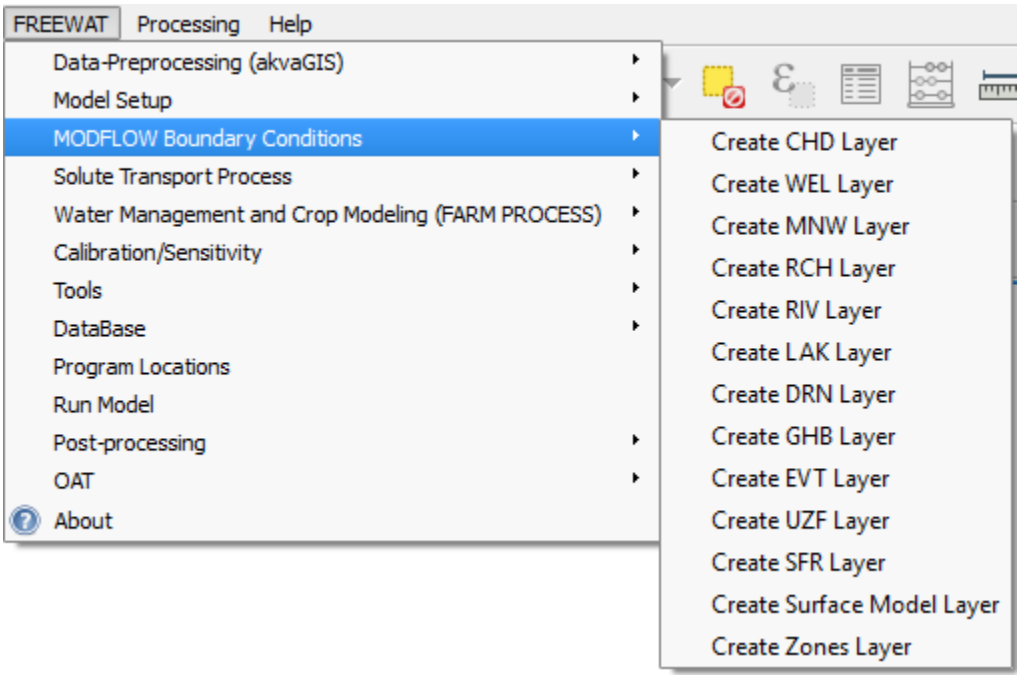
As stated in Chapter 2, in *FREEWAT* implementing each process requires translating a GIS layer into an MDO and then into a *MODFLOW* input file. Such procedure includes two or three among the following steps:

1. loading the GIS layer;
2. translating the GIS layer into an MDO;
3. generating the corresponding *MODFLOW* input file.

Note: As described in Chapter 7, the last step is automatically performed before the run procedure starts, provided that the corresponding MDO has been defined.

Boundary Condition Packages can be activated through the following menu:

FREEWAT -> MODFLOW Boundary Conditions.



Note: Once created an MDO through this menu, it will be saved in the DB and loaded in the LP with a specific extension (e.g., *_chd* for an MDO related to the CHD Package). Such extension must not be changed in the LP and neither in the DB, as the related MDO will be filtered in the **Run Model** window according to such extension.

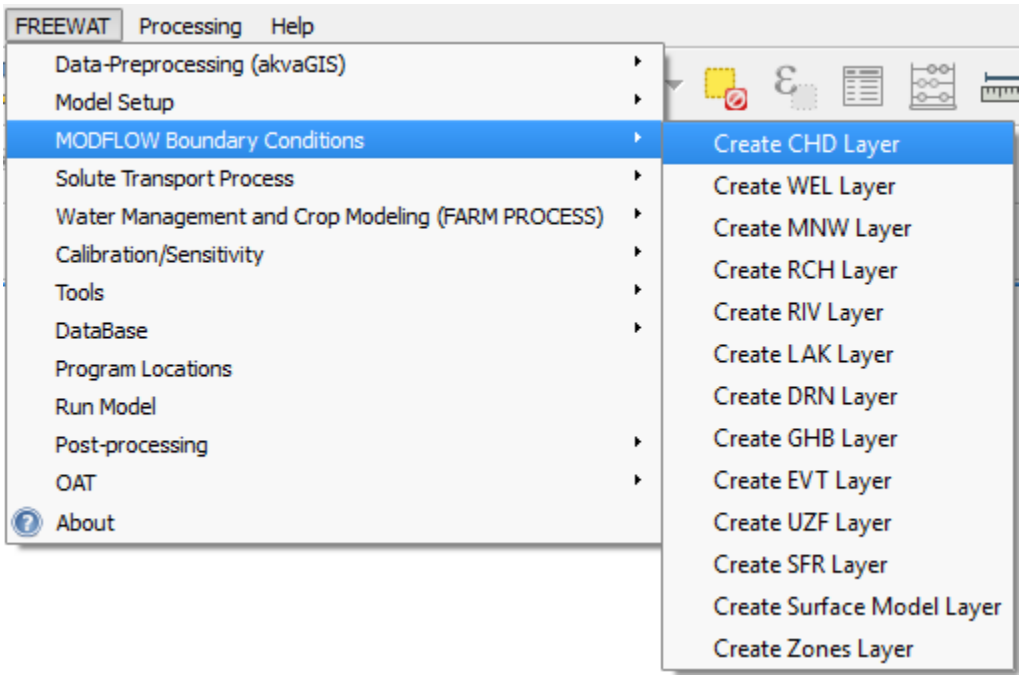
Time Variant Specified Head - CHD

MODFLOW CHD Package allows to simulate a specified-head boundary condition.

Activating this Package requires selecting cells from the grid MDO to which such boundary condition has to be assigned. To achieve this purpose, the *QGIS* selection tools presented in Chapter 5 can be used.

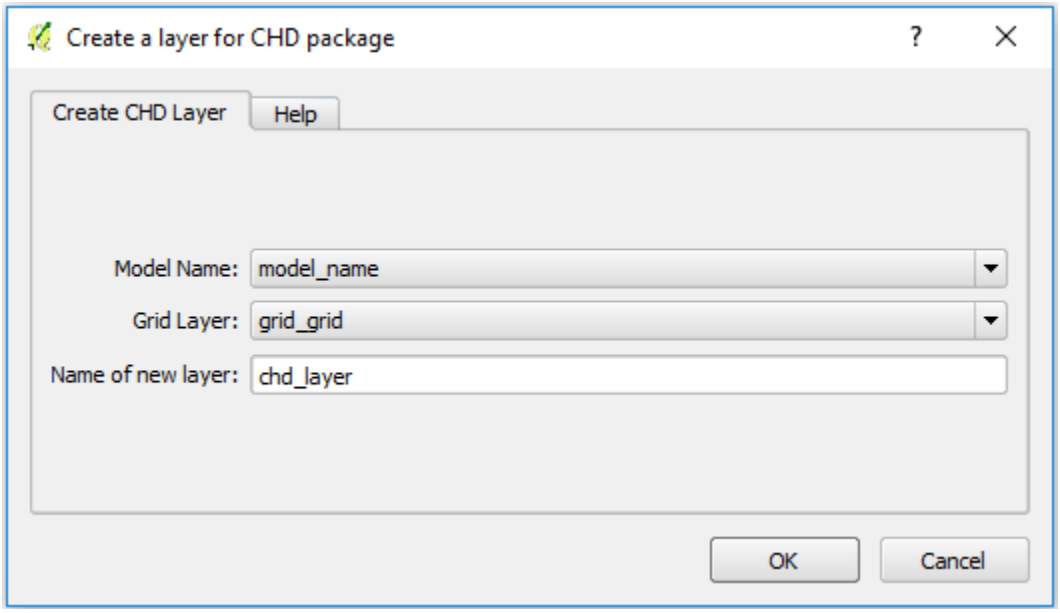
To activate the *CHD Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create CHD Layer.



The following data are required in the **Create a layer for CHD package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Name of new layer*: name of the chd MDO which has to be created.



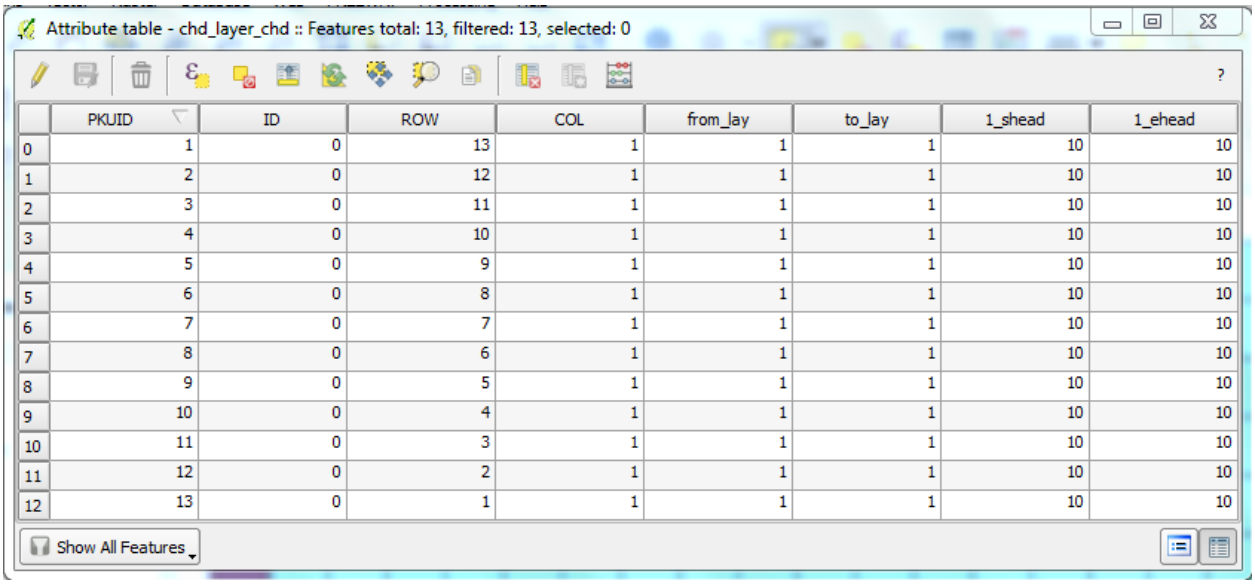
A new MDO, named *chd_layer_chd*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);

- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *from_lay*: number of the uppermost layer where the boundary condition must be assigned;
- *to_lay*: number of the deepest layer where the boundary condition must be assigned;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *n_shead*: specified head [L] at the beginning of the *n*-th SP;
  - *n_ehead*: specified head [L] at the end of the *n*-th SP.

The fields *from_lay*, *to_lay*, *n_shead* and *n_ehead* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5.



	PKUID	ID	ROW	COL	from_lay	to_lay	1_shead	1_ehead
0	1	0	13	1	1	1	10	10
1	2	0	12	1	1	1	10	10
2	3	0	11	1	1	1	10	10
3	4	0	10	1	1	1	10	10
4	5	0	9	1	1	1	10	10
5	6	0	8	1	1	1	10	10
6	7	0	7	1	1	1	10	10
7	8	0	6	1	1	1	10	10
8	9	0	5	1	1	1	10	10
9	10	0	4	1	1	1	10	10
10	11	0	3	1	1	1	10	10
11	12	0	2	1	1	1	10	10
12	13	0	1	1	1	1	10	10

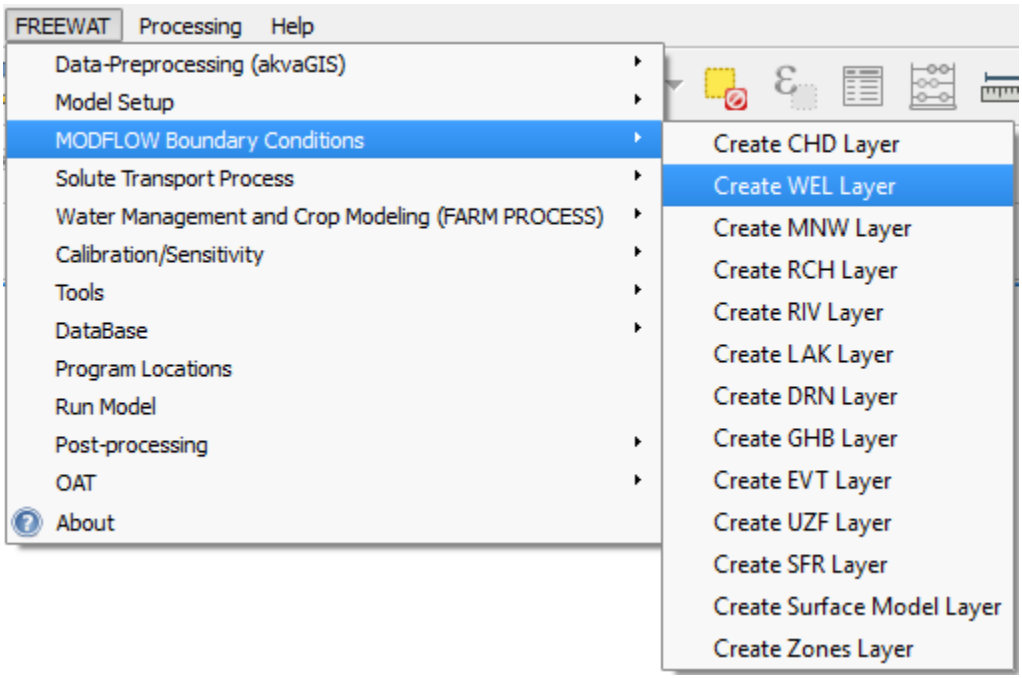
Well - WEL (specified-flux)

MODFLOW WEL Package allows to simulate recharge to the aquifer or extraction of groundwater, defining a specified positive or negative flux, respectively, to individual cells.

Activating this Package requires prior processing of a point shapefile, containing the location of recharge/pumping wells within the study area. Once the point shapefile is loaded in the Layers Panel, cells intersected by these points must be selected from the grid MDO. To achieve this purpose, the *QGIS* selection tools presented in Chapter 5 can be used.

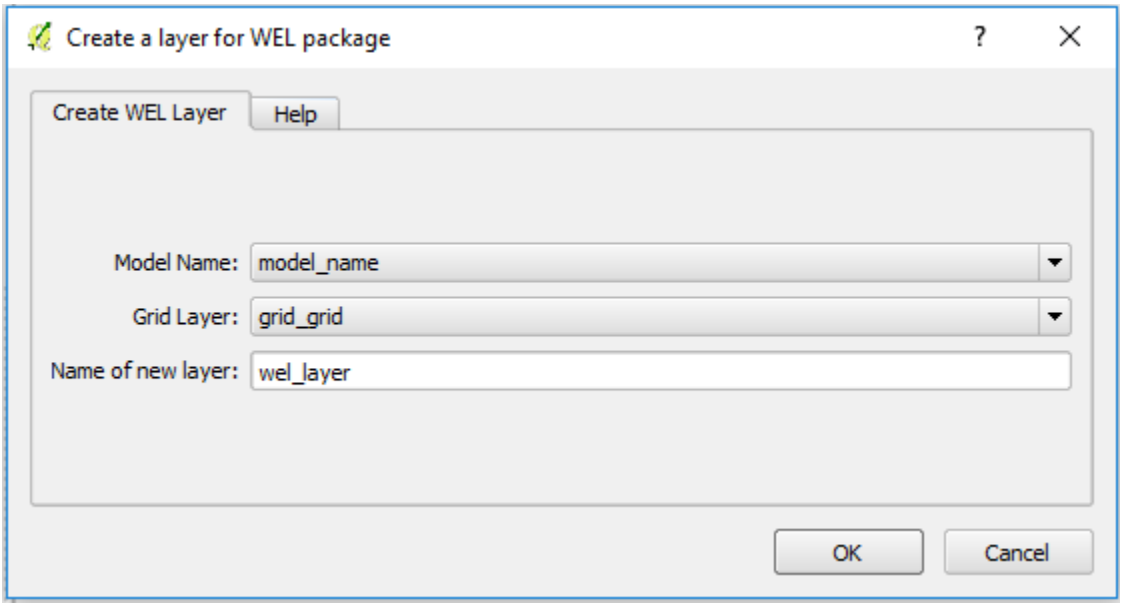
To activate the *WEL Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create WEL Layer.



The following data are required in the **Create a layer for WEL package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Name of new layer*: name of the wel MDO which has to be created.



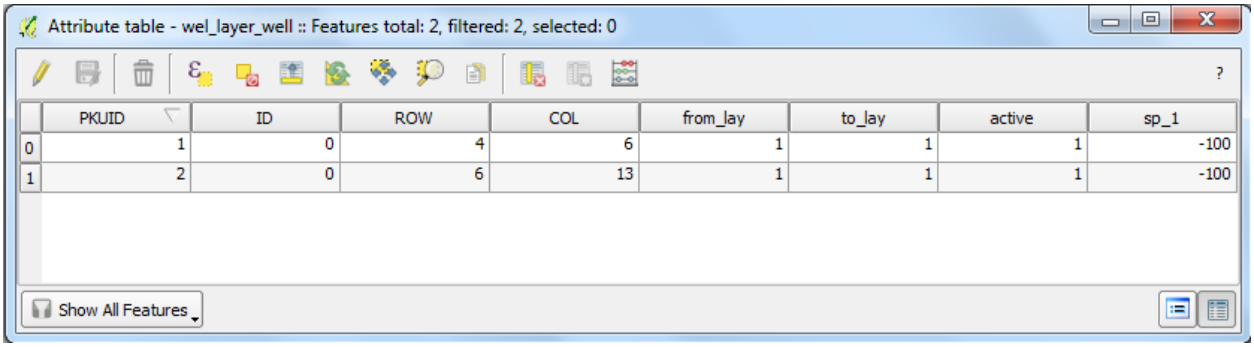
A new MDO, named *wel_layer_well*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);

- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *from_lay*: number of the uppermost layer where the boundary condition must be assigned;
- *to_lay*: number of the deepest layer where the boundary condition must be assigned;
- *active*: integer flag to activate (*active=1*) or not (*active=0*) the corresponding well during the simulation (not yet implemented in the current version);
- the following field is repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *sp_n*: specified positive/negative flux $[L^3/T]$ during the *n*-th SP.

The fields *from_lay*, *to_lay*, *active* and *sp_n* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5.



	PKUID	ID	ROW	COL	from_lay	to_lay	active	sp_1
0	1	0	4	6	1	1	1	-100
1	2	0	6	13	1	1	1	-100

Note: If the recharge/pumping flow is assigned to more than one model layer, the specified flux is equally distributed among the model layers involved.

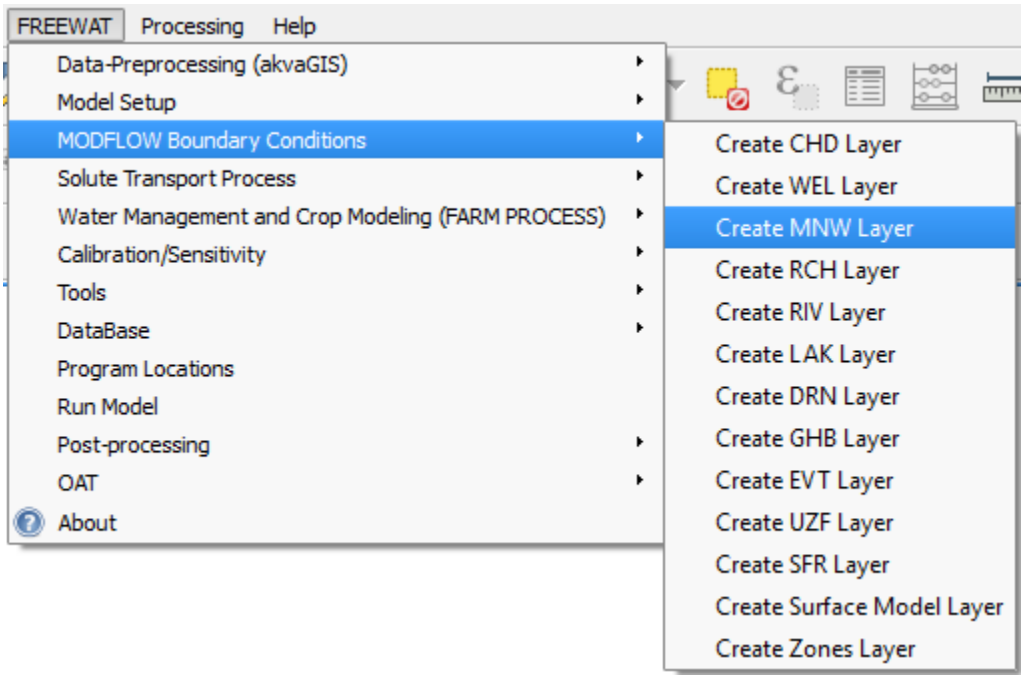
Multi-Node Well - MNW (head-dependent flux)

MODFLOW MNW Package allows to simulate screened wells, that are connected to more than one node of the model grid.

Activating this Package requires prior processing of a point shapefile, containing the location of multi-node wells within the study area. Once the point shapefile is loaded in the Layers Panel, cells intersected by these points must be selected from the grid MDO. To achieve this purpose, the *QGIS* selection tools presented in Chapter 5 can be used.

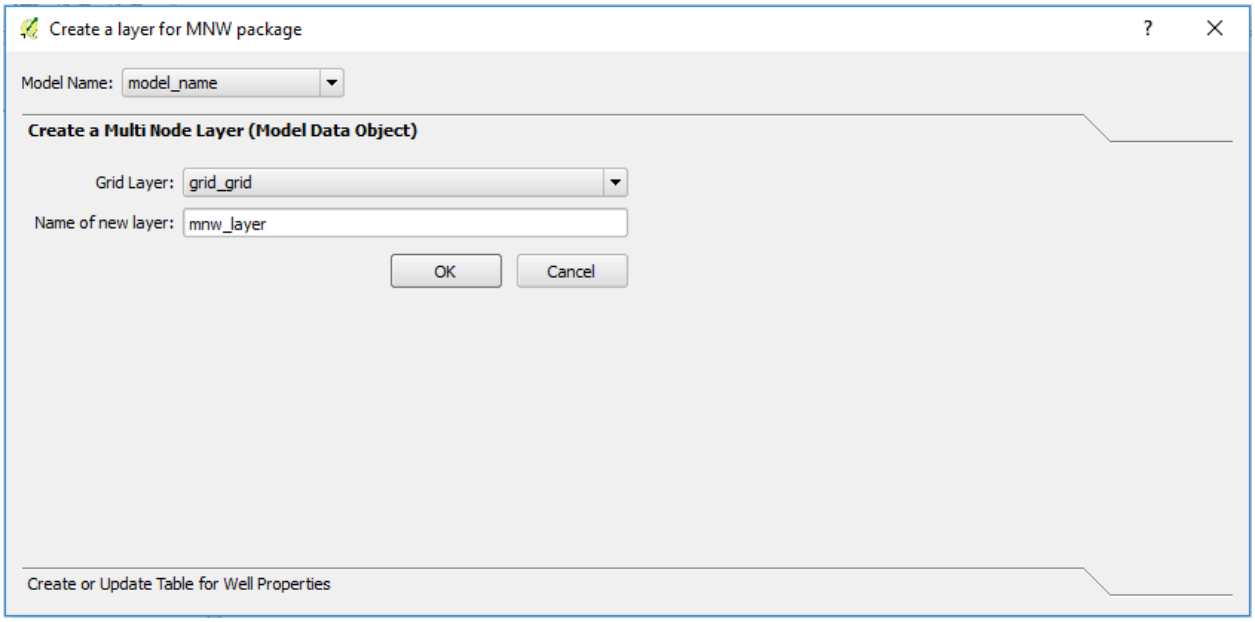
To activate the *MNW Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create MNW Layer.



The following data are required in the **Create a layer for MNW package** window:

- *Model Name*: name of the hydrological model;
- in the *Create a Multi Node Layer (Model Data Object)* section:
  - *Grid Layer*: grid MDO;
  - *Name of new layer*: name of the mnw MDO which has to be created.



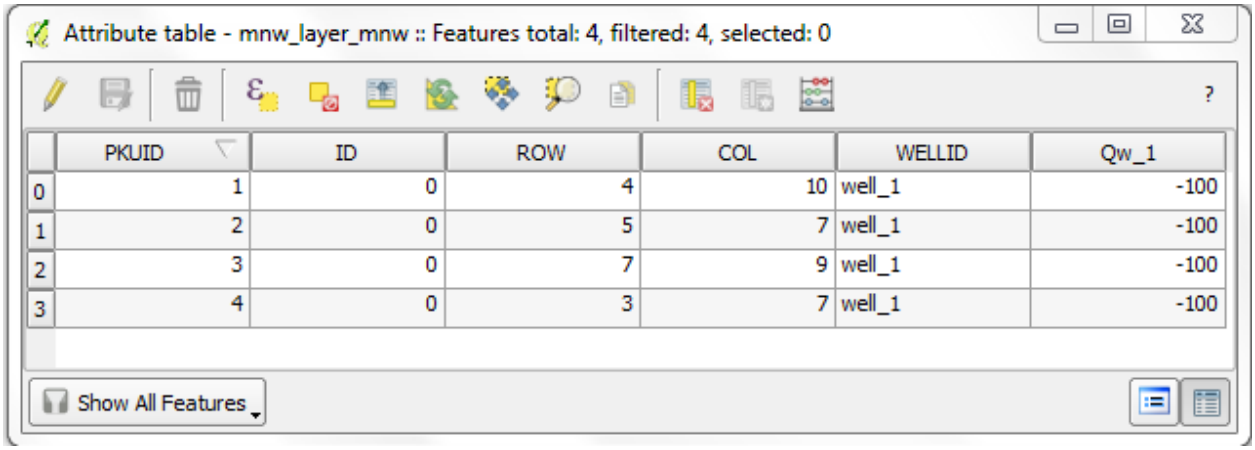
A new MDO, named *mnw_layer_mnw*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- *PKUID*: database primary key (it must not be modified);

- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *WELLID*: name assigned to each multi-node well;
- the following field is repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *Qw_n*: actual volumetric pumping rate (negative for withdrawal or positive for injection) at each well $[L^3/T]$ during the *n*-th SP.

The fields *WELLID* and *Qw_n* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5.



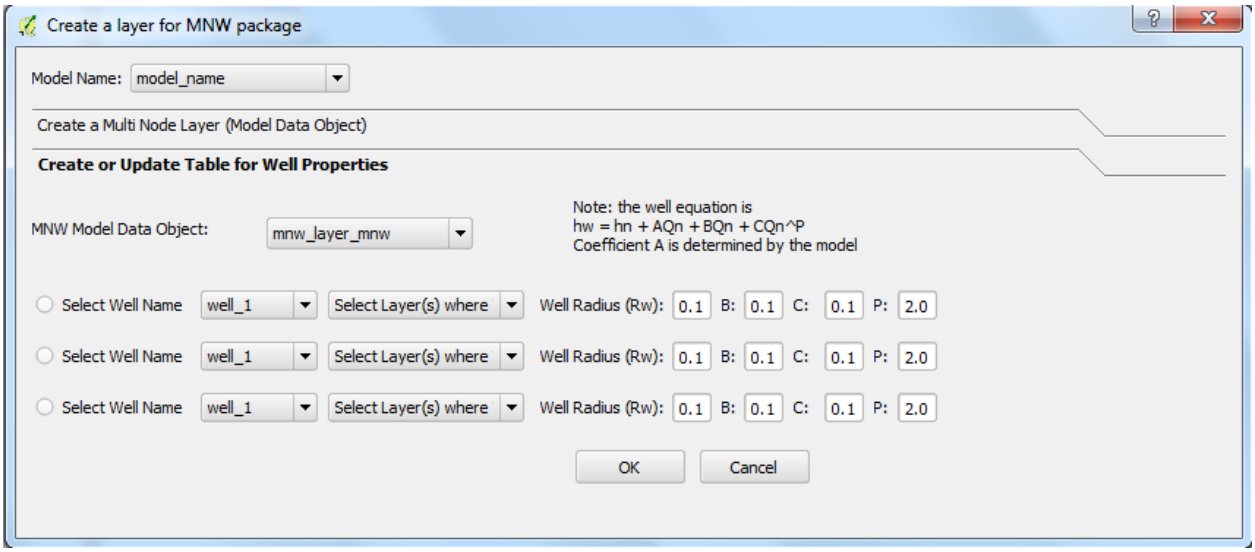
	PKUID	ID	ROW	COL	WELLID	Qw_1
0	1	0	4	10	well_1	-100
1	2	0	5	7	well_1	-100
2	3	0	7	9	well_1	-100
3	4	0	3	7	well_1	-100

Once the mnw MDO is created, the **Create a layer for MNW Package** window must be opened again by using the menu:

FREEWAT -> MODFLOW Boundary Conditions -> Create MNW Layer.

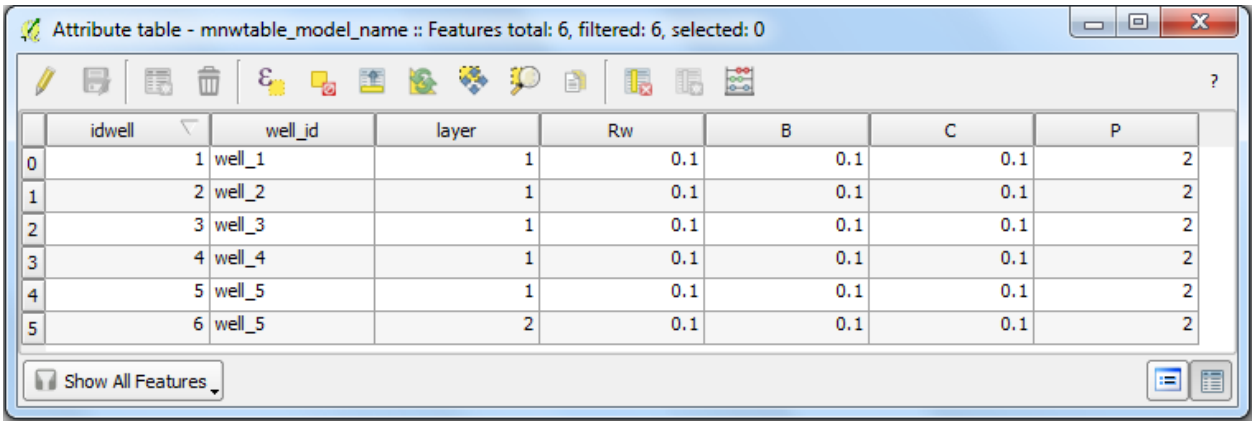
In the *Create or Update Table for Well Properties* section, the following data are required for each multi-node well:

- *MNW Model Data Object*: name of the mnw MDO created;
- for each multi-node well:
  - the *WELLID* must be selected from the drop-dowm menu near to *Select Well Name*;
  - the number of model layer(s) to which the multi-node well is screened must be checked in the drop-dowm menu *Select Layer(s) where Well is active*;
  - *Well Radius (Rw)* is the radius of the well;
  - *B*, *C* and *P* are coefficients used in the general well-loss equation (for details the reader is referred to the *MNW2* manual, Konikow et al., 2009).



A table named *mnwtable_model_name* is created, stored in the model DB and loaded in the Layers Panel. It may contain several records, according to the number of multi-node wells, and the following fields:

- *idwell*: progressive ID of each record;
- *well_id*: name assigned to each multi-node well as assigned in the *WELLID* when creating the mnw MDO;
- *layer*: number of the model layer(s) to which the multi-node well is screened; if the multi-node well is screened to more than one model layer, multiple lines are repeated for the same *well_id*;
- *Rw*: radius of the multi-node well as assigned in the *Well Radius (Rw)* when editing the *Create or Update Table for Well Properties* section;
- *B*, *C* and *P* as defined when editing the *Create or Update Table for Well Properties* section.



	idwell	well_id	layer	Rw	B	C	P
0	1	well_1	1	0.1	0.1	0.1	2
1	2	well_2	1	0.1	0.1	0.1	2
2	3	well_3	1	0.1	0.1	0.1	2
3	4	well_4	1	0.1	0.1	0.1	2
4	5	well_5	1	0.1	0.1	0.1	2
5	6	well_5	2	0.1	0.1	0.1	2

Note: In the *Create or Update Table for Well Properties* section, it is possible to define *Well Radius (Rw)* and coefficients *B*, *C* and *P* for a maximum of three multi-node wells at once. Anyway, the *mnwtable_model_name* automatically updates when parameters are defined for more wells.

Limitations

The *MODFLOW* flag *LOSSTYPE* to determine the user-specified model for well loss is set to *GENERAL*, i.e., head loss is defined by the following equation: $h_{WELL} = h_n + AQ_n + BQ_n + CQ_n^P$ (for details the reader is referred to the

MNW2 manual, Konikow et al., 2009).

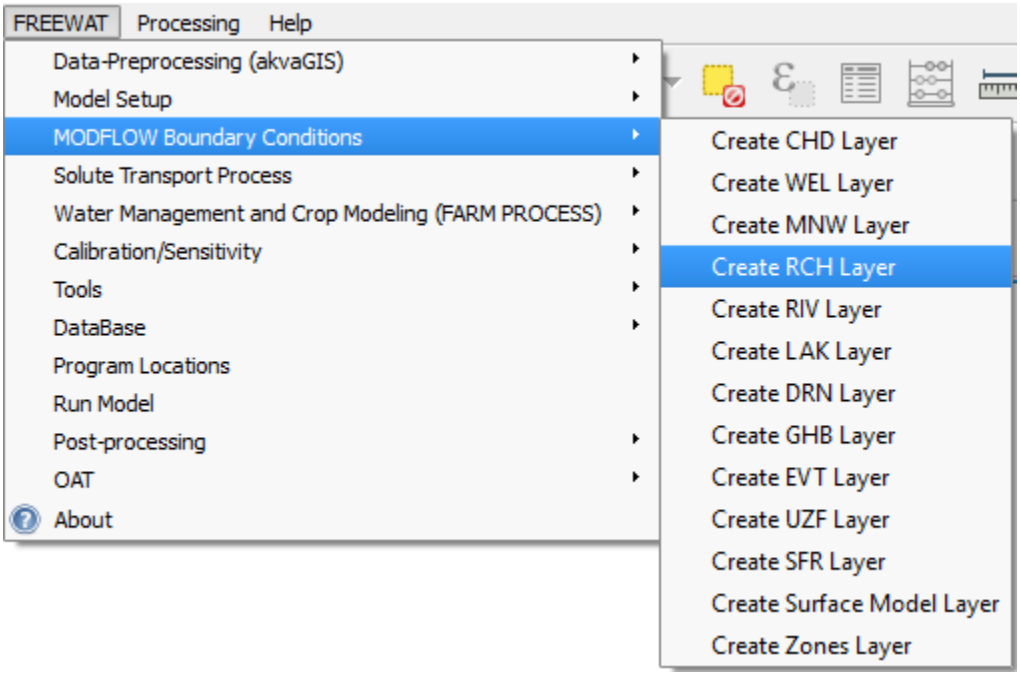
Recharge - RCH (specified-flux)

MODFLOW RCH Package allows to simulate areally-distributed recharge.

Activating this Package does not require prior processing of a polygon shapefile, as this condition can be applied to all grid cells and it is possible to deactivate recharge at some grid cells, by using *QGIS* selection and editing tools described in Chapter 5.

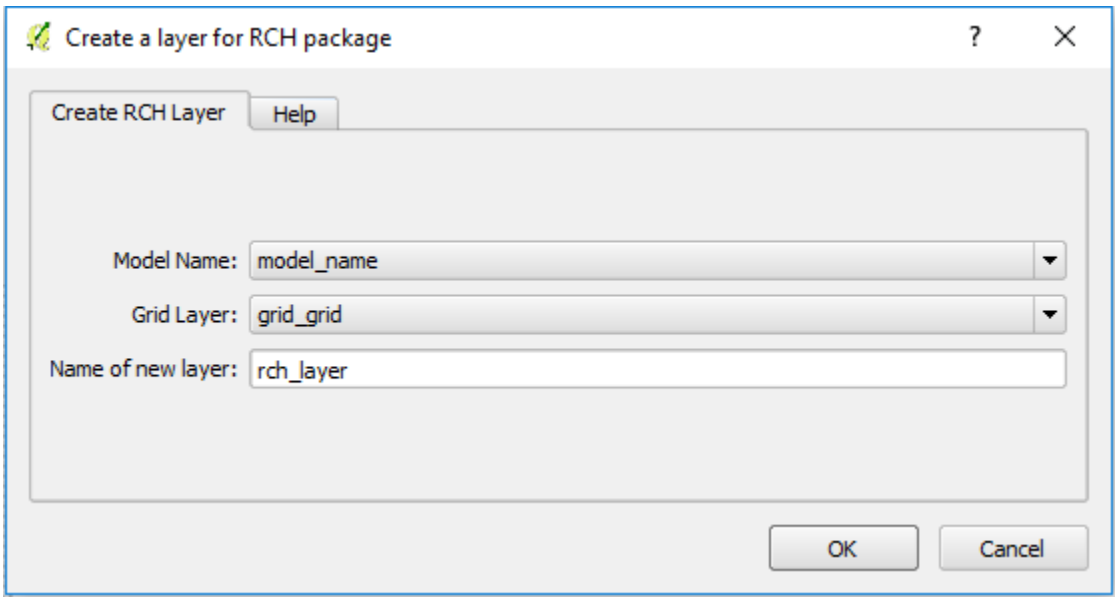
To activate the *RCH Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create RCH Layer.



The following data are required in the **Create a layer for RCH package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Name of new layer*: name of the rch MDO which has to be created.

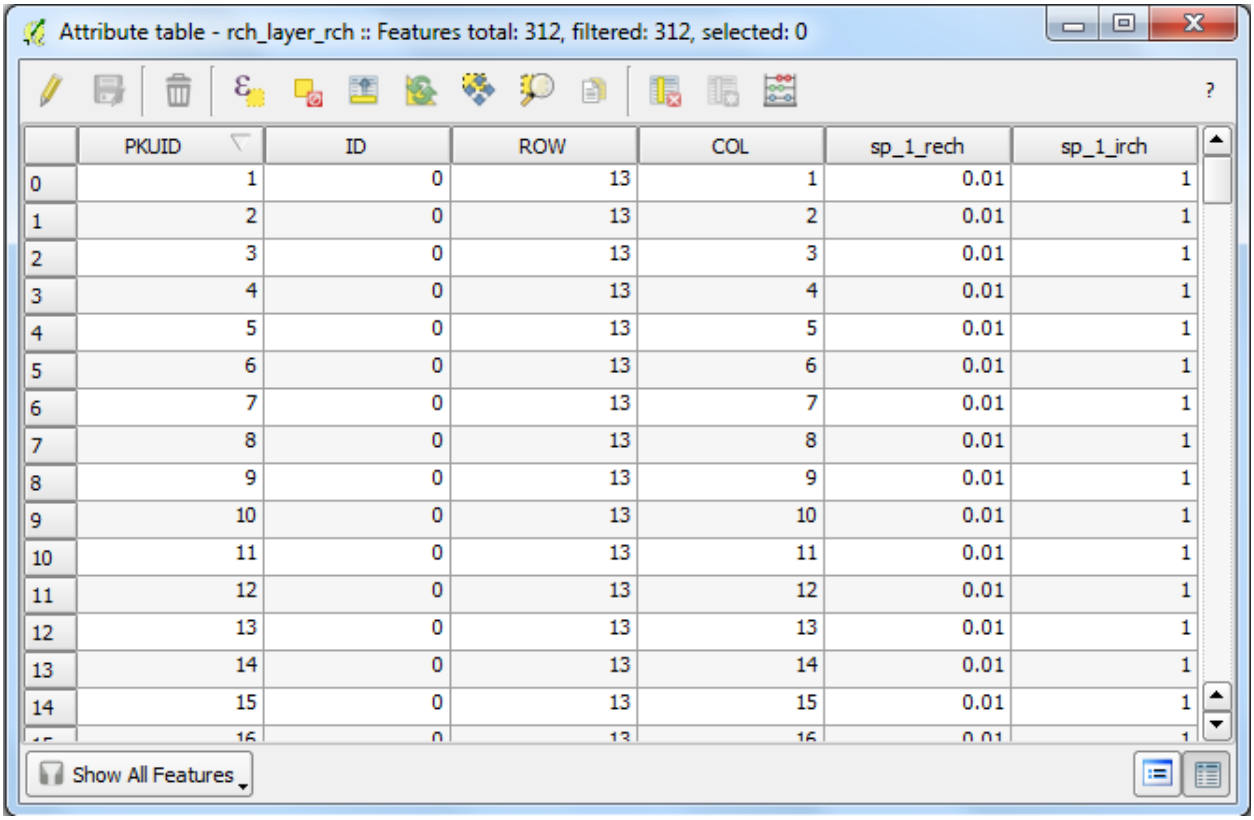


A new MDO, named *rch_layer_rch*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *sp_n_rech*: specified flux [L/T] during the *n*-th SP;
  - *sp_n_irch*: number of the model layer where the recharge will be applied during the *n*-th SP.

The fields *sp_n_rech* and *sp_n_irch* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5.



	PKUID	ID	ROW	COL	sp_1_rech	sp_1_irch
0	1	0	13	1	0.01	1
1	2	0	13	2	0.01	1
2	3	0	13	3	0.01	1
3	4	0	13	4	0.01	1
4	5	0	13	5	0.01	1
5	6	0	13	6	0.01	1
6	7	0	13	7	0.01	1
7	8	0	13	8	0.01	1
8	9	0	13	9	0.01	1
9	10	0	13	10	0.01	1
10	11	0	13	11	0.01	1
11	12	0	13	12	0.01	1
12	13	0	13	13	0.01	1
13	14	0	13	14	0.01	1
14	15	0	13	15	0.01	1
15	16	0	13	16	0.01	1

Note: Notice that *sp_n_rech* is actually a specified rate, rather than a flux. This is because recharge is usually used to simulate rainfall infiltration and rainfall is expressed as a rate [L/T]. Such specified rate is then automatically multiplied by the area of the grid cell [L^2] to get a specified flux [L^3/T].

Note: To deactivate recharge at some cells during SP *n*, it is necessary to select the involved cells and set *sp_n_rech* to *0*.

Note: Editing *sp_n_irch* is only required when recharge has to be applied to a grid cell other than the one belonging to model layer 1 or the uppermost active one in the vertical column. More details will be provided in Chapter 7.

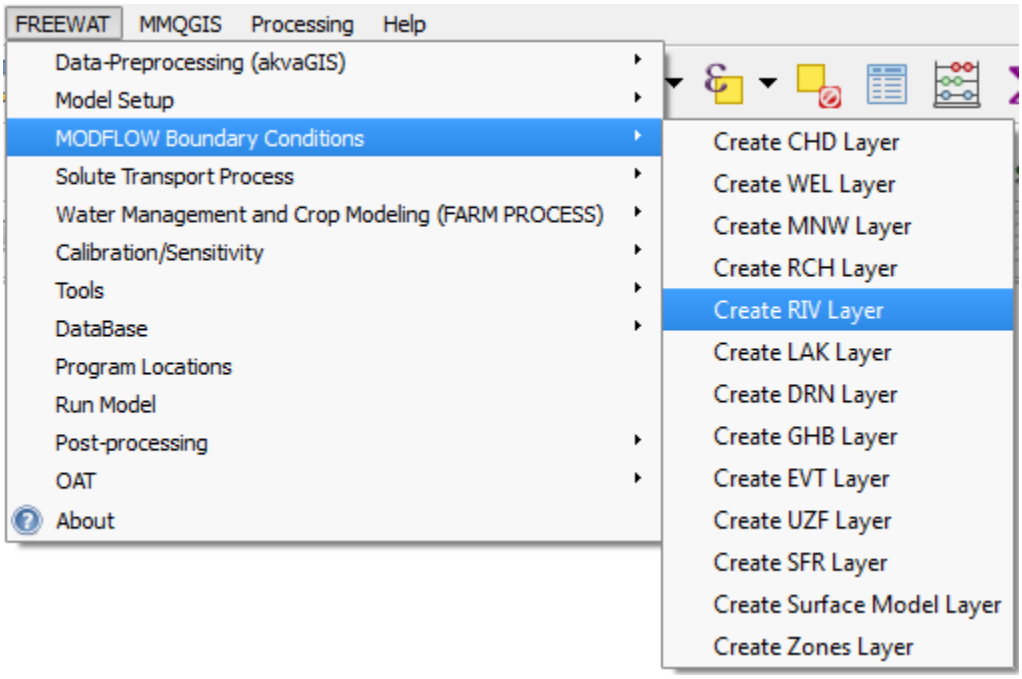
River - RIV (head-dependent flux)

MODFLOW RIV Package allows to simulate river/aquifer seepage, depending on the head gradient between the river and the groundwater system.

Activating this Package requires prior processing of a line shapefile, containing the profile of the river within the study area.

Once the line shapefile is loaded in the Layers Panel, to activate the *RIV Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create RIV Layer.



Two alternative options are available:

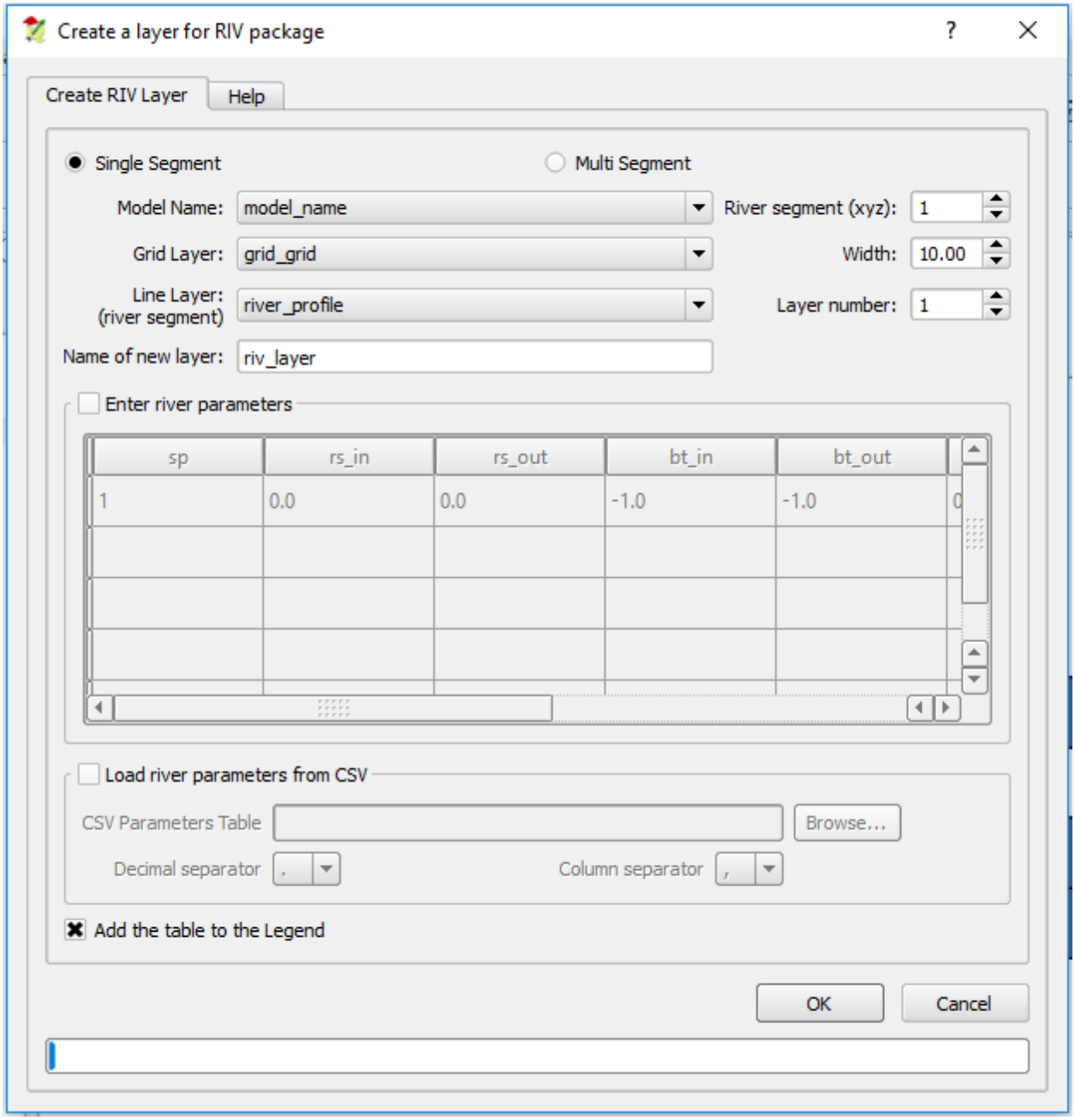
- *Single Segment*, if the river profile develops over one single line;
- *Multi Segment*, if the river profile develops over a multi-line.

Note: The option *Single Segment*, allows the User to assign river properties (i.e., river stage, river width, river bed bottom and thickness, hydraulic conductivity of the river bed sediments), as required in the *MODFLOW RIV Package*. On the contrary, the option *Multi Segment* allows to define the river profile only and the required properties must be assigned by the User at each cell once the riv MDO is created. Anyway, the option *Single Segment* may still be applied even if the river develops over more than one segment. In this case, the multi-line shapefile must be splitted into several single segments. The latter will be used one by one to create several riv MDOs through the *Single Segment* option. All these MDOs will then be merged using the *Merge SpatiaLite layers* tool, as described below.

If the *Single Segment* option is checked, the following data are required in the **Create a layer for RIV package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer (river segment)*: line shapefile containing the profile of the single river segment;
- *Name of new layer*: name of the riv MDO which has to be created;
- *River segment (xyz)*: number of the single river segment;
- *Width*: width [L] of the river;
- *Layer number*: number of the model layer to which the river is in contact;
- if *Enter river parameters* is checked, the user can fill manually the table with all the necessary parameters to be assigned to grid cells where the river is located;
- if *Load river parameters from CSV* is checked, the user can load a csv file containing parameters to be assigned to grid cells where the river is located, using the *Browse...* button (field *CSV Parameters Table*). In this case, the user must define the *Decimal separator* and *Column separator* used in the csv file loaded;

- if *Add the table to the Legend* is checked, a table containing the river parameters assigned is loaded in the Layers Panel.



Parameters required when creating the riv MDO are related to the geometry and hydraulic conductivity of the river bed sediments and must be assigned at the upstream and downstream cells of the river segment and for each SP:

- *sp*: SP number;
- *rs_in*: river stage [L] at the upstream cell of the river segment;
- *rs_out*: river stage [L] at the downstream cell of the river segment;
- *bt_in*: height [L] of the river bed bottom at the upstream cell of the river segment;
- *bt_out*: height [L] of the river bed bottom at the downstream cell of the river segment;

- *hc_in*: hydraulic conductivity [L/T] of the river bed sediments at the upstream cell of the river segment;
- *hc_out*: hydraulic conductivity [L/T] of the river bed sediments at the downstream cell of the river segment;
- *thick_in*: thickness [L] of the river bed sediments at the upstream cell of the river segment;
- *thick_out*: thickness [L] of the river bed sediments at the downstream cell of the river segment.

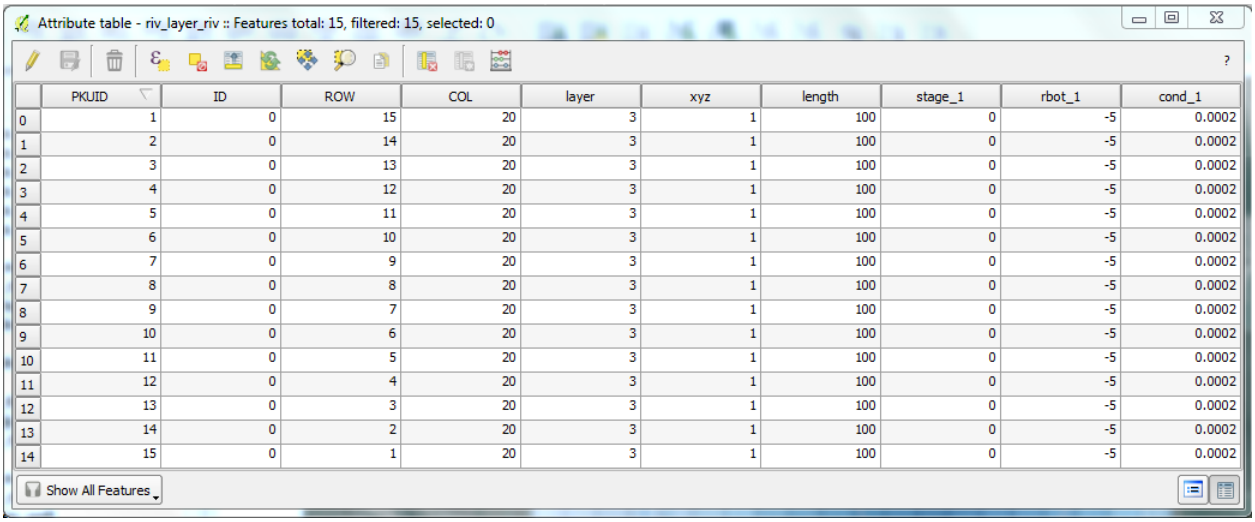
If loaded, the csv file must follow this structure.

A new MDO, named *riv_layer_riv*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

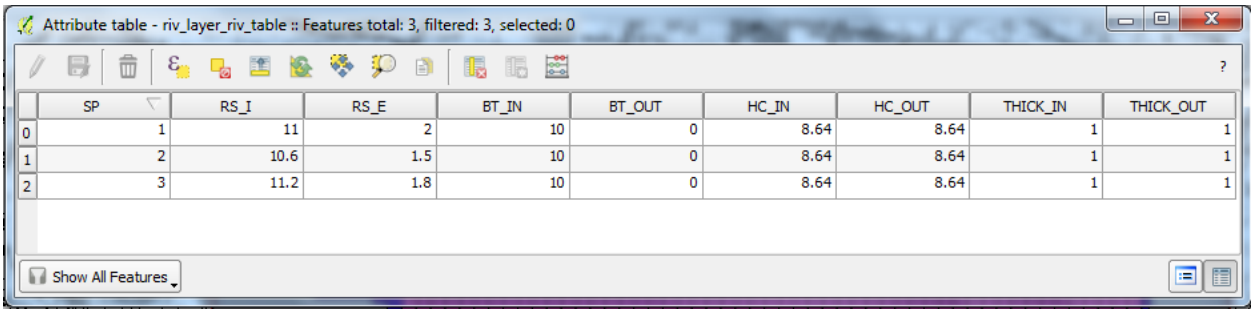
- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *layer*: number of the model layer to which the river is in contact;
- *xyz*: number of the river segment;
- *length*: length [L] of the river segment within a grid cell;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *stage_n*: river stage [L] during the *n*-th SP;
  - *rbot_n*: height of the river bottom [L] during the *n*-th SP;
  - *cond_n*: conductance of the rever bed sediments [L^2/T] during the *n*-th SP.

The fields *layer*, *xyz*, *stage_n*, *rbot_n* and *cond_n* are filled with values assigned by the User when the *riv_layer_riv* MDO is created. The values of *length* within each grid cell are automatically calculated according to the portion of the river segment which intersects a grid cell. Also, *cond_n* is automatically calculated depending on the river bed geometry and its hydraulic conductivity (for details the reader is referred to the *MODFLOW-2005* manual, Harbaugh, 2005).



	PKUID	ID	ROW	COL	layer	xyz	length	stage_1	rbot_1	cond_1
0	1	0	15	20	3	1	100	0	-5	0.0002
1	2	0	14	20	3	1	100	0	-5	0.0002
2	3	0	13	20	3	1	100	0	-5	0.0002
3	4	0	12	20	3	1	100	0	-5	0.0002
4	5	0	11	20	3	1	100	0	-5	0.0002
5	6	0	10	20	3	1	100	0	-5	0.0002
6	7	0	9	20	3	1	100	0	-5	0.0002
7	8	0	8	20	3	1	100	0	-5	0.0002
8	9	0	7	20	3	1	100	0	-5	0.0002
9	10	0	6	20	3	1	100	0	-5	0.0002
10	11	0	5	20	3	1	100	0	-5	0.0002
11	12	0	4	20	3	1	100	0	-5	0.0002
12	13	0	3	20	3	1	100	0	-5	0.0002
13	14	0	2	20	3	1	100	0	-5	0.0002
14	15	0	1	20	3	1	100	0	-5	0.0002

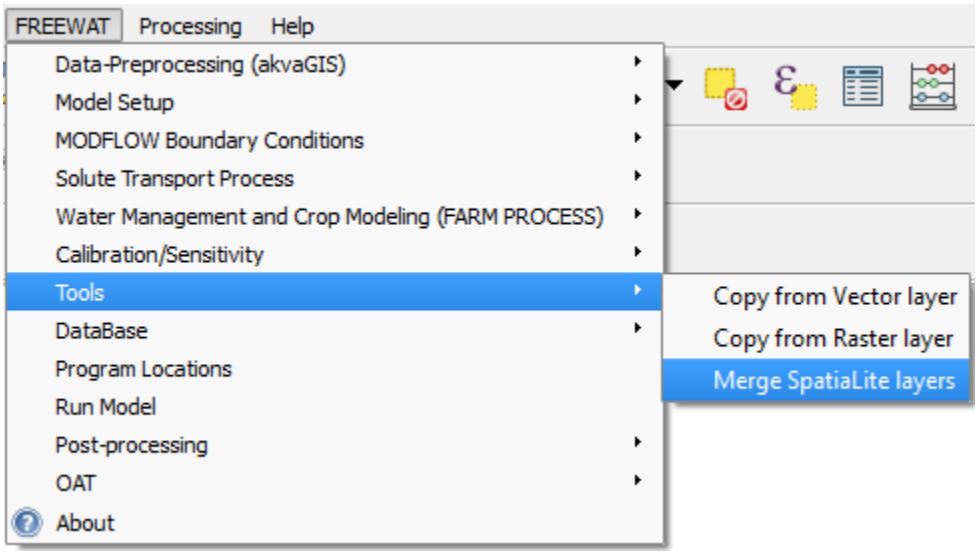
A table named *riv_layer_riv_table* is created with the riv MDO, stored in the model DB and possibly loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters listed above.

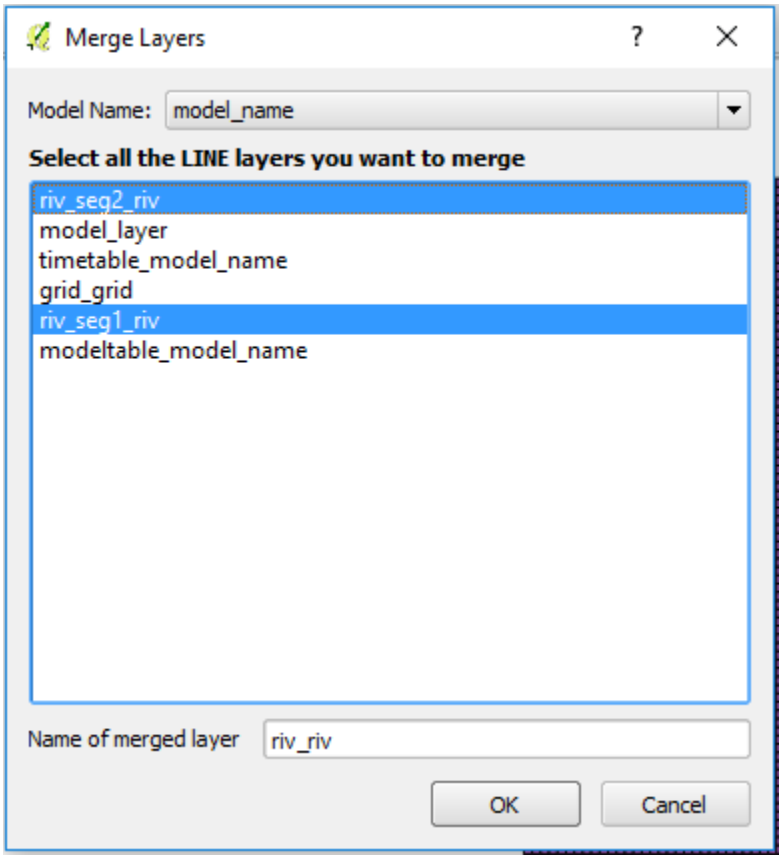


	SP	RS_I	RS_E	BT_IN	BT_OUT	HC_IN	HC_OUT	THICK_IN	THICK_OUT
0	1	11	2	10	0	8.64	8.64	1	1
1	2	10.6	1.5	10	0	8.64	8.64	1	1
2	3	11.2	1.8	10	0	8.64	8.64	1	1

Note: If the river develops over more than one segment, the procedure described above must be repeated for each segment. In this case, pay attention to assign a different name in the *Name of new layer* field and to select the correct line shapefile in the *Line Layer (river segment)* field and use a progressive segment number in the *River segment (xyz)* field. Once all the riv MDOs have been created, the *Merge SpatiaLite layers* tool must be used to get a single MDO. The latter will then be used during the *Run* procedure.

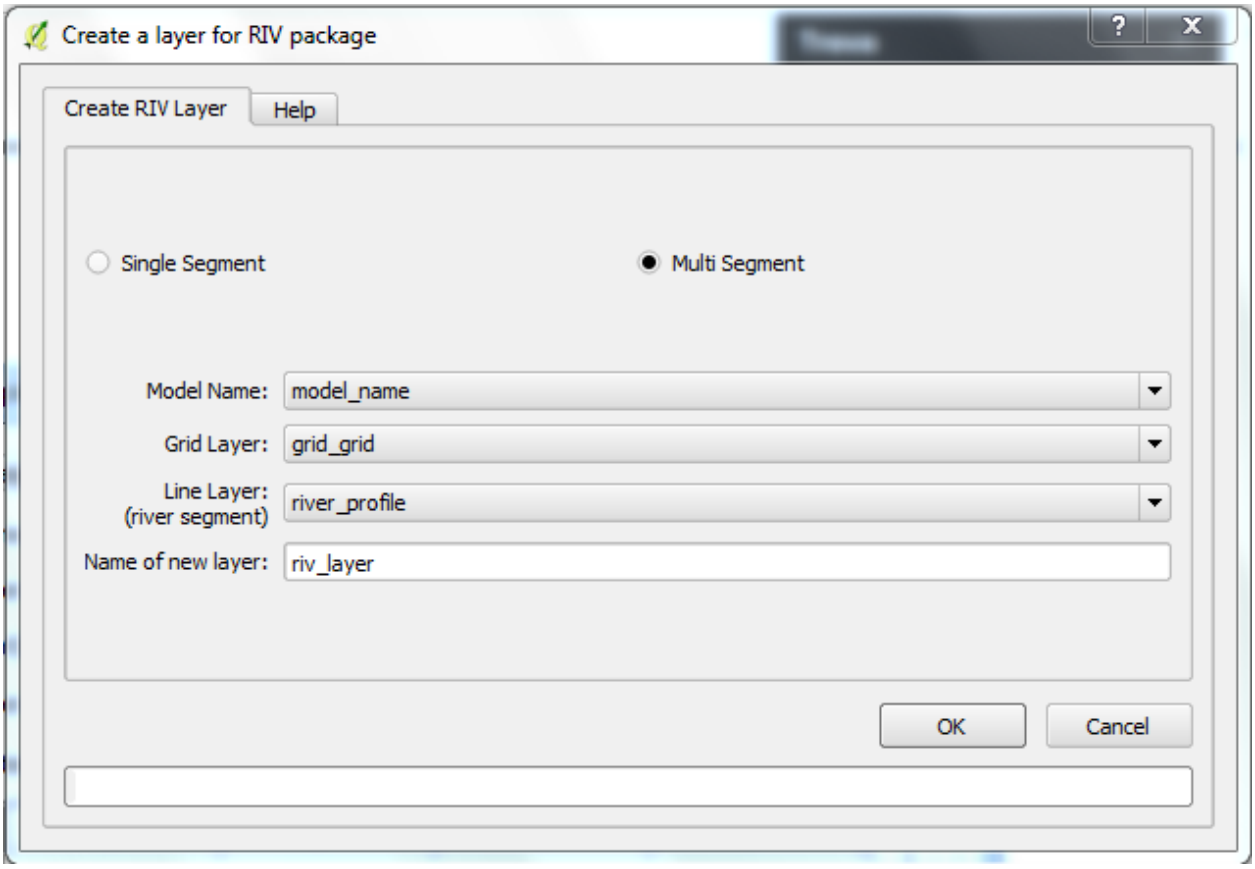
Note: The following figures refer to an application of the *Merge SpatiaLite layers* tool for two riv MDOs. In the **Merge Layers** window you must simply select the MDOs you want to merge and assign a new name to the merged MDO. The Attribute Table of the merged MDO will contain the same fields as the single MDOs, but more records, according to the number of cells intersected by *all* the river segments.





If the *Multi Segment* option is checked, the following data are required in the **Create a layer for RIV package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer (river segment)*: line shapefile containing the profile of the multi river segment;
- *Name of new layer*: name of the riv MDO which has to be created.

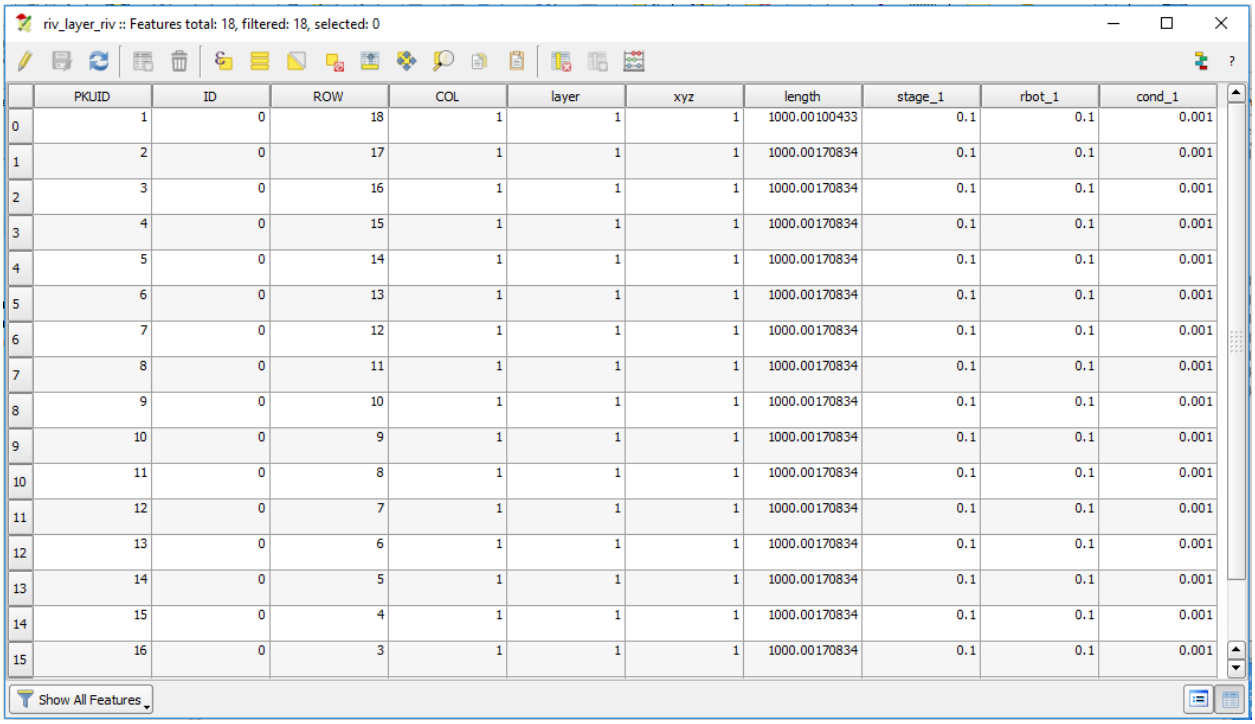


A new MDO, named *riv_layer_riv*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *layer*: number of the model layer to which the river is in contact;
- *xyz*: number of the river segment;
- *length*: length [L] of the river segment within a grid cell;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *stage_n*: river stage [L] during the *n*-th SP;
  - *rbot_n*: height of the river bottom [L] during the *n*-th SP;
  - *cond_n*: conductance of the rever bed sediments [L^2/T] during the *n*-th SP.

The fields *layer*, *stage_n*, *rbot_n* and *cond_n* are filled with default values. The values of *length* within each grid cell are automatically calculated according to the portion of the river segment which intersects a grid cell. The field *xyz* is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.



	PKUID	ID	ROW	COL	layer	xyz	length	stage_1	rbot_1	cond_1
0	1	0	18	1	1	1	1000.00100433	0.1	0.1	0.001
1	2	0	17	1	1	1	1000.00170834	0.1	0.1	0.001
2	3	0	16	1	1	1	1000.00170834	0.1	0.1	0.001
3	4	0	15	1	1	1	1000.00170834	0.1	0.1	0.001
4	5	0	14	1	1	1	1000.00170834	0.1	0.1	0.001
5	6	0	13	1	1	1	1000.00170834	0.1	0.1	0.001
6	7	0	12	1	1	1	1000.00170834	0.1	0.1	0.001
7	8	0	11	1	1	1	1000.00170834	0.1	0.1	0.001
8	9	0	10	1	1	1	1000.00170834	0.1	0.1	0.001
9	10	0	9	1	1	1	1000.00170834	0.1	0.1	0.001
10	11	0	8	1	1	1	1000.00170834	0.1	0.1	0.001
11	12	0	7	1	1	1	1000.00170834	0.1	0.1	0.001
12	13	0	6	1	1	1	1000.00170834	0.1	0.1	0.001
13	14	0	5	1	1	1	1000.00170834	0.1	0.1	0.001
14	15	0	4	1	1	1	1000.00170834	0.1	0.1	0.001
15	16	0	3	1	1	1	1000.00170834	0.1	0.1	0.001

Lake - LAK (head-dependent flux)

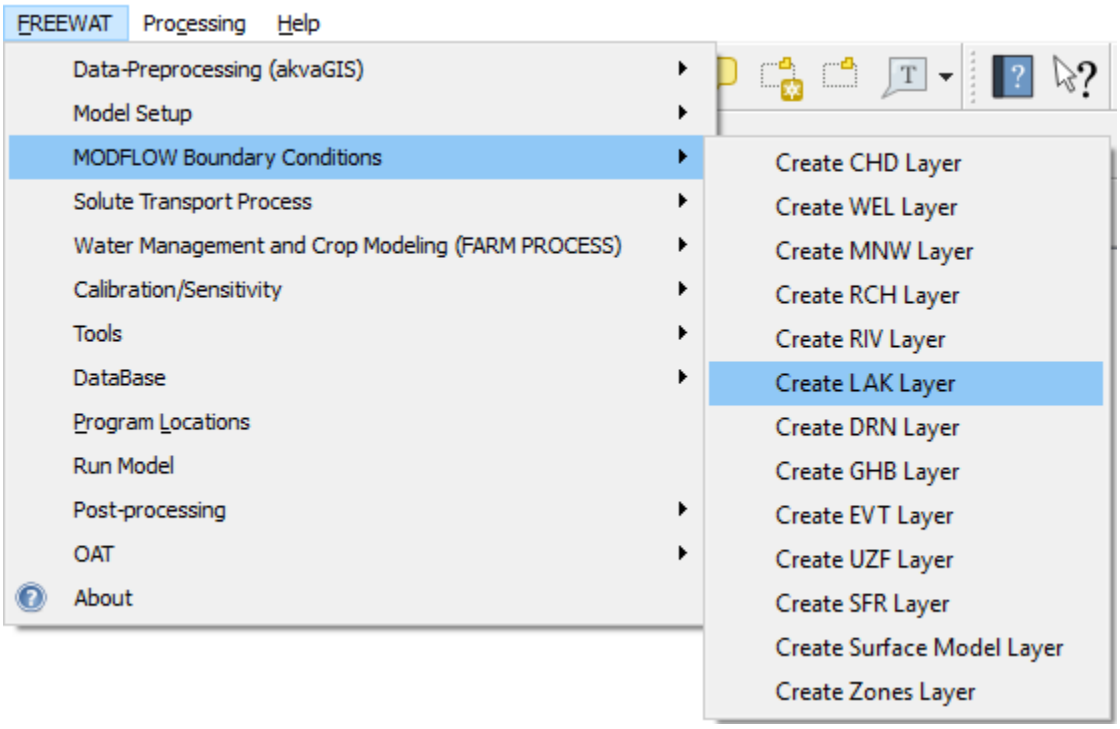
MODFLOW LAK Package allows to simulate the hydraulic interaction between a lake and groundwater in the surrounding aquifer so that the effects of the changes in the conditions of one of the two water bodies is calculated on the other.

The LAK Package calculates a separate water budget for those cells identified as lakes, removing them from the solution of the groundwater equation and setting them as inactive. Any cells in which a lake is to be simulated must be set to inactive. The integer value corresponding to the *IBOUND* flag in *MODFLOW* must be set to *0* in the model layers corresponding to the hydrostratigraphic units in which a lake is present. This corresponds with the *ACTIVE* field in the *FREEWAT* model layers, which must be changed to *0* for any cells in which a lake is to be simulated.

Any layers in which lakes are to be simulated must also be set to *convertible* and *wettable* in the *Layer Property Flow* (*LPF*) table. The “type” must be “convertible” and “laywet” must be “Yes”.

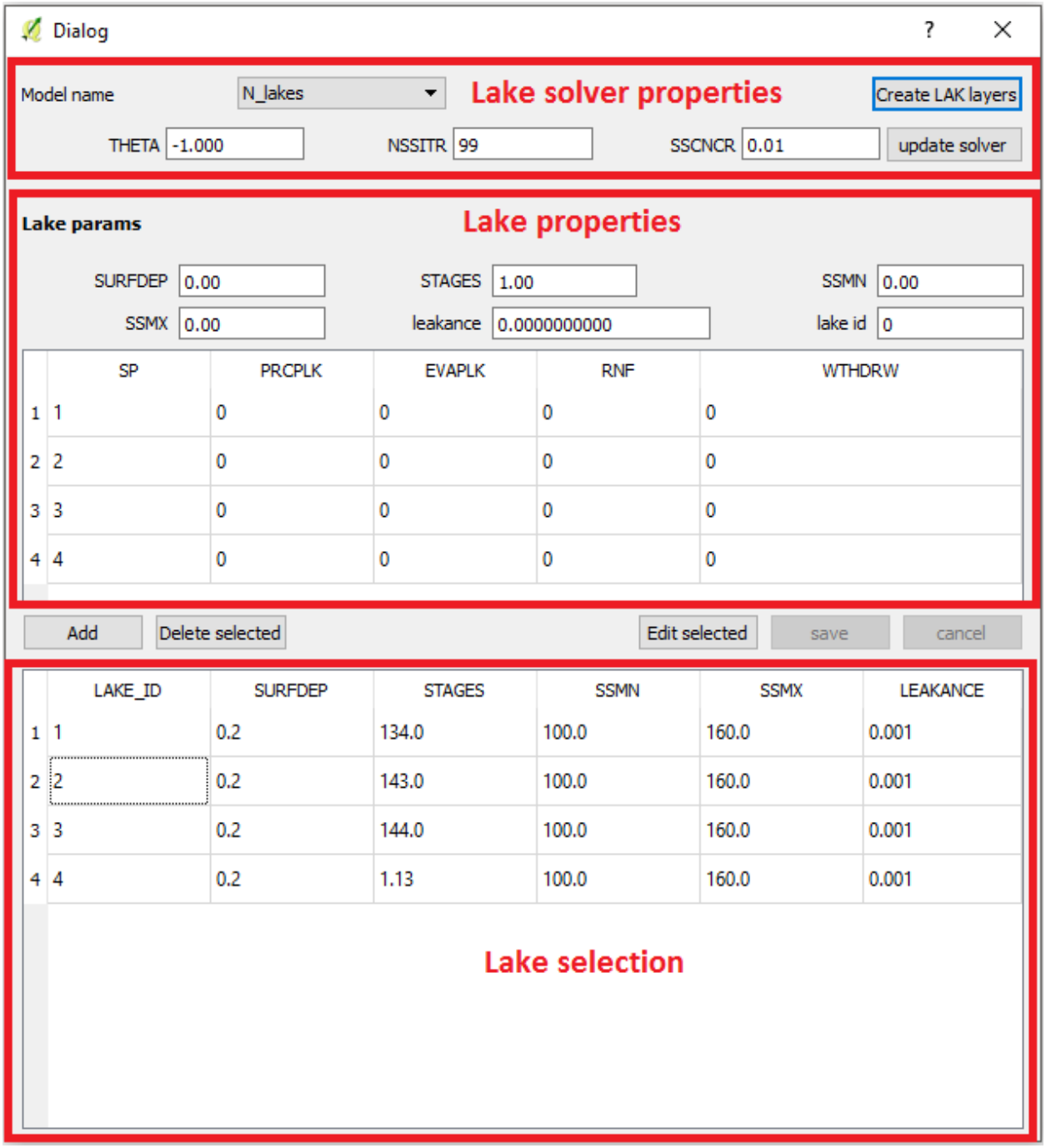
Once these conditions are met to activate the *LAK Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create LAK Layer.



Note: If lake layers already exist in the model database, the *lake layer group* will be loaded into the MDO.

The **Create Lak Layer** window can be divided into three frames:



- *Lake solver properties*: contains options for the solver of the lake budget. To be used once to create all lake layers;
- *Lake properties*: options specific to each lake;
- *Lake selection*: a summary of created lakes.

The *Lake solver properties* options apply to all the lakes within one *MODFLOW* simulation.

- *THETA*: Theta determines whether the solution for the lake package is solved implicitly (*Theta*=*1*) or semi-implicitly (*0.5*<=*Theta*<*1*);
- *NSSITR*: is the maximum number of iterations for Newton's method solution for equilibrium lake stages in each

MODFLOW iteration for steady-state aquifer head solution;

- *SSCNCR*: is the convergence criterion for equilibrium lake stage solution by Newton's method.

Note: A negative *Theta* value is used as flag for additional options in the LAK Package for transient calculations. *MODFLOW* will automatically convert it to a positive value for calculations of lake stage.

Once the *Lake solver properties* have been defined, pressing the *Create LAK layers* button will create one *_lak* layer for every model aquifer layer. These layers are used to assign the location of lakes using the *LAKE* field which corresponds to the *lake id*. Once the *_lak* layers have been created, the *update solver* button can be used to change or update the lake budget solver criteria.

The *Lake properties* are assigned to each lake individually. For each lake that is to be created, the *Lake properties* must be filled, with a unique non-zero integer for *lake id*.

- *SURFDEP*: lake bottom elevation undulations. Can be used to smooth the solution for the rewetting of the lake bottom. Values between *0.01* and *0.5* are suggested;
- *STAGES*: initial Stage of each lake at the start of the run;
- *SSMN*: minimum lake stage for steady-state simulations;
- *SSMX*: maximum lake stage for steady-state simulations;
- *leakance*: leakance term representing the lakebed sediments. Values are assumed to represent the combined leakances of the lakebed material and the aquifer material between the lake and the centers of the underlying grid cells;
- *lake id*: lake identifier for determining location, sub-lakes and stream flow routing.

The *Lake properties* frame reads the number of stress periods from the model *timetable* and displays as many rows. The table is to be filled with precipitation, evaporation, runoff and withdrawal information for the current lake, i.e. for the lake with the currently specified *lake id* in the *Lake properties*.

- *PRCPLK*: precipitation flux [L/T];
- *EVAPLK*: evaporation flux [L/T];
- *RNF*: surface runoff [L^3/T];
- *WTHDRW*: direct withdrawal from the lake [L^2/T].

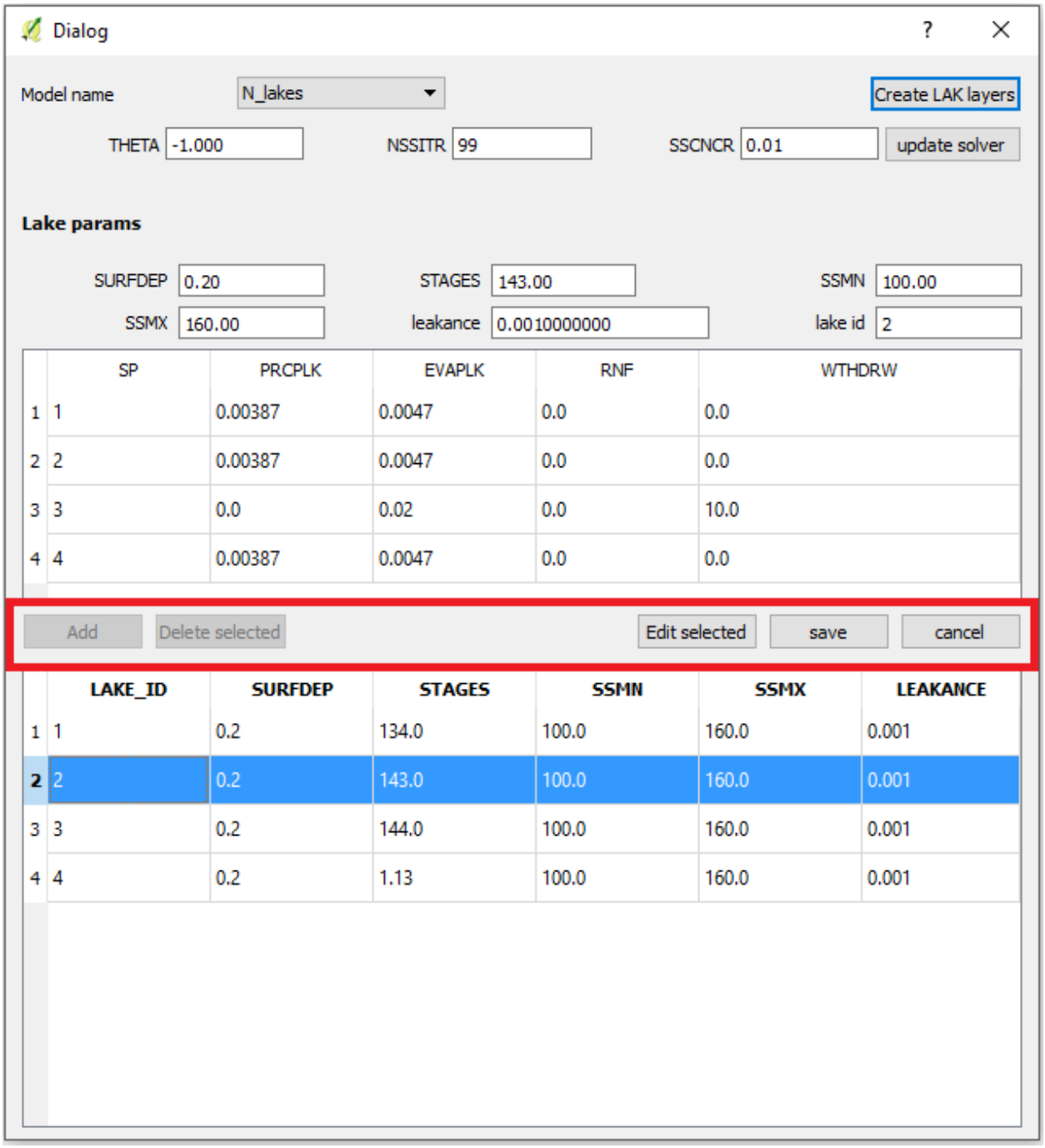
Refer to MODFLOW LAK Package for further information on these input options and parameters.

Once the *Lake properties* frame has been filled out for **one** lake, this lake is created through the *Add* button.

The lake is then added to the *Lake selection* frame.

When the *Add* button is pressed, the *Lake properties* frame is reset and, if needed, additional lakes can be added. The created lake is added to the *Lake selection* frame. This frame displays a summary of the time-constant properties of each created lake.

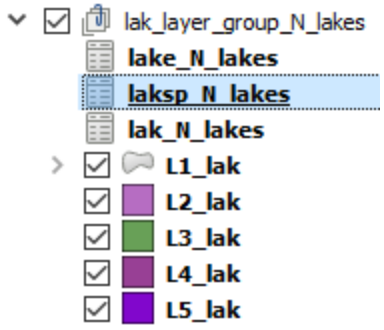
Once one or more lakes have been created, they can be deleted by selecting the relevant row in the *Lake selection* frame and using the *Delete Selected* button or edited and clicking *Edit Selected*. *Edit selected* will re-load the properties of the selected lake into the *Lake properties* frame, where they can be altered. Any changes can be applied using the *Save* button or discarded using *Cancel*. When editing a layer, the *Add* and *Delete selected* fields are locked. To use these funtions, the editing must be concluded, by *saving* or *cancelling*.



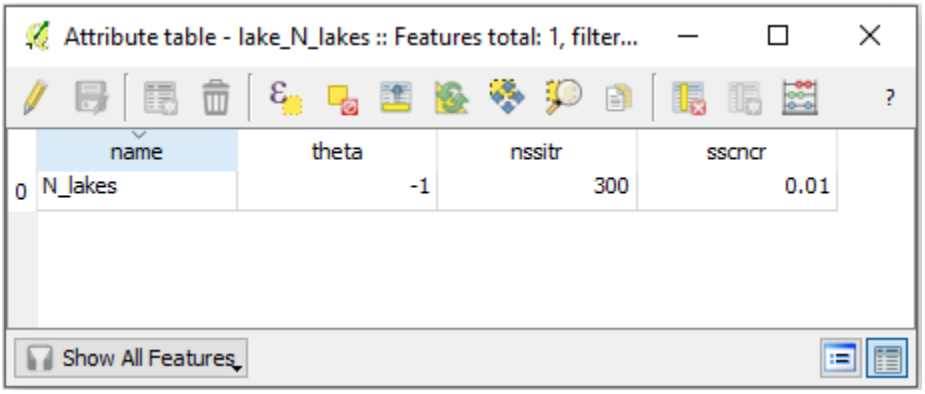
A new MDO group, named *lak_layer_group_model_name*, is created and stored within the model DB.

The *lak_layer_group_model_name* MDO group contains a *_lak* layer for every model aquifer layer, one *lak_model_name* table, one *laksp_model_name* and one *lake_model_name* table. By default, the *lak_model_name*, *laksp_model_name* and *lake_model_name* are not loaded in the Layers Panel. Modification to the lake properties can be done through the *Create LAK layers* dialog, even after they have been created. The *lak_model_name*, *laksp_model_name* and *lake_model_name* can also be added to the Layers Panel using the QGIS Database Manager.

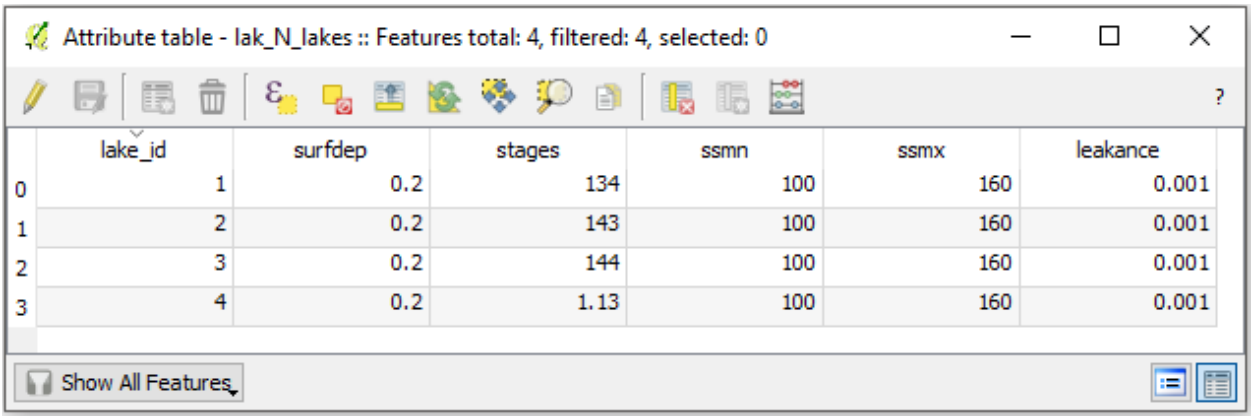
Note: The following images and attribute tables were made using example data and will differ for every model.



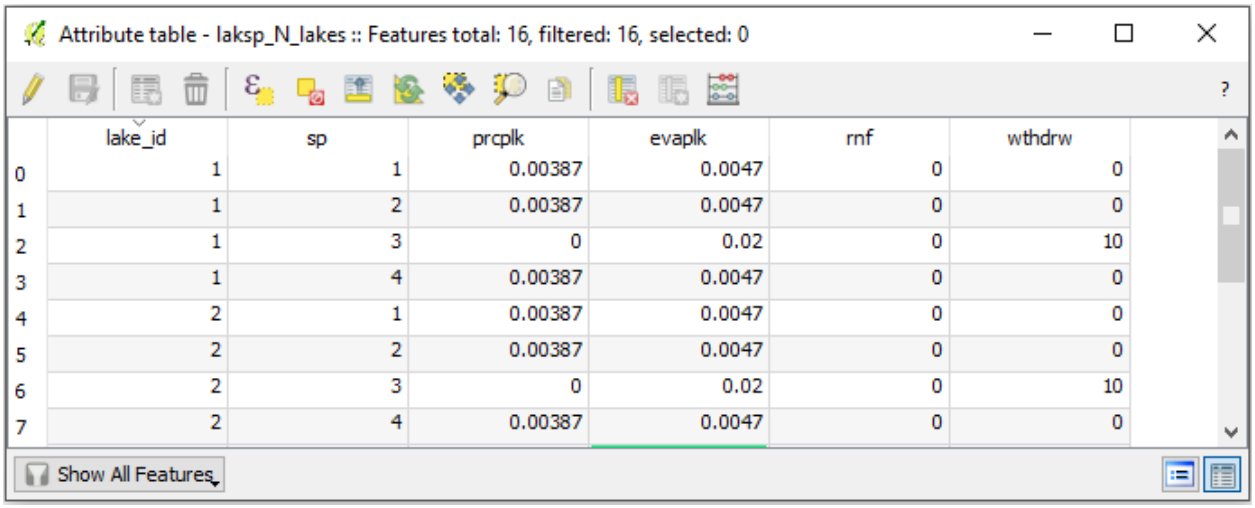
The *lake_model_name* is not automatically loaded into the lake group MDO, but is created in the model DB. The *lake_model_name* is used to save the *lake solver properties* options.



The *lak_model_name* is not automatically loaded into the lake group MDO, but is created in the model DB.The *lak_model_name* Attribute Table contains the time constant *Lake properties* information for all lakes.



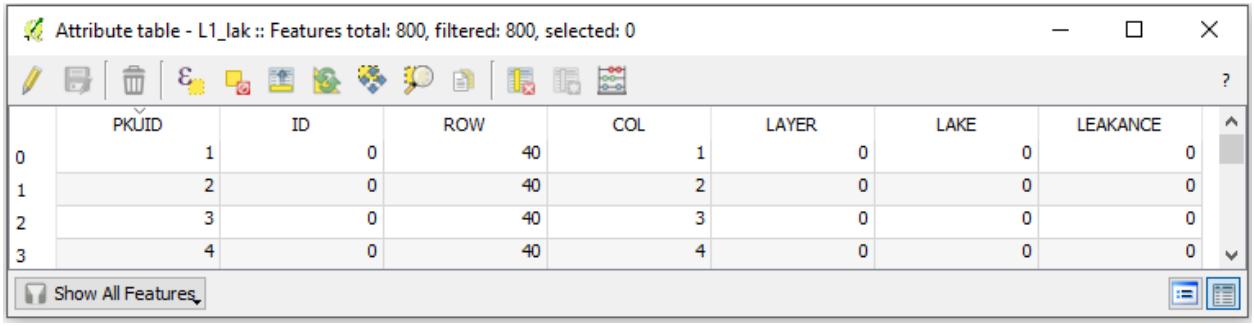
The *laksp_model_name* is not automatically loaded into the lake group MDO, but is created in the model DB. The *laksp_model_name* Attribute Table contains the time variant *Lake properties* information for all lakes, for all stress periods.



	lake_id	sp	prcplk	evaplk	rnf	wthdrw
0	1	1	0.00387	0.0047	0	0
1	1	2	0.00387	0.0047	0	0
2	1	3	0	0.02	0	10
3	1	4	0.00387	0.0047	0	0
4	2	1	0.00387	0.0047	0	0
5	2	2	0.00387	0.0047	0	0
6	2	3	0	0.02	0	10
7	2	4	0.00387	0.0047	0	0

The *lake_model_name* is automatically loaded into the lake group MDO and is created in the model DB. Each *_lak* Attribute Table may contain several records, according to the number of grid cells, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *LAYER*: number of the model layer which the *_lak* layer represents;
- *LAKE*: the *lake id* number to identify which lake is in a given cell;
- *LEAKANCE*: the leakance term for a given cell.



	PKUID	ID	ROW	COL	LAYER	LAKE	LEAKANCE
0	1	0	40	1	0	0	0
1	2	0	40	2	0	0	0
2	3	0	40	3	0	0	0
3	4	0	40	4	0	0	0

To specify the location of certain lakes within the *FREEWAT* model, the *LAKE* field must be edited to refer to the relevant non-zero *lake id*. If lake layers are created, but the *LAKE* fields are unassigned, the lakes will be not be simulated.

Limitations

The LAK Package has the following limitations, which can be overcome only by editing the lak *MODFLOW* input file and running the model independently of the *FREEWAT* platform (for details refer to Merrit and Konikow, 2000):

- the lake bathymetry cannot be specified through an external file;
- the designation for central and sub-lakes, as well as sills between lakes, for the separation and coalescence of lakes is not yet implemented in *FREEWAT*;

- *MOC3D* for solute concentrations in lakes is not implemented in *FREEWAT*, but will be replaced by *MT3DMS*.

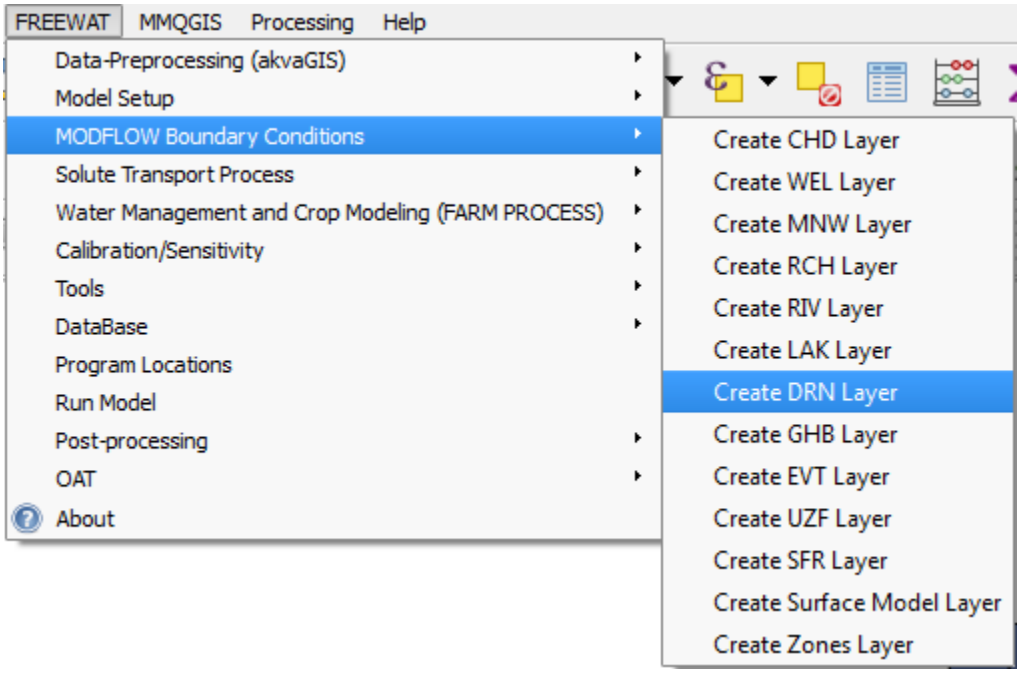
Drain - DRN (head-dependent flux)

MODFLOW DRN Package allows to simulate groundwater exchange between a drainage system and an aquifer system, depending on the difference between the drain elevation and the hydraulic head of the aquifer itself.

Activating this Package requires prior processing of a line shapefile, containing the profile of the drain system within the study area.

Once the line shapefile is loaded in the Layers Panel, to activate the *DRN Package* the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create DRN Layer.



Two alternative options are available:

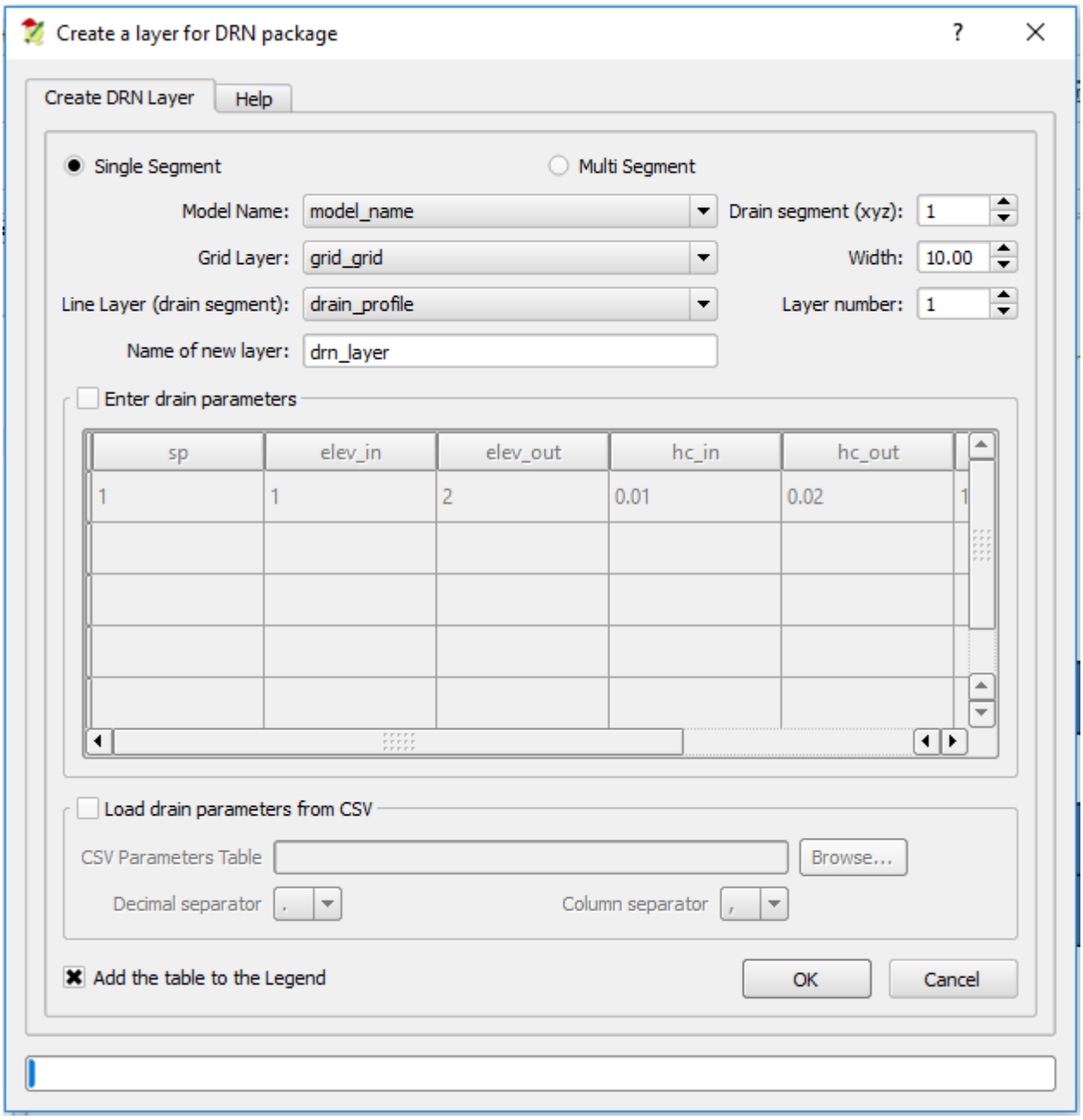
- *Single Segment*, if the drain profile develops over one single line;
- *Multi Segment*, if the drain profile develops over a multi-line.

Note: The option *Single Segment*, allows the User to assign drain properties (i.e., drain elevation, drain width, drain bed thickness, hydraulic conductivity of the drain bed sediments), as required in the *MODFLOW DRN Package*. On the contrary, the option *Multi Segment* allows to define the drain profile only and the required properties must be assigned by the User at each cell once the drn MDO is created. Anyway, the option *Single Segment* may still be applied even if the drain develops over more than one segment. In this case, the multi-line shapefile must be splitted into several single segments. The latter will be used one by one to create several drn MDOs through the *Single Segment* option. All these MDOs will then be merged using the *Merge SpatiaLite layers* tool.

If the *Single Segment* option is checked, the following data are required in the **Create a layer for DRN package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;

- *Line Layer (drain segment)*: line shapefile containing the profile of the single drain segment;
- *Name of new layer*: name of the drn MDO which has to be created;
- *Drain segment (xyz)*: number of the single drain segment;
- *Width*: width [L] of the drain;
- *Layer number*: number of the model layer to which the drain is in contact;
- if *Enter drain parameters* is checked, the user can fill manually the table with all the necessary parameters to be assigned to grid cells where the drain is located;
- if *Load drain parameters from CSV* is checked, the user can load a csv file containing parameters to be assigned to grid cells where the drain is located, using the *Browse...* button (field *CSV Parameters Table*). In this case, the user must define the *Decimal separator* and *Column separator* used in the csv file loaded;
- if *Add the table to the Legend* is checked, a table containing the drain parameters assigned is loaded in the Layers Panel.



Parameters required when creating the drn MDO are related to the geometry and hydraulic conductivity of the drain bed sediments and must be assigned at the upstream and downstream cells of the drain segment and for each SP:

- *sp*: SP number;
- *elev_in*: drain elevation [L] at the upstream cell of the drain segment;
- *elev_out*: drain elevation [L] at the downstream cell of the drain segment;
- *hc_in*: hydraulic conductivity [L/T] of the drain bed sediments at the upstream cell of the drain segment;
- *hc_out*: hydraulic conductivity [L/T] of the drain bed sediments at the downstream cell of the drain segment;
- *thick_in*: thickness [L] of the drain bed sediments at the upstream cell of the drain segment;
- *thick_out*: thickness [L] of the drain bed sediments at the downstream cell of the drain segment.

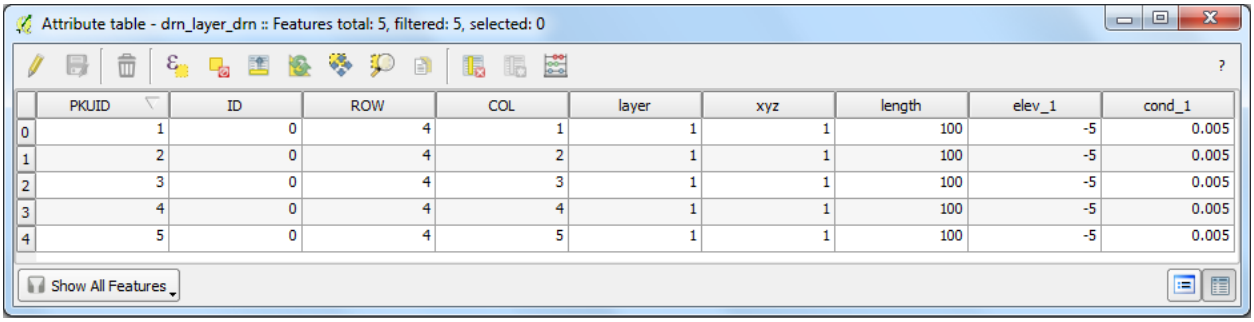
If loaded, the csv file must follow this structure.

A new MDO, named *drn_layer_drn*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

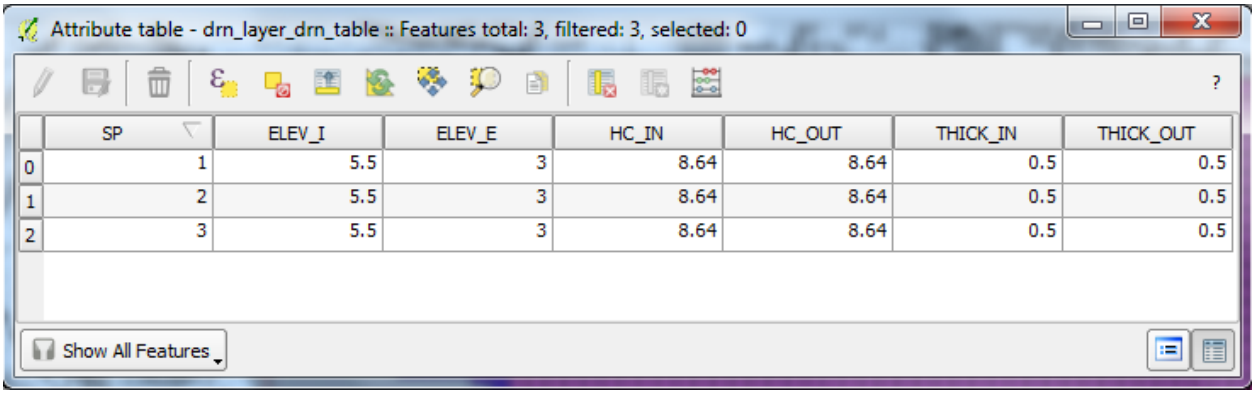
- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *layer*: number of the model layer to which the drain is in contact;
- *xyz*: number of the drain segment;
- *length*: length [L] of the drain segment within a grid cell;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *elev_n*: drain elevation [L] during the *n*-th SP;
  - *cond_n*: drain conductance [L^2/T] during the *n*-th SP.

The fields *layer*, *xyz*, *elev_n* and *cond_n* are filled with values assigned by the User when the *drn_layer_drn* MDO is created. The values of *length* within each grid cell are automatically calculated according to the portion of the drain segment which intersects a grid cell. Also, *cond_n* is automatically calculated depending on the drain bed geometry and its hydraulic conductivity (for details the reader is referred to the *MODFLOW-2005* manual, Harbaugh, 2005).



	PKUID	ID	ROW	COL	layer	xyz	length	elev_1	cond_1
0	1	0	4	1	1	1	100	-5	0.005
1	2	0	4	2	1	1	100	-5	0.005
2	3	0	4	3	1	1	100	-5	0.005
3	4	0	4	4	1	1	100	-5	0.005
4	5	0	4	5	1	1	100	-5	0.005

A table named *drn_layer_drn_table* is created with the drn MDO, stored in the model DB and possibly loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters listed above.



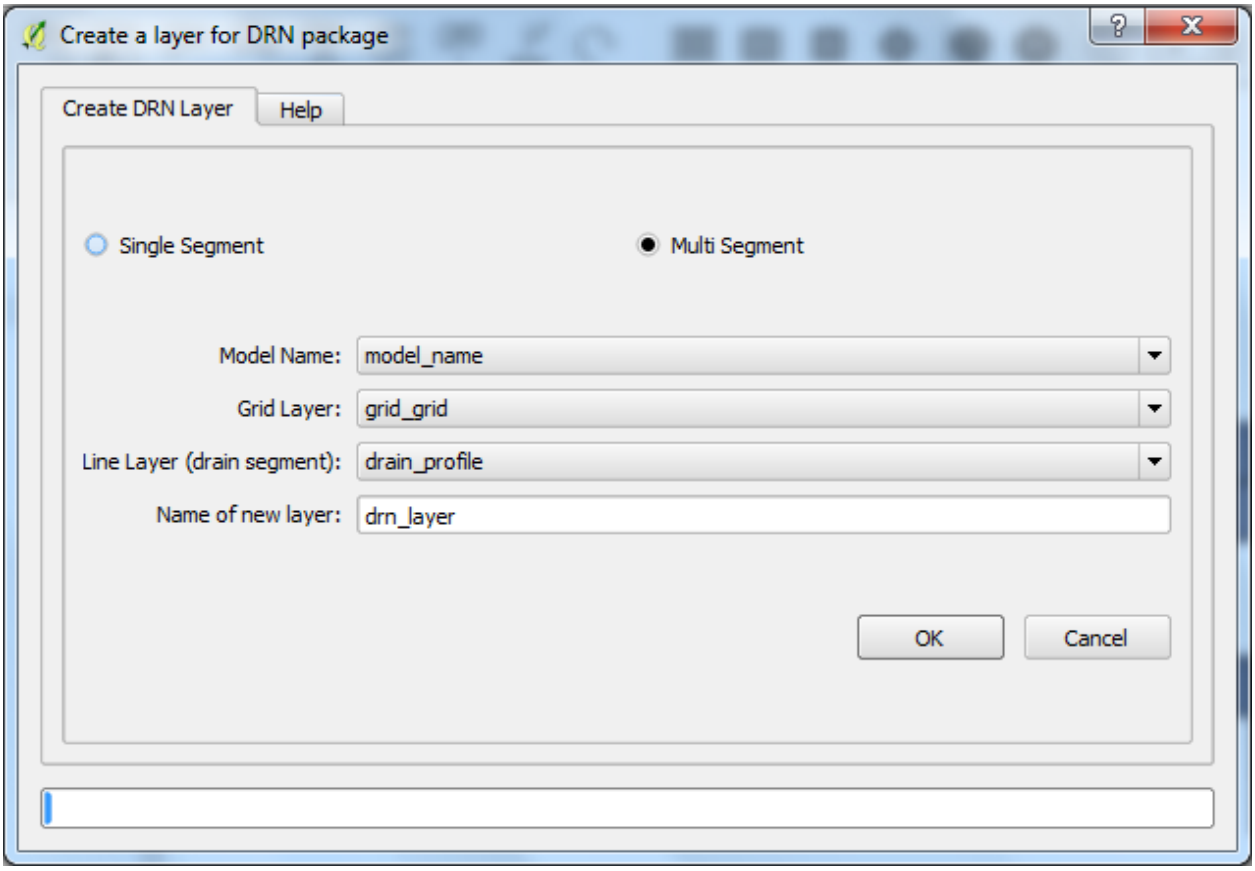
	SP	ELEV_I	ELEV_E	HC_IN	HC_OUT	THICK_IN	THICK_OUT
0	1	5.5	3	8.64	8.64	0.5	0.5
1	2	5.5	3	8.64	8.64	0.5	0.5
2	3	5.5	3	8.64	8.64	0.5	0.5

Note: If the drain develops over more than one segment, the procedure described above must be repeated for each

segment. In this case, pay attention to assign a different name in the *Name of new layer* field and to select the correct line shapefile in the *Line Layer (drain segment)* field and use a progressive segment number in the *Drain segment (xyz)* field. Once all the drn MDOs have been created, the *Merge SpatiaLite layers* tool must be used to get a single MDO. The latter will then be used during the *Run* procedure.

If the *Multi Segment* option is checked, the following data are required in the **Create a layer for DRN package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer (drain segment)*: line shapefile containing the profile of the multi drain segment;
- *Name of new layer*: name of the drn MDO which has to be created.



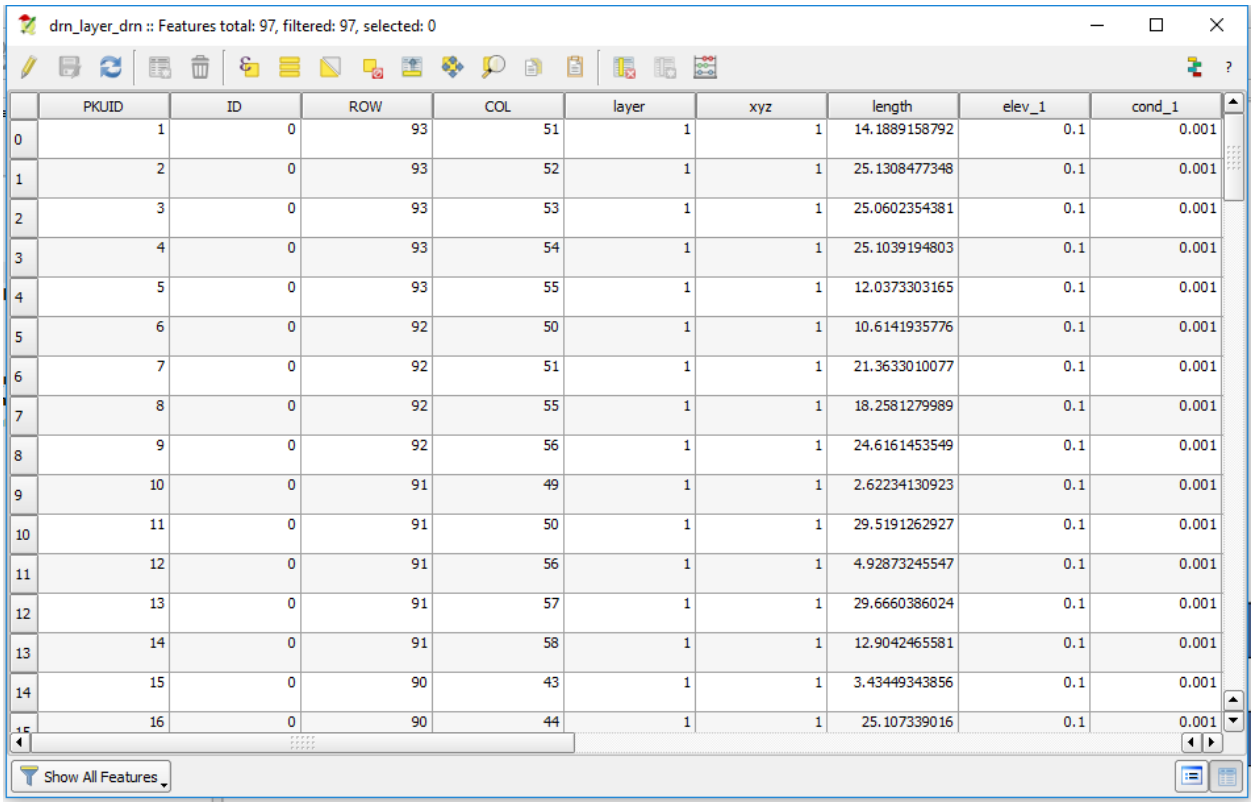
A new MDO, named *drn_layer_drn*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *layer*: number of the model layer to which the drain is in contact;
- *xyz*: number of the drain segment;

- *length*: length [L] of the drain segment within a grid cell;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *elev_n*: drain elevation [L] during the *n*-th SP;
  - *cond_n*: drain conductance [L^2/T] during the *n*-th SP.

The fields *layer*, *elev_n* and *cond_n* are filled with default values. The values of *length* within each grid cell are automatically calculated according to the portion of the drain segment which intersects a grid cell. The field *xyz* is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.



	PKUID	ID	ROW	COL	layer	xyz	length	elev_1	cond_1
0	1	0	93	51	1	1	14.1889158792	0.1	0.001
1	2	0	93	52	1	1	25.1308477348	0.1	0.001
2	3	0	93	53	1	1	25.0602354381	0.1	0.001
3	4	0	93	54	1	1	25.1039194803	0.1	0.001
4	5	0	93	55	1	1	12.0373303165	0.1	0.001
5	6	0	92	50	1	1	10.6141935776	0.1	0.001
6	7	0	92	51	1	1	21.3633010077	0.1	0.001
7	8	0	92	55	1	1	18.2581279989	0.1	0.001
8	9	0	92	56	1	1	24.6161453549	0.1	0.001
9	10	0	91	49	1	1	2.62234130923	0.1	0.001
10	11	0	91	50	1	1	29.5191262927	0.1	0.001
11	12	0	91	56	1	1	4.92873245547	0.1	0.001
12	13	0	91	57	1	1	29.6660386024	0.1	0.001
13	14	0	91	58	1	1	12.9042465581	0.1	0.001
14	15	0	90	43	1	1	3.43449343856	0.1	0.001
15	16	0	90	44	1	1	25.107339016	0.1	0.001

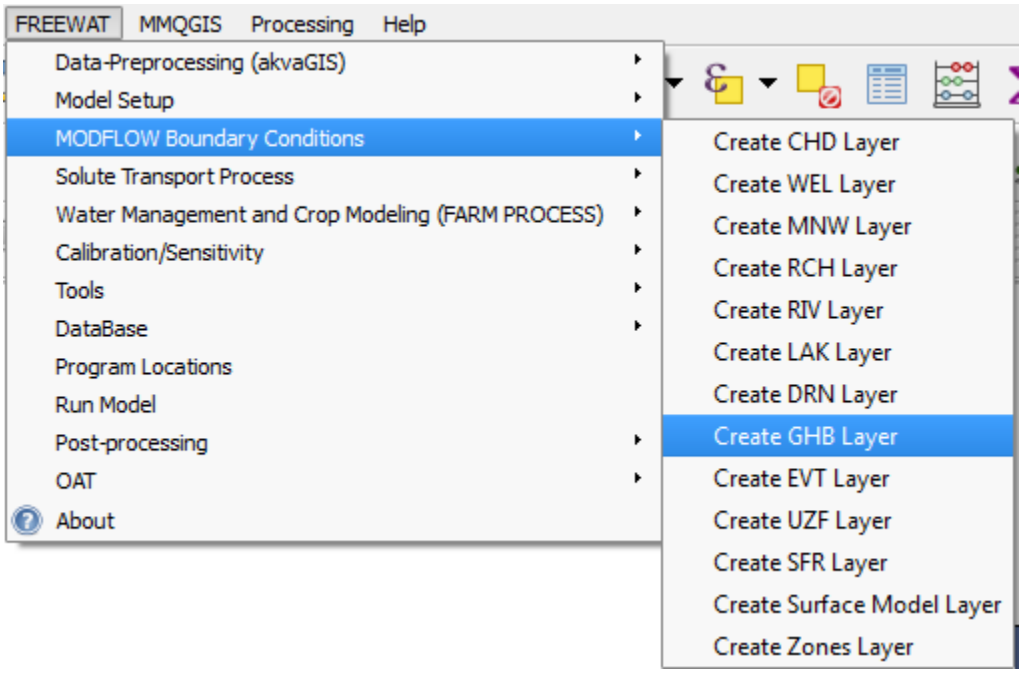
General-Head Boundary - GHB (head-dependent flux)

MODFLOW GHB Package allows to simulate groundwater exchange between an external source and an aquifer system, depending on the head gradient between the source itself and the groundwater system.

Activating this Package requires prior processing of a line shapefile, containing the profile of the general-head boundary within the study area.

Once the line shapefile is loaded in the Layers Panel, to activate the *GHB Package* the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create GHB Layer.



Two alternative options are available:

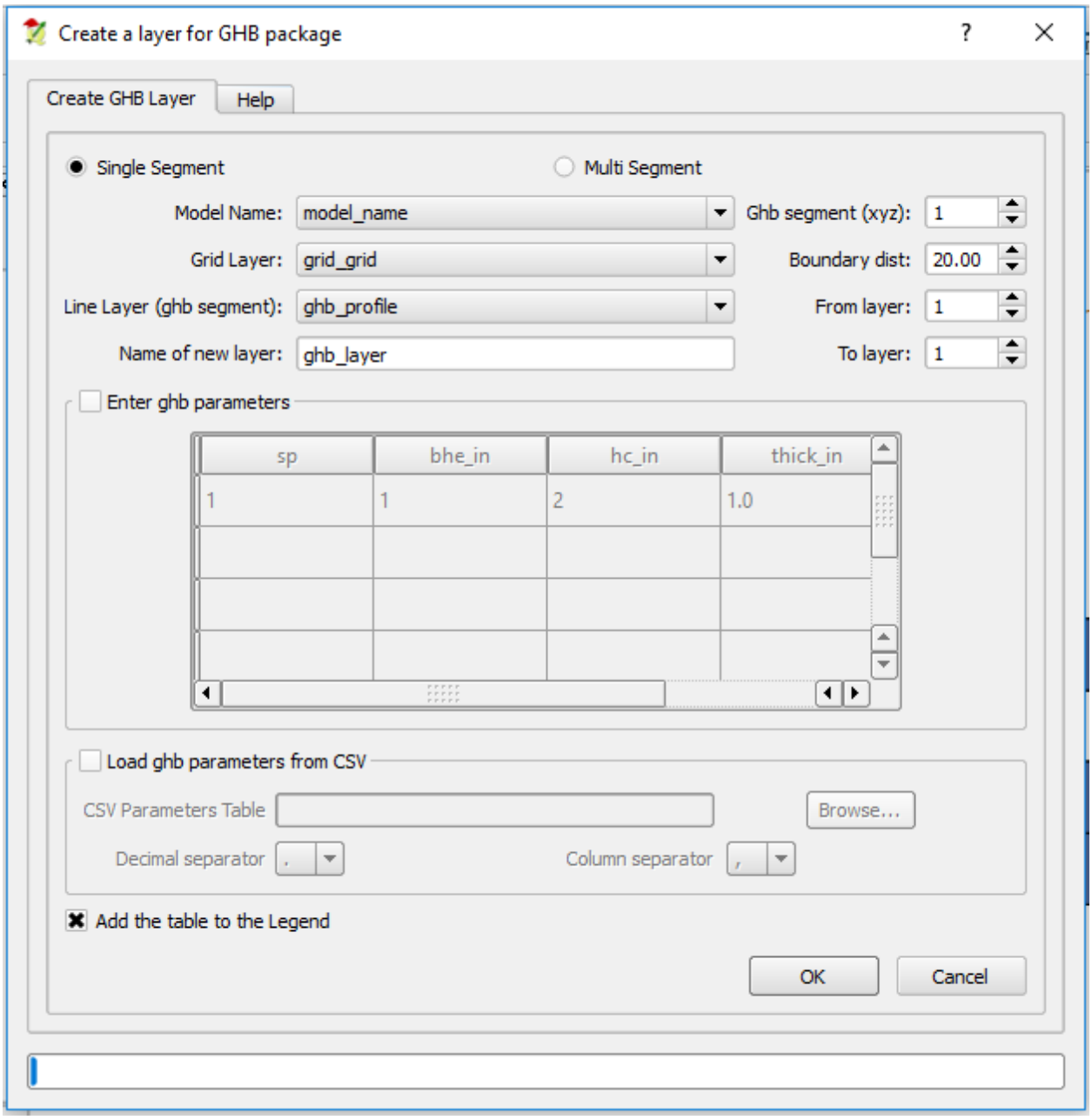
- *Single Segment*, if the general-head boundary profile develops over one single line;
- *Multi Segment*, if the general-head boundary profile develops over a multi-line.

Note: The option *Single Segment*, allows the User to assign drain properties (i.e., head assigned to the external source, hydraulic conductivity and thickness of the sediments between the external source and the grid cell), as required in the *MODFLOW GHB Package*. On the contrary, the option *Multi Segment* allows to define the general-head boundary profile only and the required properties must be assigned by the User at each cell once the ghb MDO is created. Anyway, the option *Single Segment* may still be applied even if the general-head boundary develops over more than one segment. In this case, the multi-line shapefile must be splitted into several single segments. The latter will be used one by one to create several ghb MDOs through the *Single Segment* option. All these MDOs will then be merged using the *Merge SpatiaLite layers* tool.

If the *Single Segment* option is checked, the following data are required in the **Create a layer for GHB package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer (ghb segment)*: line shapefile containing the profile of the single ghb segment;
- *Name of new layer*: name of the ghb MDO which has to be created;
- *Ghb segment (xyz)*: number of the single ghb segment;
- *Boundary dist*: distance between the external source and the general-head boundary;
- *From layer*: number of the uppermost model layer to which the ghb condition is applied;
- *To layer*: number of the deepest model layer to which the ghb condition is applied;
- if *Enter ghb parameters* is checked, the user can fill manually the table with all the necessary parameters to be assigned to grid cells where the ghb condition is applied;

- if *Load ghb parameters from CSV* is checked, the user can load a csv file containing parameters to be assigned to grid cells where the ghb condition is applied, using the *Browse...* button (field *CSV Parameters Table*). In this case, the user must define the *Decimal separator* and *Column separator* used in the csv file loaded;
- if *Add the table to the Legend* is checked, a table containing the ghb parameters assigned in loaded in the Layers Panel.



Parameters required when creating the ghb MDO are related to the geometry and hydraulic conductivity of sediments between the external source and the grid cell and must be assigned for each SP:

- *sp*: SP number;
- *bhe_in*: head assigned to the external source [L];
- *hc_in*: hydraulic conductivity [L/T] between the external source and the grid cell;

- *thick_in*: thickness [L] of the sediments between the external source and the grid cell.

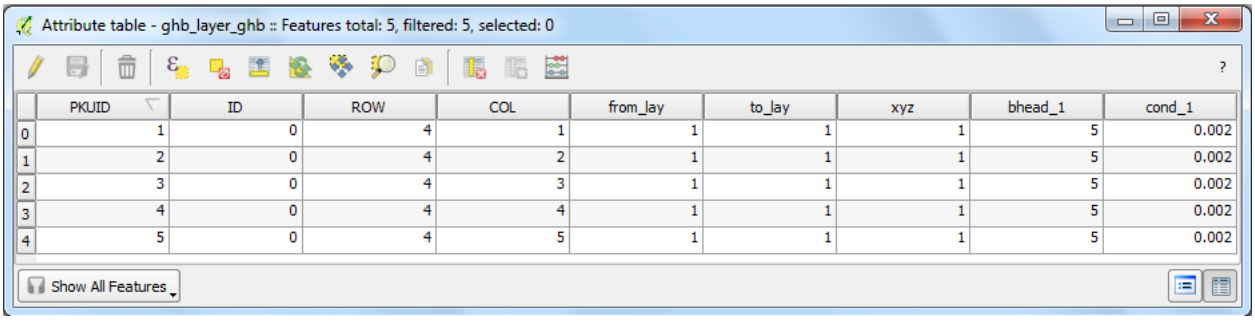
If loaded, the csv file must follow this structure.

A new MDO, named *ghb_layer_ghb*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

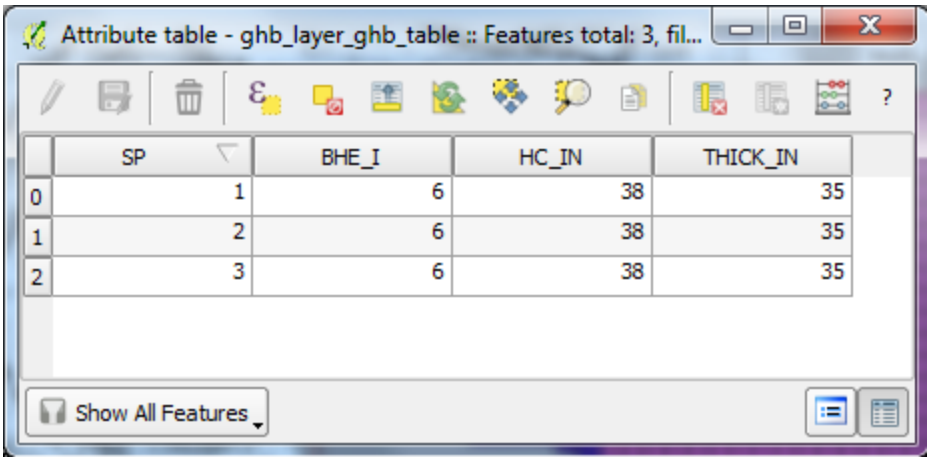
- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *from_lay*: number of the uppermost model layer to which this boundary condition is assigned;
- *to_lay*: number of the deepest model layer to which this boundary condition is assigned;
- *xyz*: number of the ghb segment;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *bhead_n*: head assigned to the external source [L] during the *n*-th SP;
  - *cond_n*: hydraulic conductance $[L^2/T]$ between the external source and each grid cell during the *n*-th SP.

The fields *from_lay*, *to_lay*, *xyz*, *bhead_n* and *cond_n* are filled with values assigned by the User when the *ghb_layer_ghb* MDO is created. The value of *cond_n* is automatically calculated depending on the cells geometry, their distance from the external source and the hydraulic conductivity between the external source and the grid cells (for details the reader is referred to the *MODFLOW-2005* manual, Harbaugh, 2005).



	PKUID	ID	ROW	COL	from_lay	to_lay	xyz	bhead_1	cond_1
0	1	0	4	1	1	1	1	5	0.002
1	2	0	4	2	1	1	1	5	0.002
2	3	0	4	3	1	1	1	5	0.002
3	4	0	4	4	1	1	1	5	0.002
4	5	0	4	5	1	1	1	5	0.002

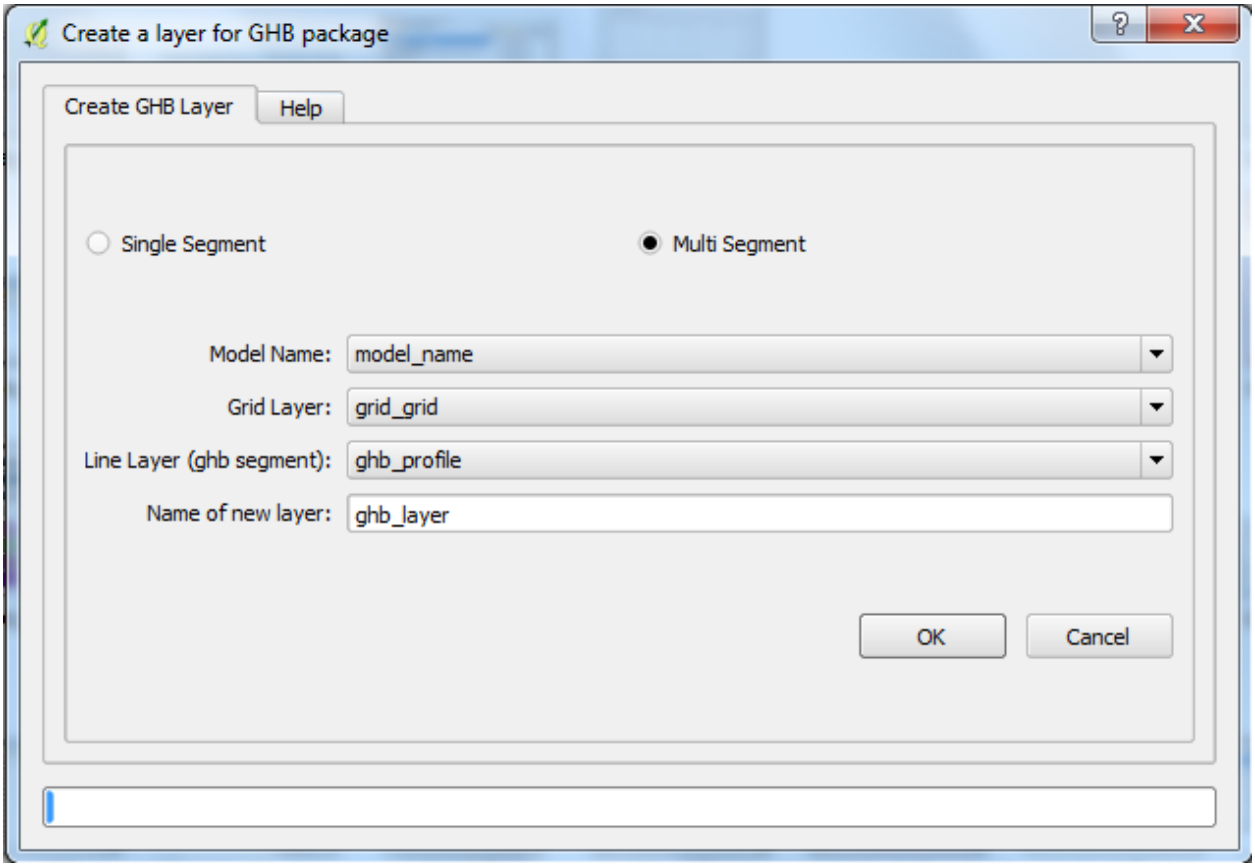
A table named *ghb_layer_ghb_table* is created with the ghb MDO, stored in the model DB and possibly loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters listed above.



Note: If the general-head boundary develops over more than one segment, the procedure described above must be repeated for each segment. In this case, pay attention to assign a different name in the *Name of new layer* field and to select the correct line shapefile in the *Line Layer (ghb segment)* field and use a progressive segment number in the *Ghb segment (xyz)* field. Once all the ghb MDOs have been created, the *Merge SpatiaLite layers* tool must be used to get a single MDO. The latter will then be used during the *Run* procedure.

If the *Multi Segment* option is checked, the following data are required in the **Create a layer for GHB package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer (ghb segment)*: line shapefile containing the profile of the multi ghb segment;
- *Name of new layer*: name of the ghb MDO which has to be created.

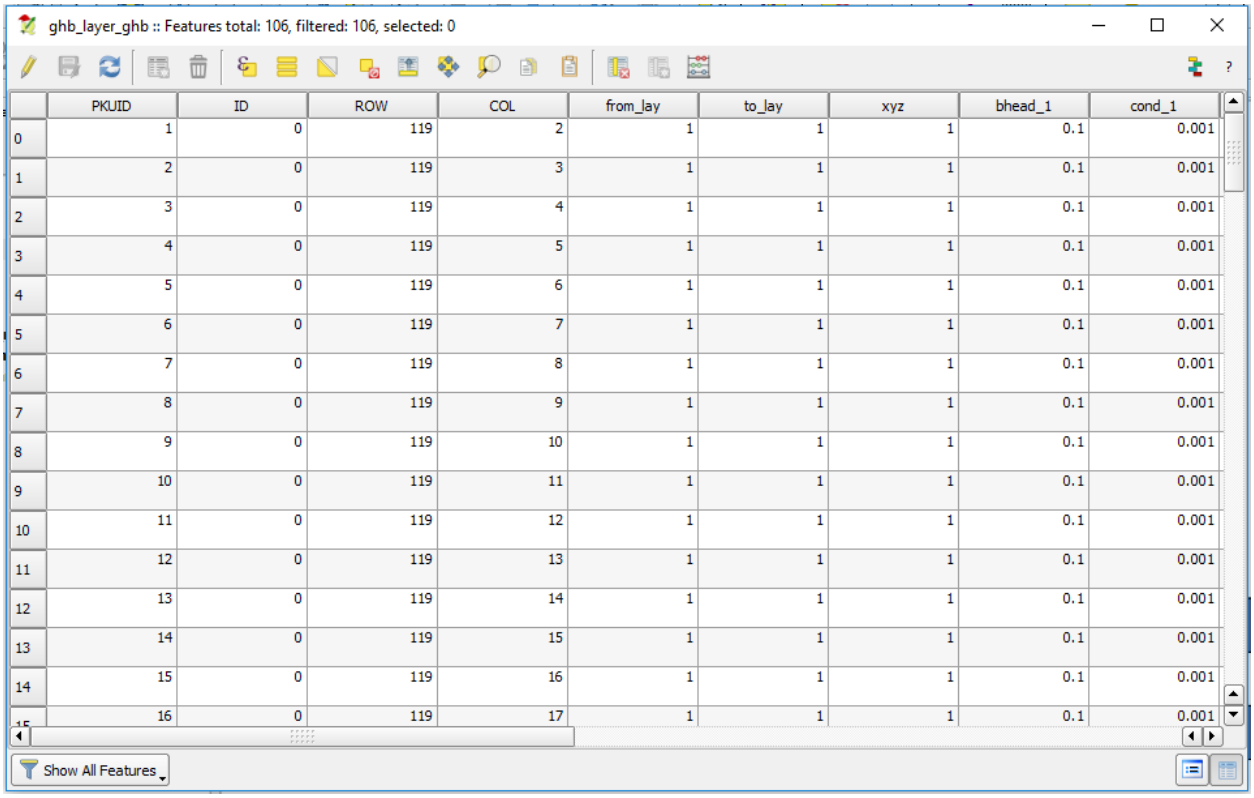


A new MDO, named *ghb_layer_ghb*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *from_lay*: number of the uppermost model layer to which this boundary condition is assigned;
- *to_lay*: number of the deepest model layer to which this boundary condition is assigned;
- *xyz*: number of the ghb segment;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *bhead_n*: head assigned to the external source [L] during the *n*-th SP;
  - *cond_n*: hydraulic conductance $[L^2/T]$ between the external source and each grid cell during the *n*-th SP.

The fields *from_lay*, *to_lay*, *elev_n* and *cond_n* are filled with default values. The field *xyz* is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.



	PKUID	ID	ROW	COL	from_lay	to_lay	xyz	bhead_1	cond_1
0	1	0	119	2	1	1	1	0.1	0.001
1	2	0	119	3	1	1	1	0.1	0.001
2	3	0	119	4	1	1	1	0.1	0.001
3	4	0	119	5	1	1	1	0.1	0.001
4	5	0	119	6	1	1	1	0.1	0.001
5	6	0	119	7	1	1	1	0.1	0.001
6	7	0	119	8	1	1	1	0.1	0.001
7	8	0	119	9	1	1	1	0.1	0.001
8	9	0	119	10	1	1	1	0.1	0.001
9	10	0	119	11	1	1	1	0.1	0.001
10	11	0	119	12	1	1	1	0.1	0.001
11	12	0	119	13	1	1	1	0.1	0.001
12	13	0	119	14	1	1	1	0.1	0.001
13	14	0	119	15	1	1	1	0.1	0.001
14	15	0	119	16	1	1	1	0.1	0.001
15	16	0	119	17	1	1	1	0.1	0.001

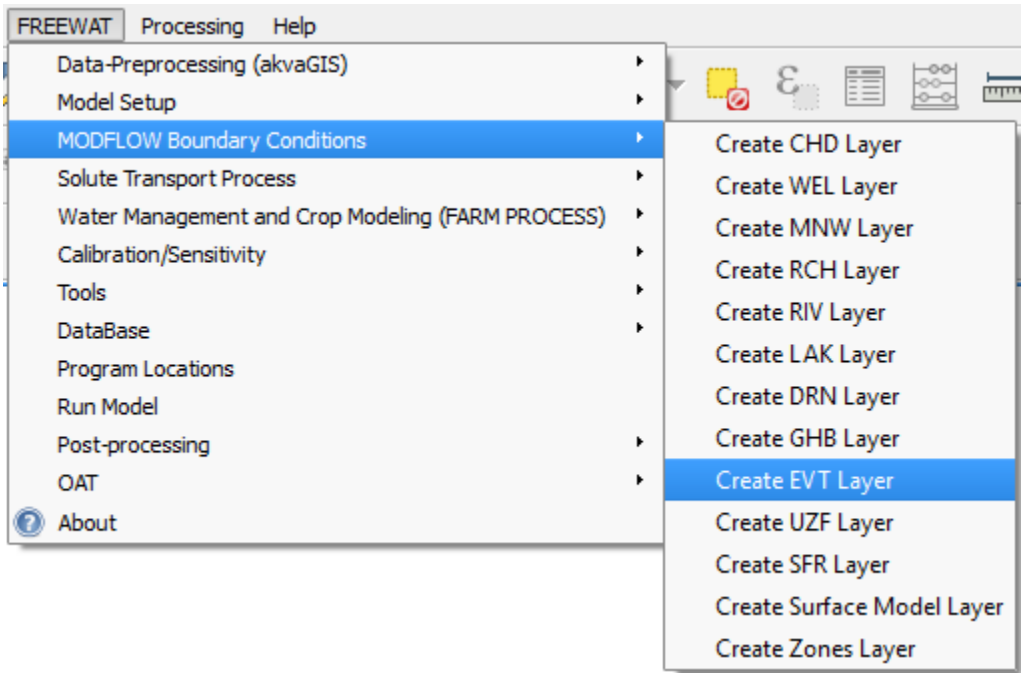
Evapotranspiration - EVT (head-dependent flux)

MODFLOW EVT Package allows to simulate areally-distributed evapotranspiration, as a result of plant transpiration and direct evaporation from groundwater.

Activating this Package does not require prior processing of a polygon shapefile, as this condition can be applied to all grid cells and it is possible to deactivate evapotranspiration at some grid cells, by using *QGIS* selection and editing tools described in Chapter 5.

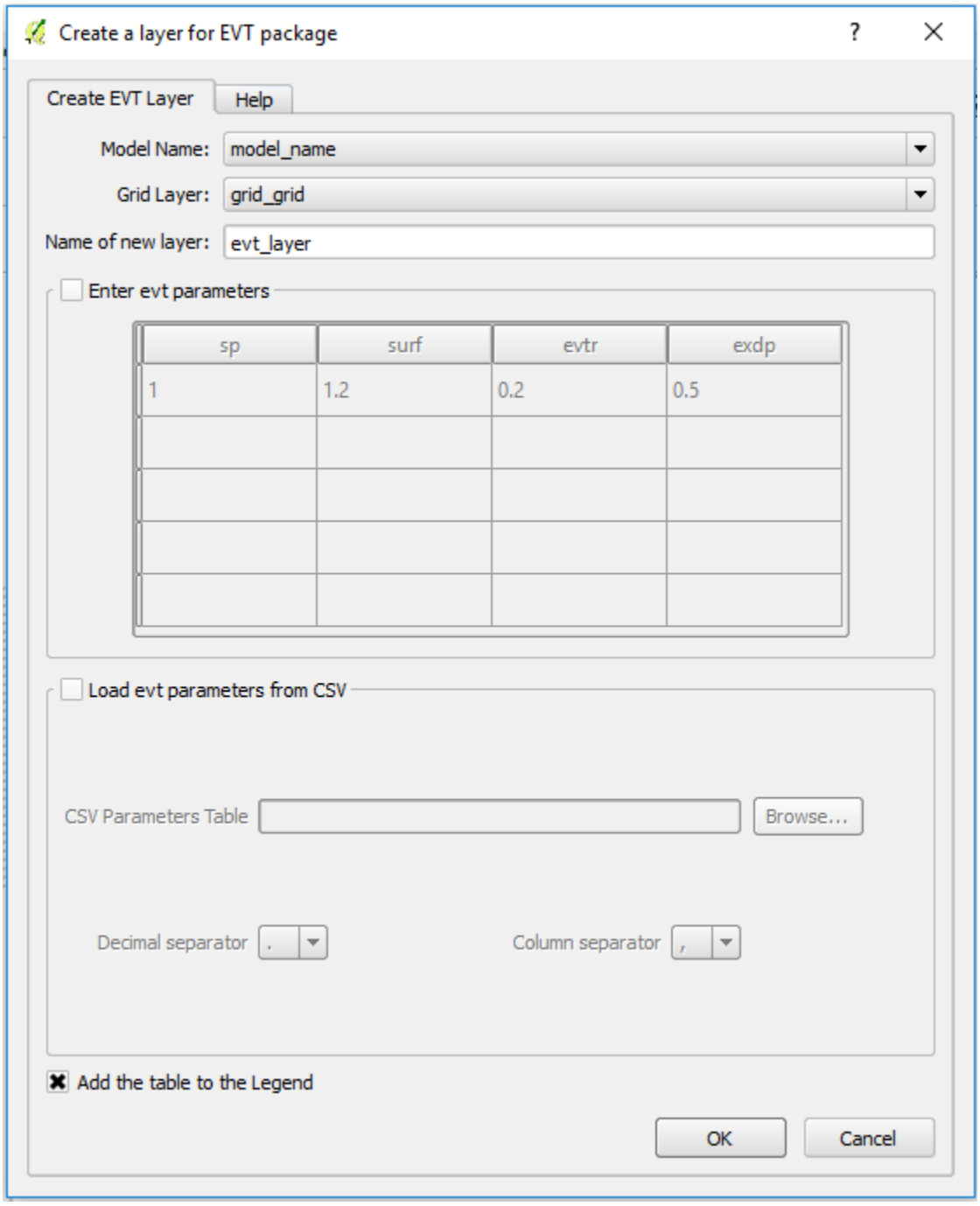
To activate the *EVT Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create EVT Layer.



The following data are required in the **Create a layer for EVT package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Name of new layer*: name of the evt MDO which has to be created;
- if *Enter evt parameters* is checked, the user can fill manually the table with all the parameters necessary to activate this Package;
- if *Load evt parameters from CSV* is checked, the user can load a csv file containing parameters necessary to activate this Package, using the *Browse...* button (field *CSV Parameters Table*). In this case, the user must define the *Decimal separator* and *Column separator* used in the csv file loaded;
- if *Add the table to the Legend* is checked, a table containing the evt parameters assigned in loaded in the Layers Panel.



Parameters required when creating the evt MDO must be assigned for each SP:

- *sp*: SP number;
- *surf*: elevation [L] of the evapotranspiration surface;
- *evtr*: maximum evapotranspiration flux [L/T];
- *exdp*: evapotranspiration extintion depth [L].

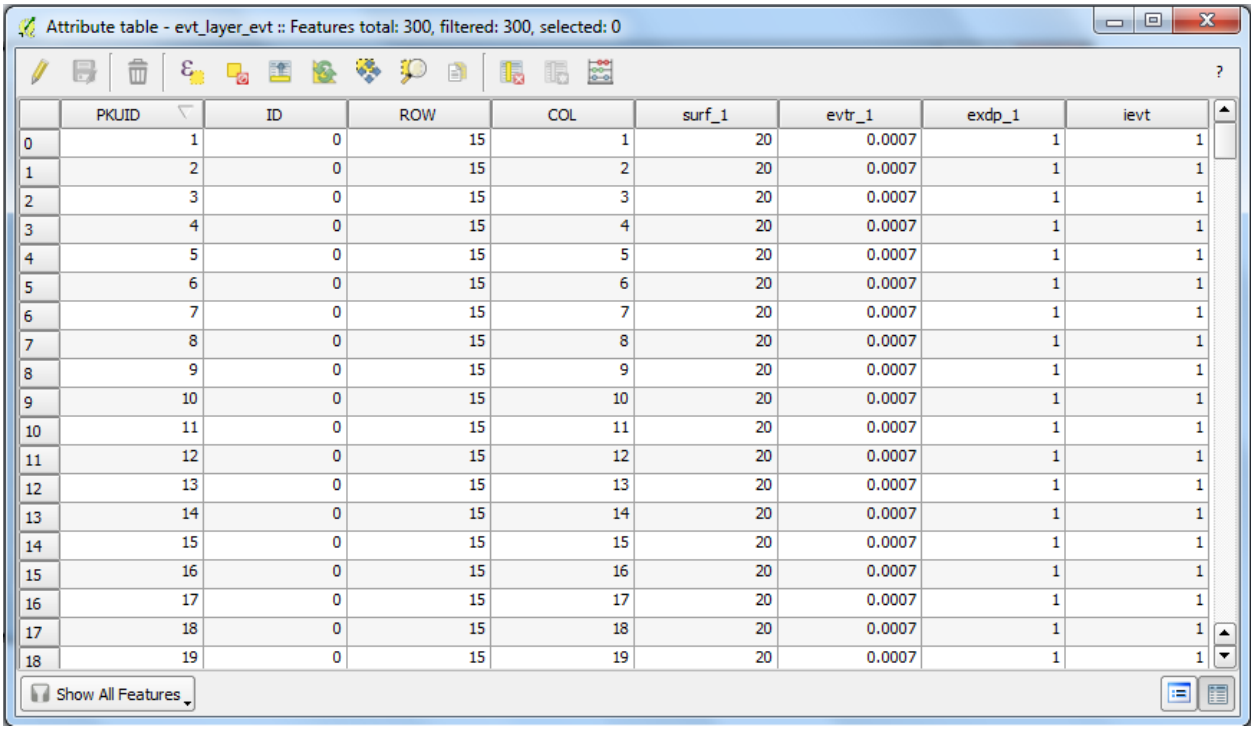
If loaded, the csv file must follow this structure.

A new MDO, named *evt_layer_evt*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *surf_n*: elevation [L] of the evapotranspiration surface during the *n*-th SP;
  - *evtr_n*: maximum evapotranspiration flux [L/T] during the *n*-th SP;
  - *exdp_n*: evapotranspiration extintion depth [L] during the *n*-th SP;
  - *ievt_n*: number of the layer where the evapotranspiration will be applied during the *n*-th SP.

The fields *surf_n*, *evtr_n*, *exdp_n* and *ievt_n* are filled with values assigned by the User when the *evt_layer_evt* MDO is created.



	PKUID	ID	ROW	COL	surf_1	evtr_1	exdp_1	ievt
0	1	0	15	1	20	0.0007	1	1
1	2	0	15	2	20	0.0007	1	1
2	3	0	15	3	20	0.0007	1	1
3	4	0	15	4	20	0.0007	1	1
4	5	0	15	5	20	0.0007	1	1
5	6	0	15	6	20	0.0007	1	1
6	7	0	15	7	20	0.0007	1	1
7	8	0	15	8	20	0.0007	1	1
8	9	0	15	9	20	0.0007	1	1
9	10	0	15	10	20	0.0007	1	1
10	11	0	15	11	20	0.0007	1	1
11	12	0	15	12	20	0.0007	1	1
12	13	0	15	13	20	0.0007	1	1
13	14	0	15	14	20	0.0007	1	1
14	15	0	15	15	20	0.0007	1	1
15	16	0	15	16	20	0.0007	1	1
16	17	0	15	17	20	0.0007	1	1
17	18	0	15	18	20	0.0007	1	1
18	19	0	15	19	20	0.0007	1	1

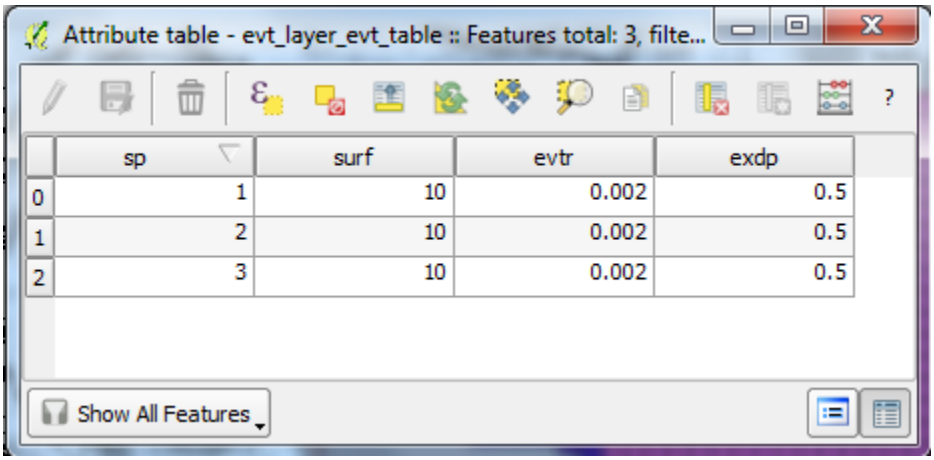
Note: Notice that *evtr_n* is actually a specified rate, rather than a flux. Such specified rate is then automatically multiplied by the area of the grid cell [L^2] to get a specified flux [L^3/T].

Note: To deactivate evapotranspiration at some cells during SP *n*, it is necessary to select the involved cells and set *evtr_n* to *0*.

Note: Editing *ievt* is only required when evapotranspiration has to be applied to a grid cell other than the one belonging

to model layer 1 or the uppermost active one in the vertical column. More details will be provided in Chapter 7.

A table named *evt_layer_evt_table* is created with the evt MDO, stored in the model DB and possibly loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters listed above.



	sp	surf	evtr	exdp
0	1	10	0.002	0.5
1	2	10	0.002	0.5
2	3	10	0.002	0.5

Unsaturated-Zone Flow Package - UZF

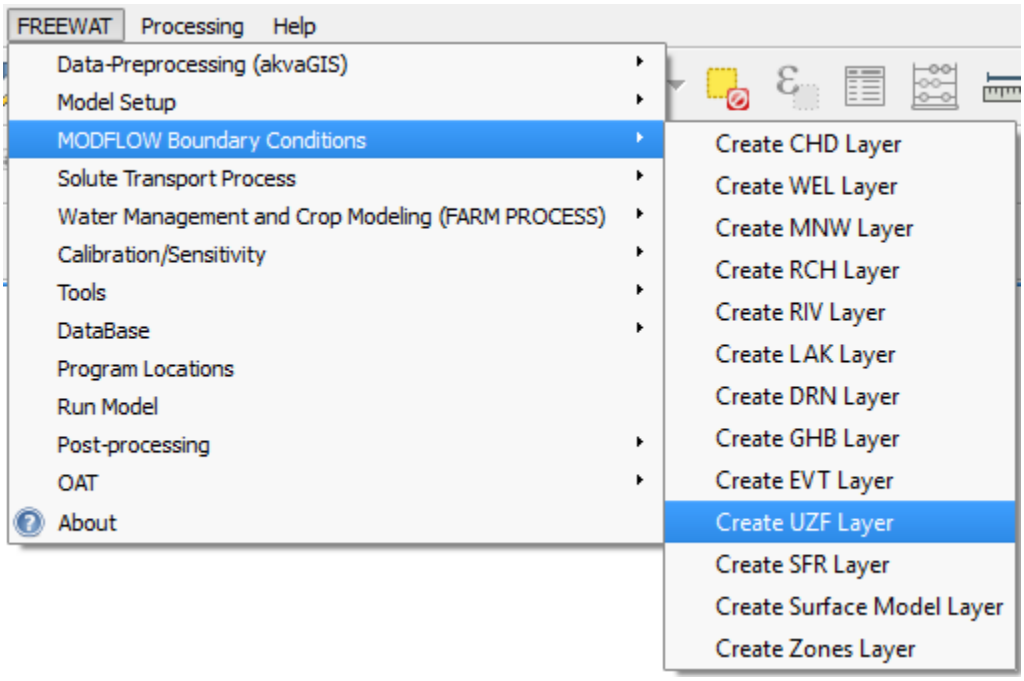
MODFLOW UZF Package allows to simulate vertical flow of water through the unsaturated zone, by etimating the evapotransporation and effective infiltration to groundwater using the land surface precipitation. This Package also allows the estimation of direct runoff to surface waterways. If the UZF Package is used, RCH and EVT Packages should not be activated. Implementing the module UZF requires the creation of two MDOs: the uzf and the Surface Model Layer MDOs.

Activating this Package does not require prior processing of a polygon shapefile, as this condition can be applied to all grid cells and it is possible to deactivate evapotranspiration and recharge at some grid cells, by using *QGIS* selection and editing tools described in Chapter 5.

Creating the uzf MDO

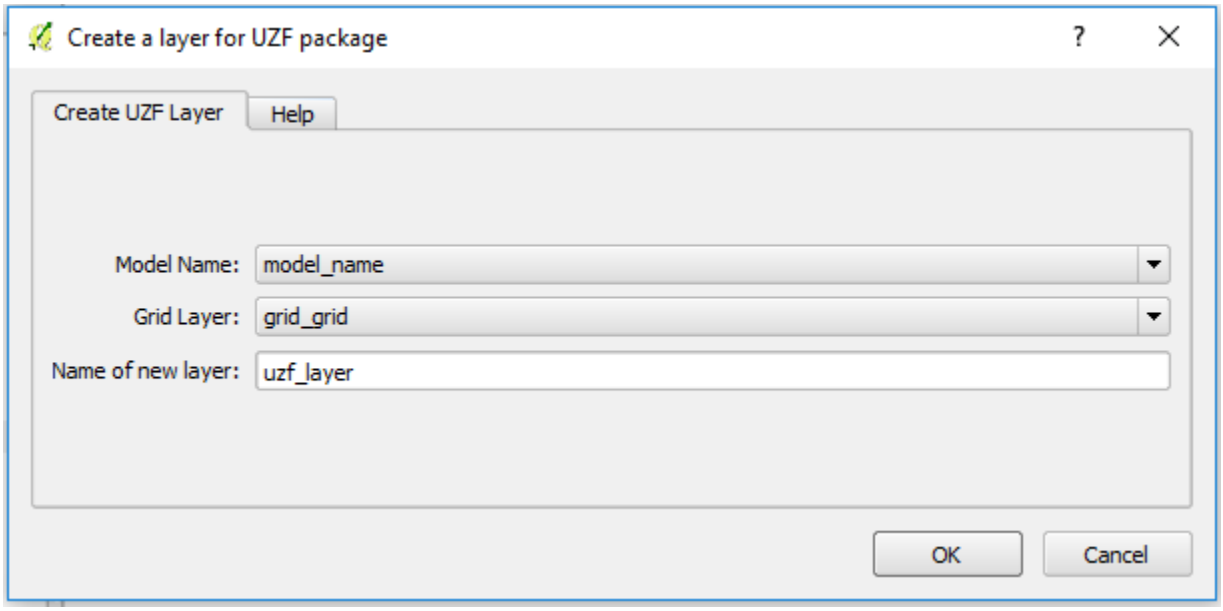
To activate the *UZF Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create UZF Layer.



The following data are required in the **Create a layer for UZF package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Name of new layer*: name of the uzf MDO which has to be created.



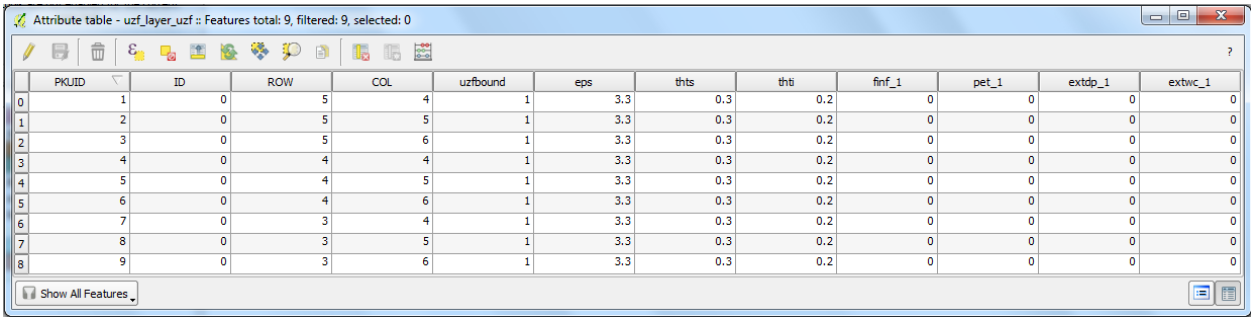
A new MDO, named *uzf_layer_uzf*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);

- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *iuzfbnd*: integer value used to define the aerial extent of the active domain in which recharge and discharge will be simulated: it must be set to *0* in cells where recharge and discharge will not be simulated, otherwise its value indicates to which model layer recharge and discharge will occur;
- *eps*: Brooks-Corey epsilon of the unsaturated zone to calculate the water content;
- *thts*: saturated water content of the unsaturated zone in units of volume of water to total volume;
- *thti*: initial water content for each vertical column of cells in units of volume of water at the beginning of simulation to total volume;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *finf_n*: infiltration rate [L/T] at land surface during the *n*-th SP;
  - *pet_n*: ET demand rate [L/T] within the ET extinction depth interval during the *n*-th SP;
  - *extdp_n*: ET extintion depth [L] during the *n*-th SP;
  - *extwc_n*: extinction water content below which ET cannot be removed from the unsaturated zone, defined during the *n*-th SP.

The fields *iuzfbnd*, *eps*, *thts*, *thti*, *finf_n*, *pet_n*, *extdp_n* and *extwc_n* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5.



	PKUID	ID	ROW	COL	uzfbound	eps	thts	thti	finf_1	pet_1	extdp_1	extwc_1
0	1	0	5	4	1	3.3	0.3	0.2	0	0	0	0
1	2	0	5	5	1	3.3	0.3	0.2	0	0	0	0
2	3	0	5	6	1	3.3	0.3	0.2	0	0	0	0
3	4	0	4	4	1	3.3	0.3	0.2	0	0	0	0
4	5	0	4	5	1	3.3	0.3	0.2	0	0	0	0
5	6	0	4	6	1	3.3	0.3	0.2	0	0	0	0
6	7	0	3	4	1	3.3	0.3	0.2	0	0	0	0
7	8	0	3	5	1	3.3	0.3	0.2	0	0	0	0
8	9	0	3	6	1	3.3	0.3	0.2	0	0	0	0

Note: Notice that *finf_n* and *pet_n* are actually specified rates, rather than fluxes. Such specified rates are then automatically multiplied by the area of the grid cell [L^2] to get specified fluxes [L^3/T].

Note: To deactivate uzf at some cells, it is necessary to select the involved cells and set *iuzfbnd* to *0*, so that recharge and discharge through the unsaturated zone will not be simulated.

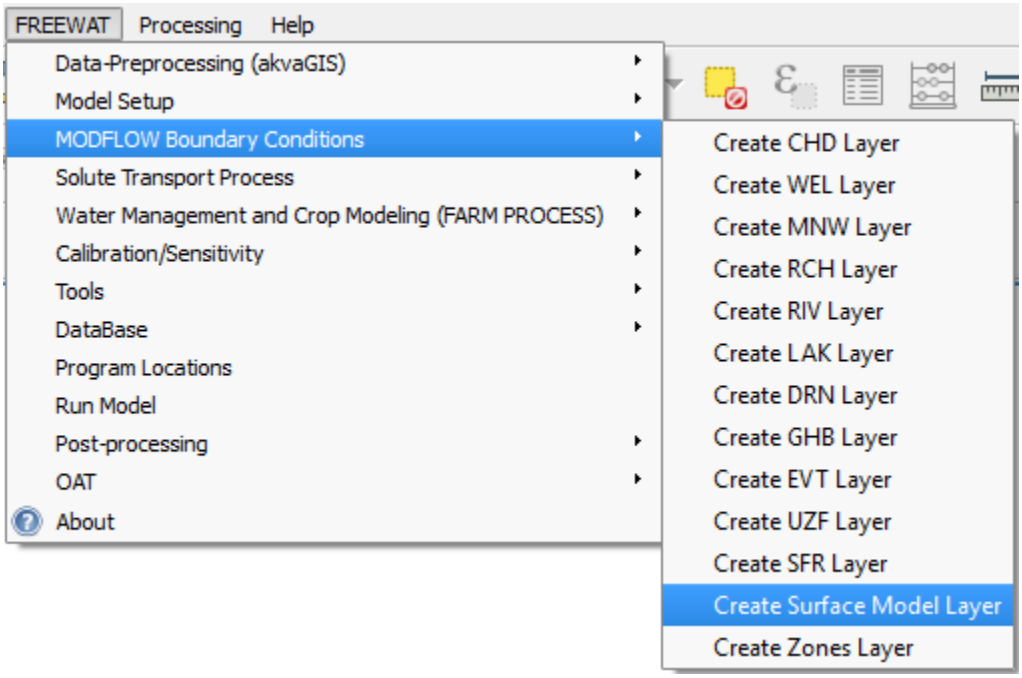
Note: Editing *iuzfbnd* is only required when recharge and discharge has to be applied to a grid cell other than the one belonging to model layer 1 or the uppermost active one in the vertical column. More details will be provided in Chapter 7.

Creating the Surface Model Layer MDO

Creating the Surface Model Layer (sml) is necessary only if the UZF Package has to be coupled with the SFR to address runoff. Of course, if the SFR Package is activated, but the Surface Model Layer is not implemented, no runoff will be relocated to the SFR segments.

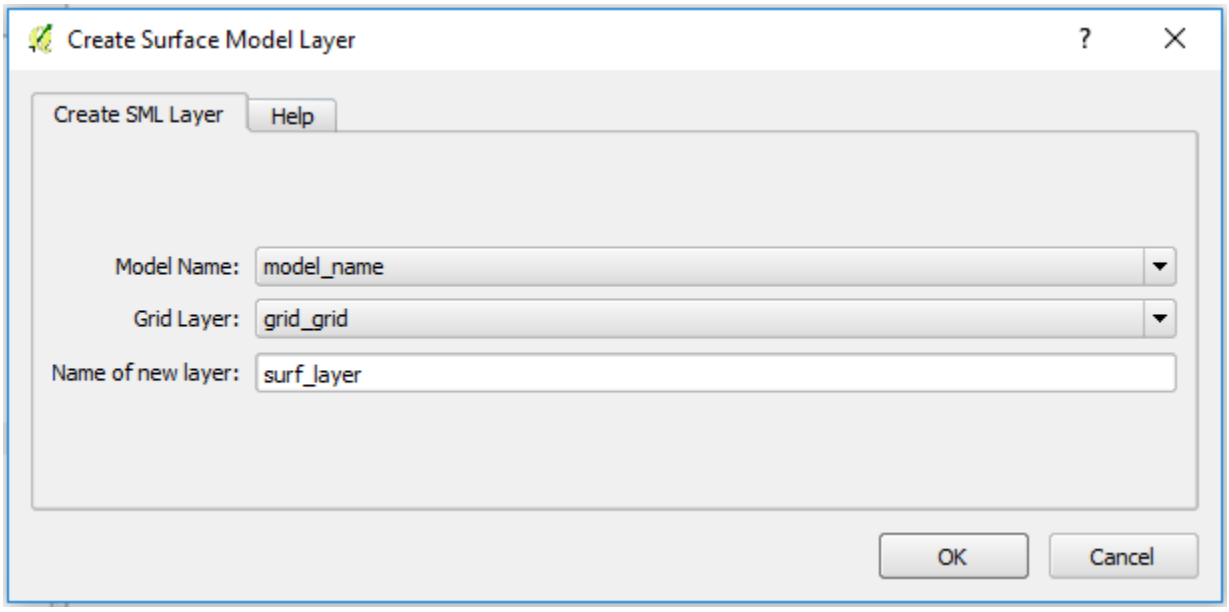
To define the *Surface Model Layer* the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create Surface Model Layer.



The following data are required in the **Create Surface Model Layer** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Name of new layer*: name of the sml MDO which has to be created.

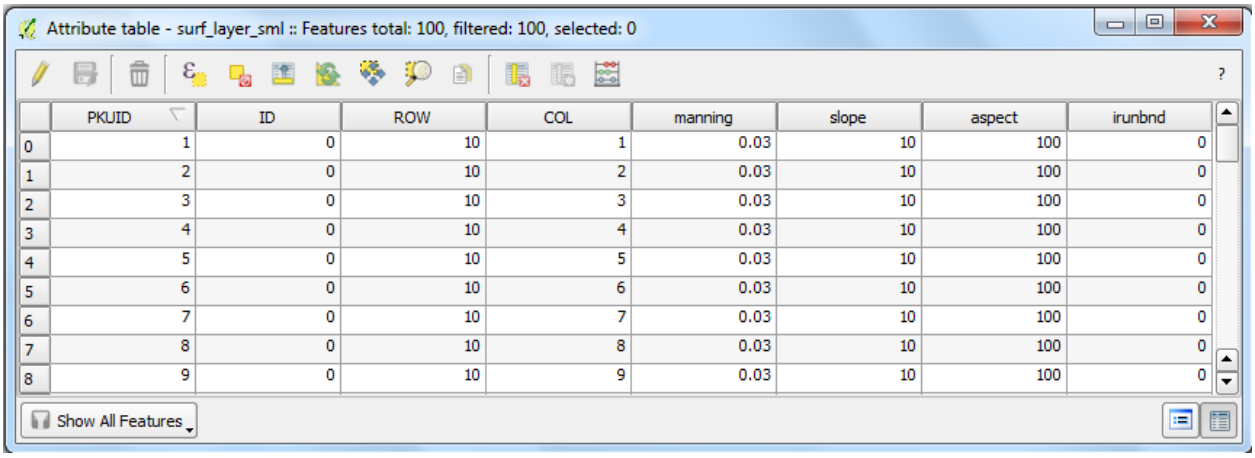


A new MDO, named *surf_layer_sml*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *manning*: Manning's roughness coefficient;
- *slope*: slope of the bottom of the cell;
- *aspect*: aspect value for the cell;
- *irunbnd*: integer value used to define the stream segment to which run off will be addressed.

The fields *manning*, *slope*, *aspect*, and *irunbnd* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5.



	PKUID	ID	ROW	COL	manning	slope	aspect	irunbnd
0	1	0	10	1	0.03	10	100	0
1	2	0	10	2	0.03	10	100	0
2	3	0	10	3	0.03	10	100	0
3	4	0	10	4	0.03	10	100	0
4	5	0	10	5	0.03	10	100	0
5	6	0	10	6	0.03	10	100	0
6	7	0	10	7	0.03	10	100	0
7	8	0	10	8	0.03	10	100	0
8	9	0	10	9	0.03	10	100	0

Limitations

The UZF Package has the following limitations, which can be overcome only by editing the uzf *MODFLOW* input file and running the model independently on the *FREEWAT* platform (for details refer to Niswonger et al., 2006):

- the vertical hydraulic conductivity is the same as defined in the *KZ* field of the relative model layer (*MODFLOW* flag *IUZFOPT=2*). As such, variables *UHC1* and *UHC2* are optional when using the SFR Package and the unsaturated-zone flow is simulated beneath the streams (refer to the *MODFLOW-2005* manual, Harbaugh, 2005);
- the number of trailing waves used to define the water-content profile following a decrease in the infiltration rate (*MODFLOW* variable *NTRAIL2*) is set to *10* as a default value;
- the number of wave sets used to simulate multiple infiltration periods (*MODFLOW* variable *NSETS2*) is set to *20* as a default value;
- the possibility to specify the number of cells for printing detailed information on the unsaturated zone water budget and water content is not available (*MODFLOW* flag *NUZGAG=0*);
- the average height of undulations in the land surface altitude (*MODFLOW* variable *SURFDEP*) is set to *0.2* m as a default value.

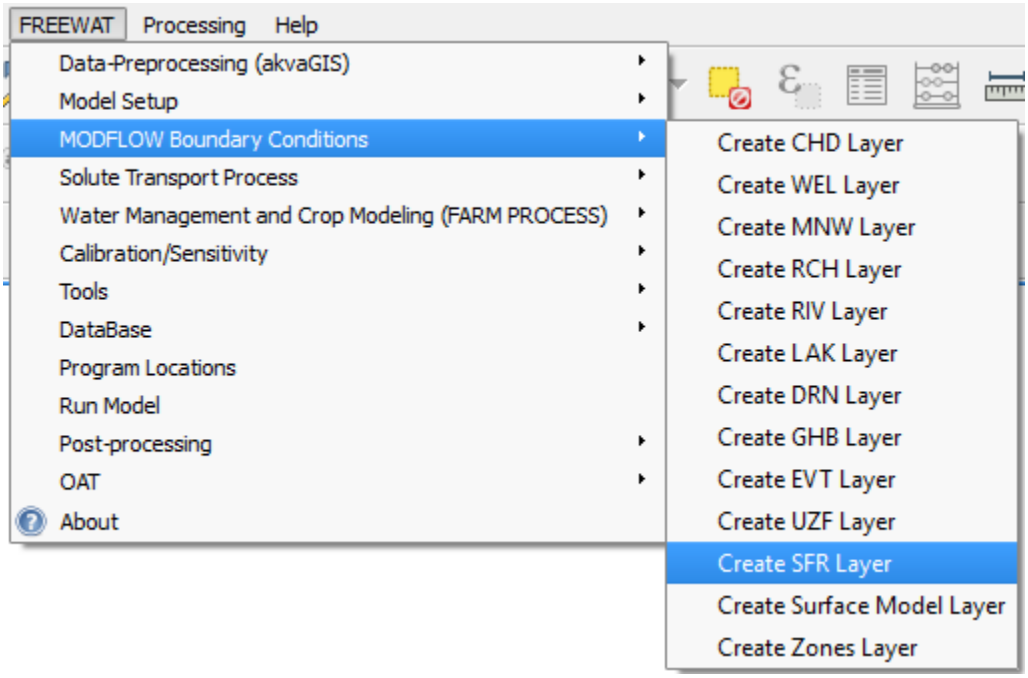
Streamflow-Routing Package - SFR

MODFLOW SFR Package allows to simulate streamflow to downstream streams using a kinematic wave equation. Unsaturated flow beneath streams can be simulated as well.

Activating this Package requires prior processing of a line shapefile, containing the profile of the stream within the study area.

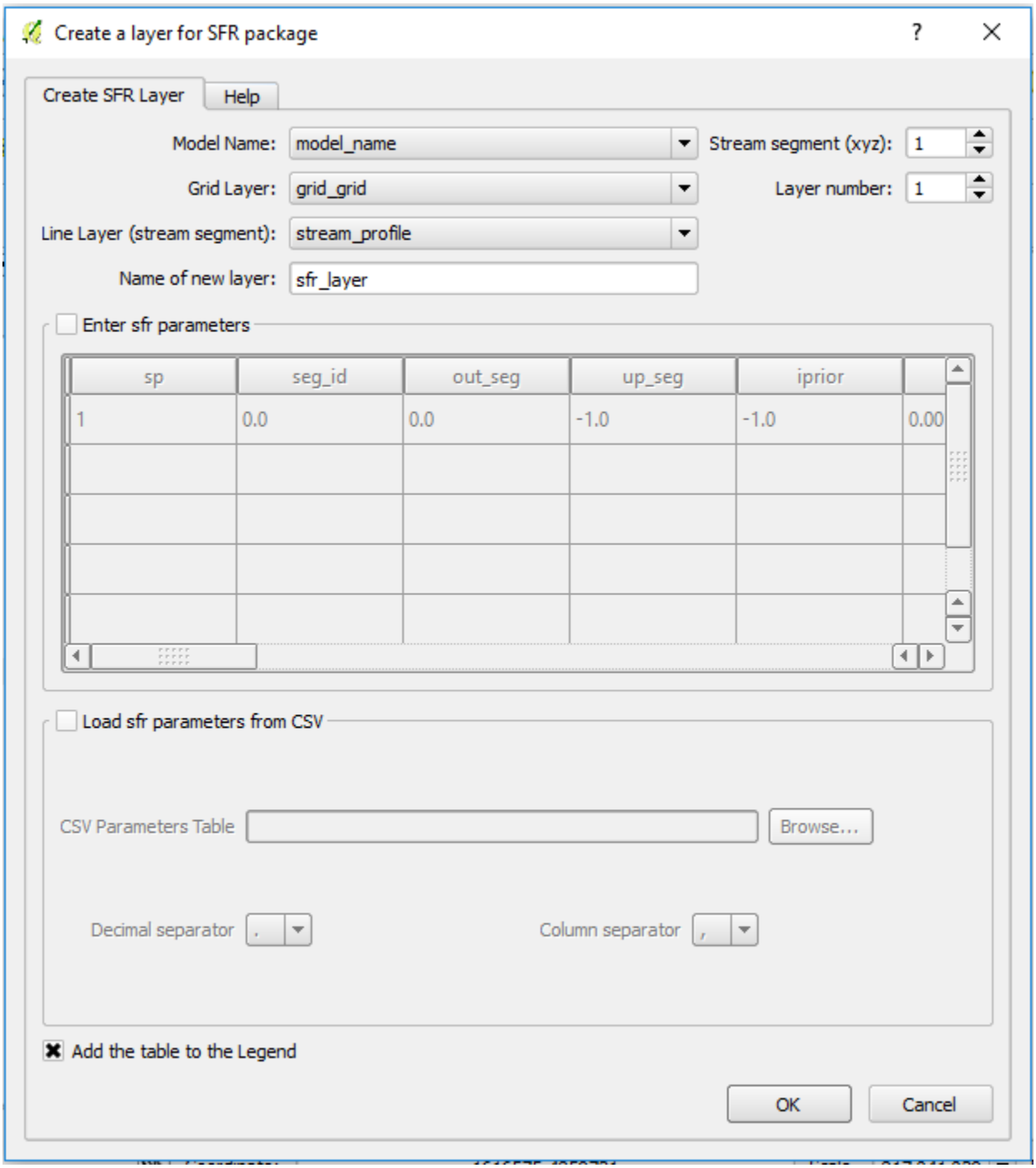
Once the line shapefile is loaded in the Layers Panel, to activate the *SFR Package* the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create SFR Layer.



The following data are required in the **Create a layer for SFR package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer (stream segment)*: line shapefile containing the profile of the stream segment;
- *Name of new layer*: name of the sfr MDO which has to be created;
- *Stream segment (xyz)*: number of the stream segment;
- *Layer number*: number of the model layer to which this Package is applied;
- if *Enter sfr parameters* is checked, the user can fill manually the table with all the necessary parameters to be assigned to grid cells where this Package is applied;
- if *Load sfr parameters from CSV* is checked, the user can load a csv file containing parameters to be assigned to grid cells where this Package is applied, using the *Browse...* button (field *CSV Parameters Table*). In this case, the user must define the *Decimal separator* and *Column separator* used in the csv file loaded;
- if *Add the table to the Legend* is checked, a table containing the sfr parameters assigned in loaded in the Layers Panel.



Parameters required when creating the sfr MDO must be assigned at the upstream and downstream cells of the stream segment and for each SP:

- *sp*: SP number;
- *seg_id*: stream segment ID;
- *out_seg*: ID of the stream segment located downstream with respect to the current stream segment;
- *up_seg*: ID of the stream segment located upstream with respect to the current stream segment;
- *iprior*: priority flag of the diversion (used only if *up_seg* is not *0*);

- *flow*: inflow [L^3/T] at the upstream reach of the current stream segment;
- *runoff*: incoming runoff [L^3/T] at each reach of the current stream segment;
- *etsw*: volumetric rate per unit area of water removed by evapotranspiration directly from the stream channel [L/T] (positive value);
- *pptsw*: volumetric rate per unit area of water added by precipitation directly on the stream channel [L/T];
- *roughch*: Manning's roughness coefficient;
- *hcond1*: hydraulic conductivity [L/T] of the streambed at the upstream reach of the current segment;
- *thickm1*: thickness [L] of streambed material at the upstream reach of the current segment;
- *elevup*: elevation [L] of the top of the streambed at the upstream reach of the current segment;
- *width1*: average width [L] of the stream channel at the upstream reach of the current segment;
- *thts1*: saturated volumetric water content in the unsaturated zone beneath the upstream reach of the current segment;
- *thti1*: initial volumetric water content beneath the upstream reach of the current segment;
- *eps1*: Brooks-Corey exponent used in the relation between water content and hydraulic conductivity within the unsaturated zone beneath the upstream reach of the current segment;
- *hcond2*: hydraulic conductivity [L/T] of the streambed at the downstream reach of the current segment;
- *thickm2*: thickness [L] of streambed material at the downstream reach of the current segment;
- *elevdn*: elevation [L] of the top of the streambed at the downstream reach of the current segment;
- *width2*: average width [L] of the stream channel at the downstream reach of the current segment;
- *thts2*: saturated volumetric water content in the unsaturated zone beneath the downstream reach of the current segment;
- *thti2*: initial volumetric water content beneath the downstream reach of the current segment;
- *eps2*: Brooks-Corey exponent used in the relation between water content and hydraulic conductivity within the unsaturated zone beneath the downstream reach of the current segment.

If loaded, the csv file must follow this structure.

A new MDO, named *sfr_layer_sfr*, is created, stored within the model DB and loaded in the Layers Panel.

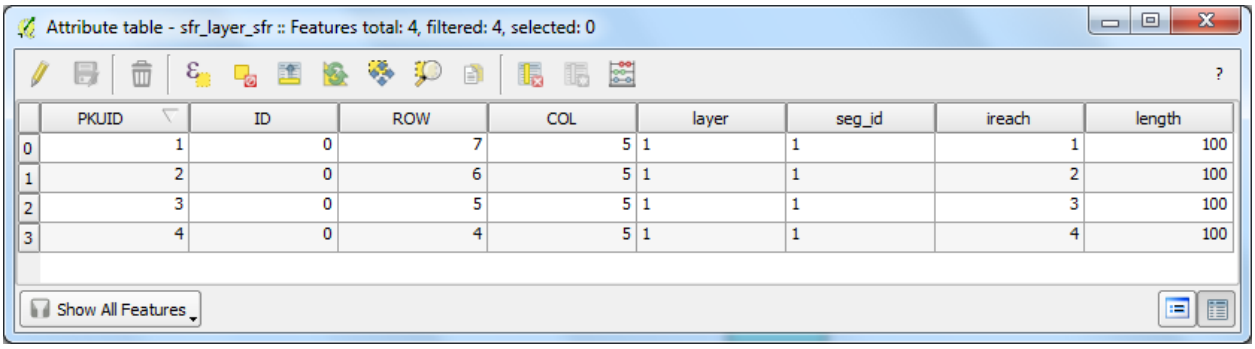
The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- *layer*: number of the model layer to which the stream is in contact;
- *seg_id*: number of the stream segment;
- *ireach*: ID number of a stream reach belonging to a certain stream segment;
- *length*: length [L] of the stream segment within a grid cell.

Note: Numbering of reaches in a segment begins with 1 for the farthest upstream reach and continues sequentially in downstream order to the last reach of the segment. For this reason, pay attention while editing the line shapefile

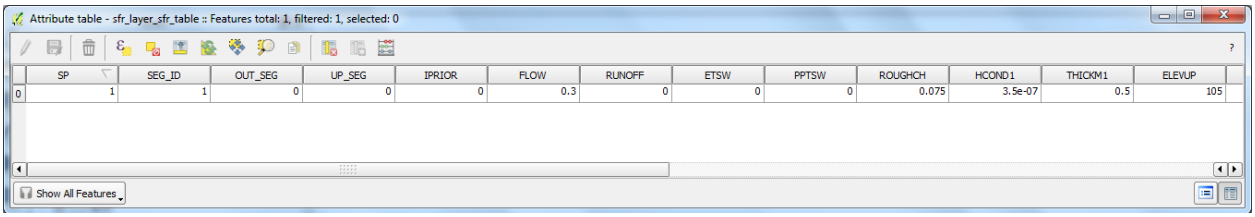
containing the profile of the stream segment: the edit must start from the farthest upstream cell and end to the last downstream one.

The fields *layer* and *seg_id*, are filled with values assigned by the user when the *sfr_layer_sfr* MDO is created. The field *ireach* is automatically filled depending on the editing order of the line shapefile. Also, the values of *length* within each grid cell are automatically calculated according to the portion of the stream segment which intersects a grid cell.



	PKUID	ID	ROW	COL	layer	seg_id	ireach	length
0	1	0	7	5	1	1	1	100
1	2	0	6	5	1	1	2	100
2	3	0	5	5	1	1	3	100
3	4	0	4	5	1	1	4	100

A table named *sfr_layer_sfr_table* is created with the sfr MDO, stored in the model DB and possibly loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters listed above.



	SP	SEG_ID	OUT_SEG	UP_SEG	IPRIOR	FLOW	RUNOFF	ETSW	PPTSW	ROUGHCH	HCOND1	THICKM1	ELEVUP
0	1	1	0	0	0	0.3	0	0	0	0.075	3.5e-07	0.5	105

Note: If the stream develops over more than one segment, the procedure described above must be repeated for each segment. In this case, pay attention assign a different name in the *Name of new layer* field and to select the correct line shapefile in the *Line Layer (stream segment)* field and use a progressive segment number in the *Stream segment (xyz)* field. Once all the sfr MDOs have been created, the *Merge SpatiaLite layers* tool must be used to get a single MDO and a single table. The latter will then be used during the *Run* procedure.

Limitations

The SFR Package has the following limitations, which can be overcome only by editing the sfr *MODFLOW* input file and running the model independently on the *FREEWAT* platform (for details refer to Niswonger and Prudic, 2005):

- stream depth is calculated using Manning's equation and assuming a wide rectangular channel (*MODFLOW* flag *ICALC=1*);
- the number of trailing waves used to define the water-content profile following a decrease in the infiltration rate (*MODFLOW* variable *NSTRAIL*) is set to *10* as a default value;
- the number of wave sets used to simulate multiple infiltration periods (*MODFLOW* variable *NSFRSETS*) is set to *30* as a default value;
- transient streamflow routing is simulated using the kinematic-wave equation (*MODFLOW* flag *IRTFLG>0*);
- if the flow in the unsaturated zone beneath stream is not simulated, streambed elevation, thickness and hydraulic conductivity must be defined at each SP (*MODFLOW* flag *ISFROPT=0*);

- if the flow in the unsaturated zone beneath stream is simulated, streambed and unsaturated zone properties must be defined at the upstream and downstream reaches of each segment and at each SP. Furthermore, saturated vertical hydraulic conductivity for the unsaturated zone is the same as the vertical hydraulic conductivity defined in the lpf *MODFLOW* input file (*MODFLOW* flag *ISFROPT=4*). If *ISFROPT=4*, values assigned to variables *thts1*, *thts2*, *thti1*, *thti2*, *eps1* and *eps2* are not read.

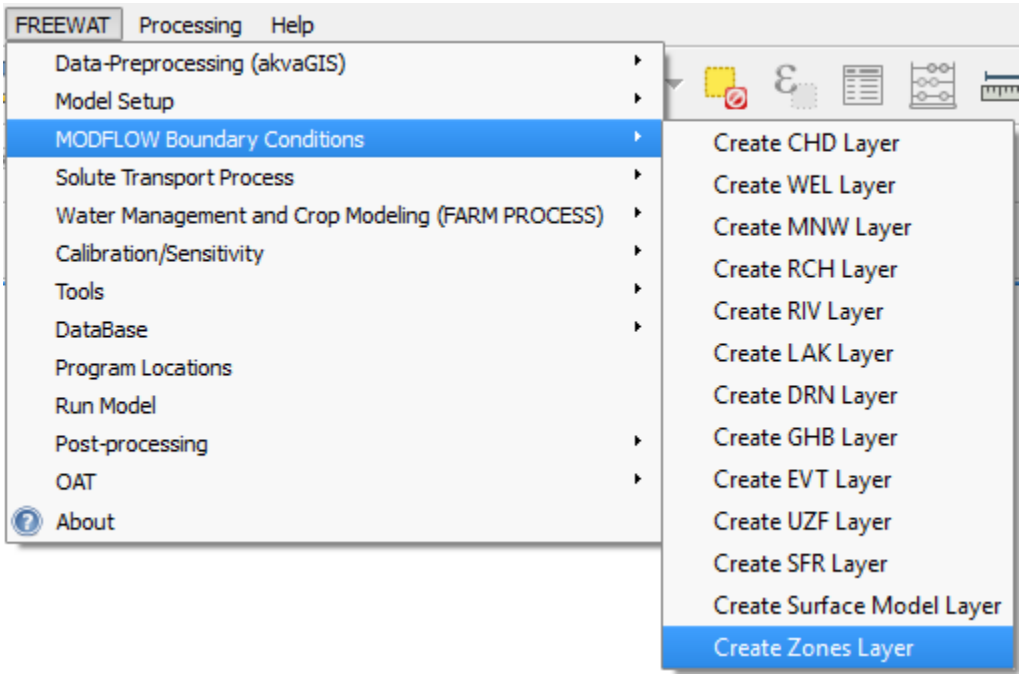
Zone Budget - ZONBUD

Zonebudget (ZONBUD) is a computer program that computes sub-regional water budgets using results from the *MODFLOW* groundwater flow model. The User must define the sub-regions by specifying zone numbers. A separate budget is computed for each zone and includes also a component of flow between each adjacent zone.

Activating this Package does not require prior processing of a polygon shapefile, as this condition can be applied to all grid cells and the User can define zones by using *QGIS* selection and editing tools described in Chapter 5.

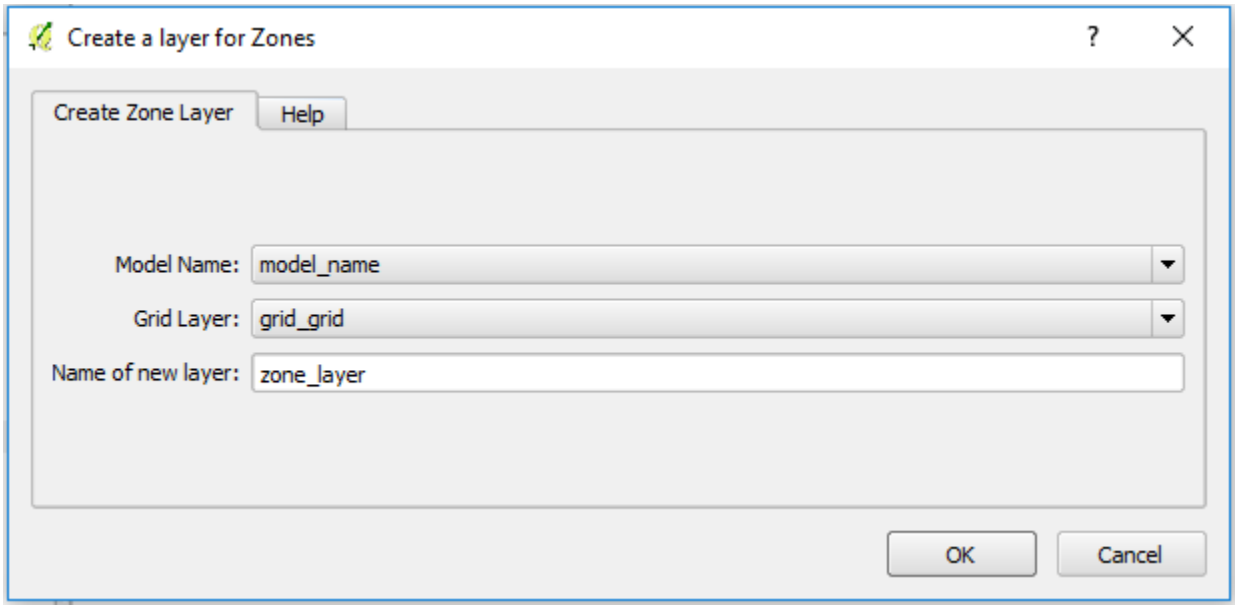
To activate the *ZONBUD*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create Zones Layer.



The following data are required in the **Create a layer for Zones** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Name of new layer*: name of the zonbud MDO which has to be created.

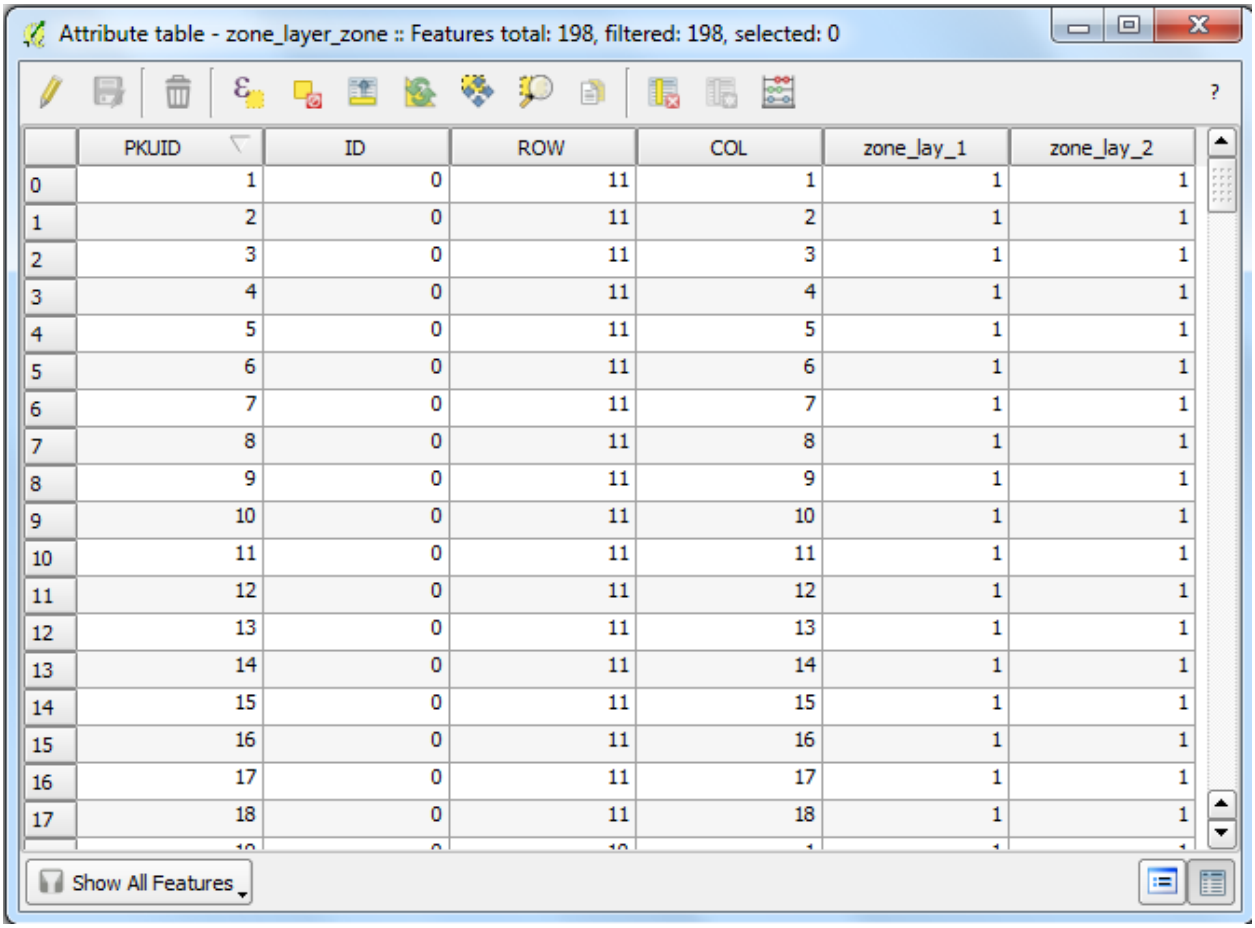


A new MDO, named *zone_layer_zone*, is created, stored within the model DB and loaded in the Layers Panel.

The Attribute Table of such MDO may contain several records, according to the number of grid cells, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row number of a grid cell;
- *COL*: column number of a grid cell;
- the following field is repeated according to the number of model layers implemented (*n* refers to the number of a model layer):
  - *zone_lay_n*: integer zone number within each cell of the *n*-th model layer.

The field *zone_lay_n* is filled with a default value, which can be modified using *QGIS selection and editing tools described in Chapter 5.



	PKUID	ID	ROW	COL	zone_lay_1	zone_lay_2
0	1	0	11	1	1	1
1	2	0	11	2	1	1
2	3	0	11	3	1	1
3	4	0	11	4	1	1
4	5	0	11	5	1	1
5	6	0	11	6	1	1
6	7	0	11	7	1	1
7	8	0	11	8	1	1
8	9	0	11	9	1	1
9	10	0	11	10	1	1
10	11	0	11	11	1	1
11	12	0	11	12	1	1
12	13	0	11	13	1	1
13	14	0	11	14	1	1
14	15	0	11	15	1	1
15	16	0	11	16	1	1
16	17	0	11	17	1	1
17	18	0	11	18	1	1

Note: To run the *Zonebudget*, a specific executable is required, as stated in Chapter 7. Further details will be provided in Chapter 8.

CHAPTER 7

MODFLOW input files and model run

All the data so far implemented (i.e., the geometry of the domain, the hydrodynamic properties of the hydrogeological system and the discretization of the involved processes) are stored within the model DB in a format which cannot be directly processed by the simulation code. Before running the model is so necessary to translate such datasets in model files which can be read by the numerical code. In *FREEWAT*, such procedure is authomatically performed when the simulation is run.

Hereinafter, a quick list of the *MODFLOW* input files which can be generated is provided. For further details the reader is suggested to refer to the MODFLOW online guide.

The following are basic model files required for any simulation:

- **Name (.NAM) file**: it contains a list of all the input and output files involved in the current simulation;
- **Basic Package (.BAS) file**: it reports the fields *ACTIVE* and *STRT* for each model layer;
- **Discretization (.DIS) file**: it reports information stored in the table *timetable_model_name* about time discretization;
- **Layer Property Flow (.LPF) file**: it reports information stored in the table *lpf_model_name* about hydraulic parameters of each model layer and the wetting capability options;
- **Preconditioned Conjugate Gradient (.PCG) file**: it contains flag options related to the numerical solver;
- **Output Control (.OC) file**: it contains flag options related to the output results to be saved.

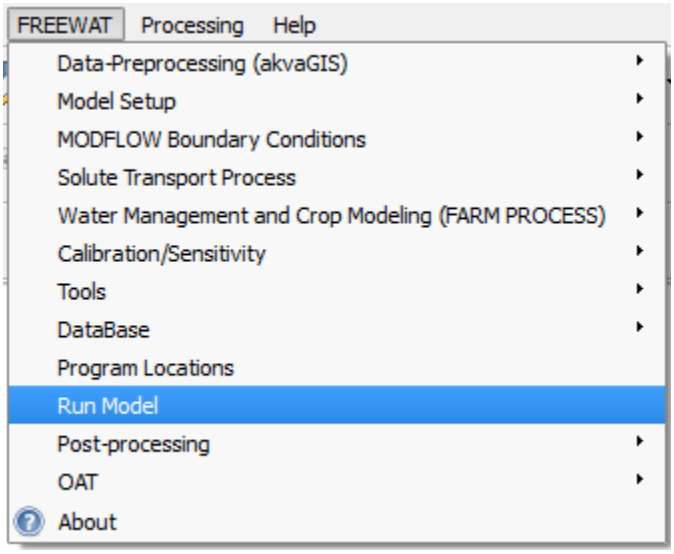
The following are boundary conditions model files, only required if the corresponding boundary condition is activated for the simulation of a particular stress:

- **Time-Variant Specified Head (.CHD) file**: it is required if the *CHD Package* is activated to define specified-head cells;
- **Well (.WEL) file**: it is required if the *WEL Package* is activated to define recharge or pumping wells;
- **Multi-Node Well (.MNW) file**: it is required if the *MNW Package* is activated to simulate screened wells;
- **Recharge (.RCH) file**: it is required if the *RCH Package* is activated to simulate areally-distributed recharge;
- **River (.RIV) file**: it is required if the *RIV Package* is activated to simulate the effects of flow between surface-water features and ground-water systems;
- **Lake (.LAK) file**: it is required if the *LAK package* is activated to simulate lake-groundwater interaction;
- **Drain (.DRN) file**: it is required if the *DRN Package* is activated to simulate the effects of features, such as agricultural drains;
- **General-Head Boundary (.GHB) file**: it is required if the *GHB Package* is activated to simulate inflow to or outflow from the ground-water system, due to the presence of an external source;

- **Evapotranspiration (.EVT) file**: it is required if the *EVT Package* is activated to simulate the effects of plant transpiration and direct evaporation from the soil;
- **Unsaturated-Zone Flow (.UZF) file**: it is required if the *UZF Package* is activated to simulate vertical flow of water through the unsaturated zone;
- **Stream Flow Routing (.SFR) file**: it is required if the *SFR Package* is activated to simulate routed runoff within surface streams.

The model run can be now performed through the following menu:

FREEWAT -> Run Model.



The processes which can be simulated are the following:

- **Groundwater Flow**;
- **Solute Transport** (see Volume 2);
- **Water Management and Crop Modeling** (see Volume 3);
- **Model Calibration** (see Volume 4).

In the **Groundwater Flow** tab, the following information is required:

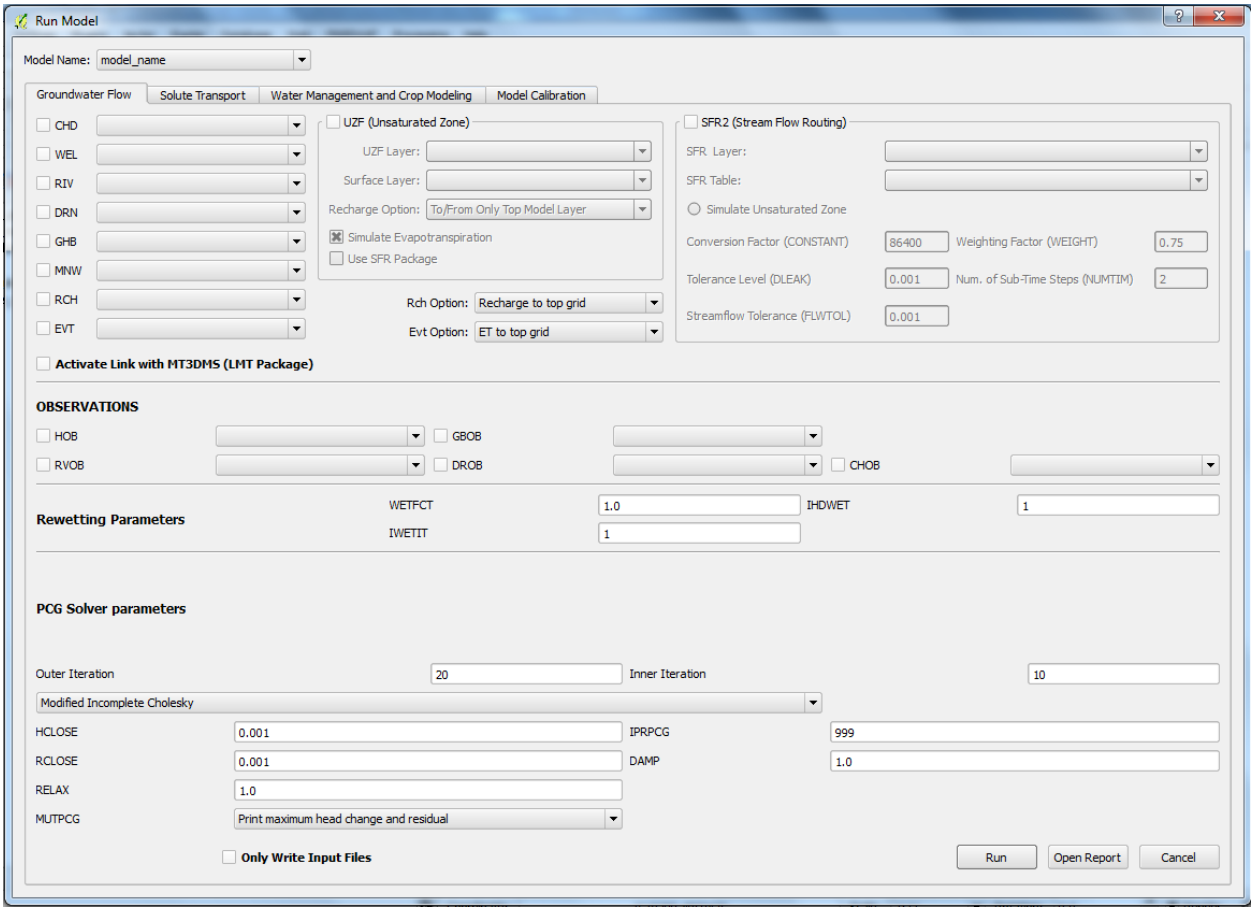
- according to which among the boundary conditions Packages listed above are activated, the corresponding box must be checked and the related MDO must be selected;
- in the *UZF (Unsaturated Zone)* section (if used) the following data are required:
  - *UZF Layer*: name of the uzf MDO;
  - *Surface Layer*: name of the sml MDO (only required if the SFR Package is activated);
  - *Recharge Option*: three options are available to define in which cell of a vertical column recharge and discharge are simulated, *To/From Only Top Model Layer*, *To/From layer specified in iuzfbnd*, *To/From Highest Active Cell*;
  - the box *Simulate Evapotranspiration* must be checked if evapotranspiration has to be simulated;
  - the box *Use SFR Package* must be checked if the SFR Package is used;
- in the *SFR2 (Stream Flow Routing)* section (if used) the following data are required:
  - *SFR Layer*: name of the sfr MDO;

  - *SFR Table*: *sfr_layer_sfr_table* containing information about time discretization of the stream parameters;
  - the option *Simulate Unsaturated Zone* must be checked if the unsaturated flow beneath streams has to be simulated;
  - *Conversion Factor (CONSTANT)*: conversion factor used to calculate stream depth for stream reach (for details refer to Harbaugh, 2005);
  - *Weighting Factor (WEIGHT)*: time weighting factor used to calculate the change in channel storage (for details refer to Harbaugh, 2005);
  - *Tolerance Level (DLEAK)*: closure tolerance for stream depth used to calculate leakage between each stream reach and active model cell (for details refer to Harbaugh, 2005);
  - *Num. of Sub-Time Steps (NUMTIM)*: number of sub-time steps used to route streamflow (for details refer to Harbaugh, 2005);
  - *Streamflow Tolerance (FLWTOL)*: streamflow tolerance for convergence of the kinematic wave equation used for transient streamflow routing (for details refer to Harbaugh, 2005);
- if the Solute Transport process has to be simulated, the link between *MODFLOW* and *MT3DMS* is required, so the box *Activate Link with MT3DMS (LMT) Package* must be checked;
- in the *OBSERVATIONS* section, according to which among the observation Packages (see Volume 6) are activated, the corresponding box must be checked and the related MDO must be selected;
- in the *Rewetting Parameters* section the following data are required:
  - *WETFCT* is a constant involved in the calculation of the hydraulic head within cells which convert from dry to wet (for details refer to Harbaugh, 2005);
  - *IWETIT* is the iteration interval for attempting to re-wet dry cells;
  - *IHDWET* is a flag allowing to determine which equation must be used to calculate the hydraulic head within cells which convert from dry to wet (for details refer to Harbaugh, 2005);
- in the *PCG Solver parameters* section the following data are required:
  - the number of *Outer Iterations* to be performed;
  - the number of *Inner Iterations* to be performed;
  - the matrix conditioning method to be used (corresponding to the *NPCOND* flag in *MODFLOW*): two options are available, *Modified Incomplete Cholesky* and *Polynomial*;
  - *HCLOSE* is the head change criterion for convergence;
  - *RCLOSE* is the residual criterion for convergence;
  - *RELAX* is the relaxation parameter to be defined if the *Modified Incomplete Cholesky* method is used;
  - *MUTPCG* is a flag that controls printing of convergence information from the solver: four options are available, *Print maximum head change and residual*, *Print only total number of iterations*, *No printing*, *Print only if convergence fails*;
  - *IPRPCG* is the printout interval;
  - *DAMP* is the damping factor.

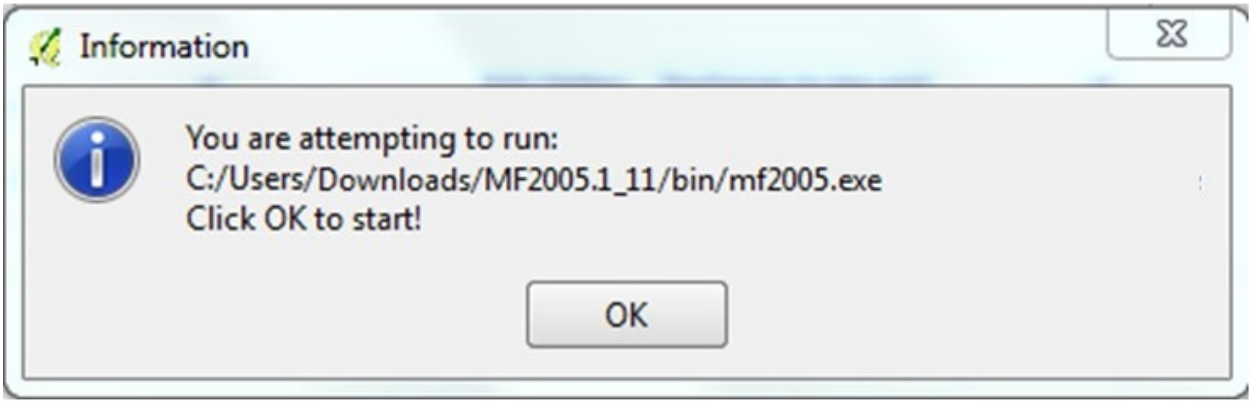
Note: If the box corresponding to the RCH and/or EVT Packages is checked, a further option must be selected (*Rch Option* and/or *Evt Option*) to properly assign the boundary condition to a specific cell along the vertical column. For the RCH Package, three options are available: *Recharge to top grid*, *Recharge layer defined in irch* and *Recharge to highest active cell*. Similarly, three options are available for the EVT Package as well: *ET to top grid*, *ET layer defined in ievt*, *ET to highest active cell*. For both Packages, through the first option the boundary condition is applied to model layer 1;

through the second one the boundary condition is applied to a certain model layer as specified in the fields *irch* and/or *ievt* in the Attribute Table of each MDO; through the third option the boundary condition is applied to the uppermost active cell in the vertical column.

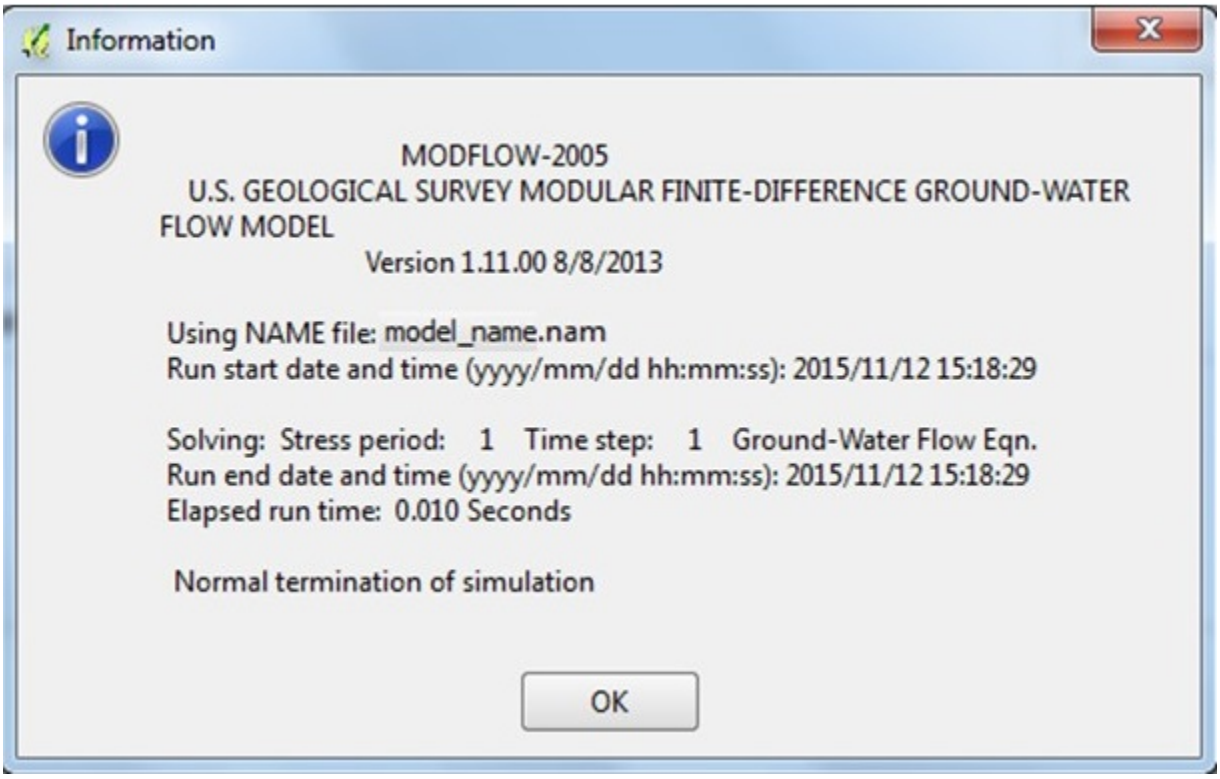
Note: In the current version, in the *SFR2 (Stream Flow Routing)* section (if used) checking *Simulate Unsaturated Zone* is mandatory. This means that it is not possible not to simulate the unsaturated zone beneath streams.



Once the required settings are defined, the *Run* button allows to start the simulation. The following **Information** window appears:



After clicking *OK* the simulation starts and, if finished successfully, the following **Information** window appears:



Note: If the aim is to create only model files, without running the simulation, in the **Run Model** window the box *Only Write Input Files* must be checked before clicking the *Run* button.

Once the simulation is successfully terminated, all the basic model files listed above are created in the working directory where the model DB is saved. The boundary conditions model files related to the activated Packages are created as well.

CHAPTER 8

Model output and post-processing

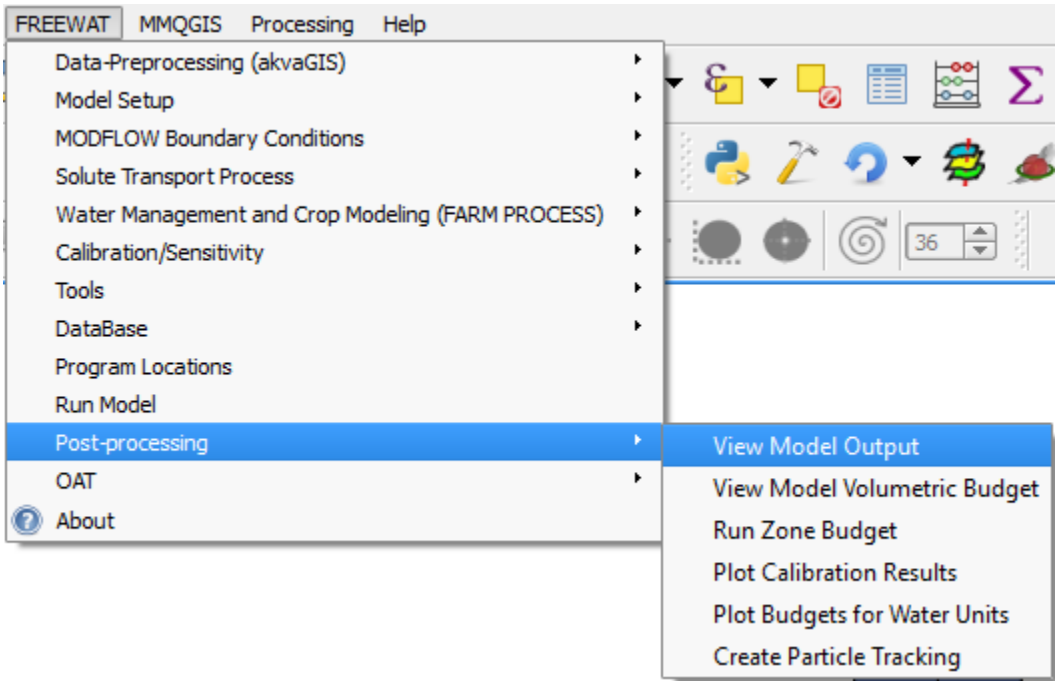
Besides the input files listed in Chapter 7, within the **model_name.nam** file the following output files are also listed:

- **model_name.hds**: binary file containing hydraulic head data;
- **model_name.ddn**: binary file containing drawdown data;
- **model_name.cbc**: binary file containing cell-by-cell budget data;
- **model_name.list**: text file containing several information about the simulation, among which the aquifer budget (for further details refer to Harbaugh, 2005); it can be open with any text editor or using the *Open Report* button in the **Run Model** window.

Display model output

Once the model run has been successfully completed, the hydraulic head simulated for each model layer can be displayed through the following menu:

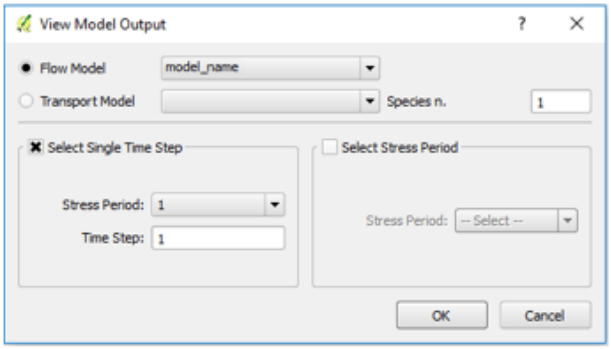
FREEWAT -> Post-processing -> View Model Output.

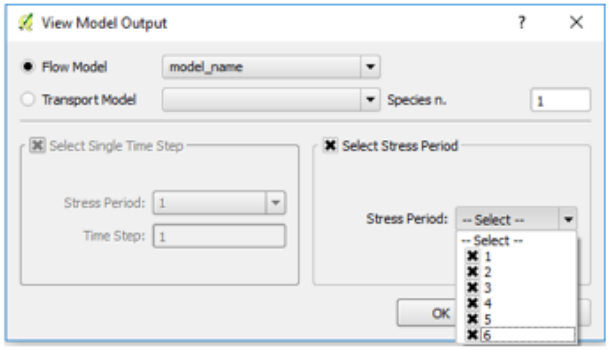


The User has the possibility to load the hydraulic head distribution for each model layer, at the end of a particular TS within a selected SP, or that simulated at the end of each TS within selected SP(s), all at once.

The following data are required in the **View Model Output** window:

- the name of the hydrological model previously built; it must be selected from the drop-down menu after checking if it is a *Flow Model* or a *Transport Model*;
- in the *Select Single Time Step* section (it must be checked if used):
  - *Stress Period*: SP number for which the simulated hydraulic head will be loaded;
  - *Time Step*: TS number, within the selected SP, for which the simulated hydraulic head will be loaded;
- alternatively, in the *Select Stress Period(s)* section (it must be checked if used):
  - the SP number(s) for which the simulated hydraulic head will be loaded must be checked from the drop-down menu near to *Stress Period*.





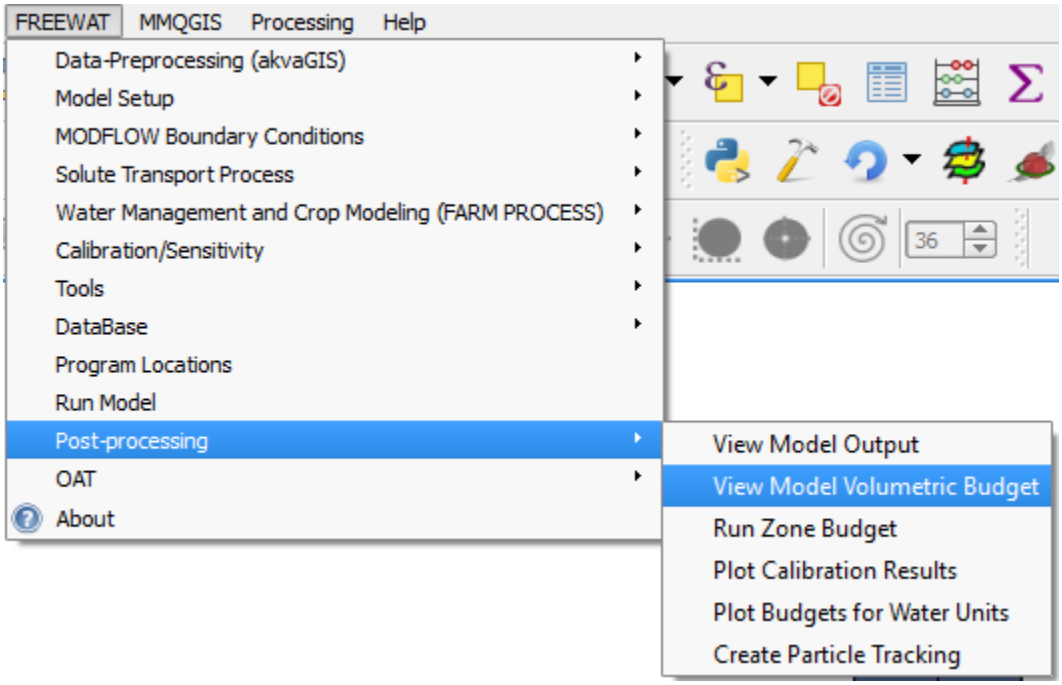
Once clicked *OK*, raster output files are created in the working folder and loaded in the Layers Panel with default names assigned. For example, the raster file containing the simulated head values for model layer 1, at the end of TS 5 within SP 2 will be named *model_name_lay_1_sp_2_ts_5.asc*.

Such outputs can be post-processed for visualization with *QGIS* tools described in Chapter 8 of the QGIS training manual. If needed, contour lines can be extracted by using the available *QGIS* plugins.

Display model budget

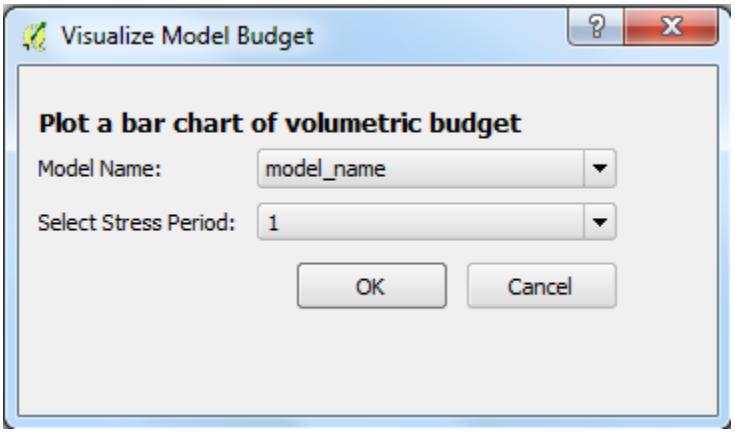
Among the model outputs, the volumetric budget can be displayed as well through the following menu:

FREEWAT -> Post-processing -> View Model Volumetric Budget.

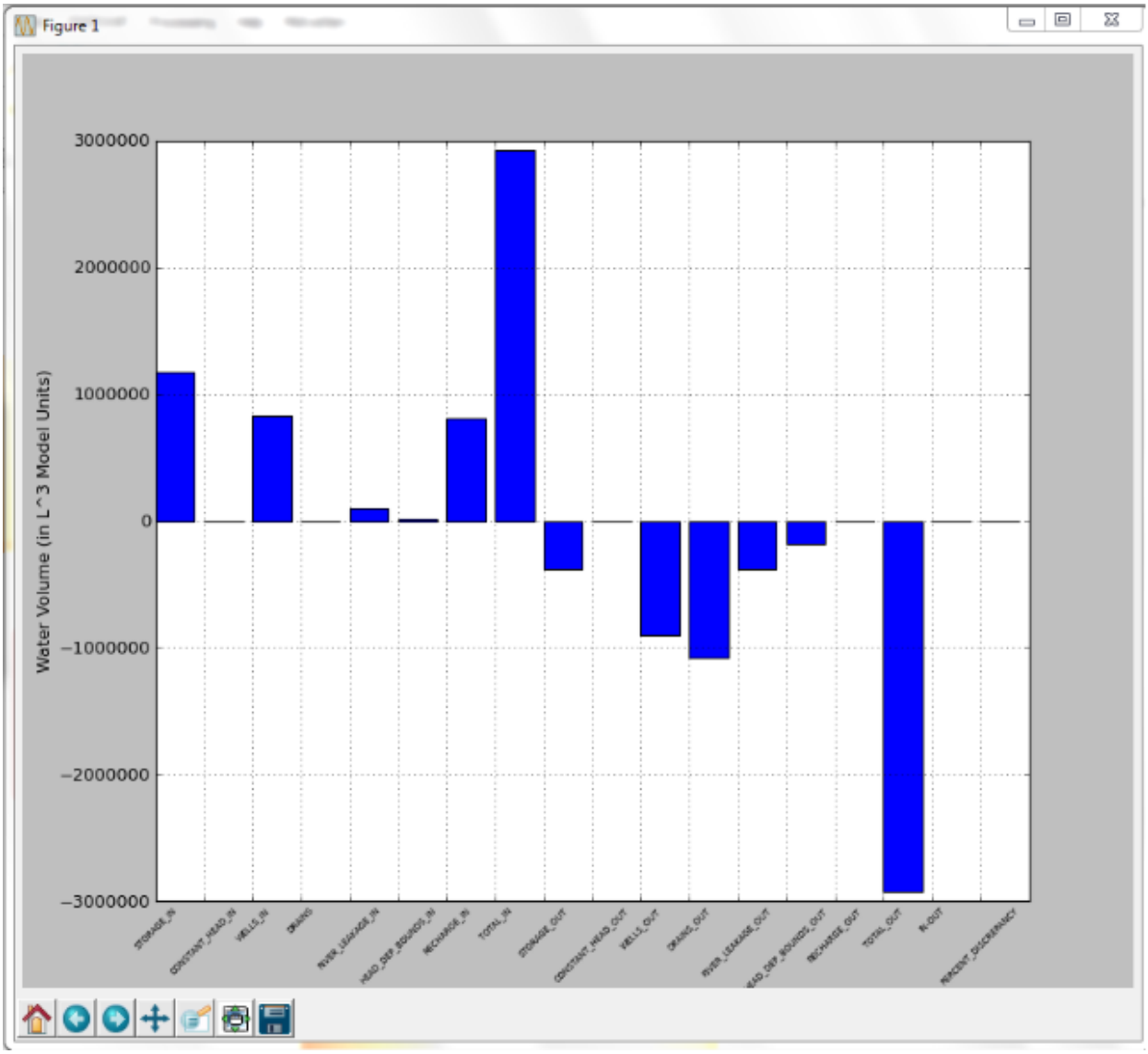


The following data are required in the **Visualize Model Budget** window:

- *Model Name*: name of the hydrological model;
- *Select Stress Period*: SP number for which the model budget will be displayed.



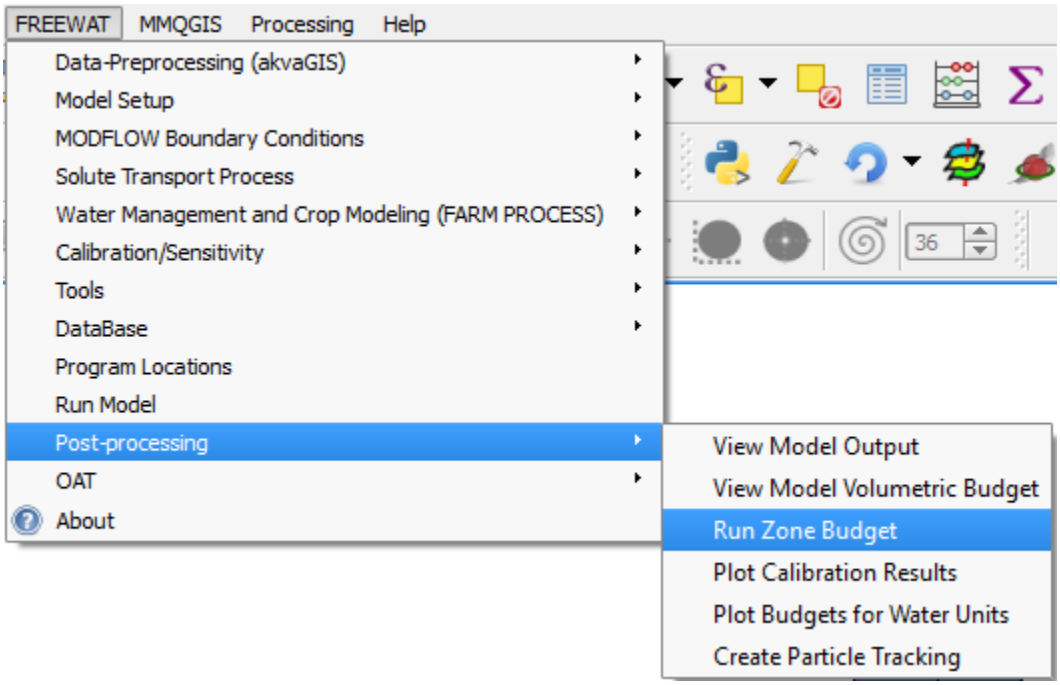
A bar chart is displayed, with cumulative volumes [L^3] along the Y axis and flow terms along the X axis:



Run ZONE BUDGET

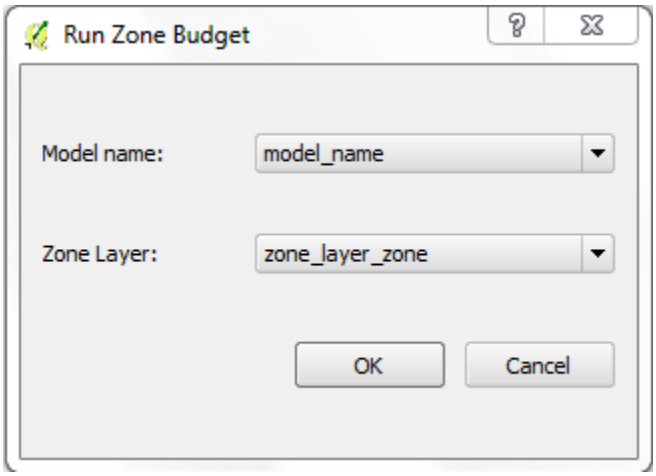
If a zonbud MDO has been created (see Chapter 6) and the ZONE BUDGET executable has been loaded (see Chapter 3), *Zone Budget* can be run through the following menu:

FREEWAT -> Post-processing -> Run Zone Budget.



The following data are required in the **Run Zone Budget** window:

- *Model Name*: name of the hydrological model;
- *Zone Layer*: name of the zonbud MDO created.



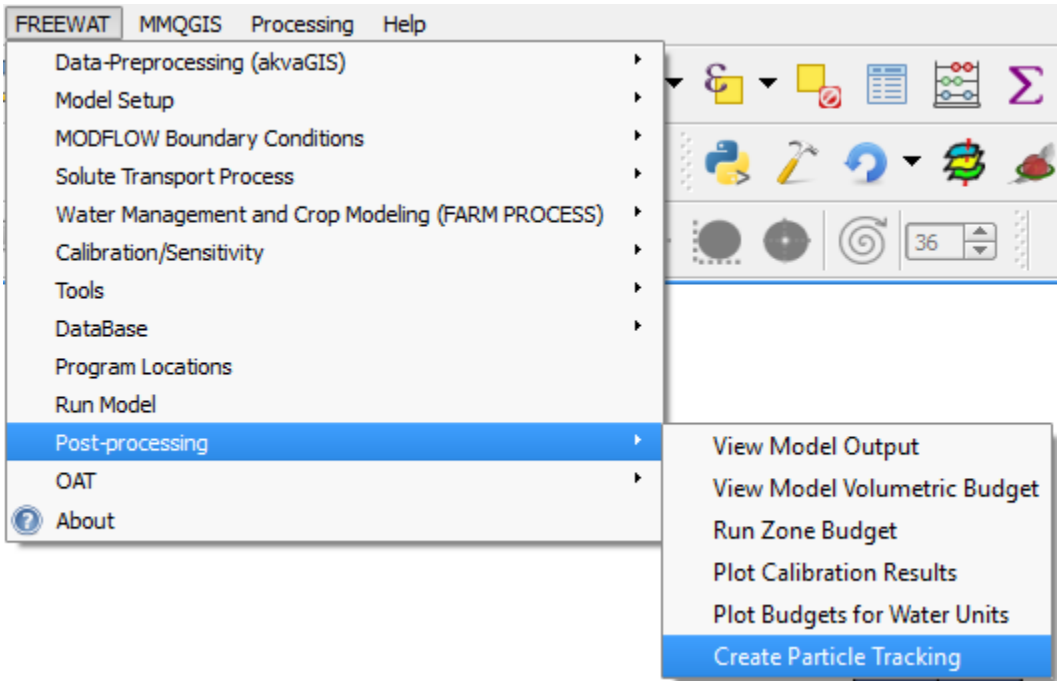
Once the run of the *Zone Budget* is completed, the *Zone Budget* input file (**.zon**) is created and stored in the working folder. It contains zone values assigned at each grid cells. An output file is saved as well (**.zbud**). It reports budgets for each zone, at all the times for which *MODFLOW* has saved flow terms.

Note: To run the *Zone Budget*, the model run must have been completed and cell-by-cell flow terms saved.

Run MODPATH

If the MODPATH executable has been loaded (see Chapter 3), *Modpath* can be run through the following menu:

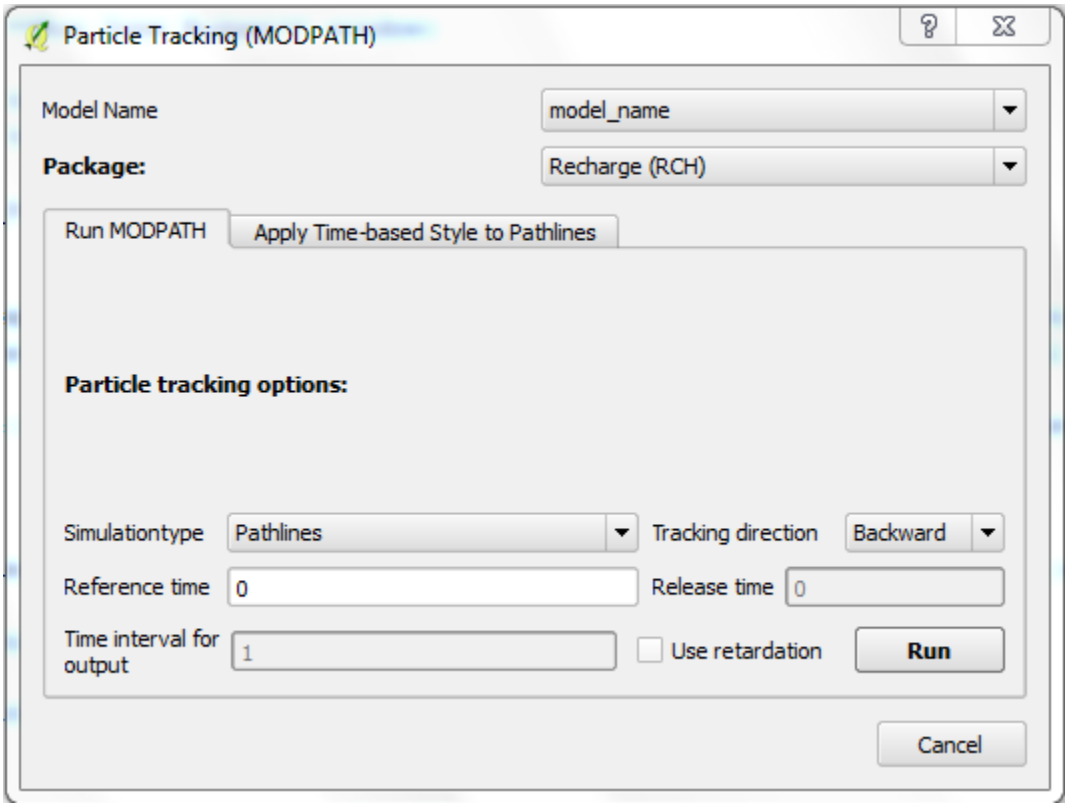
FREEWAT -> Post-processing -> Create Particle Tracking.



The following data are required in the **Particle Tracking (MODPATH)** window:

- *Model Name*: name of the hydrological model;
- *Package*: *MODFLOW* Package to which the particle tracking will be applied (two options are available: *Well (WEL)* or *Recharge (RCH)*);
- in the *Run MODPATH* section, the following *Particle tracking options* are needed:
  - *Simulationtype*: two options are available (*Pathlines*, if the User wishes to record coordinates along the path of each particle; *Endpoints*, if the end point of the path of each particle is recorded);
  - *Tracking direction*: two options are available (*Forward*, if the User wishes to track the particles in the downstream direction; *Backward*, if the particles are tracked backwards in the upstream direction);
  - *Reference time*: reference simulation time [T] (in time units), needed to identify the accumulated time during a particle-tracking analysis;
  - *Release time*: reference time [T] (in time units) when the particles are released (this option is not still available);
  - *Time interval for output*: time interval (in time units) to save the outputs (this option is not still available);
  - if the checkbox *Use retardation* is checked, linear sorption phenomena on the apparent velocity of a reactive solute can be taken into account.

Once the *Particle tracking options* are set, *Modpath* can be run clicking the *Run* button.



Note: To run *Modpath*, the model run must have been completed and cell-by-cell flow terms saved.

Once the run of *Modpath* is completed, the following input files are created and stored in the working folder:

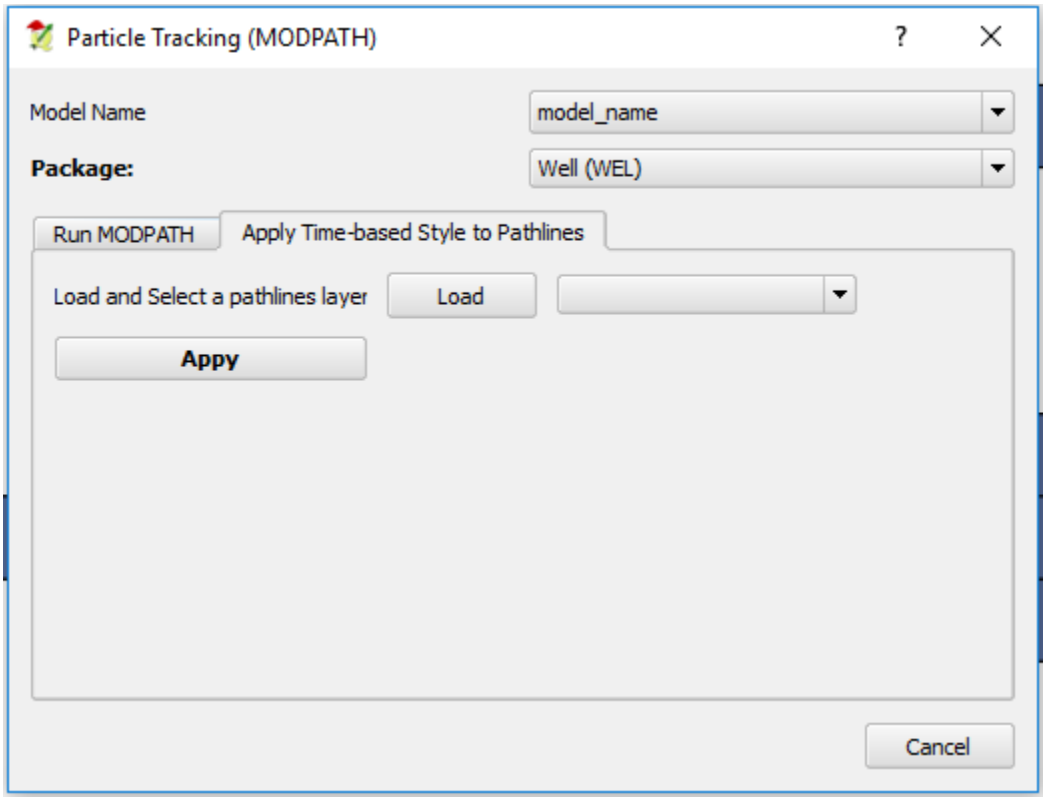
- **.mpn** contains the list of *MODFLOW*/*MODPATH* files needed for the simulation;
- **.mpbas** consists of a combination of data contained in the *MODFLOW BAS Package* data file and the *MODFLOW LPF Package* data file (see Chapter 2), plus additional data, such as porosity;
- **.mpsim** contains information about the simulation options set above;
- **.mpstrt** contains information about particle starting location.

An output file is saved as well (**.mplst**). It reports input data and results for MODPATH simulations.

Besides *MODPATH* input and output files, point and line shapefiles are created and stored in the model DB, according to the number of model layers. Such shapefiles are created with default names (*model_name_particles_lay_1.shp*, *model_name_particles_lay_2.shp*, ..., *model_name_particles_lay_n.shp* the point shapefiles and *model_name_pathlines_lay_1.shp*, *model_name_pathlines_lay_2.shp*, ..., *model_name_pathlines_lay_n.shp* the line shapefiles, where *n* is the maximum number of model layers implemented).

Note: As default values are assigned, if a new run of *Modpath* is performed, then such output shapefiles need to be deleted from the model DB.

Once these output shapefiles are created, the User can either manage the simbology or open again the **Particle Tracking (MODPATH)** window, through the menu *FREEWAT -> Post-processing -> Create Particle Tracking*, and use the *Apply Time-based Style to Pathlines* section:



Once the *Load* button is clicked, all the available line shapefiles (*model_name_pathlines_lay_1.shp*, *model_name_pathlines_lay_2.shp*, ..., *model_name_pathlines_lay_n.shp*) are loaded in the combo box. The User must choose the line shapefile to which a style will be applied and click on *Apply*.

The pathlines stored in the line shapefile just selected will be represented on the Map Canvas with labels indicating the tracking time for each *Modpath* time-step and arrows indicating the tracking direction.

Note: This process of changing simbology is a bit slow, so it is soggested to use it just for model layers of interest.

References

Hanson RT, Boyce SE, Schmid W, Hughes JD, Mehl SM, Leake SA, Maddock T, Niswonger RG (2014). One-Water Hydrologic Flow Model (MODFLOW-OWHM). U.S. Geological Survey, Techniques and Methods 6?A51, 134 p.

Harbaugh AW (2005). MODFLOW-2005, The U.S. Geological Survey Modular Ground-Water Model - the Ground-Water Flow Process. U.S. Geological Survey, Techniques and Methods 6?A16, 253 p.

Konikow LF, Hornberger GZ, Halford KJ, Hanson RT (2009). Revised multi-node well (MNW2) package for MODFLOW ground-water flow model. U.S. Geological Survey, Techniques and Methods 6?A30, 67 p.

Merritt ML and Konikow LF (2000). Documentation of a computer program to simulate lake-aquifer interation using the MODFLOW Ground-Water Flow Model and the MOC3D Solute-Transport Model. U.S. Geological Survey Water-Resources Investigations Report 00-4167, 146.

Niswonger RG and Prudic DE (2005). Documentation of the Streamflow-Routing (SFR2) Package to Include Unsaturated Flow Beneath Streams?A Modification to SFR1. U.S. Geological Survey, Techniques and Methods 6?A13, 59 p.

Niswonger RG, Prudic DE and Regan RS (2006). Documentation of the Unsaturated-Zone Flow (UZF1) Package for Modeling Unsaturated Flow Between the Land Surface and the Water Table with MODFLOW-2005. U.S. Geological Survey, Techniques and Methods 6?A19, 71 p.

Schmid W, Hanson RT, Maddock T, Leake SA (2006). User Guide for the Farm Process (FMP1) for the U.S. Geological Survey?s Modular Three-Dimensional Finite-Difference Ground-Water Flow Model, MODFLOW-2000. U.S. Geological Survey, Techniques and Methods 6?A17, 140 p.

Release history

31/07/2016 release of vesion 0.1

15/10/2016 release of version 0.2

(new abstract inserted; minor changes in the text)

5/12/2016 release of version 0.3

(new installation procedure; possibility to use multi segments to implement RIV, DRN and GHB *MODFLOW* Packages; new post-processing tool (*MODPATH*) to simulate particle tracking)