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)

Version 1.0.2
March 31st, 2018

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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. Latest Version of FREEWAT is 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)

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FOREWORD

FREEWAT is a 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.

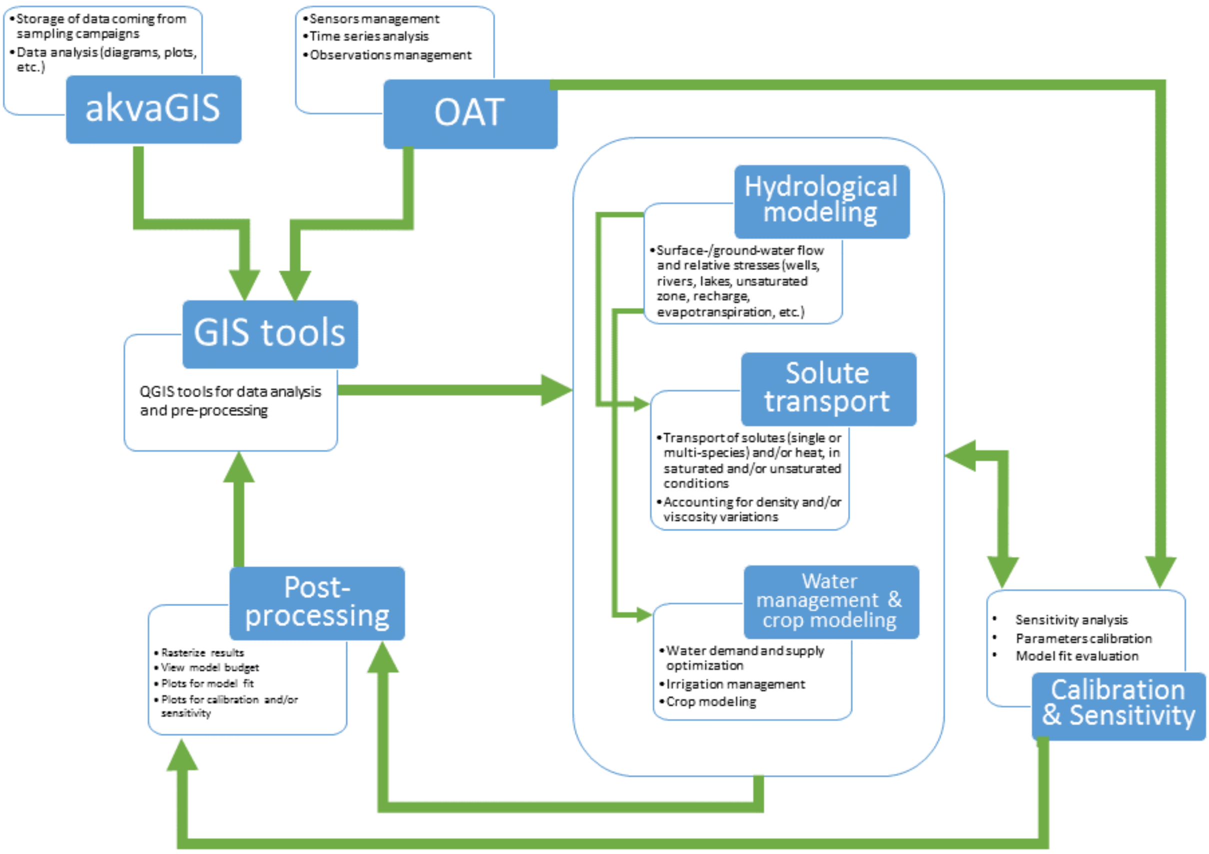
The open source characteristics of the platform allow considering this an initiative "ad includendum", as further research institutions, private developers etc. may contribute to the platform development.

FREEWAT is conceived as a composite plugin for the well-known GIS open source desktop software QGIS (http://qgis.org). The selected reference version of QGIS is the latest LTR (Long Term Release), namely QGIS 2.14: even if this release will be maintained as the reference one, it is worth mentioning that any test performed so far with subsequent versions (e.g. 2.16 and 2.18) worked without experiencing any problem.

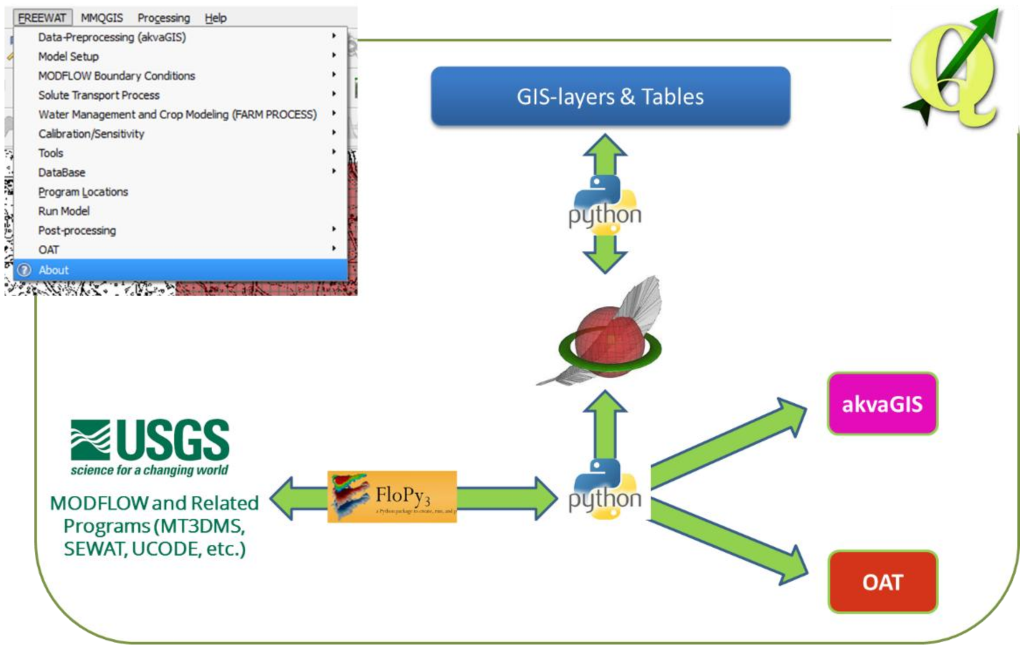
As composite plugin, FREEWAT is designed as a modular ensemble of different tools: some of them can be used independently, while some modules require the preliminary execution of other tools. Capabilities integrated in FREEWAT are:

- Simulation of models related to the hydrological cycle (Volume 1)
- A module for simulating solute transport in the unsaturated/saturated zone, including density and viscosity dependent flow (Volume 2)
- A module for water resource management and optimization of conjunctive use, including issues related to irrigation management in rural environment (Volume 3)
- Tools for the analysis, interpretation and visualization of hydrogeological and hydrochemical data and quality issues (Volume 4)
- A module for time-series processing to support input data processing and advanced model calibration (Volume 5)
- A module for calibration, uncertainty and sensitivity analysis (Volume 6)

The following diagram shows how these different modules are interconnected, taking as reference a standard modeling procedure.



FREEWAT architecture is based on the integration of different software tools (the so called FREEWAT pillars): SQLITE relational database manager, external (free and open source) codes like MODFLOW and MODFLOW-related programs as well as codes specifically developed for the FREEWAT. The way of interconnecting such tools is done via Python programming language, with extensive use of the Python library FloPy. A schematic representation of FREEWAT pillars and their interconnection is showed in the following figure.



Contents

Abstract

The *FREEWAT* platform integrates a hydrological model 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 management and planning processes.

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

In *FREEWAT*, the simulation of the water cycle is performed through the application of two versions of *MODFLOW*, 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 or square cells. Flow associated with external stresses, such as wells, areal recharge, evapotranspiration, drains, rivers, and lakes can be simulated as well.

The two versions of *MODFLOW* integrated within the *FREEWAT* platform are: *MODFLOW-2005* (Harbaugh, 2005) and the latest version *MODFLOW-OWHM* (*One-Water Hydrologic flow Model*; Hanson et al., 2014).

MODFLOW-OWHM is a free and open source 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 simulating 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 coupling *MODFLOW-2005* and the *Farm Process* module, which is described in Volume 3 (Water management and crop-growth modeling) of the FREEWAT User Manual.

This Volume describes requirements and the steps needed to download and install the *FREEWAT* plugin (Chapter 1), and it provides instructions to set up and run a hydrological model.

In Chapter 2, the workflow to be followed to create and set up a new hydrological model is described. Possible limitations and default options are reported.

Starting from Chapter 3, the procedure needed to create a new hydrological 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 by means of the *UZF* Package. Among the 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), which can be used also to simulate farm wells in *Farm Process* (refer to Volume 3), and the *Lake* Package (*LAK*; Merrit and Konikow, 2000) for the simulation of lake-aquifer interaction.

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

CHAPTER 1

FREEWAT Installation & Requirements

Install 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*, which is at present version 2.14 *Essen*, or later (either version 2.16 or 2.18).

Note: The present version of the *FREEWAT* plugin is NOT compatible with *QGIS 3*.

FREEWAT has been tested within the following *QGIS* versions:

- 2.8 *Wien*;
- 2.10 *Pisa*;
- 2.12 *Lyon*;
- 2.14 *Essen*;
- 2.16 *Nodebo*;
- 2.18 *Las Palmas*.

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

Note: In order to avoid conflicts during *FREEWAT* installation, having ONLY ONE VERSION OF *QGIS* installed is highly recommended. However, Users having *QGIS* versions 2.18 and 3.0 installed on the same pc did not experience any problem. Furthermore, having *QGIS* and *ArcGIS* jointly installed on the same pc is strongly discouraged.

Note: Screenshots of *QGIS* interfaces reported in the following were made with *QGIS* version 2.18 *Las Palmas*.

Install the FREEWAT plugin

Information on how to download the last version of the *FREEWAT* plugin can be found at this web page. Once the download area of the FREEWAT web site has been accessed, it will be possible to download the zip file `freewat_v.x.x.zip` (`x.x` indicates the most updated version of the plugin), along with User Manuals and training material.

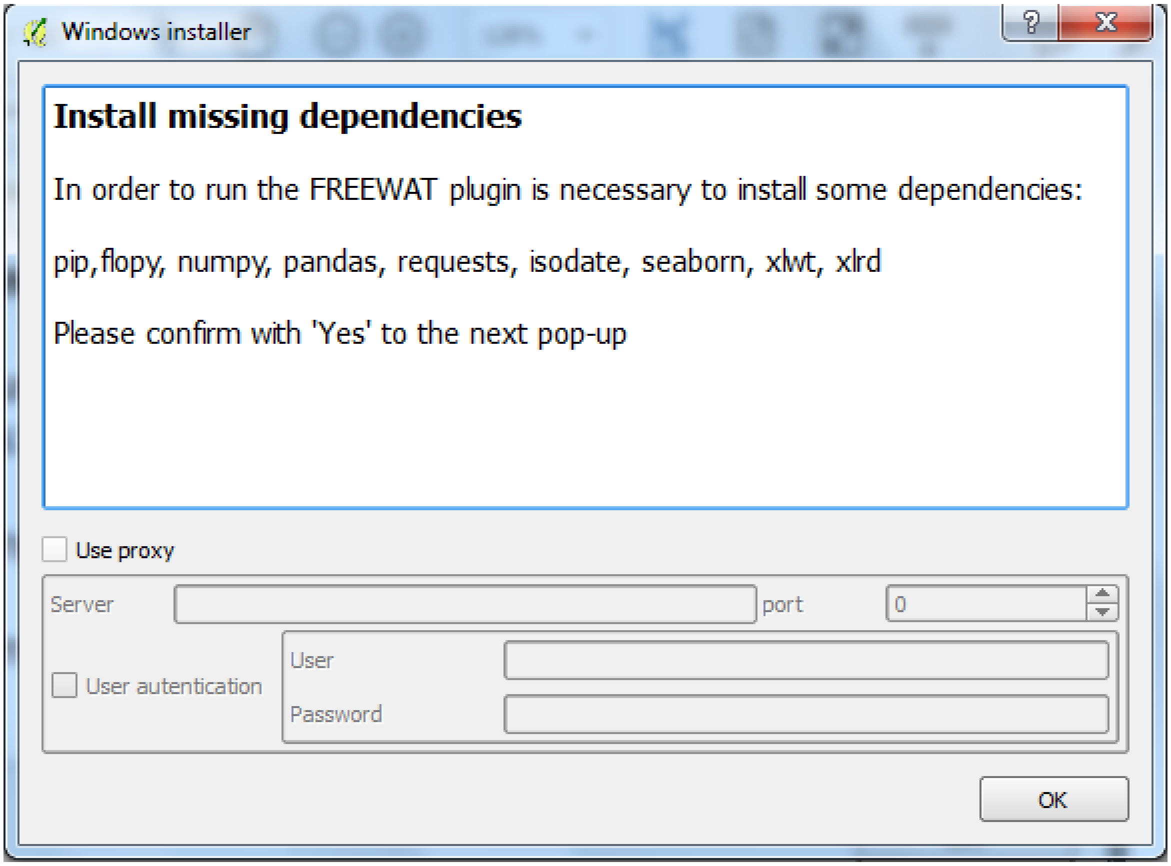
Note: The *FREEWAT* plugin can not be installed on *MAC* OS machines.

In all the other Operative Systems (*Windows* and *Linux*), once *QGIS* is run for the first time, the `.qgis2` folder is created.

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

Note: Spaces and/or special characters (e.g., accents) must be avoided in the path of the `C:\Users\your_name\.qgis2` or `/home/user/.qgis2` folders.

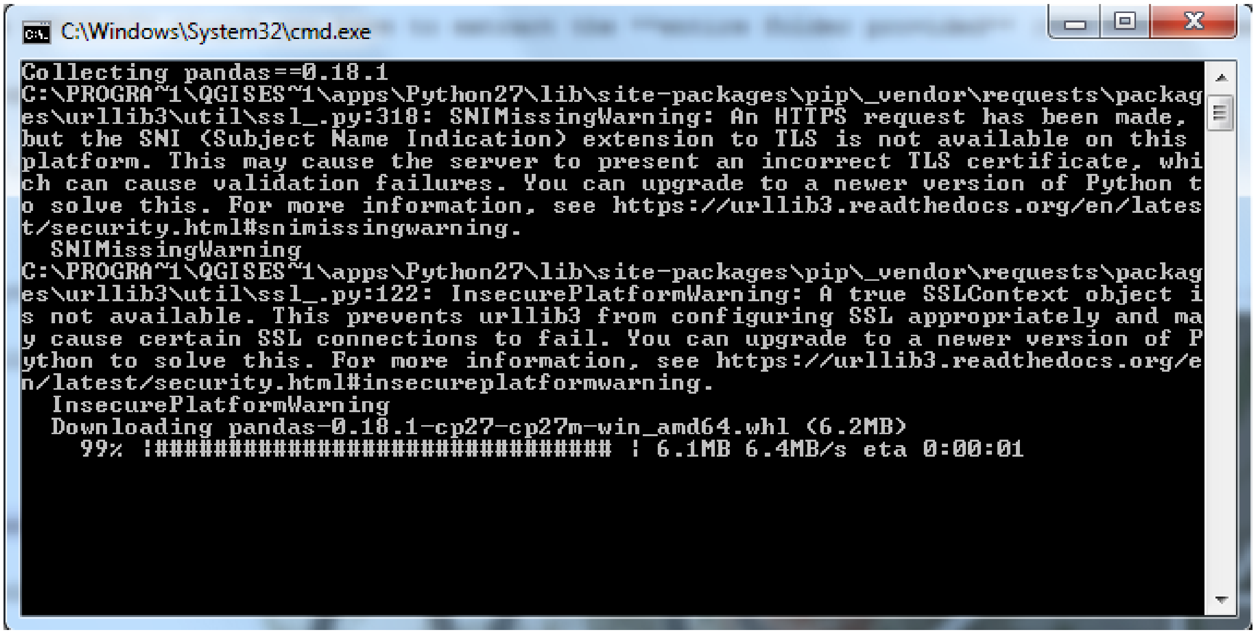
- **Step 1.** In order to install the *FREEWAT* plugin, you have to extract the **provided plugin folder** (its name is `freewat`, it is located within the downloaded `freewat_v.x.x.zip` file) in `C:\Users\your_name\.qgis2\python\plugins` (for *Windows* machines) or `/home/user/.qgis2/python/plugins` (for *Linux* machines). Sometimes the `plugins` folder could not exist. In such case, you can just create it (its name must be exactly `plugins`, lower case letters).
- **Step 2.** You must now run *QGIS*.
- **Step 3.** The **Installer** window appears, reporting that the following dependencies are needed:
  - *pip*;
  - *flopy*;
  - *numpy*;
  - *pandas*;
  - *requests*;
  - *isodate*;
  - *seaborn*;
  - *xlwt*;
  - *xlrd*.



Note: Installing all the libraries listed above requires connection to the Internet.

Note: If the checkbox *Use proxy* is checked, you can insert all the information related to any proxy set on your machine.

- **Step 4.** Once you click *OK*, several pop-up windows will appear and all the missing dependencies will be automatically installed:

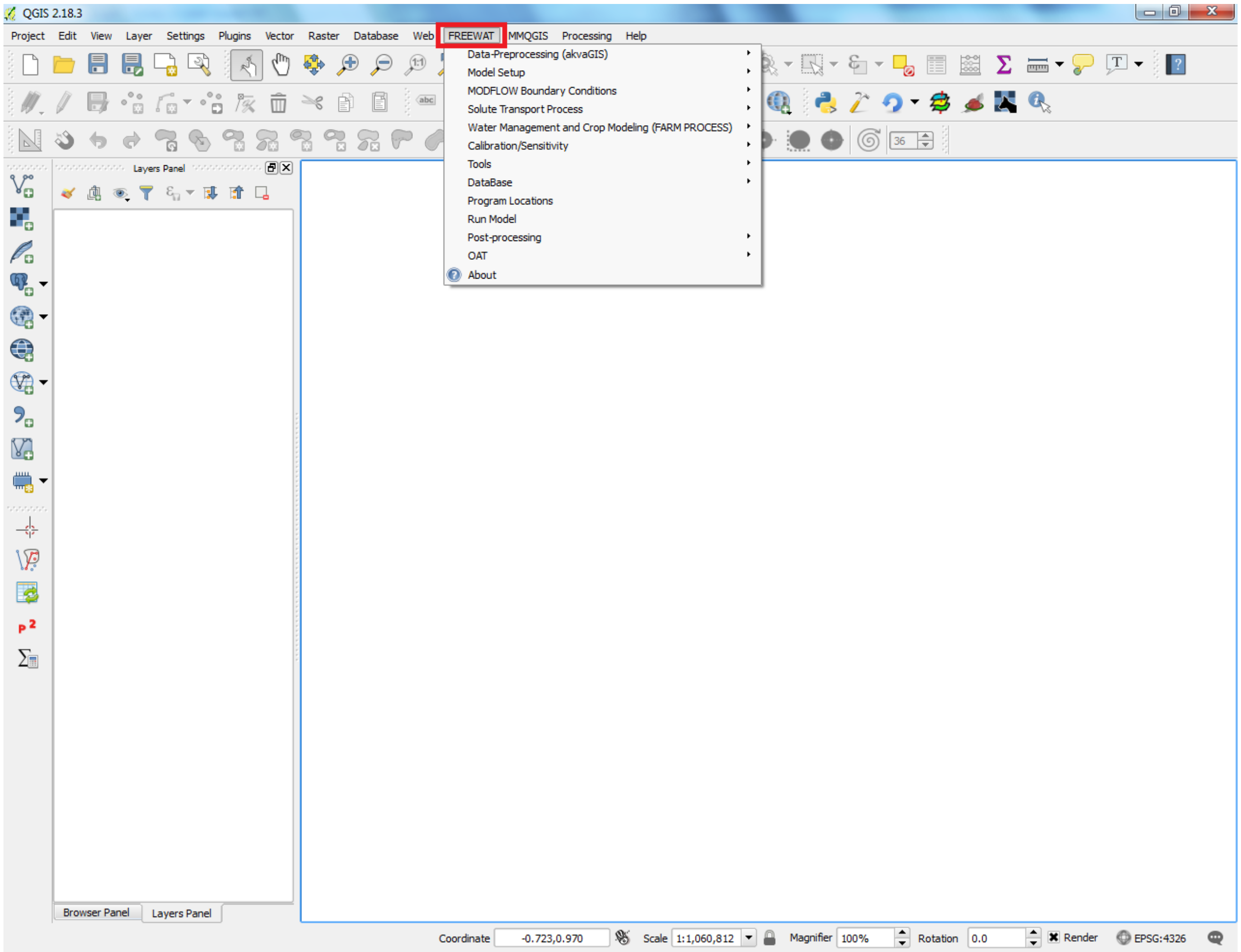


Note: Installing each missing dependency requires authorization, so you will be asked to enter a password so that each pop-up window is run as administrator.

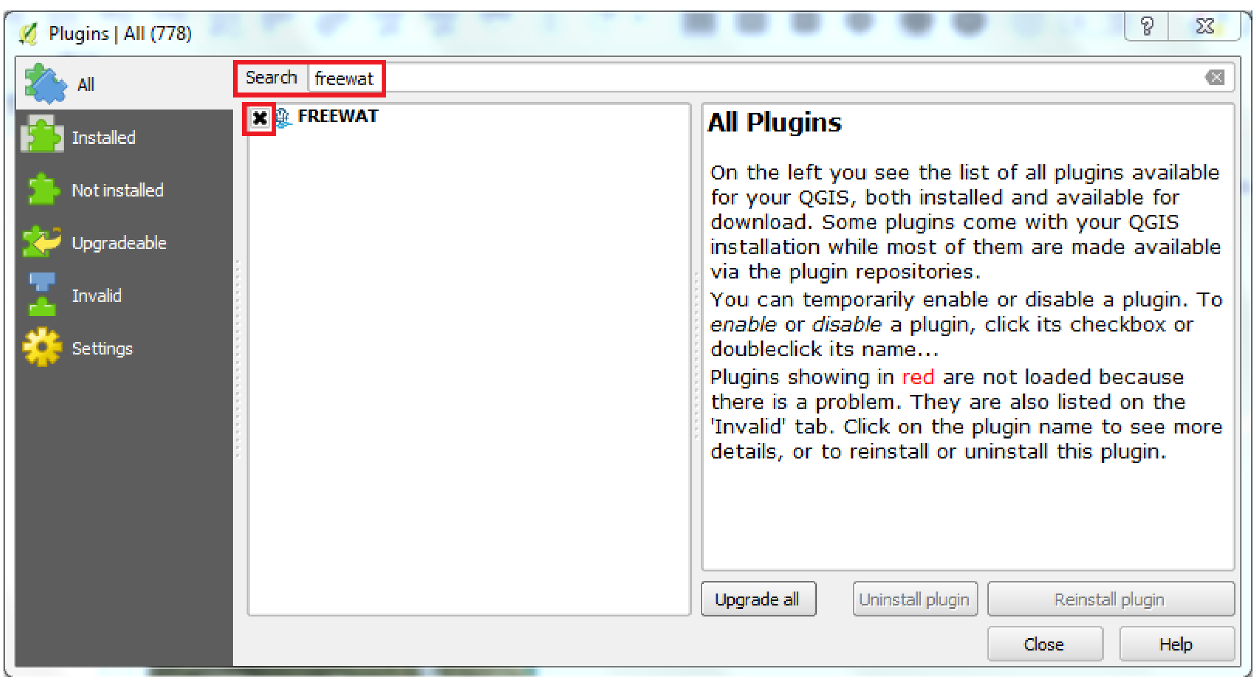
Start FREEWAT

After *QGIS* and all the needed dependencies have been correctly installed, run *QGIS*.

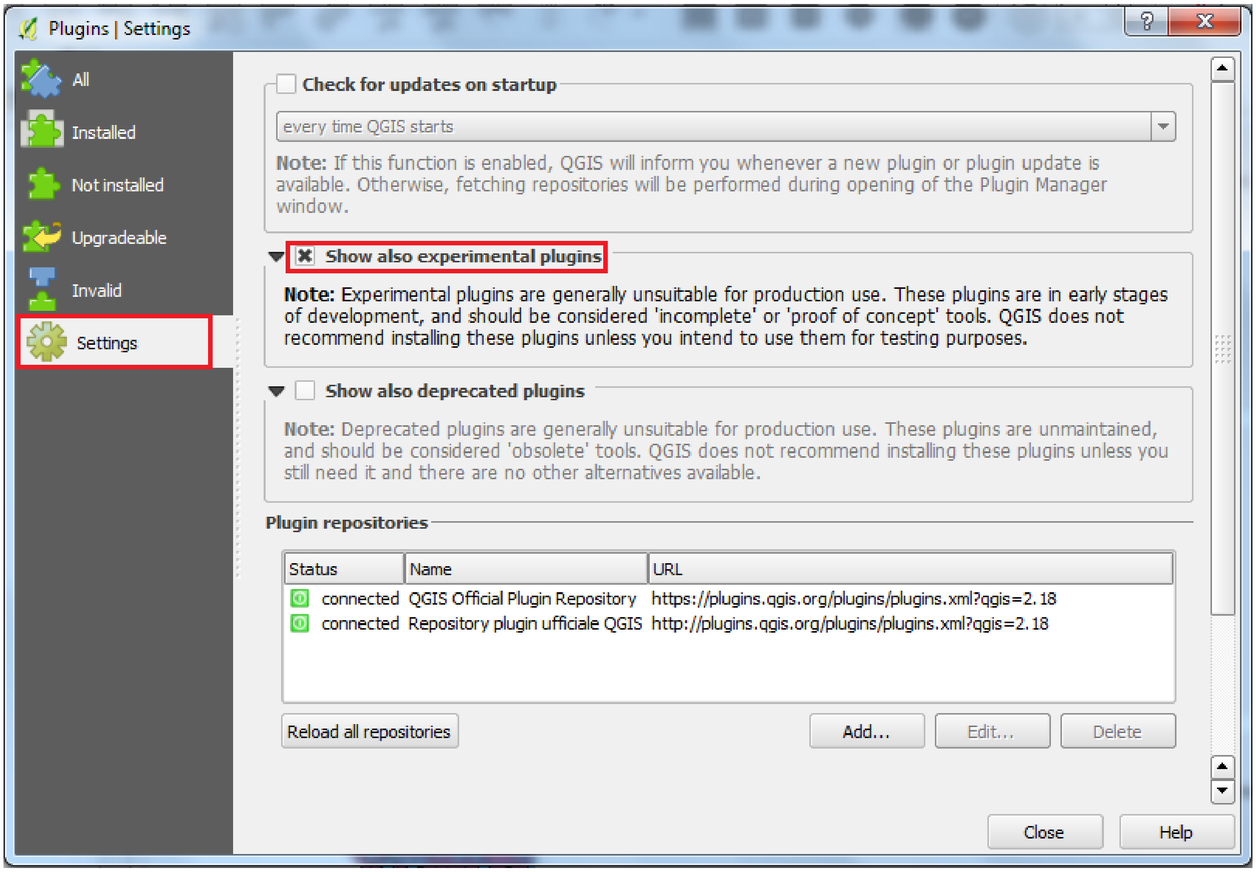
FREEWAT should appear as a drop-down menu in the toolbar of the *QGIS* Graphical User Interface (GUI).



If not, just go to *Plugins -> Manange and Install Plugins..*, type **FREEWAT** in the *Search* bar and click on the corresponding checkbox to activate the plugin, as shown in the picture below:

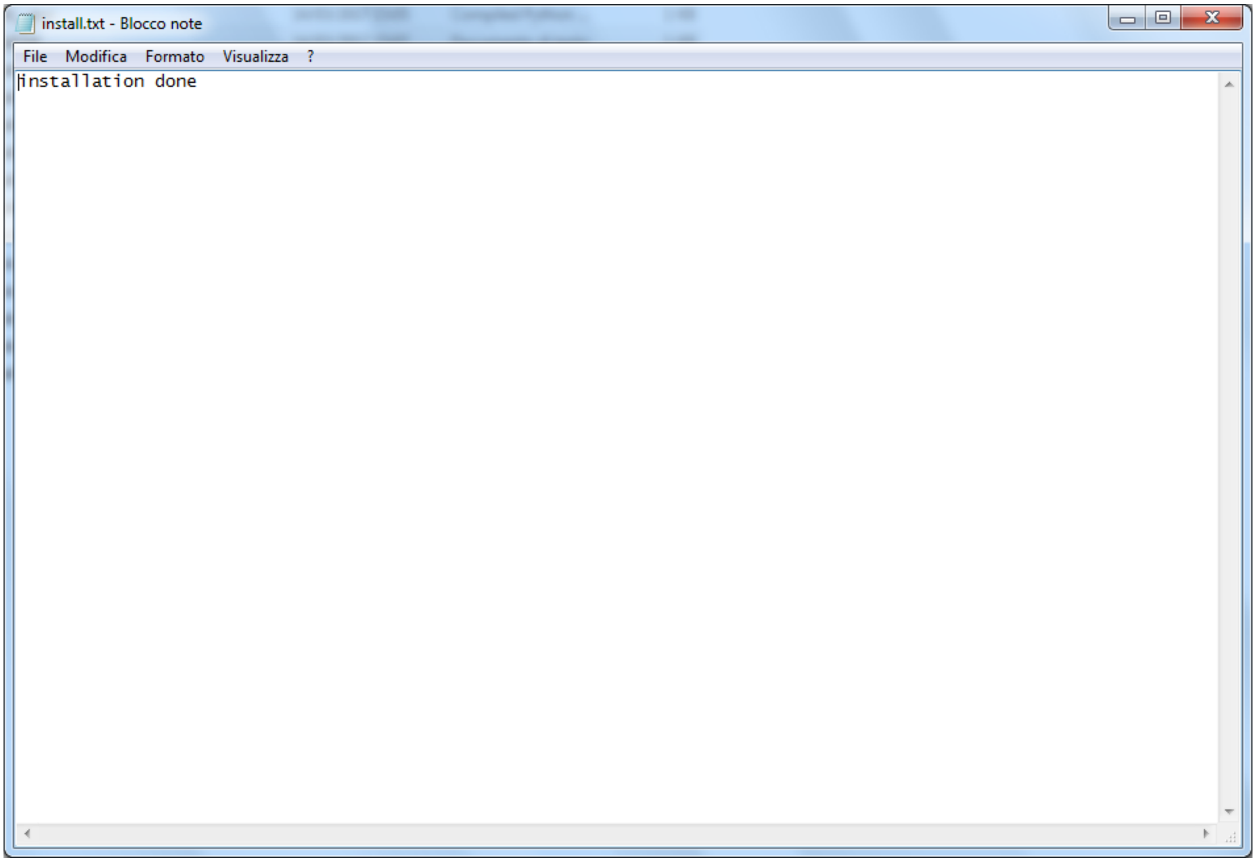


Note: Should *FREEWAT* not be present among the installed plugins, switch to the *Settings* tab and check *Show also experimental plugins*. Search again the *FREEWAT* plugin.



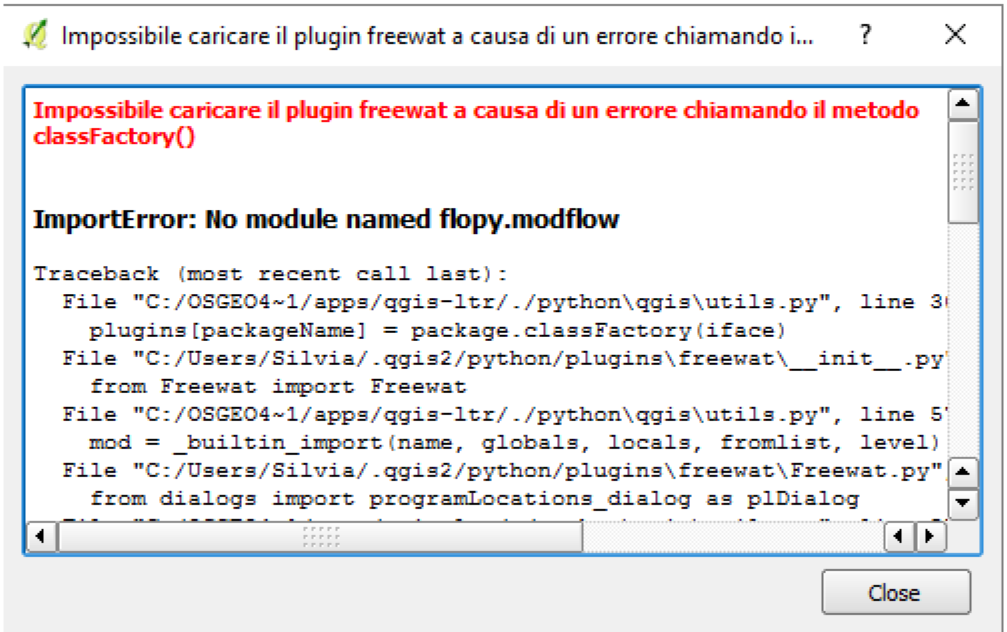
The *FREEWAT* platform can now be used by following the logical workflow presented in the following Chapters.

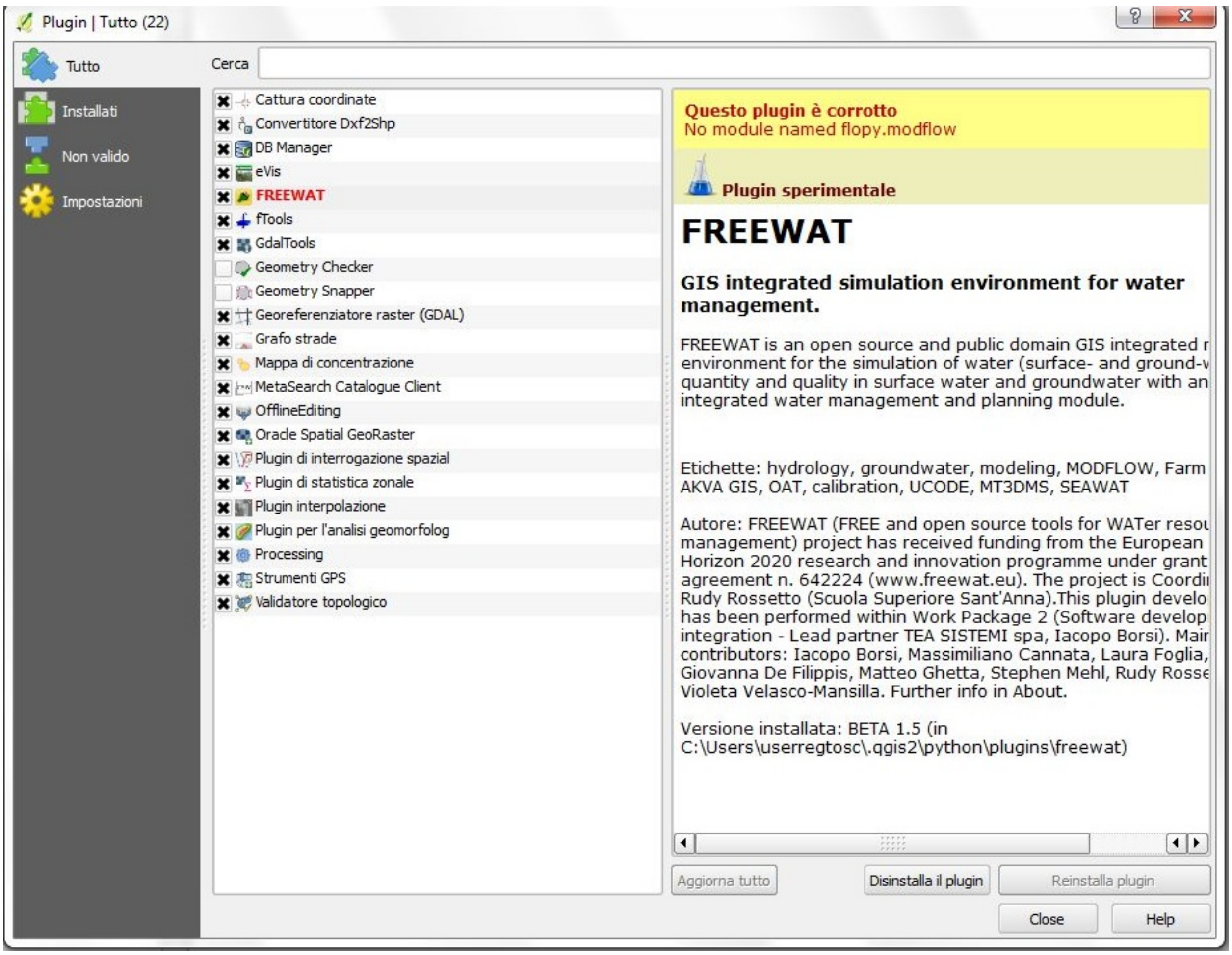
Note: It can happen that, even if all the needed dependencies have been correctly installed (and *FREEWAT* appears in the toolbar of the *QGIS* GUI), installation procedure starts each time you re-run *QGIS*. If this happens, a txt file renamed `install.txt` must be created manually in `C:\Users\your_name\.qgis2\python\plugins\freewat\install`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



Manual installation procedure

Should you experience any error when you open *QGIS* or when you try to activate the *FREEWAT* plugin through the *Plugins -> Manange and Install Plugins...* menu (see, e.g., the following figures), please try the manual installation procedures described below.





Manual procedure

- Close *QGIS* if it is open;

- From the START button search *OSGeo4W Shell* -> right click on it and **Run as administrator**;
- Type the following instructions one by one (please, respect the spaces and click Enter each time and wait some seconds until the installation of the library is completed):

python –m pip install numpy==1.11.0 -> press Enter

python –m pip install pandas==0.18.0 -> press Enter

python –m pip install setuptools -> press Enter

python –m pip install isodate -> press Enter

python –m pip install requests -> press Enter

python –m pip install matplotlib -> press Enter

python –m pip install flopy==3.2.6 -> press Enter

python –m pip install xlrd -> press Enter

python –m pip install xlwt -> press Enter

python –m pip install seaborn -> press Enter

for 64-bit Windows machines only

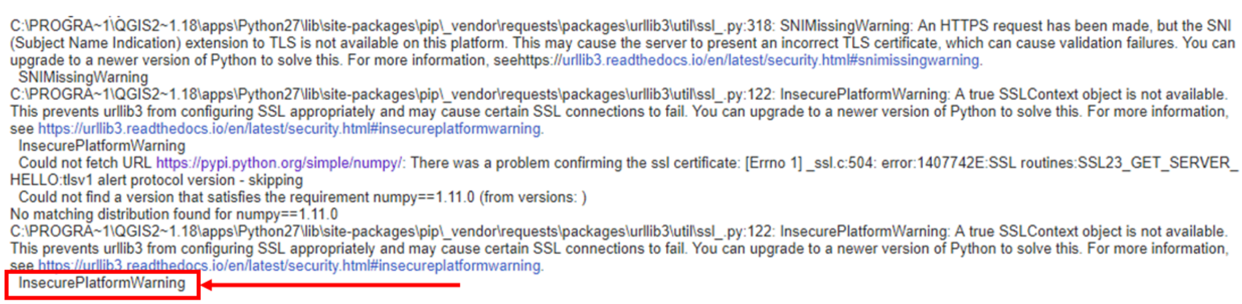
python -m pip install –upgrade http://www.silx.org/pub/wheelhouse/old/numpy-1.11.1+mkl-cp27-cp27m-win_amd64.whl -> press Enter

for 32-bit Windows machines only

python -m pip install –upgrade http://www.silx.org/pub/wheelhouse/old/numpy-1.11.1+mkl-cp27-cp27m-win32.whl -> press Enter

- A txt file renamed `install.txt` must be created manually in `C:\Users\your_name\.qgis2\python\plugins\freewat\install` or `/home/user/.qgis2/python/plugins`. This txt file must contain only the sentence `installation done`;
- Open *QGIS* and you should see *FREEWAT* as a drop-down menu in the toolbar of *QGIS*;
- If not, just go to *Plugins -> Manange and Install Plugins..*, type **FREEWAT** in the *Search* bar and click on the checkbox to activate the plugin.

NOTE: Should you experience the following error when typing the above instructions, please do the following.



```
C:\PROGRA~1\QGIS2~1.18\apps\Python27\lib\site-packages\pip\_vendor\requests\packages\urllib3\util\ssl_.py:318: SNIMissingWarning: An HTTPS request has been made, but the SNI (Subject Name Indication) extension to TLS is not available on this platform. This may cause the server to present an incorrect TLS certificate, which can cause validation failures. You can upgrade to a newer version of Python to solve this. For more information, seehttps://urllib3.readthedocs.io/en/latest/security.html#snimissingwarning.
  SNIMissingWarning
C:\PROGRA~1\QGIS2~1.18\apps\Python27\lib\site-packages\pip\_vendor\requests\packages\urllib3\util\ssl_.py:122: InsecurePlatformWarning: A true SSLContext object is not available. This prevents urllib3 from configuring SSL appropriately and may cause certain SSL connections to fail. You can upgrade to a newer version of Python to solve this. For more information, see https://urllib3.readthedocs.io/en/latest/security.html#insecureplatformwarning.
  InsecurePlatformWarning
  Could not fetch URL https://pypi.python.org/simple/numpy/: There was a problem confirming the ssl certificate: [Errno 1] _ssl.c:504: error:1407742E:SSL routines:SSL23_GET_SERVER_HELLO:tlsv1 alert protocol version - skipping
  Could not find a version that satisfies the requirement numpy==1.11.0 (from versions: )
No matching distribution found for numpy==1.11.0
C:\PROGRA~1\QGIS2~1.18\apps\Python27\lib\site-packages\pip\_vendor\requests\packages\urllib3\util\ssl_.py:122: InsecurePlatformWarning: A true SSLContext object is not available. This prevents urllib3 from configuring SSL appropriately and may cause certain SSL connections to fail. You can upgrade to a newer version of Python to solve this. For more information, see https://urllib3.readthedocs.io/en/latest/security.html#insecureplatformwarning.
  InsecurePlatformWarning
```

- Download the *freewat_dep.zip* file from the *Download area* of the *FREEWAT* website;
- Extract the content of this zip file in whatever folder;
- Close *QGIS* if it is open;
- From the START button search *OSGeo4W Shell* -> right click on it and **Run as administrator**;

- Browse to the *freewat_dep* folder using the `cd` command (e.g., if you extracted the *freewat_dep* folder under `C:\Users`, you must type `cd C:\Users\freewat_dep`);
- Type `installer_32bit.bat` (for 32-bit machines) or `installer_64bit.bat` (for 64-bit machines) and wait until all the required libraries are installed;
- A txt file renamed `install.txt` must be created manually in `C:\Users\your_name\.qgis2\python\plugins\freewat\install` or `/home/user/.qgis2/python/plugins`. This txt file must contain only the sentence `installation done`;
- Open *QGIS* and you should see *FREEWAT* as a drop-down menu in the toolbar of *QGIS*;
- If not, just go to *Plugins -> Manange and Install Plugins..*, type **FREEWAT** in the *Search* bar and click on the checkbox to activate the plugin.

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 bodies (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).

Application of *MODFLOW-OWHM* for rural water management is described in Volume 3.

Simulated processes

MODFLOW has a wide range of different Packages for simulating 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) integrated in *FREEWAT*, 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)

The following *MODFLOW* Packages are not included in the current version of the *FREEWAT* plugin:

- BCF (Block-Centered Flow; Harbaugh et al., 2000);
- HFB (Horizontal Flow Barrier; Harbaugh et al., 2000);
- SWI (Seawater Intrusion; Bakker et al., 2013);
- FHB (Flow and Head Boundary; Leake and Lilly, 1997);
- ETS (Evapotranspiration Segments; Banta, 2000);
- RES (Reservoir; Fenske et al., 1996);
- STR (Stream; Prudic, 1989);
- any solver Package other than the PCG.

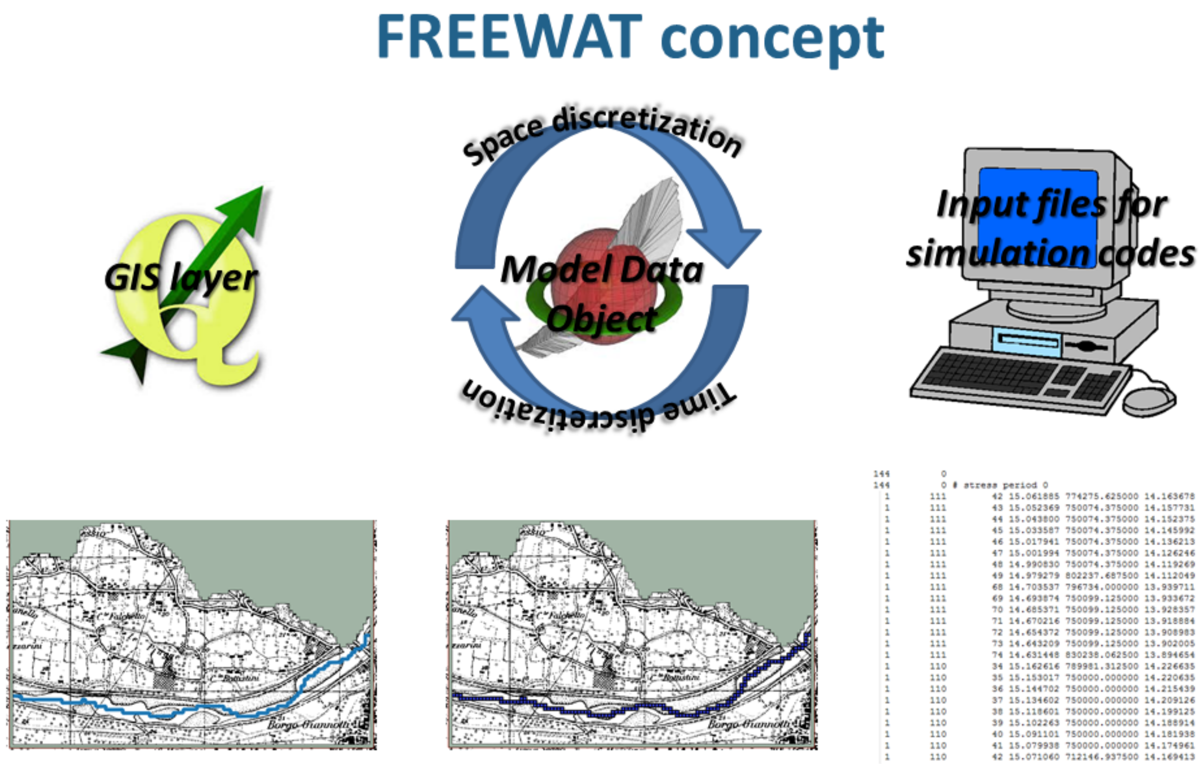
Workflow of the FREEWAT plugin

The modeler can use the *FREEWAT* plugin to implement the model, execute simulations and view and process results within a unique GIS environment (i.e., the *QGIS* Desktop).

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 programs executables.

The *FREEWAT* terminology is the following:

- *GIS layer* - it indicates a generic geographic informative layer (i.e., a vector/raster 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 nothing but 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 of the model;
- *model file* - it is a text file generated from an MDO and required to run the simulation.



Model layers and MDOs are permanently stored within a *SpatiaLite* geodatabase.

As a first step, 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, as described in Chapter 3.

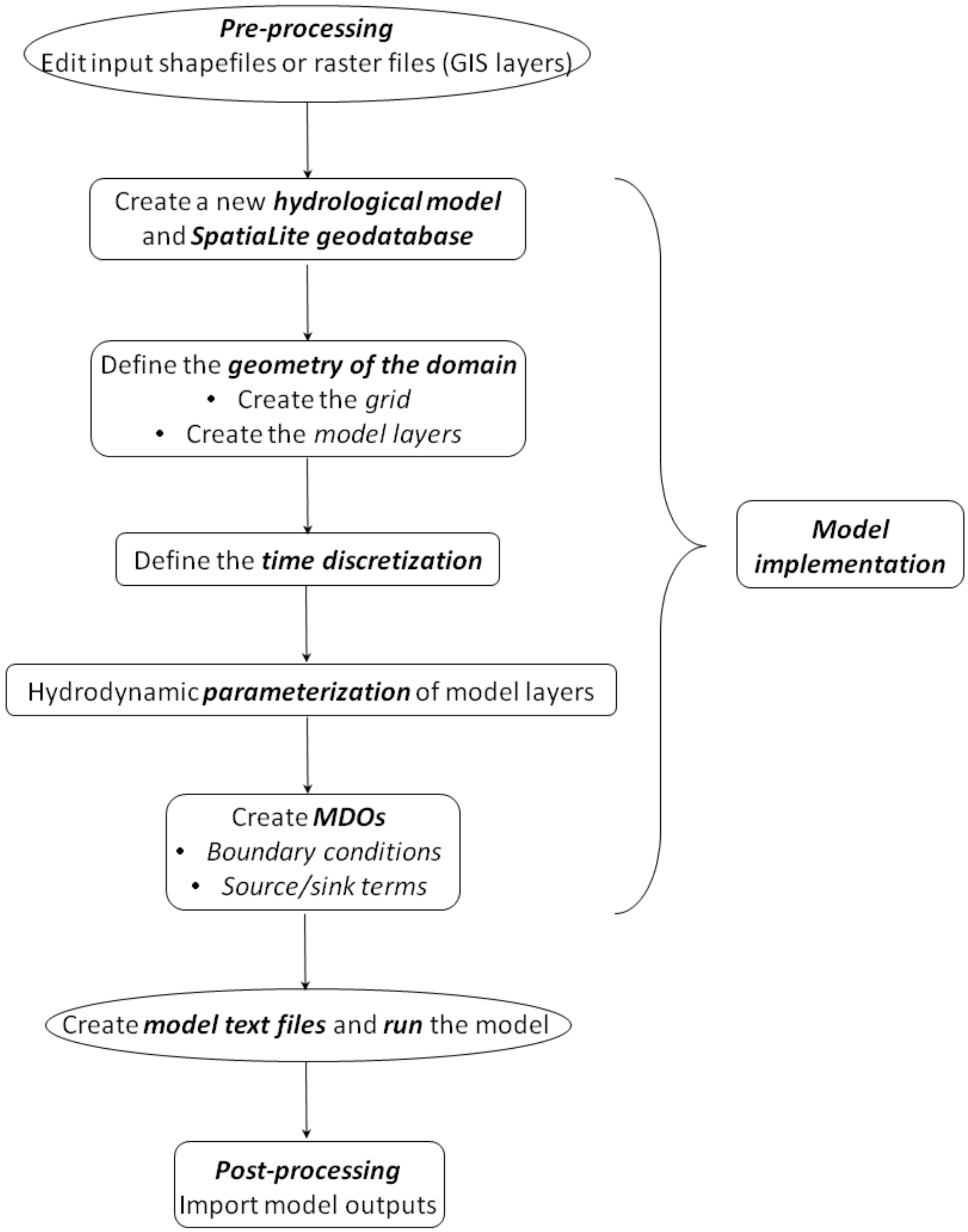
Then, the spatial and time discretizations of the model will be defined, including parameterization of the hydrodynamic properties of each model layer (Chapters 4 and 5).

Boundary conditions and sink/source terms will be defined as well, creating the related MDOs from the available GIS layers (Chapter 6).

Finally, once selecting 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, as described in Chapter 7.

Note: This step is performed automatically and internally to the *FREEWAT* code.

Visualization and post-processing of model results (e.g., the simulated hydraulic head) are described in Chapter 8.


Pre-processing
Edit input shapefiles or raster files (GIS layers)
Create a new hydrological model and SpatiaLite geodatabase
Define the geometry of the domain
• Create the grid
• Create the model layers
Define the time discretization
Hydrodynamic parameterization of model layers
Create MDOs
• Boundary conditions
• Source/sink terms
Model implementation
Create model text files and run the model
Post-processing
Import model outputs

Limitations

About creation of model files for *MODFLOW*, *FREEWAT* has some limitations related to some flags and options, assuming default values which the User cannot change. The aim is to make the model implementation easier.

Such limitations, specifically related to 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* as a default: this means that confining beds cannot be simulated;
- the default options set for the Layer Property Flow (LPF) file are the following:
  - the value -1E+30 m is assigned by default as hydraulic head of grid cells which get dry at convertible model layers at the end of the simulation. This could cause an inconvenience in visualizing the hydraulic head distribution of that model layer as a color scale map, as that particular value (-1e+30) is not recognized in *QGIS* as a no-data value. If this occurs, the User must define such value as an additional no-data value, thus assigning a 100% transparency to all the dry grid cells where it has been assigned;
  - the flag *CHANI* is set to *1* as a default: this means that isotropic conditions occur at each model layer along the X and Y axis. As such, the hydraulic conductivity along the Y axis (KY) will be automatically set equal to that along the X axis, whatever value the User will input for KY in the Attribute Table of a model layer (see Chapter 4);
  - the flag *LAYVKA* is set to *0* as a default: this means that no vertical anisotropy can be defined. As such, the User has to input value for both horizontal and vertical hydraulic conductivity at each grid cell and for each model layer (see Chapter 4);
- the default options set for the Output Control Option (OC) file are the following:
  - hydraulic head, drawdown and cell-by-cell flow are all of them stored at the end of each Time Step (TS) within external binary files;
  - either model balance and the simulated hydraulic head are printed in the output Listing (LST) file at the end of each TS. This could sometimes result in an oversized file.

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

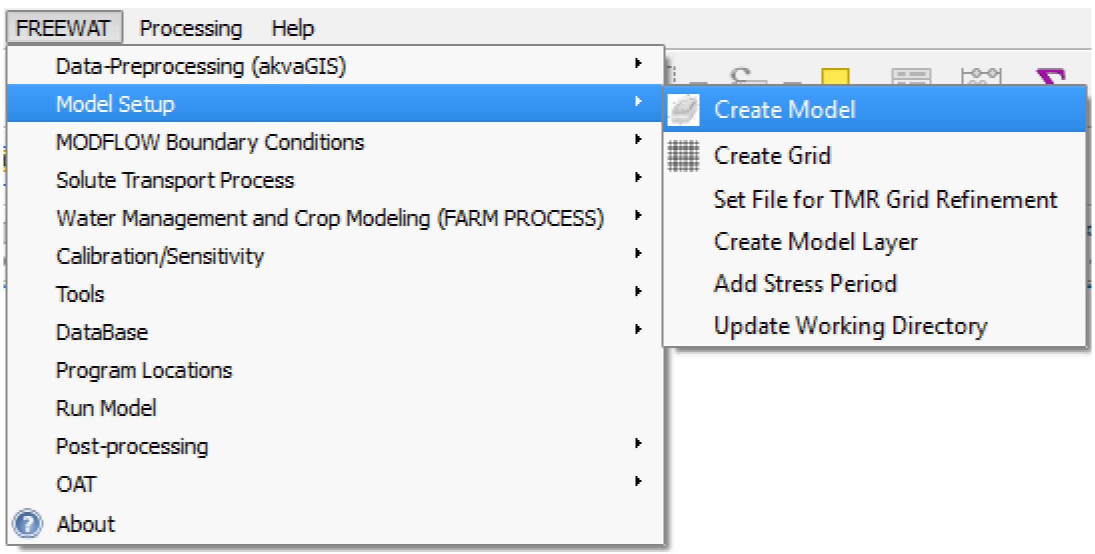
CHAPTER 3

Create a new hydrological model and geodatabase

Simulating a new hydrological scenario requires creating a new hydrological model and a model DataBase (DB).

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

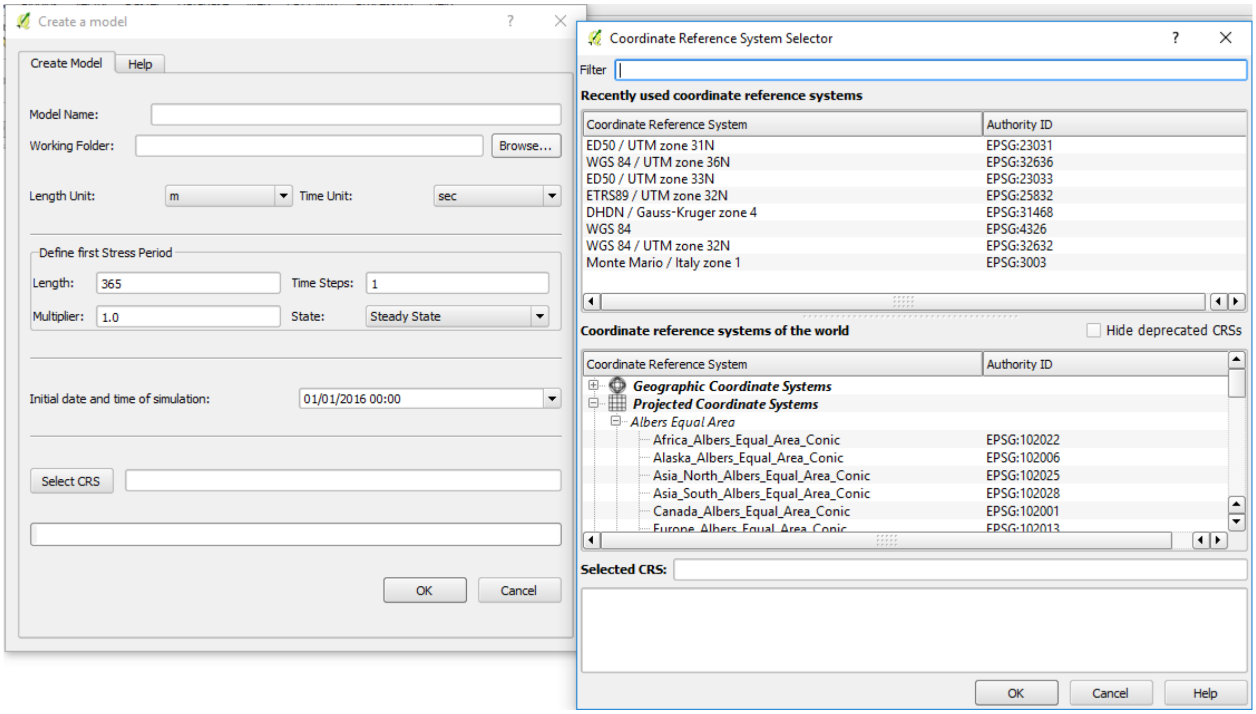
FREEWAT -> Model Setup -> Create Model



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*: length unit to be used throughout the simulation; four options are available (*m*, *cm*, *ft*, *undefined*);
- *Time Unit*: time unit to be used throughout the simulation; 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 each TS within the first SP;
  - *State*: two options are available (*Steady State*, if the solution of the model, i.e. the hydraulic head, does not change in time, and *Transient*, if the evolution of the hydraulic head over time is simulated);

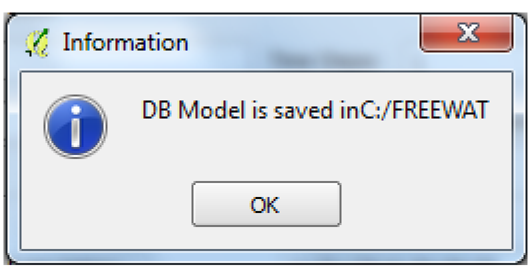
- *Initial date and time of simulation*: starting date and time of the simulation, using formats dd/mm/YYYY and hh:mm:ss, respectively (it is also possible to choose the starting date from a drop-down calendar);
- by clicking on *Select CRS*, it is possible to select the Coordinate Reference System (CRS)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



Note: Once *Length Unit* and *Time Unit* are defined, 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. Anyway, the selected options can be then modified (details are provided below).

Note: The User **MUST AVOID** spaces and/or special characters (e.g., accents) in the path of the *Working Folder*.

Once the new model is created, an **Information** window appears reporting that the corresponding *SpatiaLite* model DB has been created and stored within the selected *Working Folder* as *model_name.sqlite* (where *model_name* is the name assigned to the new hydrological model in the *Model Name* field of the **Create a model** window).

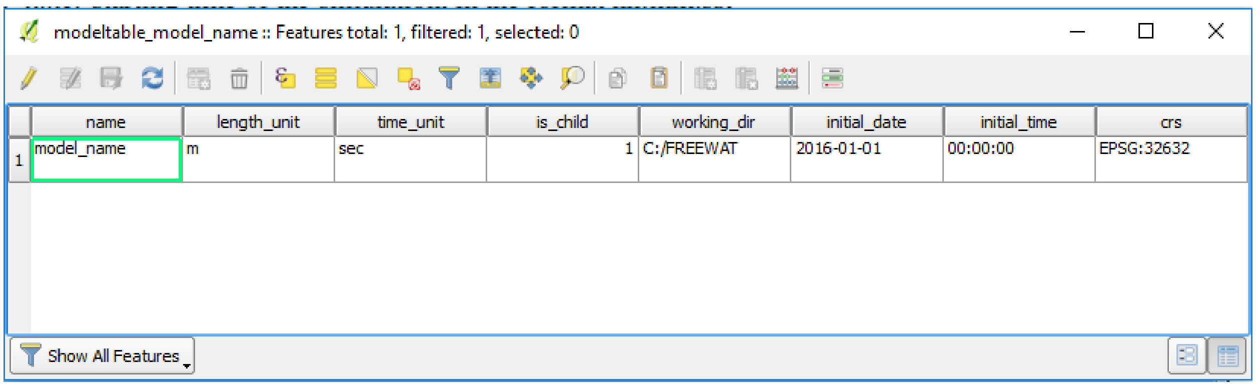


All the tables, model layers and MDOs created are permanently stored within this model DB, even if they are deleted by mistake from the Layers Panel. The model DB can be explored by using *QGIS* tools. For example, with the *DB Manager* plugin, each table, or model layer, or MDO stored within the *SpatiaLite* model DB can be simply renamed, deleted or added to the Map Canvas as needed. Such plugin should be already available in the *QGIS* interface, if not it can be found and activated within the official *QGIS* repository. Details about how to use the *DB Manager* plugin are provided in section *Import an existing DB* below.

Once the new model is created, three tables renamed *modeltable_model_name*, *timetable_model_name* and *prg_locations_model_name* are created, loaded in the Layers Panel and stored within the model DB.

The model table contains the following fields:

- *name*: name of the hydrological model just created (what appears in this field and the name of the *.sqlite* file is, **and MUST stay**, the same);
- *length_unit*: length unit defined through the *Length Unit* field above (*m*, *cm*, *ft* or *undefined*);
- *time_unit*: time unit defined through the *Time Unit* field above (*sec*, *min*, *hour*, *day*, *month*, *year* or *undefined*);
- *is_child*: this field is not relevant for the current version of the *FREEWAT* plugin, 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*: path of the selected *Working Folder*;
- *initial_date*: starting date of the simulation, in the format YYYY-mm-dd;
- *initial_time*: starting time of the simulation, in the format hh:mm:ss;
- *crs*: CRS set for the hydrological model just created (please, be sure that all your input *GIS* layers (vector and raster files) have been produced in the same CRS. If not, conversion is needed).



Each of these fields can be modified manually, activating the *Toggle editing mode* (refer to Chapter 5).

Note: For fields *length_unit* and *time_unit*, only the above listed options can be used (e.g., *undefined*; no capital letters). For fields *initial_date*, *initial_time* and *crs*, the only format to be used is the one shown in the above figure.

Note: The field *working_dir* can be modified either manually (the only format to be used is the one shown in the above figure, i.e., slash must be used, backslash is not recognized) or through the menu *FREEWAT -> Model Setup -> Update Working Directory* (see details in section *Import an existing DB*).

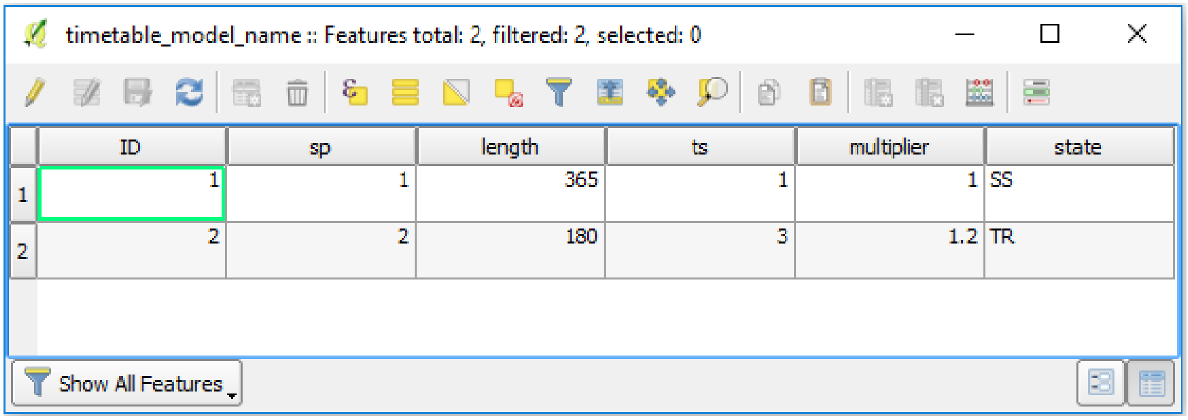
If the model table is accidentally deleted from the Layers Panel, it can be retrieved from the model DB (where it is permanently stored) by using the *DB Manager* plugin.

If the model table is accidentally deleted either from the Layers Panel, a new model need to be created.

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 (for details refer to Harbaugh, 2005);
- *state* with indication of the *State* for each SP (*SS* for *Steady State*, *TR* for *Transient*).



	ID	sp	length	ts	multiplier	state
1	1	1	365	1	1	SS
2	2	2	180	3	1.2	TR

Each of these fields can be modified manually, activating the *Toggle editing mode* (refer to Chapter 5).

Note: For the field *state*, only the above listed options can be used (*SS* or *TR*; capital letters only).

Note: If more SPs are defined later, as described in Chapter 4, the time table is automatically updated.

If the time table is accidentally deleted from the Layers Panel, it can be retrieved from the model DB (where it is permanently stored) by using the *DB Manager* plugin.

If the time table is accidentally deleted either from the Layers Panel, a new model need to be created.

The table of program locations is needed to define the paths of the simulation codes executables to be used to simulate specific processes. It contains the following fields:

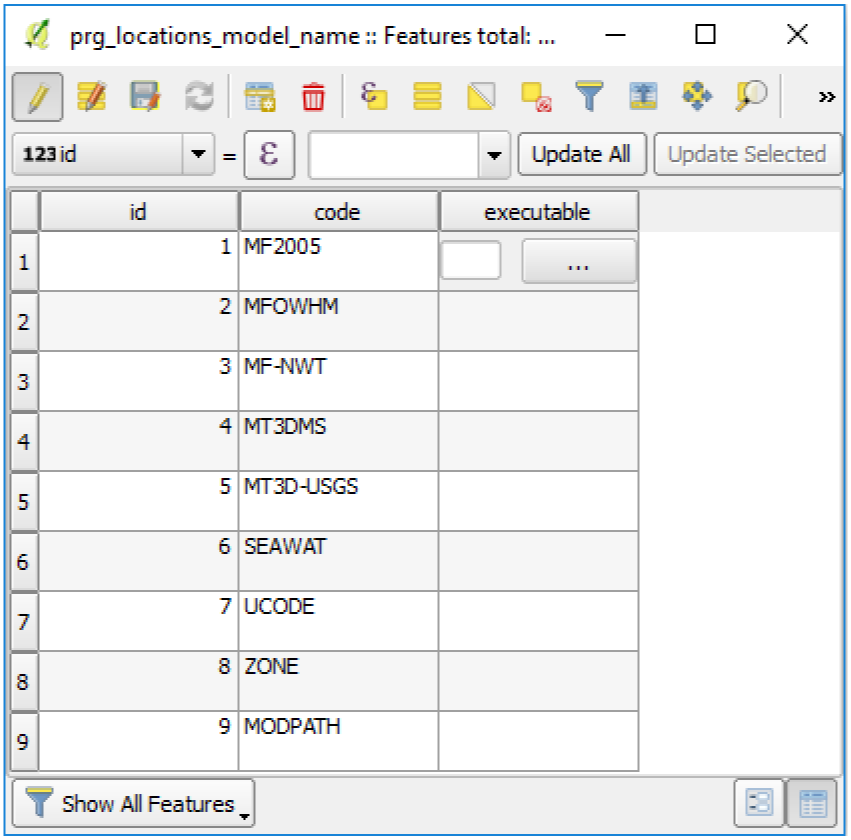
- *id*: progressive ID of each executable;
- *code*: name of the software code to be executed;
- *executable*: path defined for each executable.

A path for the needed executables can be set using the browse button which appears at each cell of the field *executable*, by single-clicking or double-clicking within it.

The following software codes can be run, according to the processes to be simulated (the folder *executables* is downloadable from the *FREEWAT* website, and it contains the executables for all the software codes listed below):

- *MF2005* for groundwater flow modeling with *MODFLOW-2005* (Harbaugh, 2005);
- *MFOWHM* for groundwater flow modeling and water management with *MODFLOW-OWHM* (Hanson et al., 2014);
- *MF-NWT* for groundwater flow modeling with *MODFLOW-NWT* (Niswonger et al., 2011);
- *MT3DMS* for transport modeling in the saturated zone with *MT3DMS* (Zheng and Wang, 1999);
- *MT3D-USGS* for transport modeling in the unsaturated zone with *MT3D-USGS* (Bedekar et al., 2016);
- *SEAWAT* for simulating viscosity-/density- dependent flow with *SEAWAT* (Langevin et al., 2007);

- *UCODE* for sensitivity analysis and model parameters estimation with *UCODE* (Poeter et al., 2014);
- *ZONE* to explicit the water budget at sub-regions of the active domain with *ZONE BUDGET* (Harbaugh, 1990);
- *MODPATH* for particle-tracking with *MODPATH* (Pollock, 2016).



Note: Once all the executables needed are loaded through the browse button, it is necessary to click wherever out of the corresponding cell, so that the path of that executable is correctly stored.

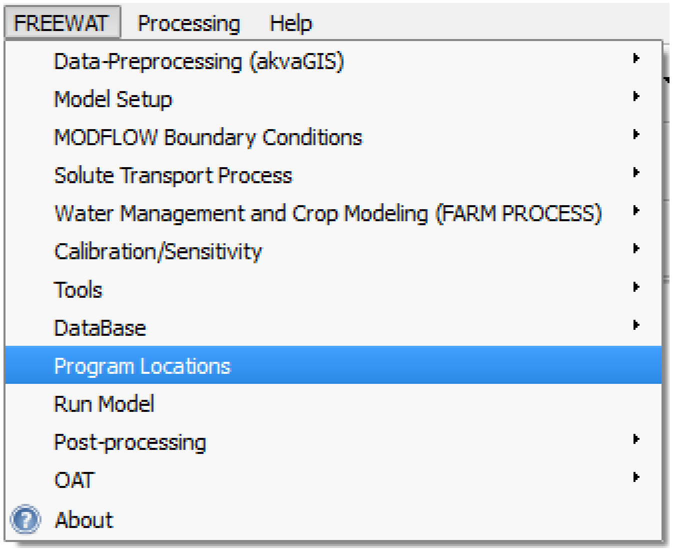
Note: Version 6.0.01 is needed for the *MODPATH* executable.

Note: The executables provided in the *executables* folder **DO NOT** need to be installed (e.g., double-clicking on them), but they **only** need to be saved somewhere and then loaded in the *prg_locations_model_name* table.

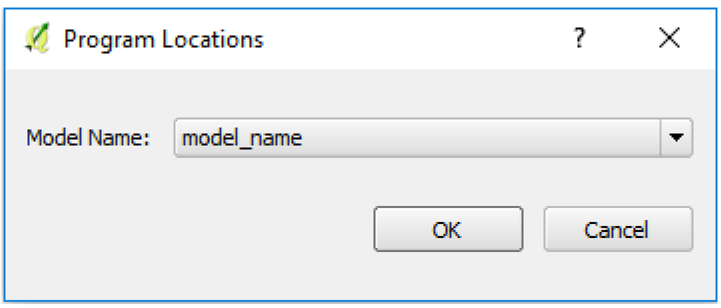
If the table *prg_locations_model_name* is accidentally deleted from the Layers Panel, it can be retrieved from the model DB (where it is permanently stored) by using the *DB Manager* plugin.

If the table *prg_locations_model_name* is accidentally deleted either 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* only (i.e., the name of the hydrological model created) is required:



Import an existing DB

Importing an existing DB requires having the *.sqlite* file in a selected 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*.

In the following, two methods are described for importing an existing DB:

- the first method is useful if the User wishes to import an existing DB and keep working on it without renaming it;
- the second method is useful if the User wishes to import an existing DB after renaming it (e.g., in order to create a new version of the original DB).

Steps to import an existing DB without renaming the *.sqlite* file

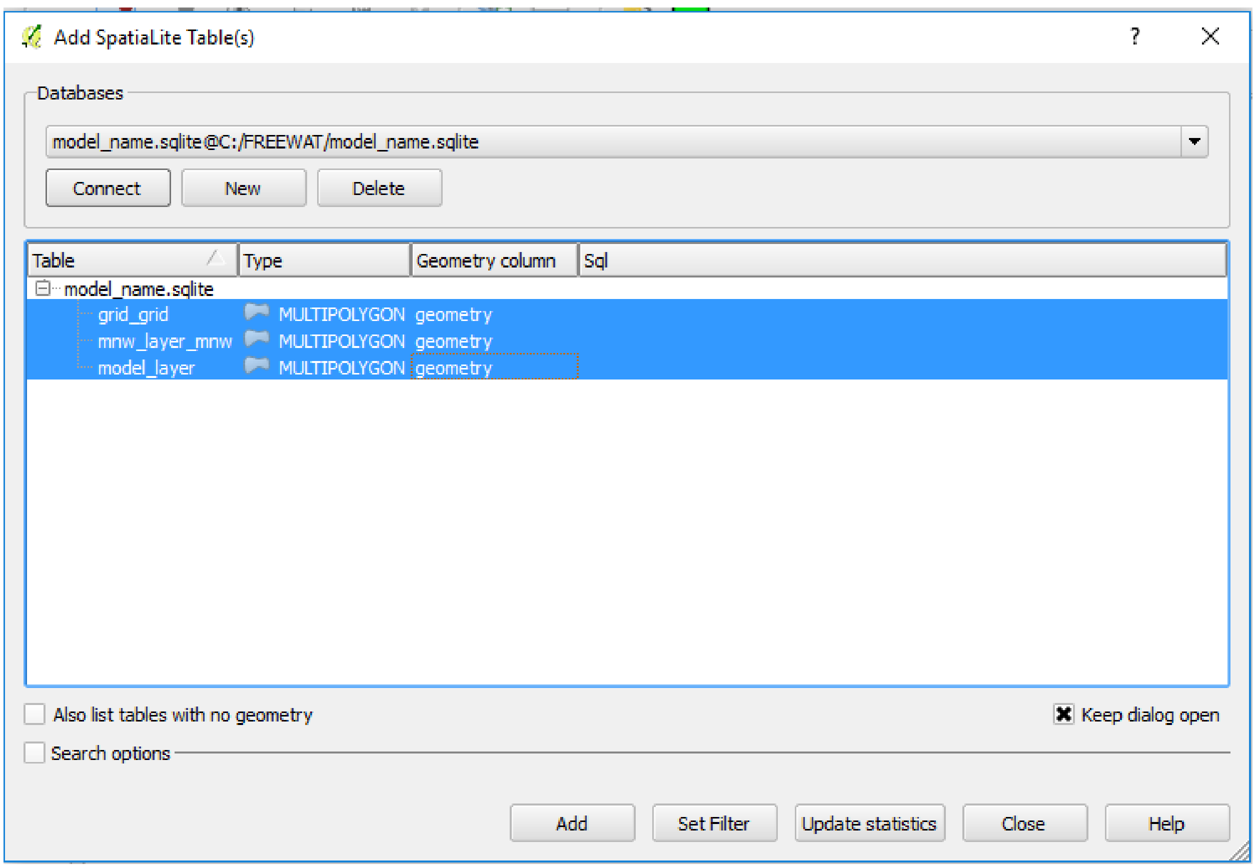
To import the existing DB, the User must use the button *Add SpatiaLite Layer* in the *QGIS* GUI, which can be found next to the Layers Panel.

In the **Add SpatiaLite Layer(s)** window, 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 connected in advance, the User can either delete the connection to the old *.sqlite* file, or assign a different name to the new connection (NOTE: opting for this last choice **DOES NOT** change the name of the *.sqlite* file, but of the connection **ONLY**).

Before to proceed with the next steps, the User should check the *Keep dialog open* checkbox (at the lower right corner of the **Add SpatiaLite Layer(s)** window).

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



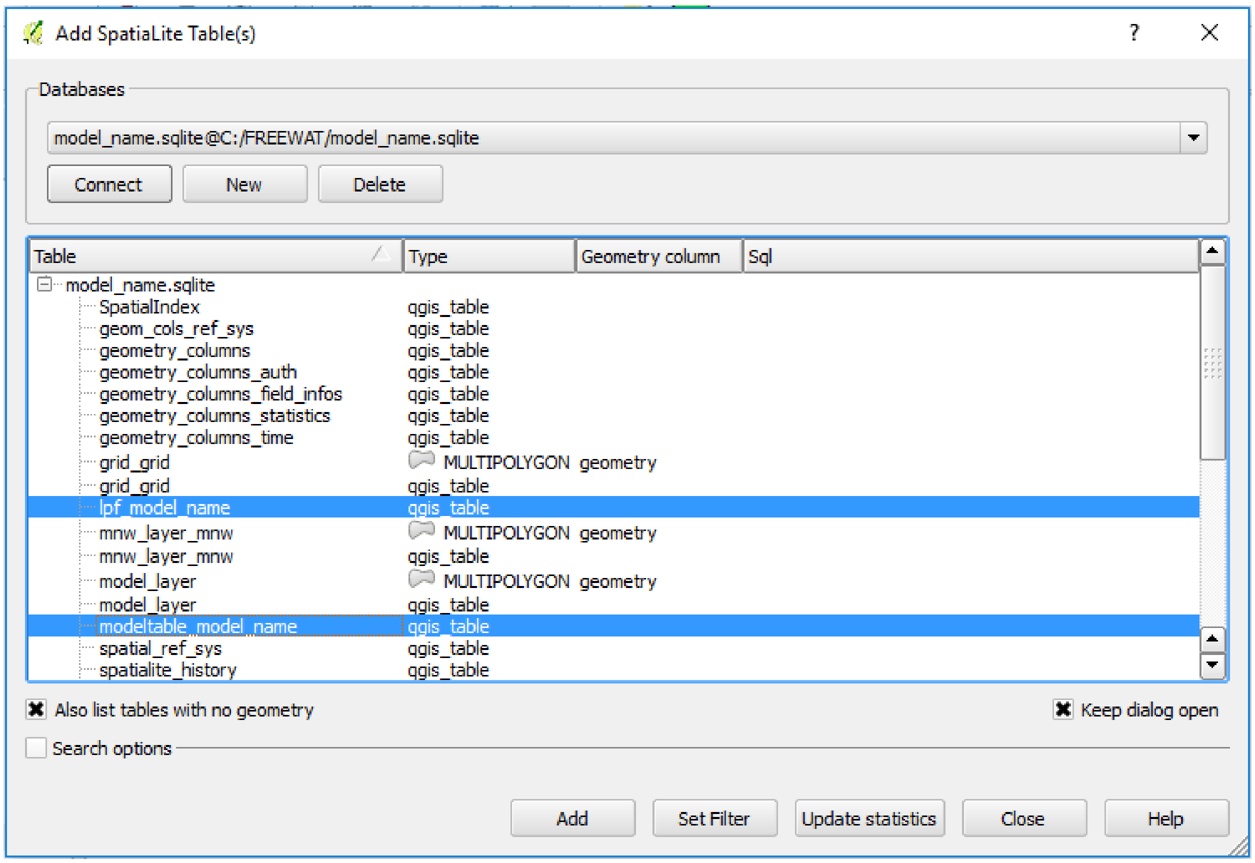
As some tables are also needed, the User must check the *Also list tables with no geometry* checkbox (at the lower left corner of the **Add SpatiaLite Layer(s)** window), select the tables needed (see below) and click on *Add* to add them to the Layers Panel.

The following tables are **mandatory**:

- *model table*;
- *time table*;
- *lpf table* (see Chaper 4);
- *program locations*.

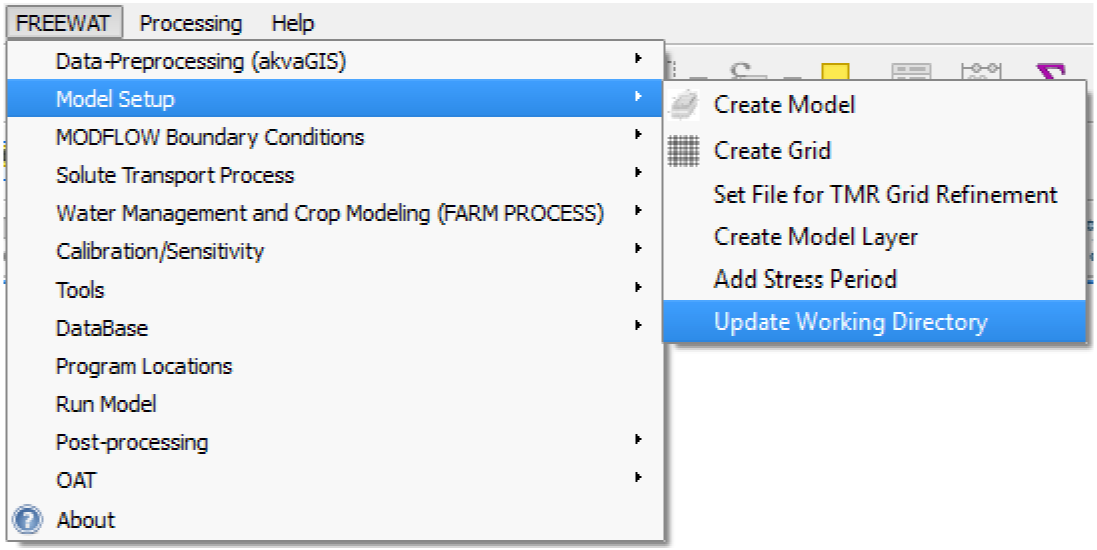
Furthermore, if the *SFR Package* is implemented, the related table must be loaded (further details will be provided in Chapter 6).

Note: These four mandatory tables (plus the table associated with the _*sfr* MDO, if implemented, see Chapter 6) are referred to the groundwater flow process described in this Volume. If any other process is to be simulated (e.g., solute transport, calibration, etc.), some other tables are needed to be loaded in the Layers Panel. For further information, the User has to refer to the related Volumes.



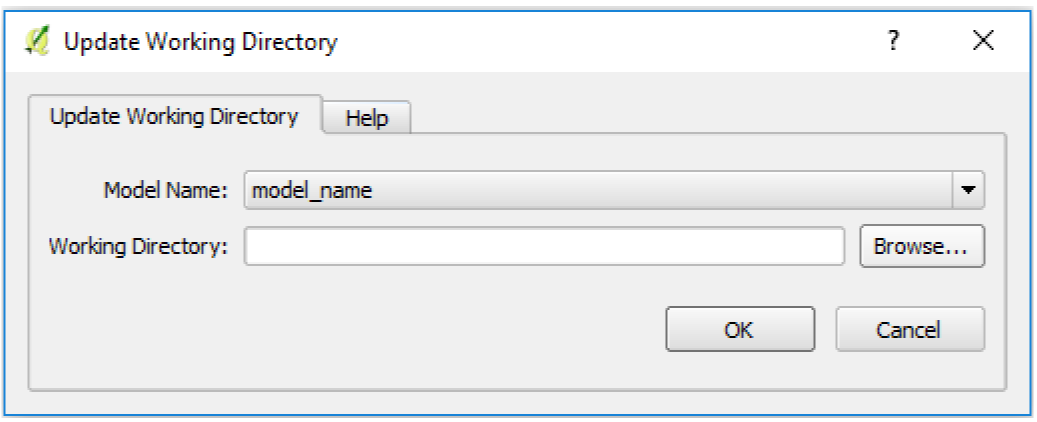
Once all the needed tables, model layers and MDOs are loaded in the Layers Panel, the path of the *Working Directory* in the model table must be updated through the following menu:

FREEWAT -> Model Setup -> Update Working Directory



In the **Update Working Directory** window, the following data are required:

- *Model Name*: name of the hydrological model (it is the same appearing in the *name* field of the model table);
- *Working Directory*: folder within which the *.sqlite* file has been saved and where the *MODFLOW* input and 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 field *executable* in the table of program locations. Please, notice that in such case the browse button could not appear. As such, the User must edit the path manually (using slashes instead of backslashes; the path must end with the name of the needed executable, e.g., C:/FREEWAT/executables/mf2005.exe) or deleting the table of program locations both from the Layers Panel and from the model DB and create it from scratch through the menu *FREEWAT* -> *Program Locations*.

Note: If the *.sqlite* file is provided along with the whole *.qgis* project, using this method (i.e., importing the DB *without* renaming the *.sqlite* file) is manadatory, otherwise the paths of all the objects loaded in the Layers Panel will not be recognized anymore.

Steps to import an existing DB after renaming the *.sqlite* file

If the *.sqlite* file has to be renamed before importing the existing DB, the steps reported above must be slightly revised.

First of all, the *.sqlite* file must be renamed as needed.

The renamed *.sqlite* file can then be imported exactly as explained above, through the *Add SpatiaLite Layer* tool.

In the model table, the following fields must be updated **manually**:

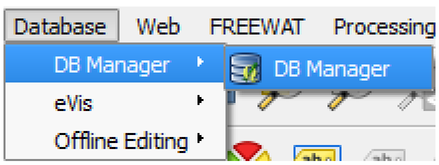
- *name*: the name of the hydrological model must be the same as the *.sqlite* file just renamed);
- *working_dir*: the whole path of the folder where the *.sqlite* is stored must be input (no spaces and/or special characters; slashes instead of backslashes).

Once saving the edits above, the model table, the time table, the lpf table and the table of program locations must be deleted from the Layers Panel, as the final part of their name (which corresponds to the old name of the hydrological model) must be modified. To do so, the *SpatiaLite* DB (the one renamed) must be accessed through the *DB Manager* plugin.

The *DB Manager* plugin can be found at:

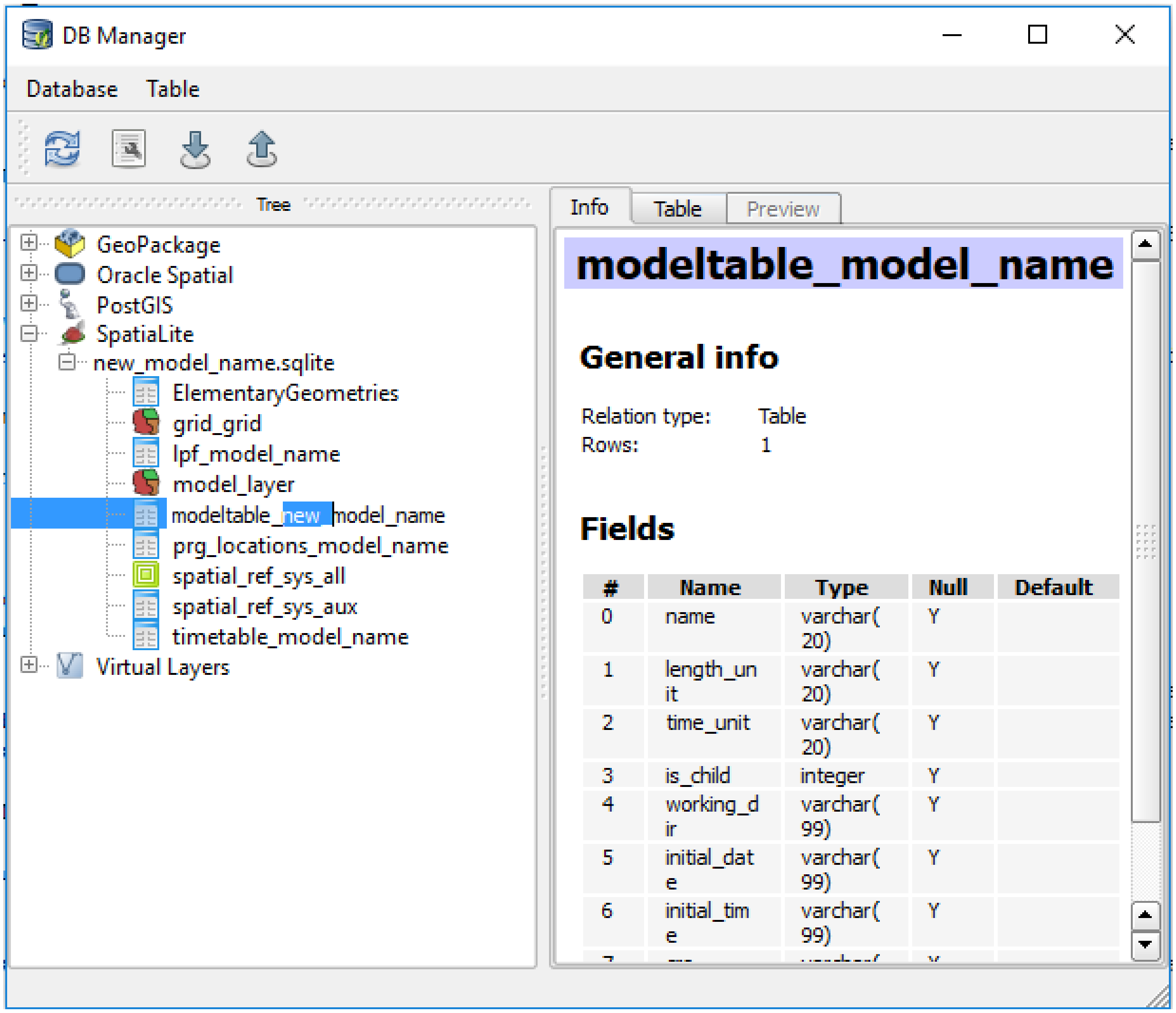
Database -> DB Manager -> DB Manager

If not, it can be found and activated within the official *QGIS* repository



In the **DB Manager** window, *SpatiaLite* must be expanded and also the item corresponding to the *.sqlite* file just renamed.

All the tables, model layers and MDOs created are listed, along with some default *QGIS* tables. By right-clicking on each of the above-mentioned tables (i.e., model table, time table, lpf table and the table of program locations), the User can rename them modifying the last part of their names (e.g., from *modeltable_model_name* to *modeltable_new_model_name*).



Once done, these tables must be added again to the Layers Panel (right-click on each of them -> *Add to canvas*).

Finally, the path for all the needed executables must be updated, editing the field *executable* in the table of program locations, exactly as described above.

CHAPTER 4

Space and time discretization

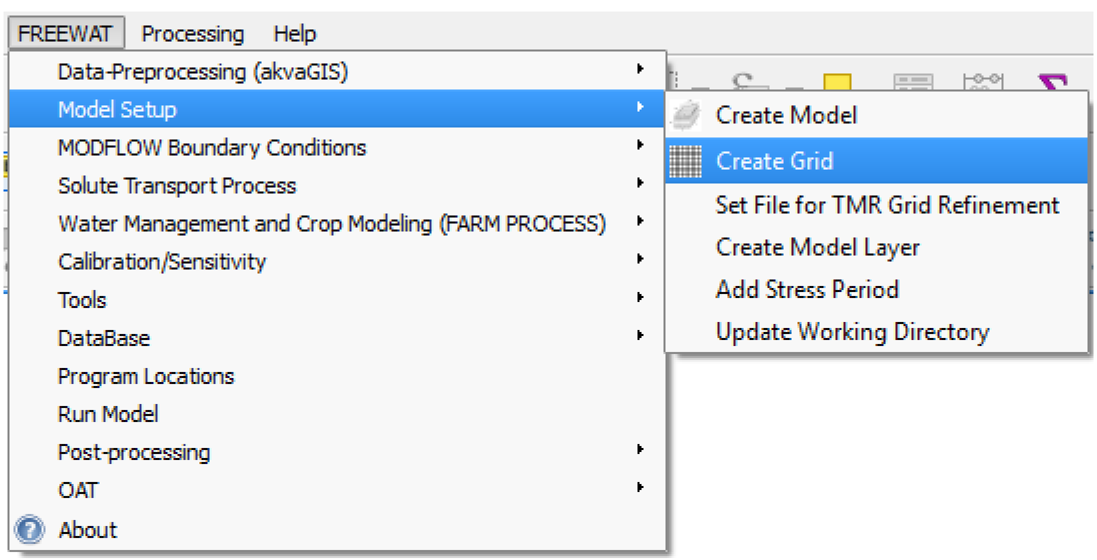
Once the input GIS files are ready and the conceptual model is defined, it is necessary to set up the 3D geometry of the aquifer system (i.e., the finite-difference horizontal grid and the vertical discretization) and the time discretization of the simulation.

Create the finite-difference grid

To create the finite-difference grid, the extent of the study area must be known. For this purpose, a polygon shapefile, which bounds the study area and within which the grid will be created, may be useful. 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 is a square with a side length of 100 m, each border of the polygon shapefile can extend for 1000 m, but not for 1025 m). Such polygon shapefile must be created in the correct CRS, coeherently with that chosen when the hydrological model has been created. Alternatively, a background map cut to the study area extent can be used.

To create the grid, the following menu must be used:

FREEWAT -> Model Setup -> Create Grid

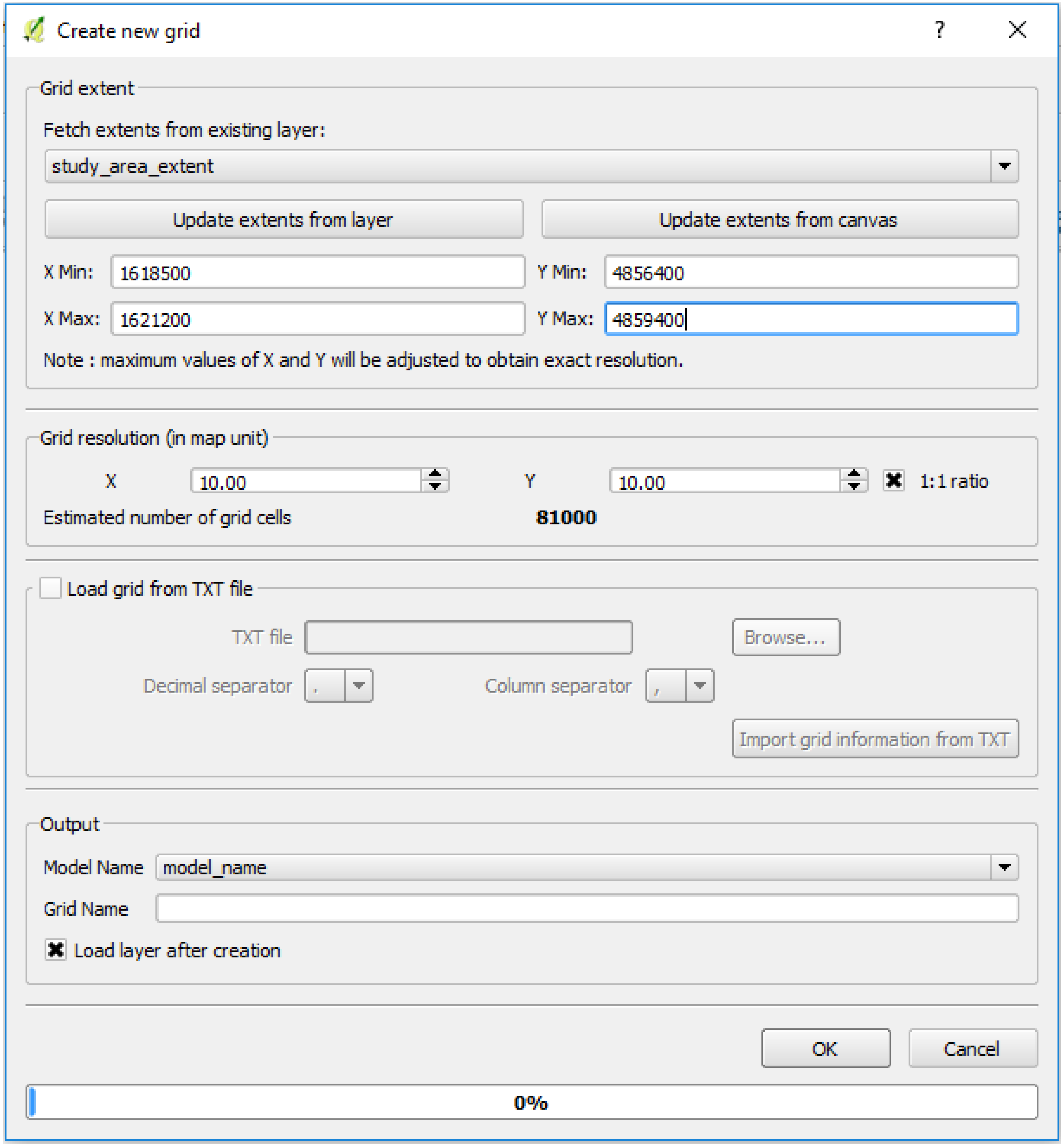


The following data are required in the **Create new grid** window:

- in the *Grid extent* section:
  - if available, the polygon shapefile previously created, containing the extent of the study area, or a background map cut to the study area extent must be selected under *Fetch extents from existing layer*;

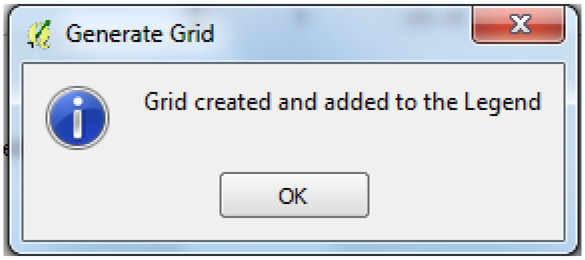
- *X Min*, *X Max*, *Y Min* and *Y Max* are the spatial coordinates of the vertices of the polygon containing the study area and within which the finite-difference grid will be created. There are three options to specify them:
    - they can be loaded from the above-mentioned polygon shapefile containing the extent of the study area, or a background map cut to the study area extent (*Update extents from layer*);
    - they can be updated based on the view extent of the Map Canvas (*Update extents from canvas*);
    - they can be input manually by the User;

- in the *Grid resolution (in map unit)* section:
  - the grid resolution (in length units) along *X* and *Y* directions. If the box *1:1 ratio* is checked, square grid cells will be generated;
- the *Load grid from TXT file* section is only needed to create a refined grid (further details in section *Telescopic Mesh Refinement*);
- 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*).

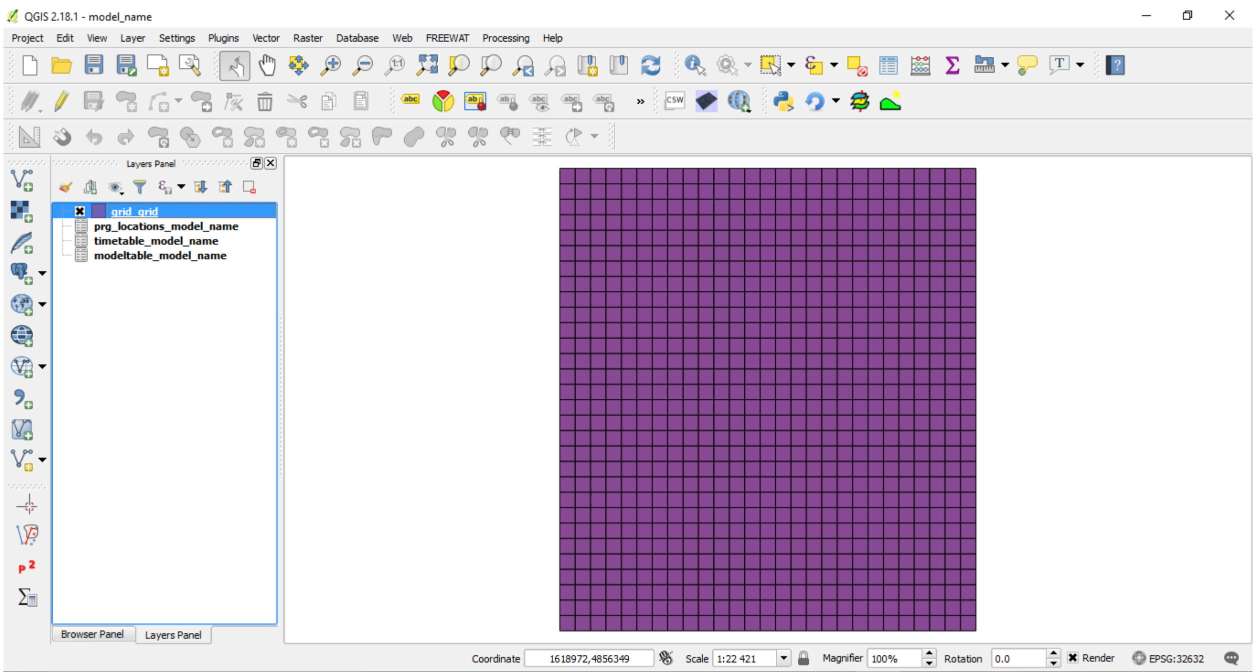
An information window **Generate Grid** appears reporting that the model grid has been successfully created.



Once the grid MDO is created, it is stored within the model DB with the name assigned by the User in the *Grid Name* field and eventually loaded in the Layers Panel.

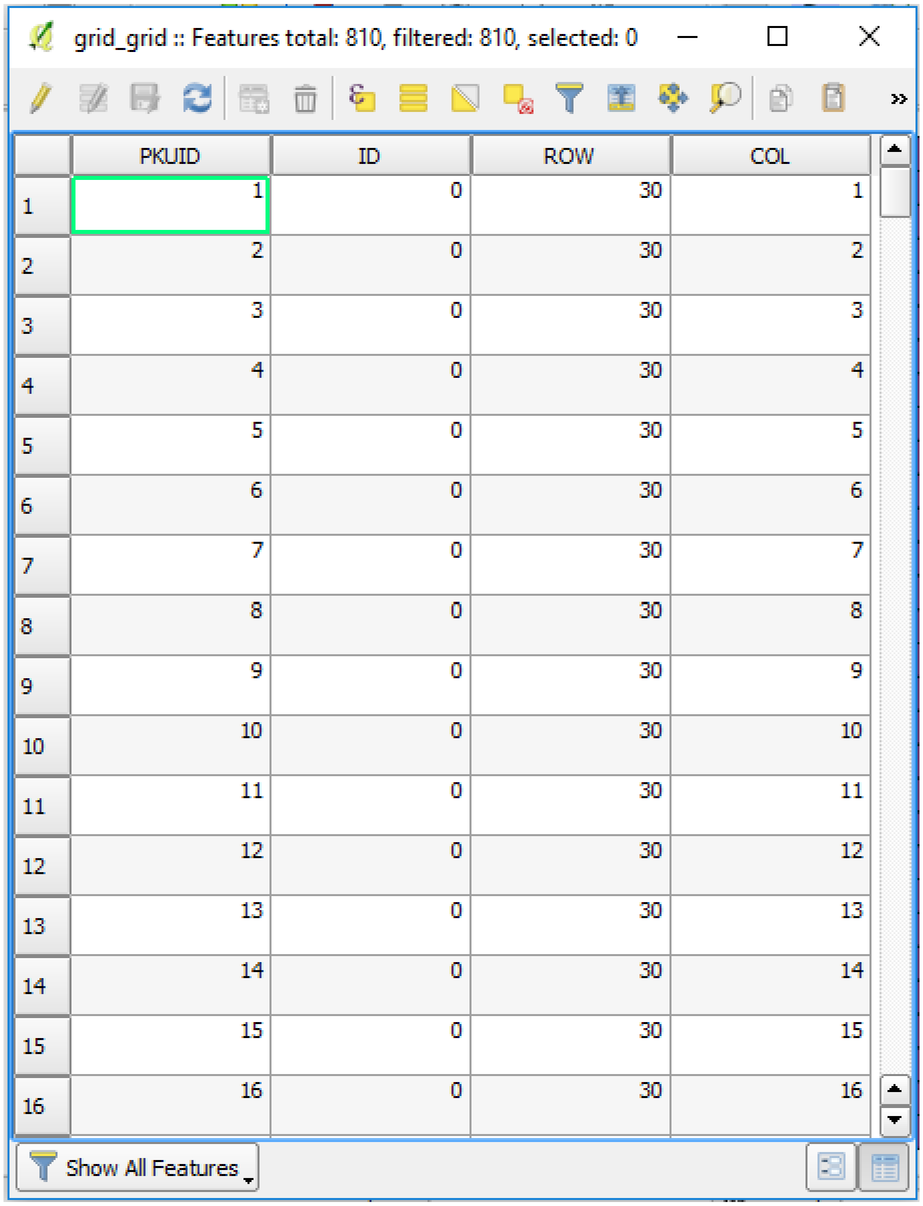
Note: The extension *_grid* is automatically added at the end of the name assigned by the User in the *Grid Name* field of the **Create new grid** window. It must not be changed in the Layers Panel and neither in the DB, as the grid MDO will be filtered in each dialog according to such extension.

The view of the grid MDO in the Map Canvas is provided in the figure below.



The Attribute Table of the grid MDO contains 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 index of a grid cell;
- *COL*: column index of a grid cell.



grid_grid :: Features total: 810, filtered: 810, selected: 0

	PKUID	ID	ROW	COL
1	1	0	30	1
2	2	0	30	2
3	3	0	30	3
4	4	0	30	4
5	5	0	30	5
6	6	0	30	6
7	7	0	30	7
8	8	0	30	8
9	9	0	30	9
10	10	0	30	10
11	11	0	30	11
12	12	0	30	12
13	13	0	30	13
14	14	0	30	14
15	15	0	30	15
16	16	0	30	16

Show All Features

Note: The row and column indexes must not be modified in the grid MDO, nor in any grid-based MDO created in the following.

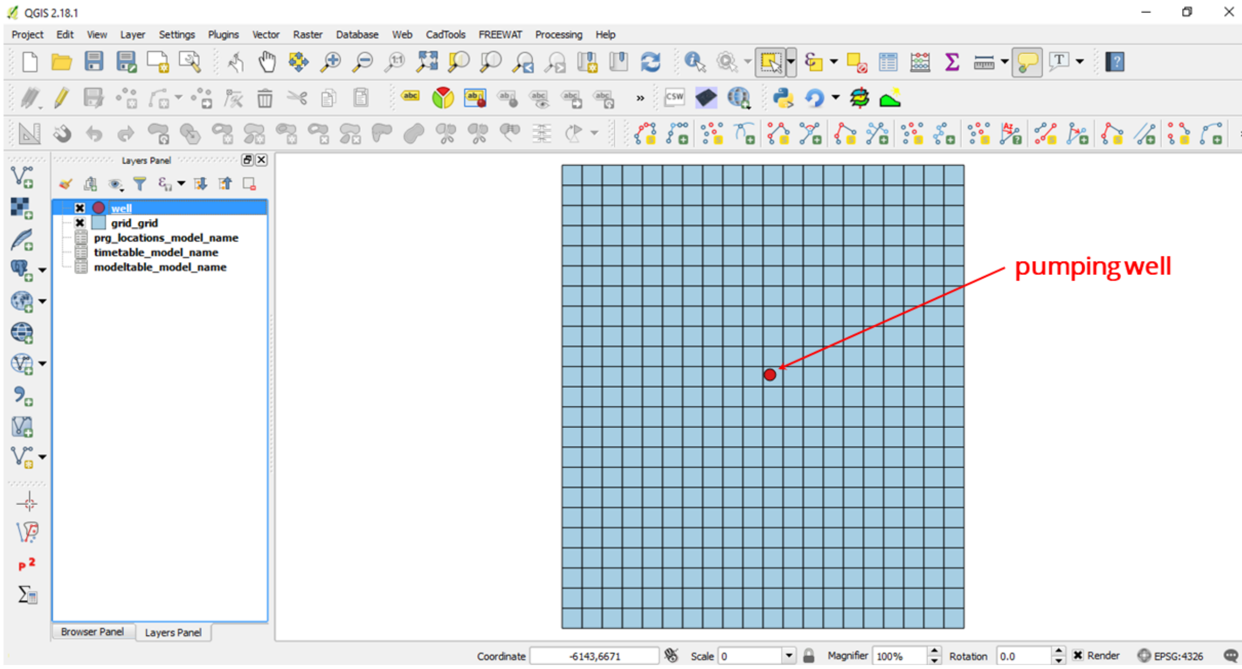
Once created, the finite-difference grid will be used to create model layers and further MDOs (e.g., the areally distributed recharge).

Telescopic Mesh Refinement

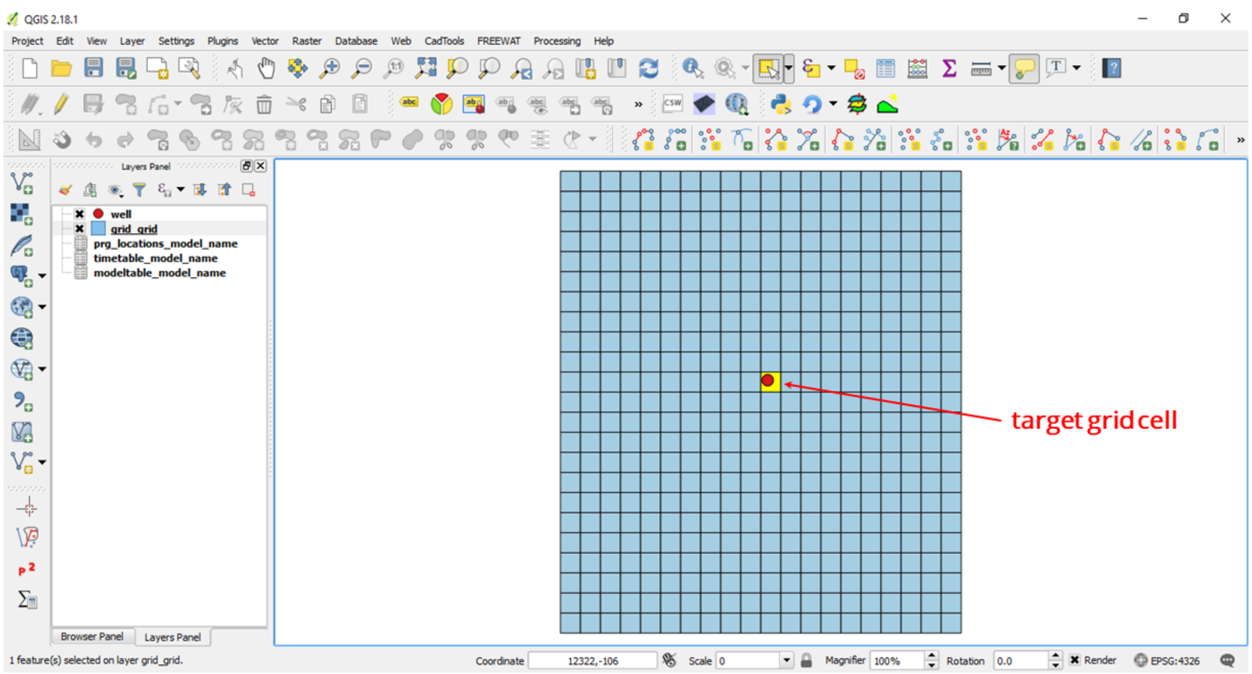
Telescopic Mesh Refinement (*TMR*) is a common application in groundwater modeling when one wishes to refine the model grid at some location within the study area (e.g., nearby a pumping well). The *TMR* tool integrated in the present version of the *FREEWAT* plugin allows the User to split a selected grid cell, and the related row and column, into different parts. The width of the adjoining rows and columns will be adapted accordingly, by setting a multiplier to increase their size from the target cell towards the borders.

The steps which have to be performed to get a grid refined around a certain cell are listed below.

Step 1. Let's suppose to have a regular grid, created using the *FREEWAT* tool *Create Grid*, and a pumping well in the middle of the study area. We want to refine the grid around the grid cell where the pumping well is located.



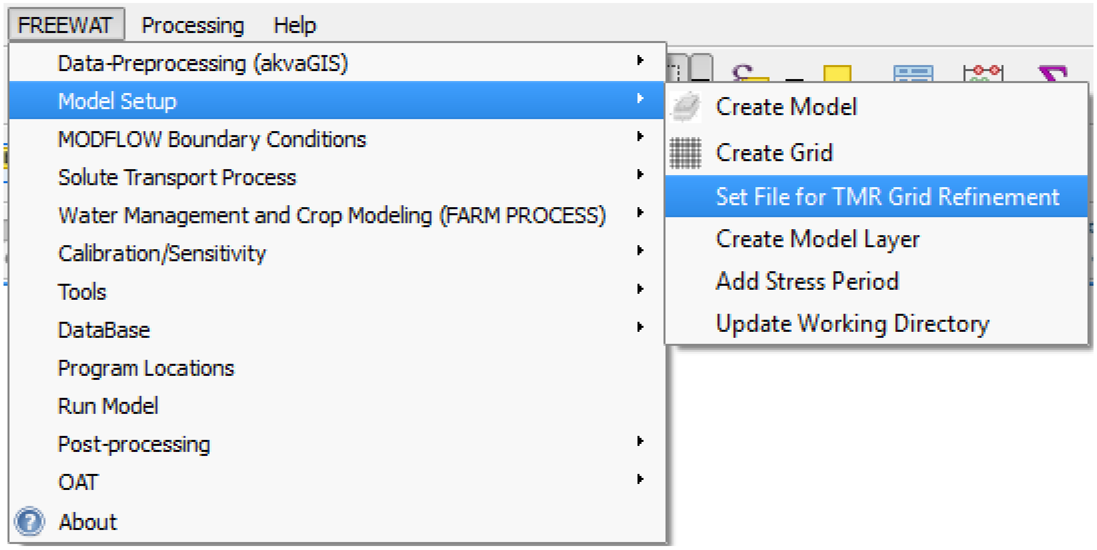
Step 2. The target cell (i.e., the one where the pumping well is located) must be selected from the grid MDO.



The refined grid will be built starting from the centroid of the target cell in the regular grid. Specifically, the target cell, and the related row and column, will be resized around its centroid, according to User-defined sizing settings reported below.

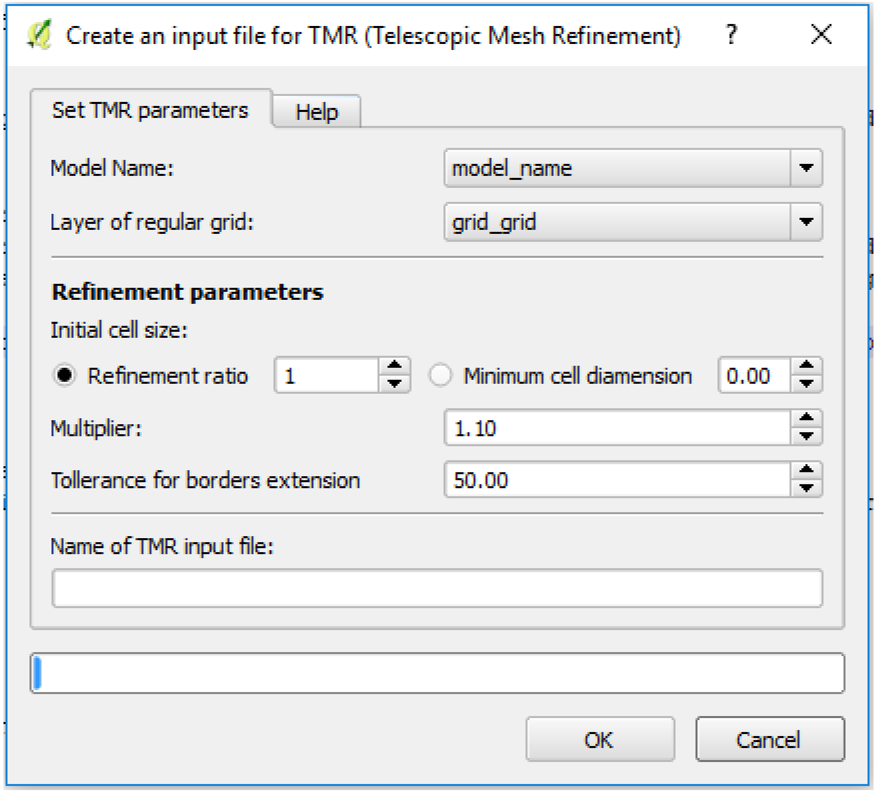
Step 3. Define the refinement options using the *TMR* tool, which can be accessed through the following menu:

FREEWAT -> Model Setup -> Set File for TMR Grid Refinement



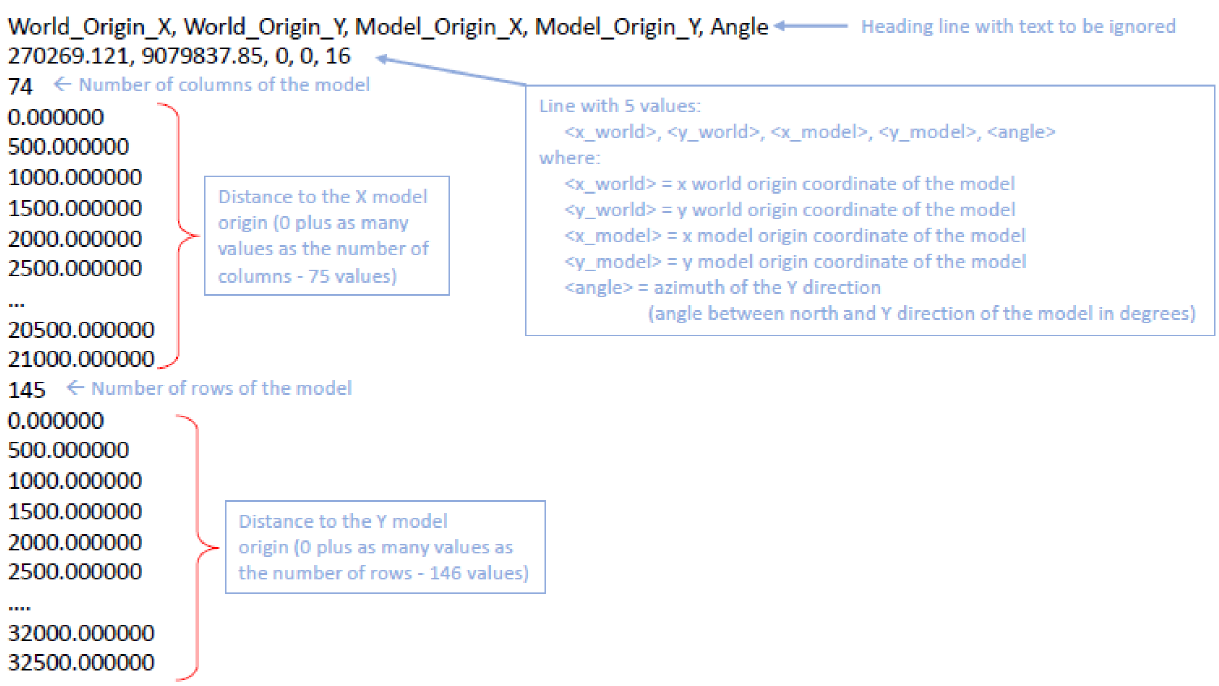
The following data are required in the **Create an input file for TMR (Telescopic Mesh Refinement)** window:

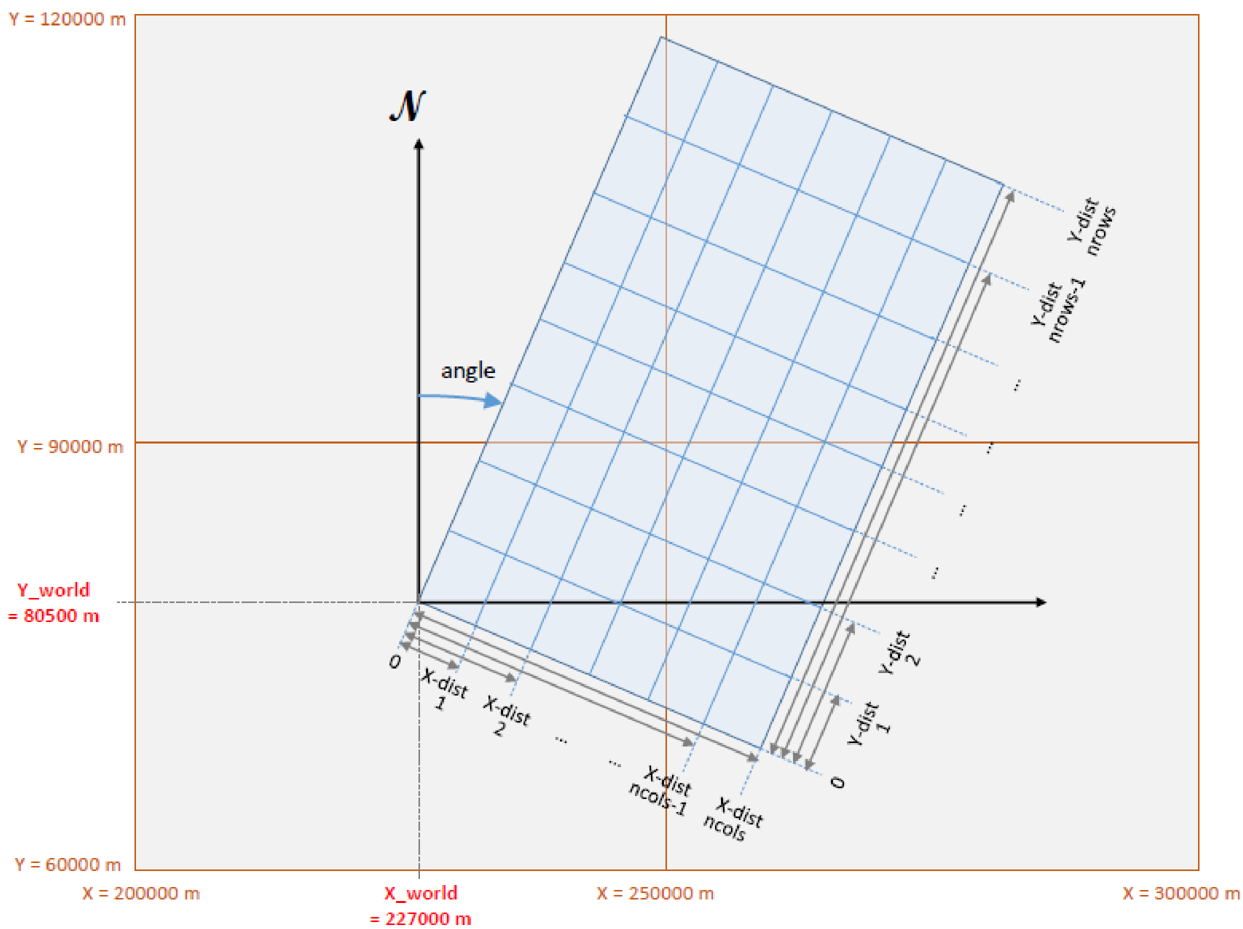
- *Model Name*: name of the hydrological model;
- *Layer of regular grid*: name of the regular grid MDO, created using the *FREEWAT* tool *Create Grid*;
- in the *Refine parameters* section:
- in the sub-section *Initial cell size*, information about resizing of the target grid cell must be input. Two options are available: *Refinement ratio* is an integer corresponding to the ratio between the size of the target cell in the regular grid and the size of the corresponding cell in the refined grid (e.g., if the side length of the target cell in the regular grid is 100 m and we want to halve its size in the refined grid, we need to set *Refinement ratio* = *2*); *Minimum cell dimension* [L] is the side length of the target cell in the refined grid (e.g., if the side length of the target cell in the regular grid is 100 m and we want to halve its size in the refined grid, we need to set *Minimum cell dimension* = *50* m);
- *Multiplier*: ratio between the size of a certain cell and that of the adjoining cell moving towards the borders of the refined grid (e.g., if the side length of the cell (ROW;COL) in the refined grid is 10 m and we want the cell (ROW+1;COL) to have a side 15 m long, we need to set *Multiplier* = *1.5*);
- *Tolerance for borders extension* is a tolerance factor [L] for determining the extent of the refined grid with respect to the extent of the regular one. Specifically, let's suppose to have a rectangular grid as the one in the figures above, and let's focus on the extreme western boundary. If the extreme western boundary of the refined grid fits outside the extent of the regular grid and the distance between the boundaries of the two grids is larger than a certain distance (the *Tolerance for borders extension* indeed), then the cells of the refined grid along column 1 will be cut and the extent of the refined grid will be smaller than that of the regular grid. Conversely, if the extreme western boundary of the refined grid fits outside the extent of the regular grid but the distance between the two boundaries is lower than the tolerance factor, then the cells of the refined grid along column 1 will not be cut and the extent of the refined grid will be larger than that of the regular one;
- *Name of TMR input file*: name of a txt file which will be created within the *Working Folder*, containing information about the size of each row and column of the refined grid.



Note: *Minimum cell dimension* and *Tolerance for borders extension* values must be expressed in model units.

Note: The txt file created through the *TMR* tool has the following structure:





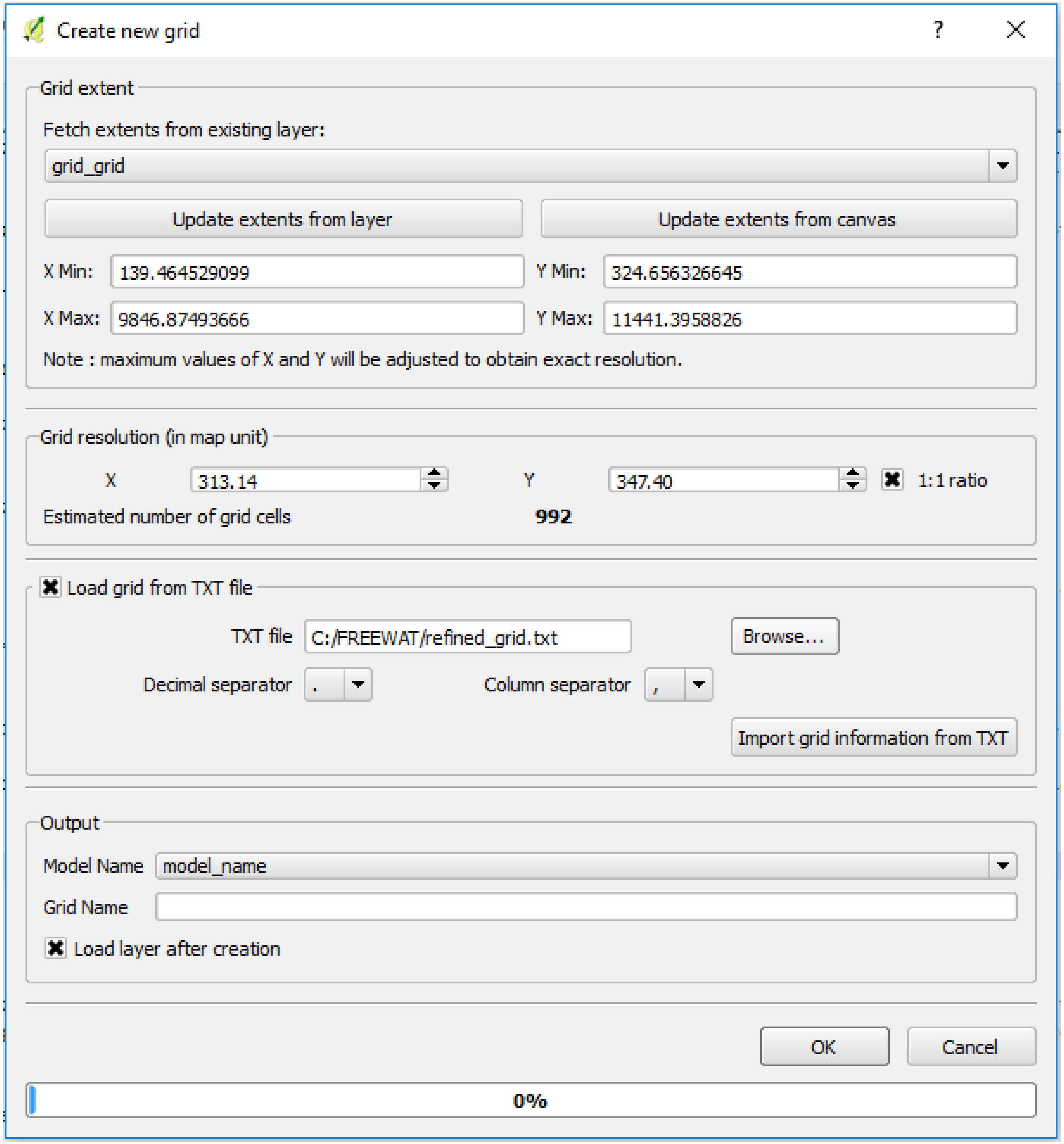
Step 4. Create now the refined grid, using the txt file just generated. To do that, the following menu must be used:

FREEWAT -> Model Setup -> Create Grid

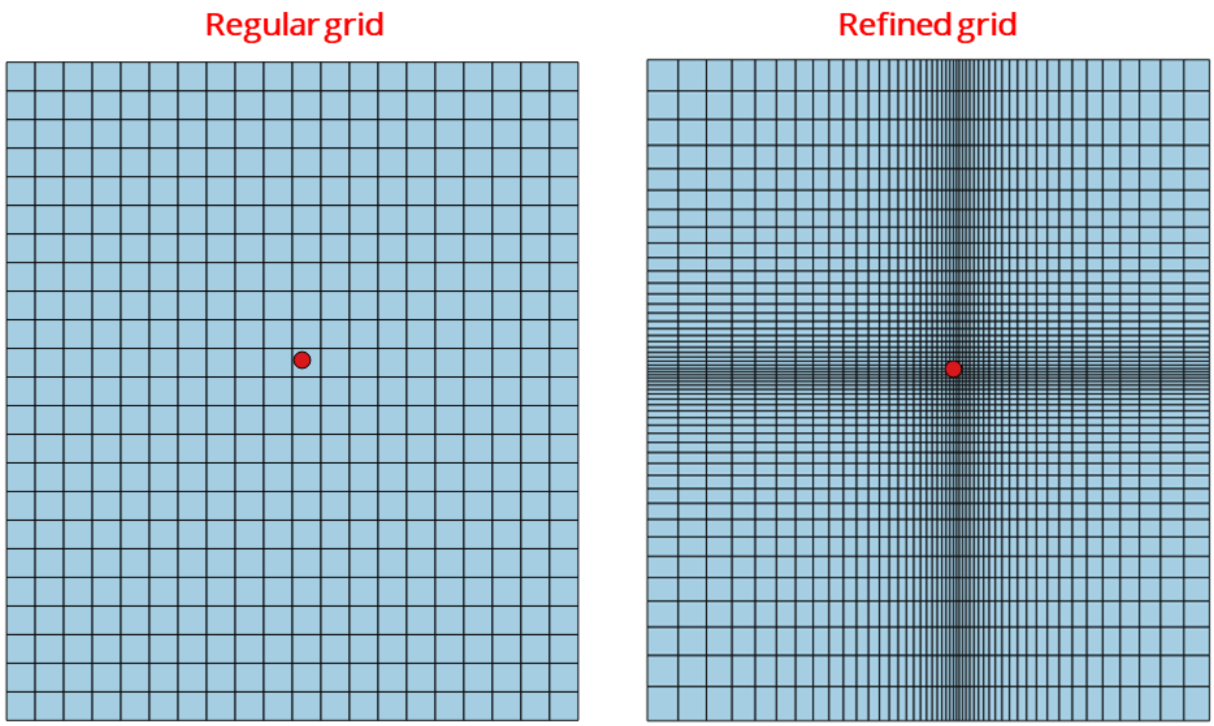
In the **Create new grid** window, check the *Load grid from TXT file* section to load the txt file just created, usign the *Browse...* button next to *TXT file*, defining the proper *Decimal separator* and *Column separator* used in the txt file.

Then click on *Import grid information from TXT*, and you will see that *X Min*, *X Max*, *Y Min* and *Y Max* coordinates, the *Grid resolution* and the *Estimated number of grid cells* are automatically updated.

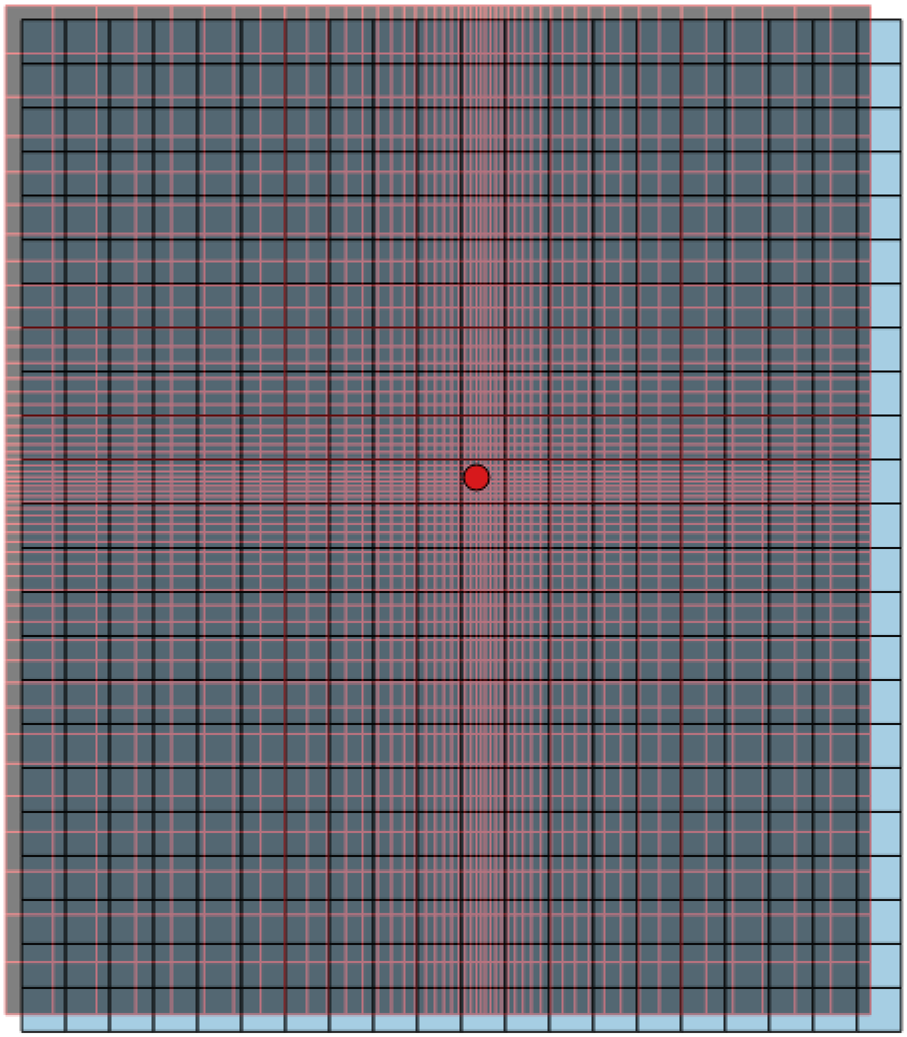
Finally, assign a *Grid Name* in the *Output* section to generate the new refined grid.



An example of application of the *TMR* tool is reported below (the regular grid is made of square cells with 500 m of side length; in the refined grid, the following was set: *Minimum cell dimension*: 50 m; *Multiplier*: 1.10; *Tolerance for borders extension*: 150 m):



Note: Please, notice that some shifts between the regular grid and the refined one could occur, due to the *Tolerance for borders extension* option and to origin coordinate settings adopted in the *TMR* tool for the refined grid. This can be easily inferred from the figure below, where the regular grid and the refined one shown in the above figure are represented overlapped:



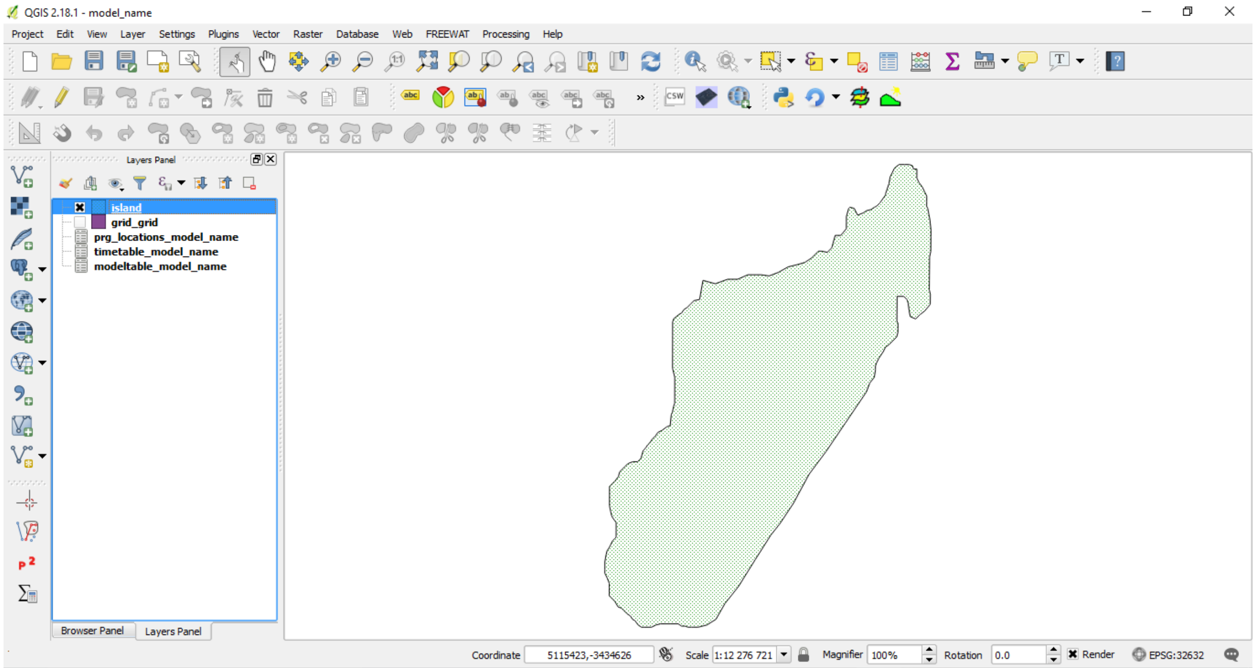
Rotated grid

It is also possible to build a model based on a rotated grid. Two alternative procedures will be presented to do this: the first procedure can be used with simple grids, while the second one is needed for grids with hundreds of thousands cells.

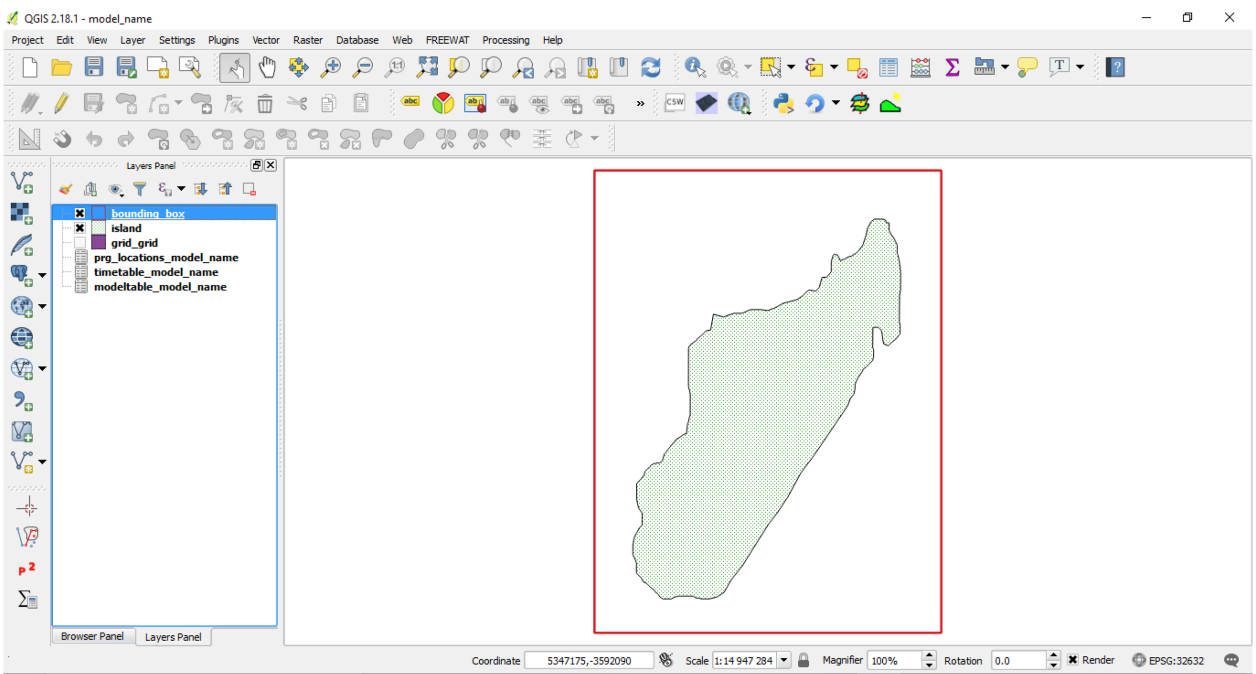
Procedure 1 (for simple grids)

The steps which have to be performed to get a simple grid rotated by 30° are listed below.

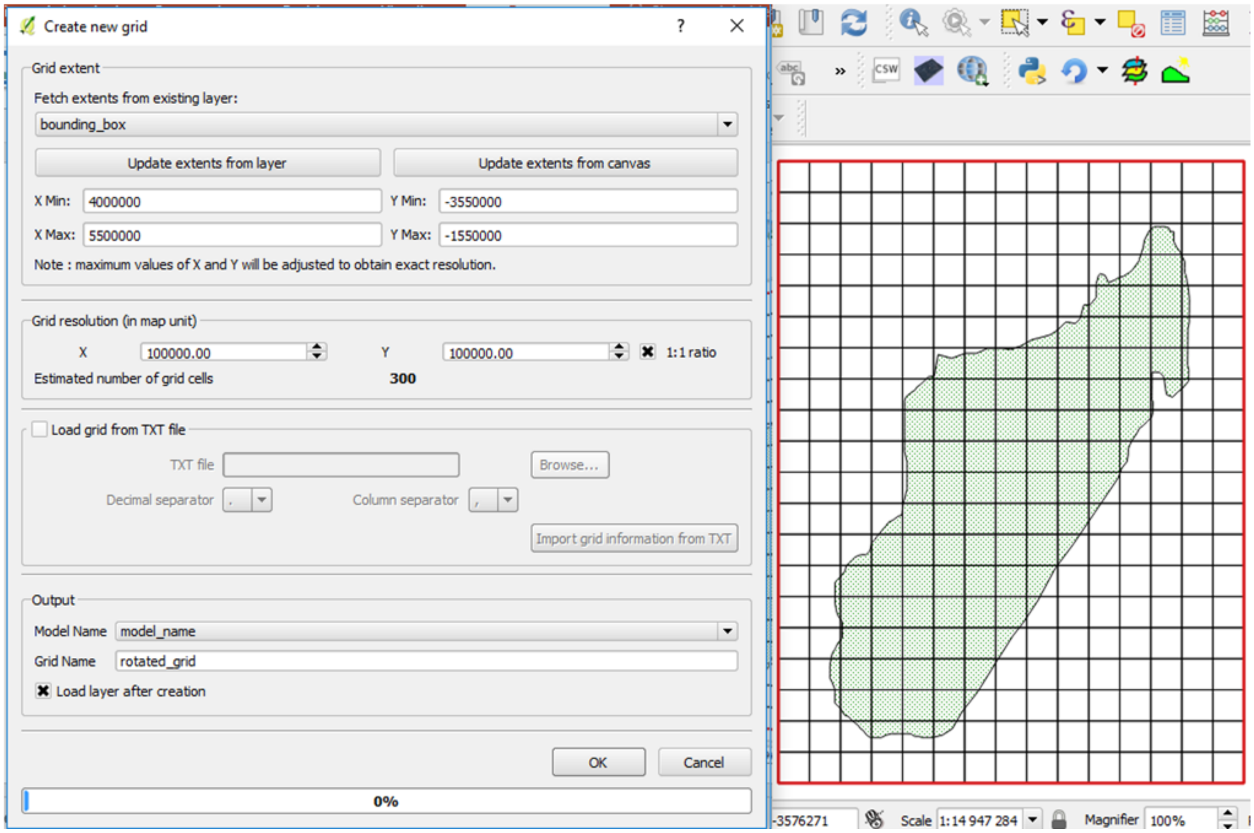
Step 1. Let's suppose to have an island, which has to be discretized using a grid rotated by 30°.



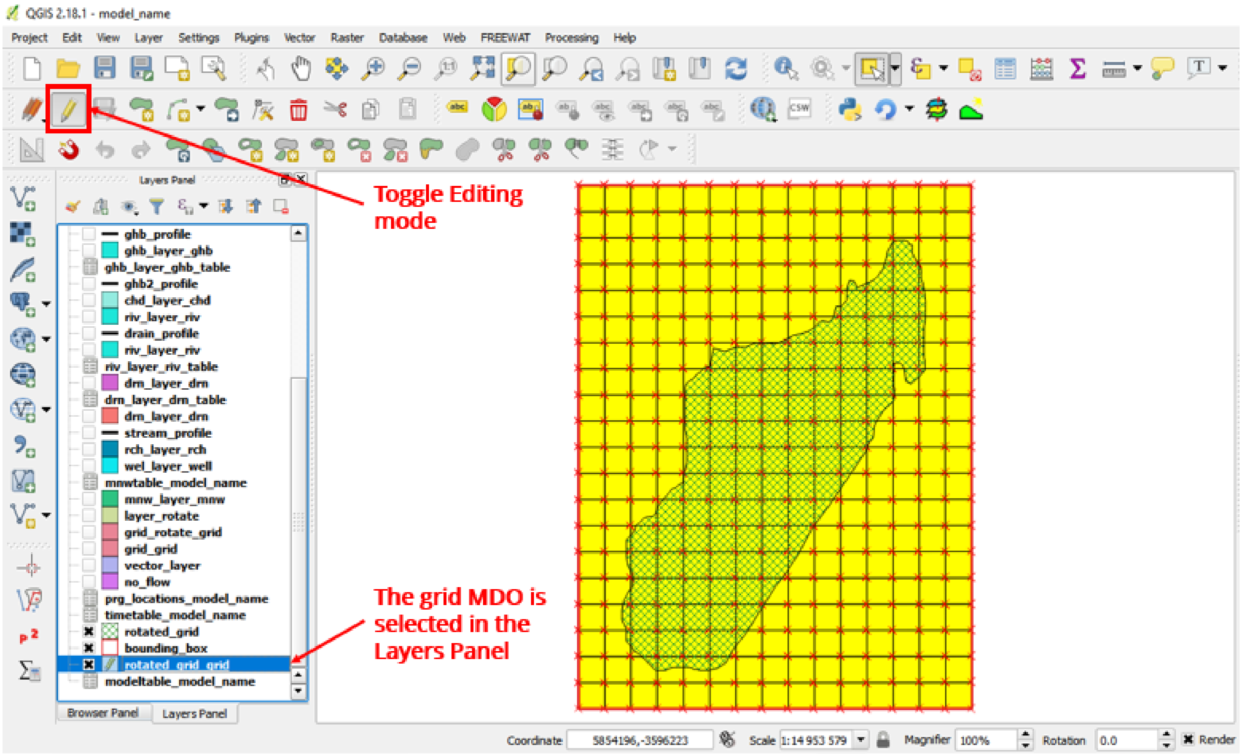
Step 2. A bounding box must be built. It should be larger than the minimum extent of the polygon bounding the island and, as mentioned before, we suggest to edit such polygon so that each border size (both along the X and Y directions) is a multiple of the cell size.



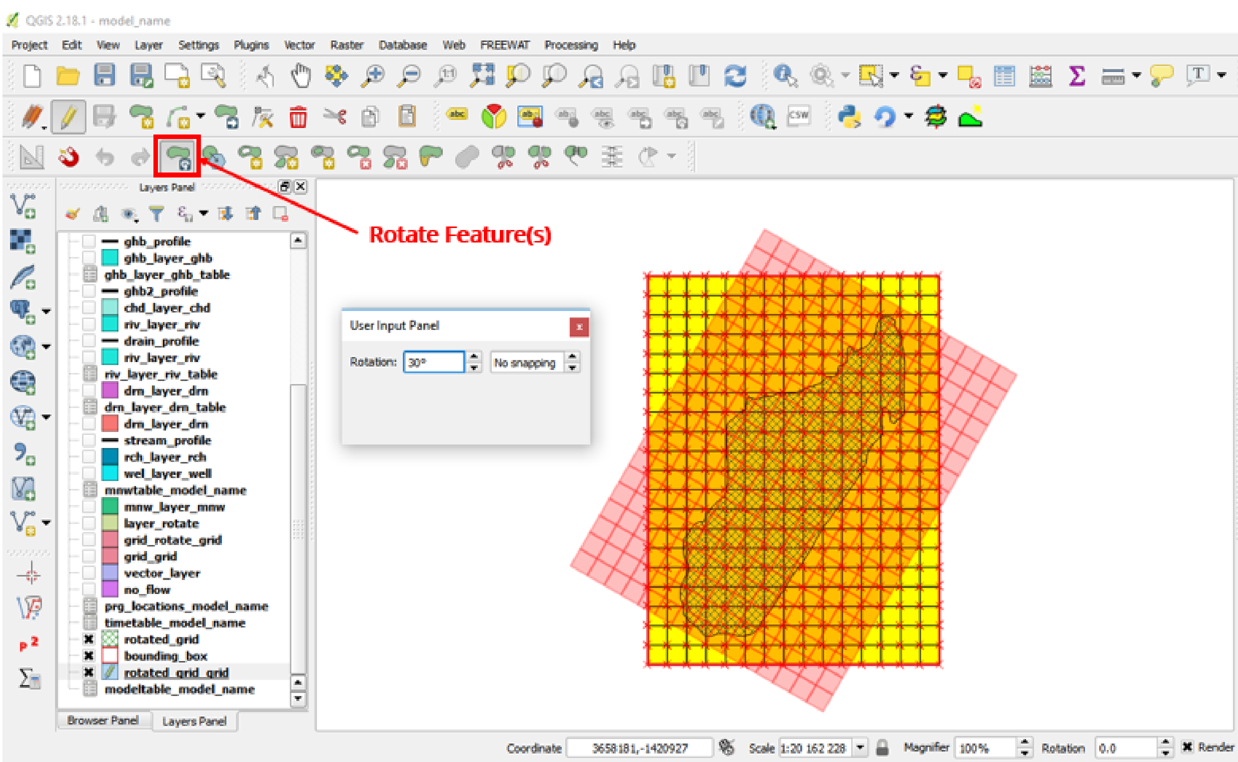
Step 3. Create the model grid within this bounding box, using the *FREEWAT* tool *Create Grid*.



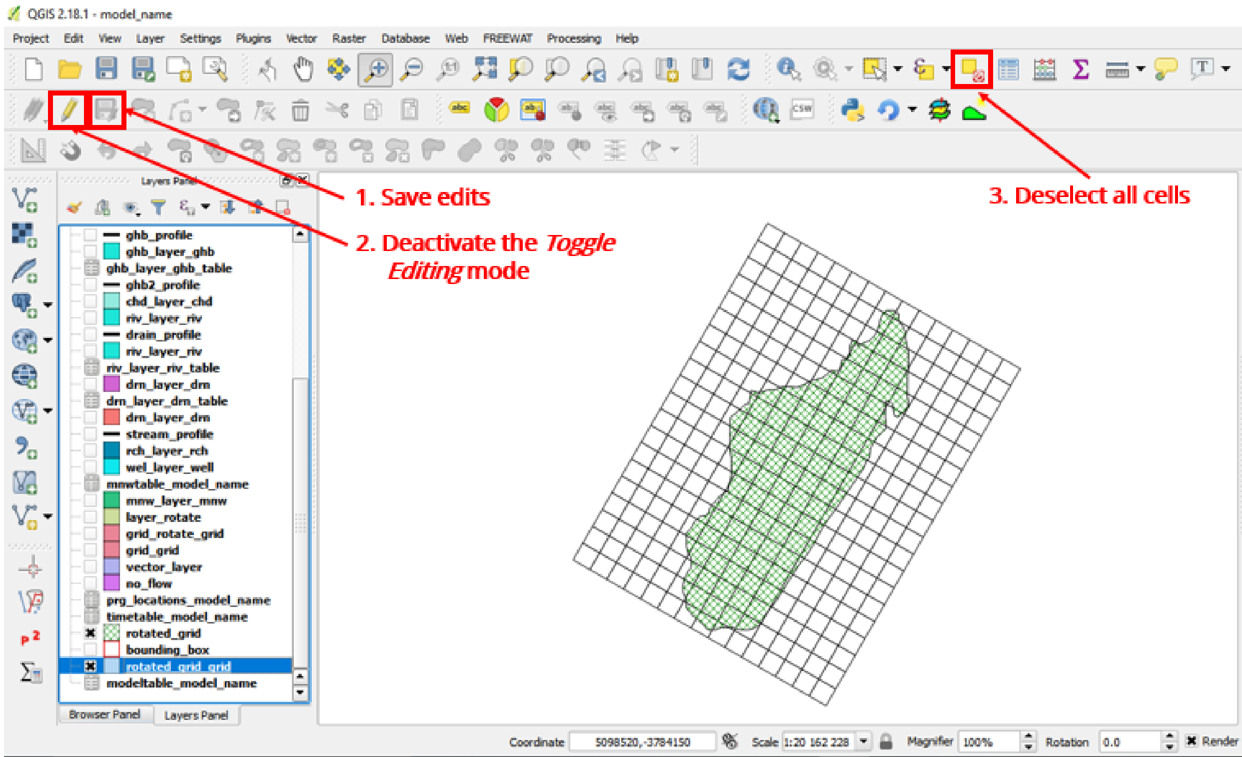
Step 4. Be sure that the grid MDO is selected in the Layers Panel (it must be highlithed in blue in the Layers Panel). Use one of the selection tools described in Chapter 5 (e.g., the *Select Features by Polygon* tool) to select the whole model grid (the grid cells should appear yellow) and activate the *Toggle Editing* mode.



Step 5. Click on *Rotate Feature(s)* and click once wherever within the grid polygon. It should become red and the *User Input Panel* should appear. Type 30° in the *Rotation* field and press *Enter*.

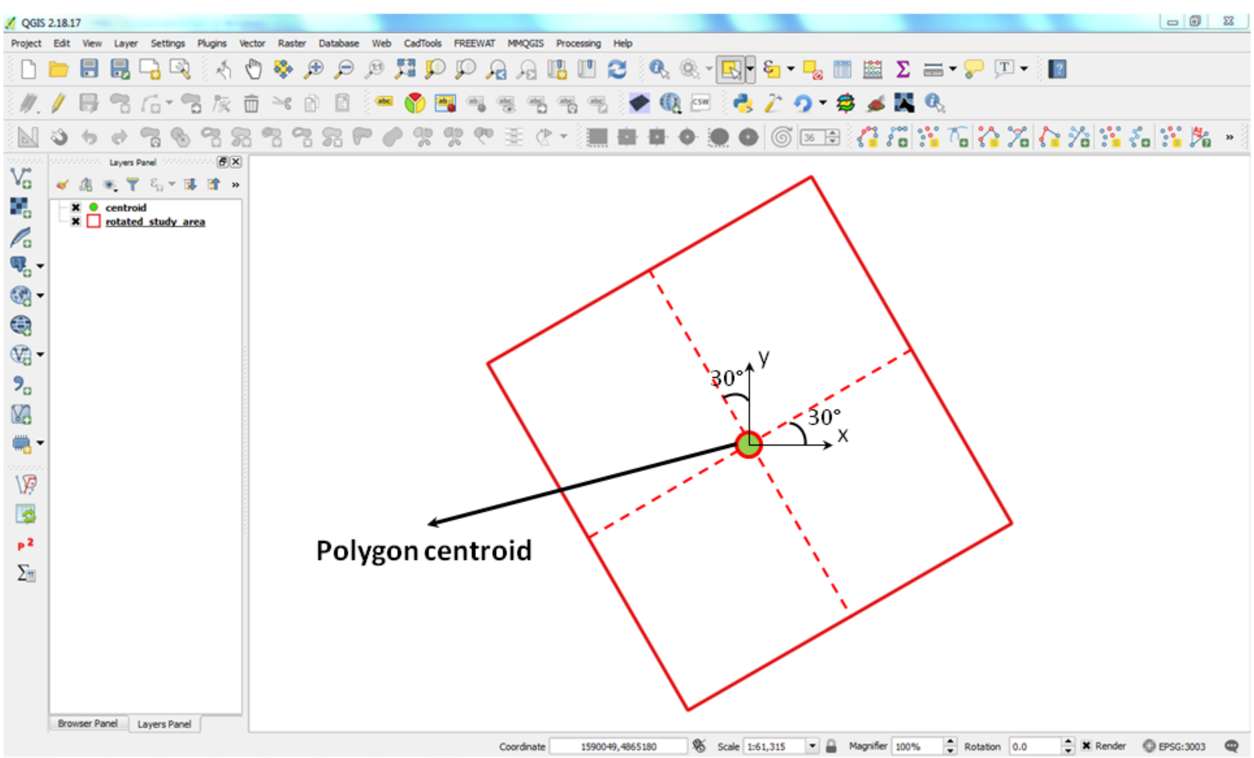


Step 6. Save your edits, deactivate the *Toggle Editing* mode and deselect all cells.

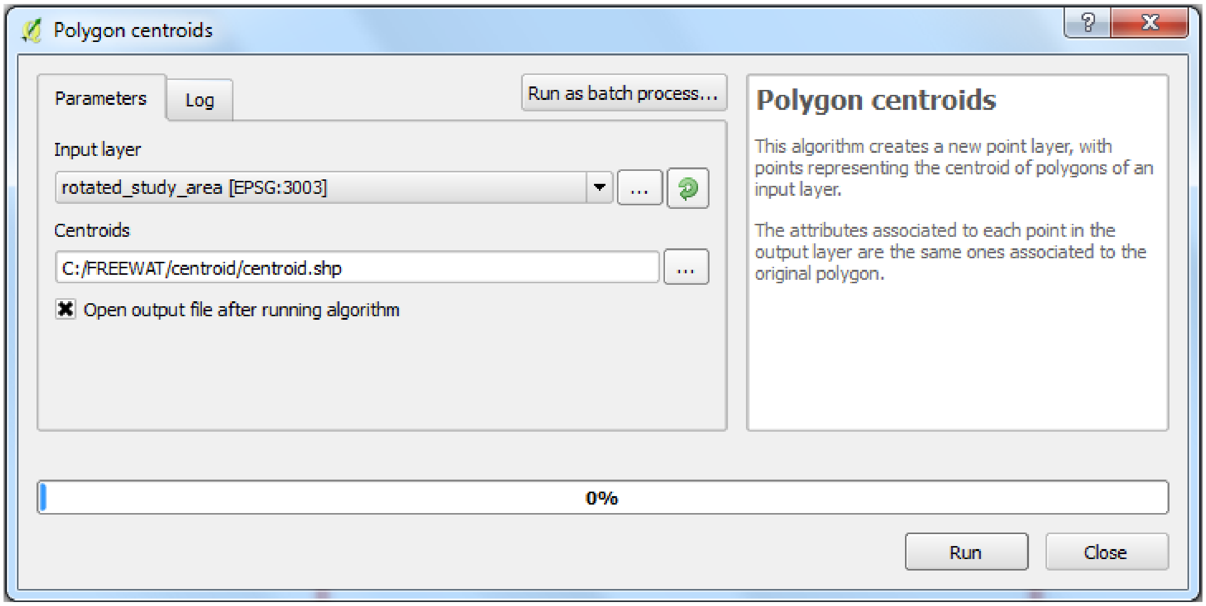


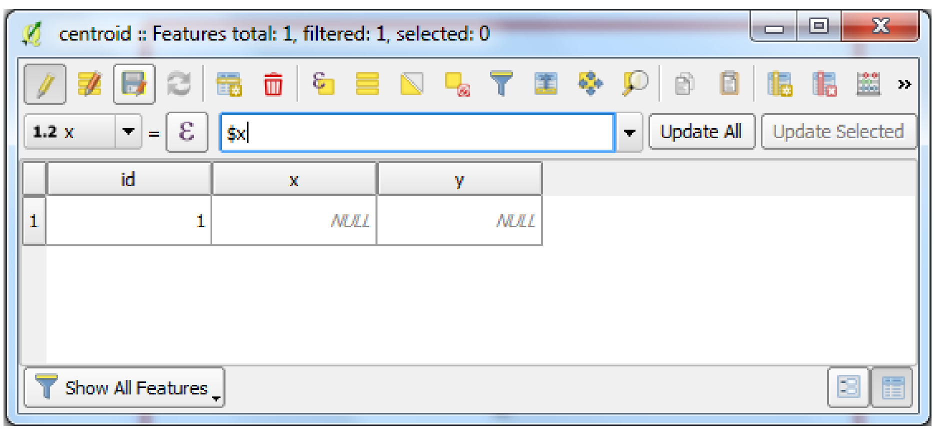
Procedure 2 (for grids with hundreds of thousands cells)

Step 1. Let's suppose that we want to create a grid within the polygon represented in the following figure. And let's suppose that such polygon is rotated by 30° counterclockwise with respect to the x and y Cartesian axes centered in the polygon centroid.



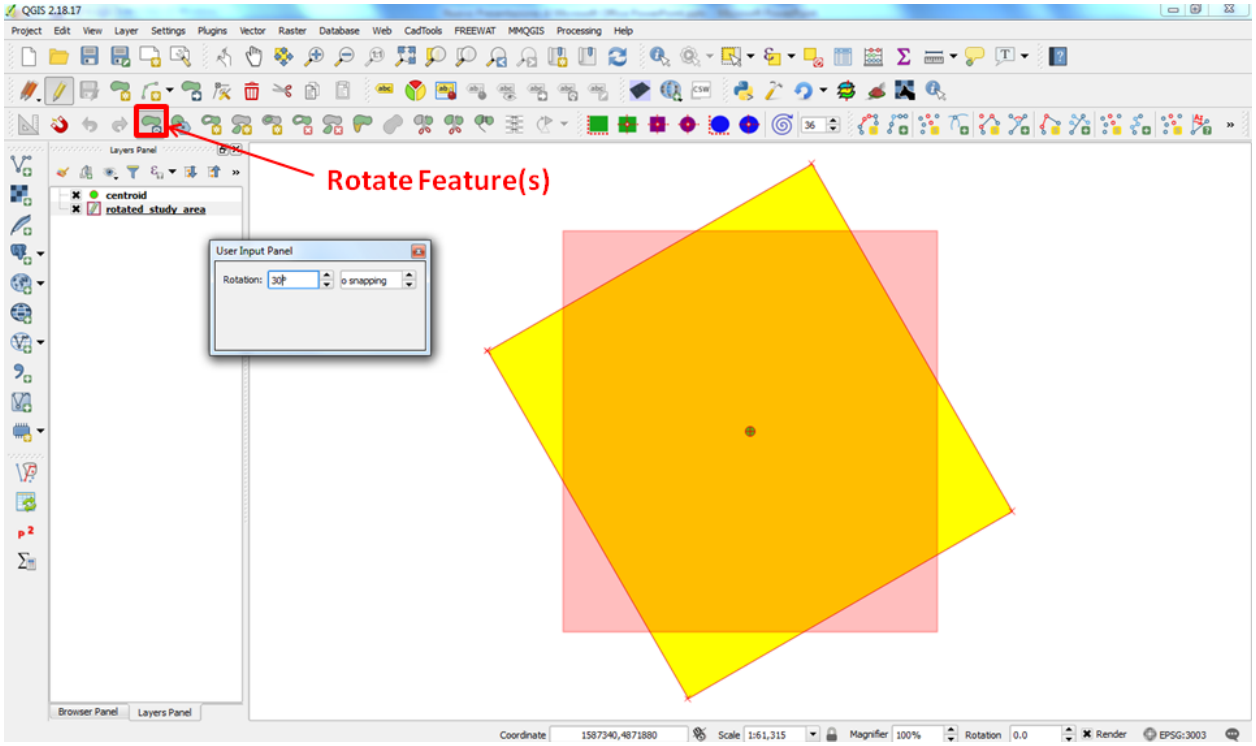
Step 2. Extract the polygon centroid using the *QGIS* plugin *Polygon centroids* (it can be found throught the *QGIS Toolbox*). Then, in the Attribute Table of the point shapefile containing this centroid, calculate its x and y coordinates using functions *$x* and *$y*.



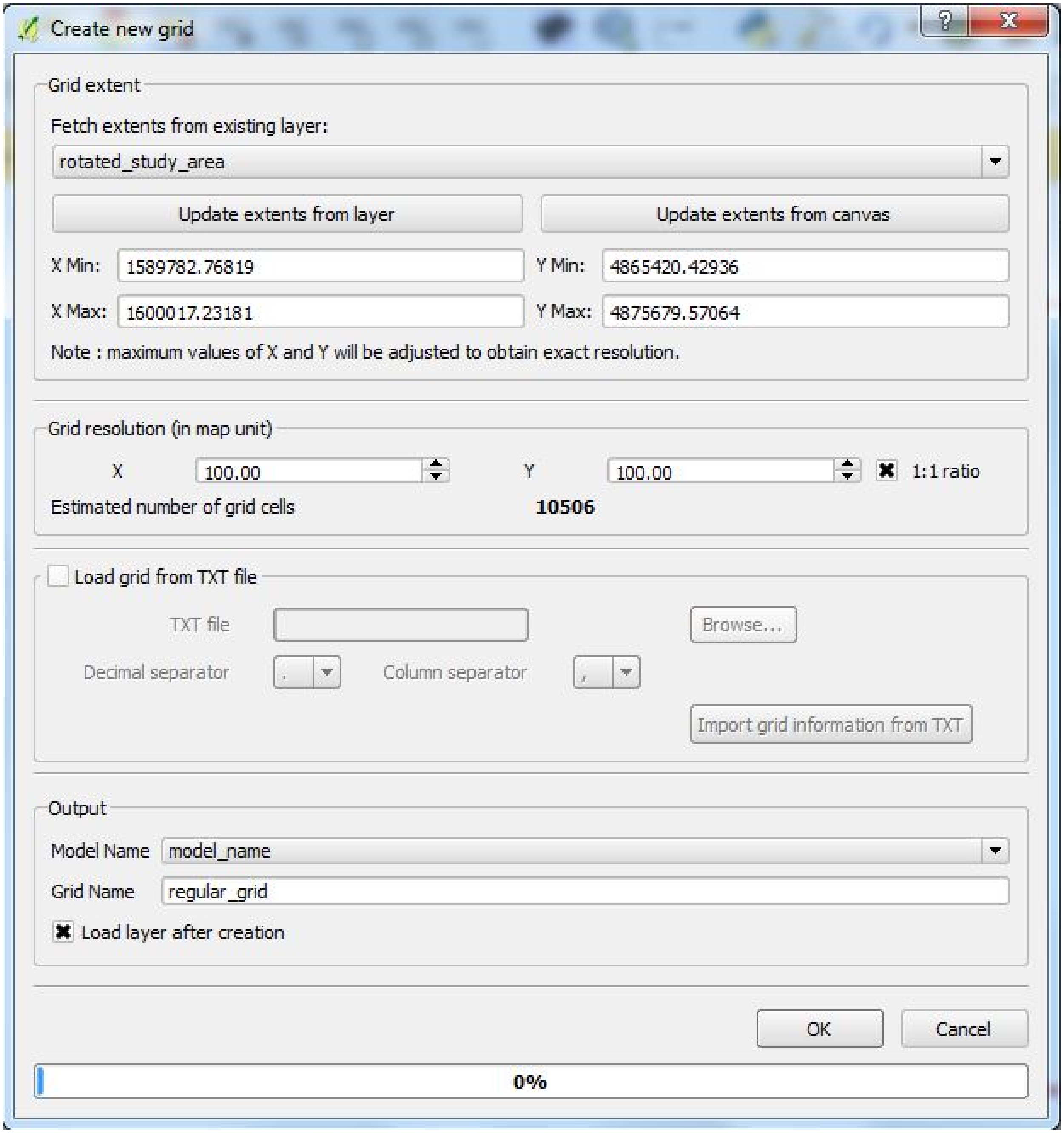


Step 3. Use the *QGIS* tool *Rotate Feature(s)* to rotate the above polygon by 30° clockwise around its centroid. As explained in the above **Procedure 1**, to use the *QGIS* tool *Rotate Feature(s)*, you must:

- be sure that the polygon is selected in the Layers Panel (it must be highlithed in blue in the Layers Panel);
- use one of the selection tools described in Chapter 5 (e.g., the *Select Feature(s)* tool) to select the polygon (it should appear yellow) and activate the *Toggle Editing* mode;
- click on *Rotate Feature(s)* and click once wherever within the polygon. It should become red and the *User Input Panel* should appear. Type 30° in the *Rotation* field and press *Enter*;
- save your edits, deactivate the *Toggle Editing* mode and deselect the polygon.



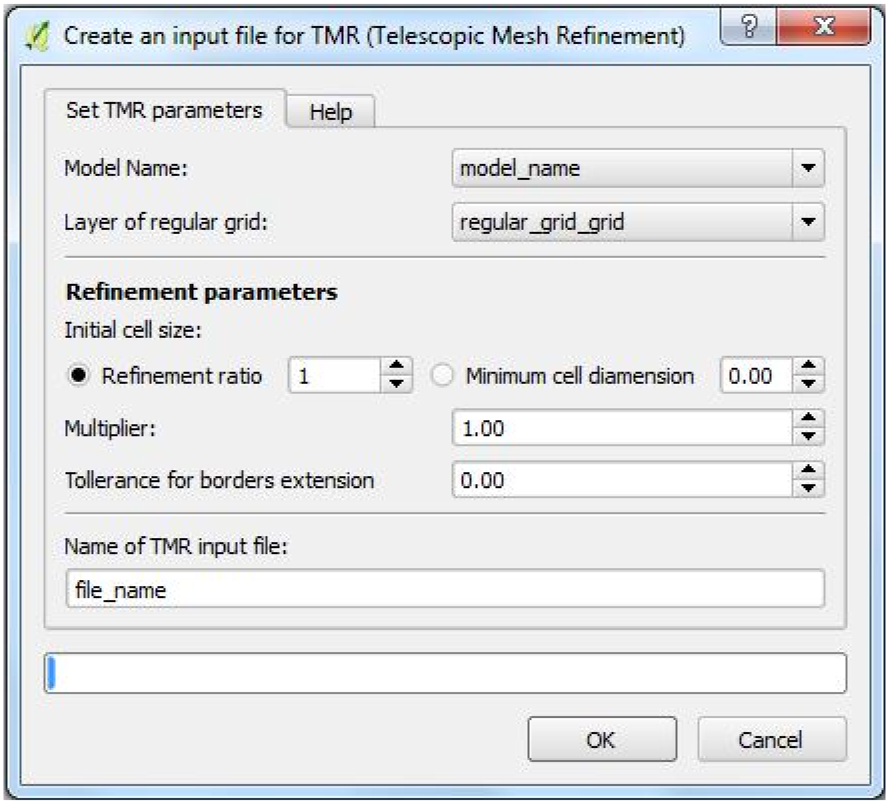
Step 4. Create a grid (hereinafter referred to as the regular grid) within this new polygon, using the *FREEWAT* tool *Create Grid*.



Step 5. Use the *TMR* tool described above with the following settings:

- *Refinement ratio* =1;
- *Multiplier* =1.00;
- *Tollerance for borders extension* =0.00.

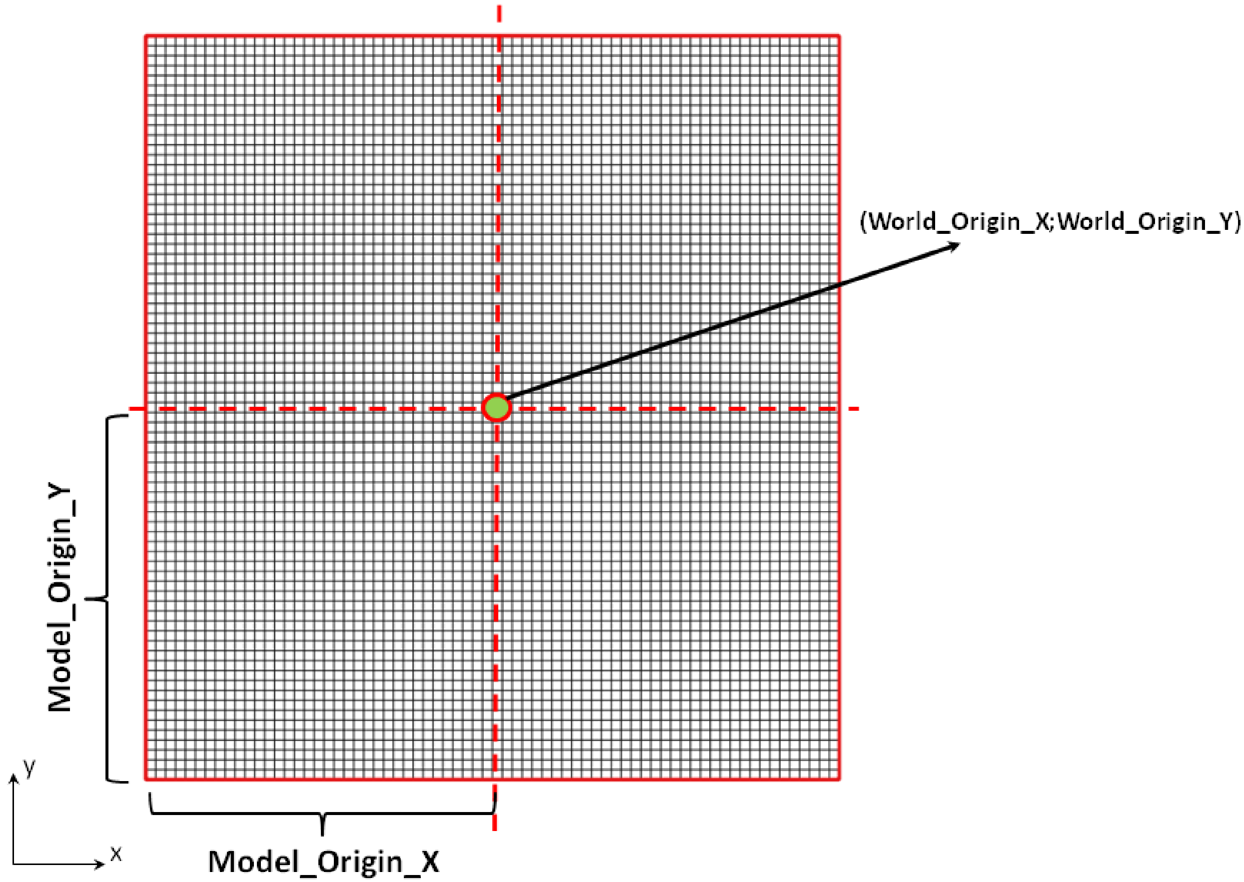
The *.txt* file created contains nothing but information on the regular grid (i.e., its origin and row and column size and number; please, notice that with the above settings, no refinement will occur).



Step 6. Open the *.txt* file just created and modify manually its second line as described below:

- *World_Origin_X* and *World_Origin_Y* are nothing but the x and y coordinates of the polygon centroid, as calculated in **Step 2**;
- *Model_Origin_X* and *Model_Origin_Y* represent the distance, along both Cartesian directions, between the x and y coordinates of the polygon centroid (as calculated in **Step 2**) and the x and y coordinates of the lower left corner of the regular grid (these can be inferred from the polygon where the regular grid has been inscribed);
- *Angle* is the desired angle of rotation (positive value for clockwise rotation; negative value for counterclockwise rotation).

The figure below explains the meaning of *World_Origin_X*, *World_Origin_Y*, *Model_Origin_X* and *Model_Origin_Y*.

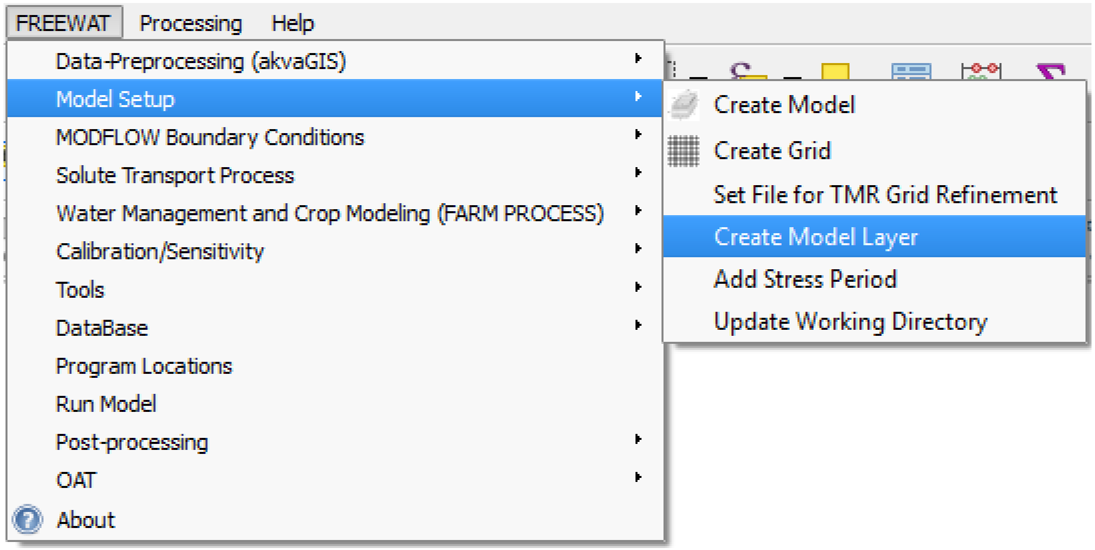


Define model layers

Once the model grid has been generated, 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 a grid-related MDO, meaning that its properties (specifically geometry and hydrodynamic parameters) are assigned at each grid cell.

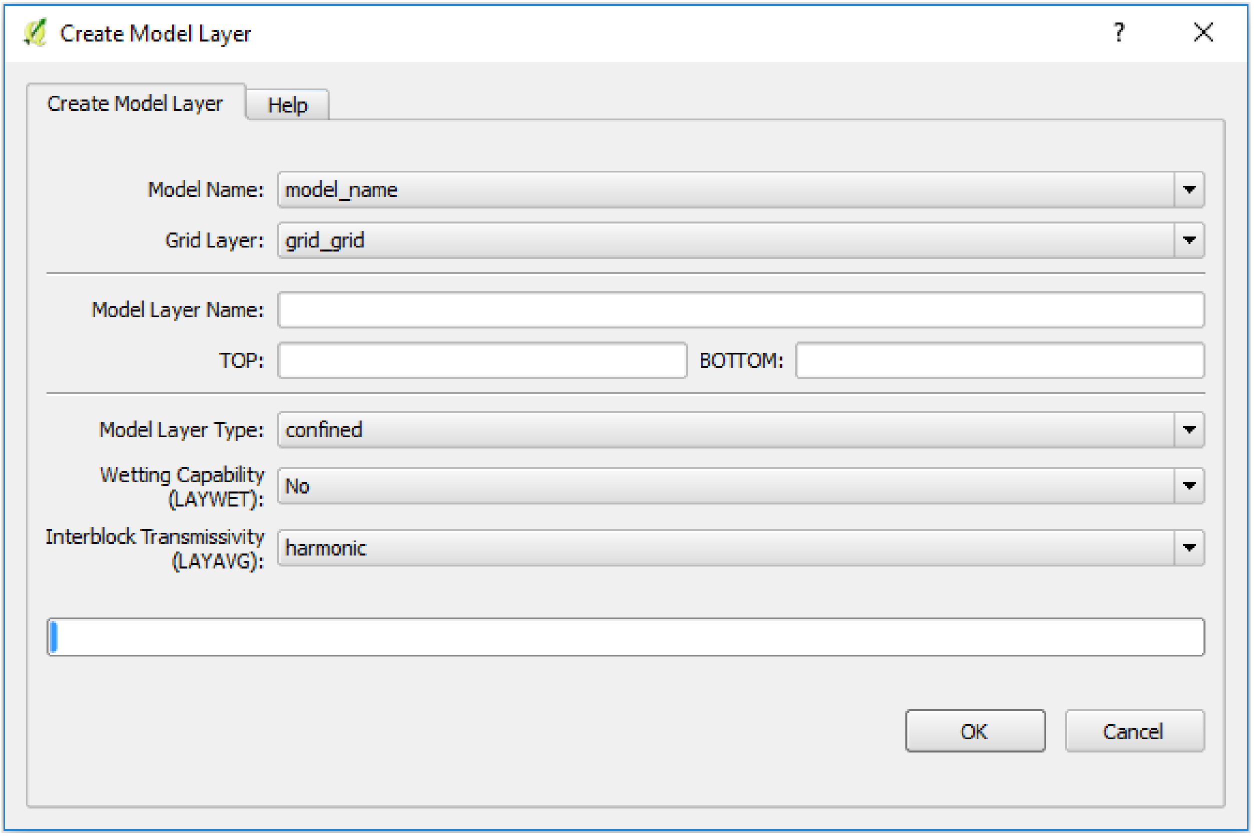
To create a model layer, the following menu must be used:

FREEWAT -> Model Setup -> Create Model Layer



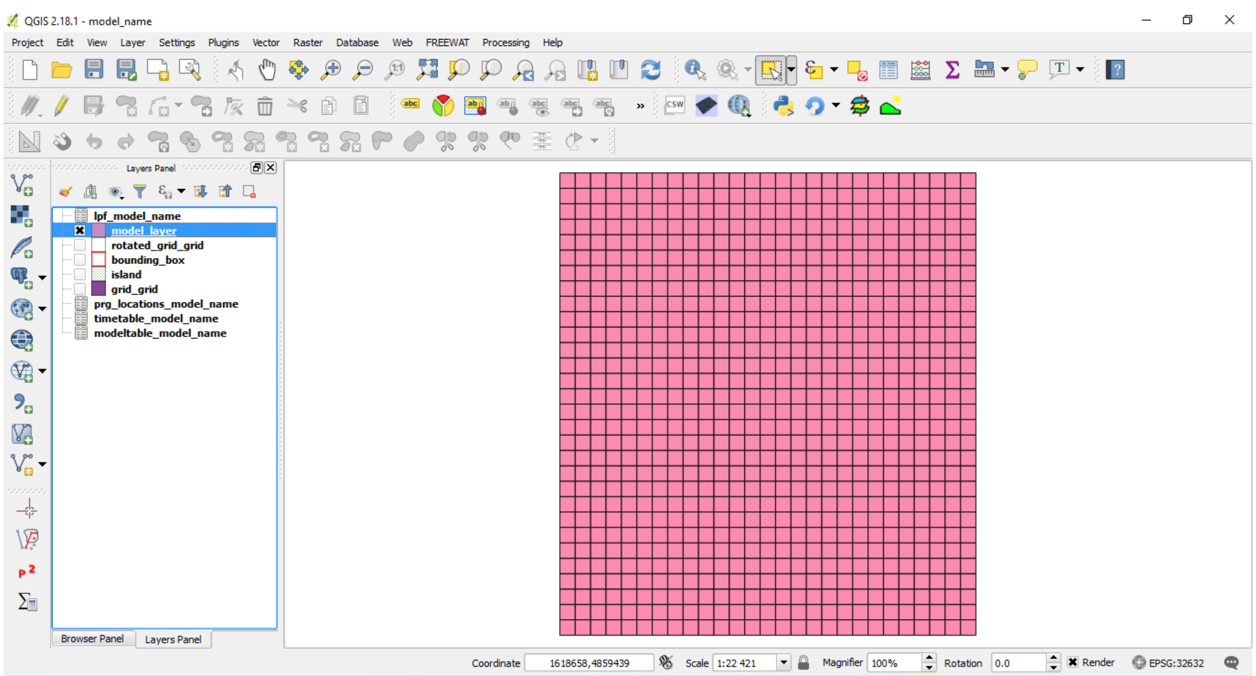
The following data are required in the **Create Model Layer** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: name of the grid MDO;
- *Model Layer Name*: name to be assigned to the model layer which has to be created;
- *TOP*: height of the top surface of the model layer [L] with respect to a reference plane;
- *BOTTOM*: height of the bottom surface of the model layer [L] with respect to a reference plane;
- *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 at 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).



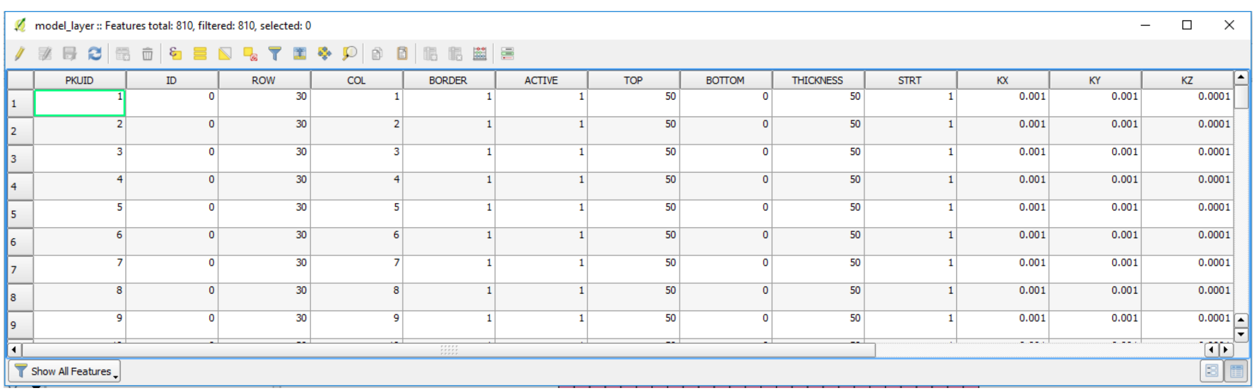
Note: Since only constant values can be assigned to *TOP* and *BOTTOM* in the **Create Model Layer** window, at this stage the corresponding model layer is limited by flat horizontal sufaces. These fields can be edited later.

For each model layer, a new MDO is created, stored within the model DB and loaded in the Layers Panel.



The Attribute Table of each model layer contains 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 index of a grid cell;
- *COL*: column index 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 computed 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 does not vary throughout the simulation - *ACTIVE=-1*);
- *TOP*: height of the top surface of the model layer at each cell [L] with respect to a reference plane;
- *BOTTOM*: height of the bottom surface of the model layer at each cell [L] with respect to a reference plane;
- *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 a cell which gets dry during the simulation can be re-wetted thanks to water exchanges 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.



	PKUID	ID	ROW	COL	BORDER	ACTIVE	TOP	BOTTOM	THICKNESS	STRT	KX	KY	KZ
1	1	0	30	1	1	1	50	0	50	1	0.001	0.001	0.0001
2	2	0	30	2	1	1	50	0	50	1	0.001	0.001	0.0001
3	3	0	30	3	1	1	50	0	50	1	0.001	0.001	0.0001
4	4	0	30	4	1	1	50	0	50	1	0.001	0.001	0.0001
5	5	0	30	5	1	1	50	0	50	1	0.001	0.001	0.0001
6	6	0	30	6	1	1	50	0	50	1	0.001	0.001	0.0001
7	7	0	30	7	1	1	50	0	50	1	0.001	0.001	0.0001
8	8	0	30	8	1	1	50	0	50	1	0.001	0.001	0.0001
9	9	0	30	9	1	1	50	0	50	1	0.001	0.001	0.0001

Note: All the dimensional variables must be expressed in model units.

Note: Top and bottom surfaces cannot intersect. As such, *THICKNESS* values cannot be negative.

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 they are used in solute transport simulations (Volume 2).

The fields *ACTIVE*, *TOP*, *BOTTOM*, *THICKNESS*, *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 model layer. They can be edited using standard *QGIS* tools and procedures described in Chapter 5.

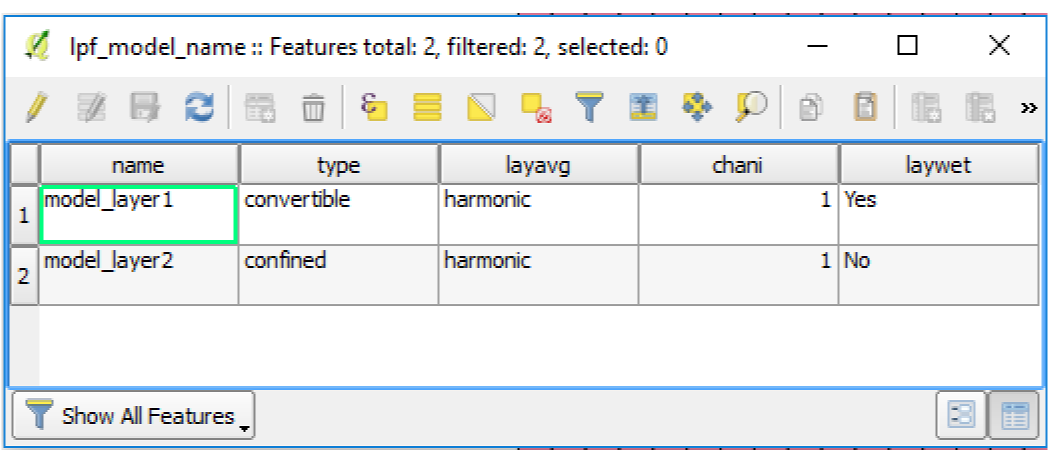
Note: If fields *TOP* and *BOTTOM* are edited, the *THICKNESS* field is not automatically updated. Editing the *THICKNESS* field, computing the difference between *TOP* and *BOTTOM*, is highly recommended each time that *TOP* and *BOTTOM* are modified, in order to check if intersection between top and bottom surfaces occurs at some grid cells.

After the first model layer is generated, 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 is created.

Such table may contain several records, according to the number of model layers created, and the following fields:

- *name*: name of each model layer;
- *type*: *Layer Type* (*confined* or *convertible*) defined during the creation of the corresponding model layer;
- *layavg*: method used to calculate the horizontal *Interblock Transmissivity (LAYAVG)* (*harmonic*, *logarithmic* or *arithmetic-mean*), defined during the creation of the corresponding model layer;
- *chani*: integer value, which defines the horizontal anisotropy for the corresponding model layer (it is not actually used in the current version of the *FREEWAT* plugin; refer to the *Limitations* section at the end of Chapter 2);
- *laywet*: flag indicating if the *Wetting Capability (LAYWET)* is active (*Yes*) or not (*No*), according to what defined during the creation of the corresponding model layer.

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



Note: If the User wishes to rename a model layer in the Layers Panel, its name **must** be modified in the *name* field of the lpf table as well. Pay attention: the *name* field is **case-sensitive**.

Note: Model layers listed within the lpf table cannot be sorted (the first model layer of the list represents the shallow hydrostratigraphic unit and the last model layer in the list represents the deepest one). As such, if a model layer has to be defined between two existing model layers, the lpf table must be edited accordingly or model layers must be deleted from the Layers Panel, from the lpf table and from the model DB and created again in the correct order.

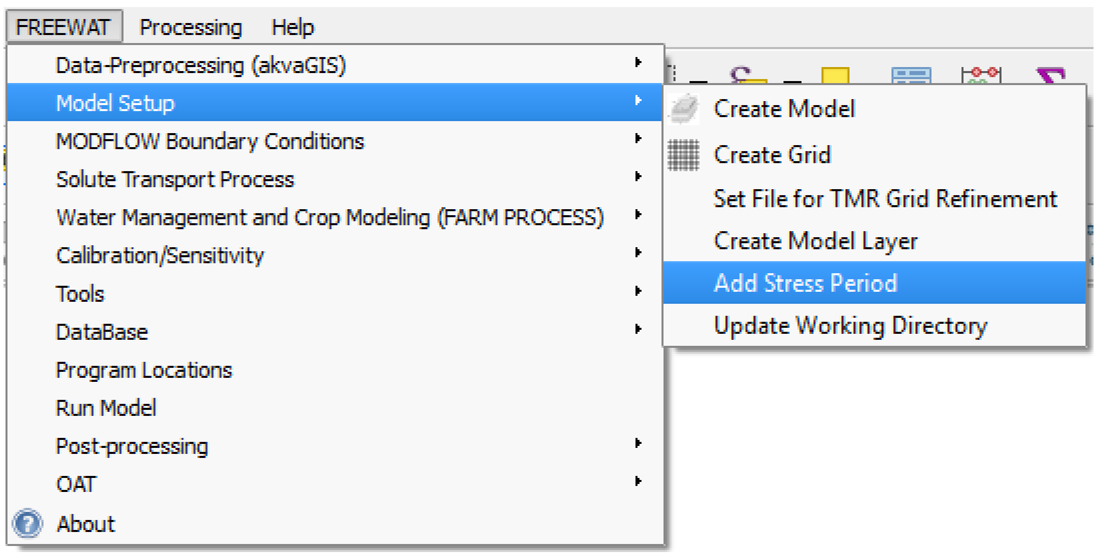
Time discretization

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* (*TSs*), namely shorter time intervals which allow to evaluate the time evolution of the solution (e.g., the hydraulic head in case of groundwater flow).

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

To add a SP, the following menu must be used:

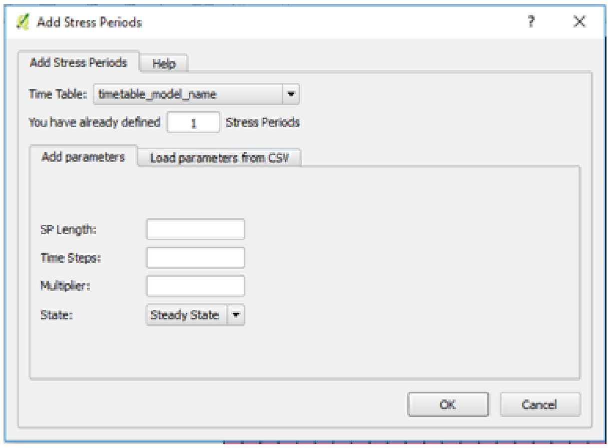
FREEWAT -> Model Setup -> Add Stress Period

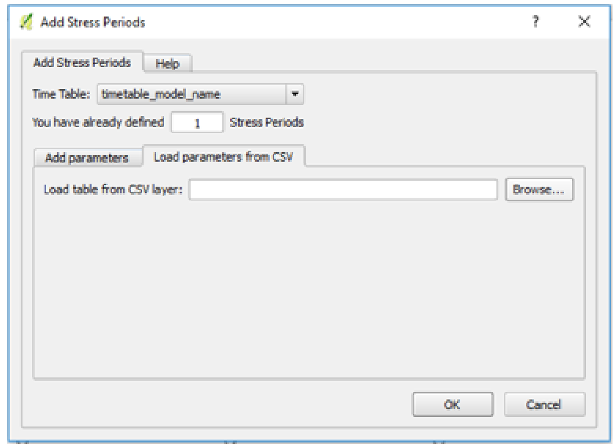


The following data are required in the **Add Stress Periods** window:

- *Time Table*: name of the time table (see Chapter 3);
- in the *Add parameters* section:
  - *SP Length*: length of the SP [T] which is being added;
  - *Time Steps*: number of TSs within the SP which is being added;
  - *Multiplier*: multiplier to calculate the length [T] of each TS within the SP which is being added;
  - *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 CSV layer* bar.





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

Note: For steady state SPs, only one TS can be defined and the multiplier must equal *1*. For details, the reader is referred to *MODFLOW-2005* User Manual (Harbaugh, 2005).

Note: If *n* SPs have been already defined, such information is reported in the **Add Stress Periods** window (*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 [T] which is being added;
- *ts*: number of TSs within each SP which is being added;
- *multiplier*: multiplier to calculate the length of each TS within each SP which is being added;
- *state*: two options are available for each SP which is being added (*SS* for *Steady State* or *TR* for *Transient*).

The CSV file must have the following scheme (the template file *stress_periods.csv* is provided within the *FREEWAT* plugin folder `freewat\csv_templates\stress_periods`):

stress_periods.csv

```
length,ts,multiplier,state
10,1,1.0,SS
60,15,1.3,TR
180,15,1.3,TR
```

As mentioned in Chapter 3, if one or more SPs are added, the time table is automatically updated.

If needed, the User can edit any SPs property within the time table, activating the *Toggle editing mode* (refer to Chapter 5).

CHAPTER 5

Tools for model layers parameterization

Once the model layers have been created, the following data are required for each of them: the height of their top and bottom surfaces (usually corresponding to those of the hydrostratigraphic units) with respect to a reference plane, the *ACTIVE* flag to distinguish between active, inactive and specified-head cells, their hydrodynamic properties (i.e., hydraulic conductivity along the three Cartesian directions, specific storage, specific yield), the *WETDRY* flag to define if the rewetting option is active or not (this is only needed for convertible model layers).

The Attribute Table of each model layer can be edited either manually and/or with the available *QGIS* selection tools, or with two specific assignment methodologies integrated in *FREEWAT* (further details in sections *Copy from vector layer* and *Copy from raster layer*).

Manual editing with selection tools

This editing methodology requires using the available *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. Such procedure can be applied to any parameter defined in the Attribute Table of the model layer. Hereinafter, we describe, as an example, how to edit the *ACTIVE* field to distinguish between active, inactive and specified-head cells.

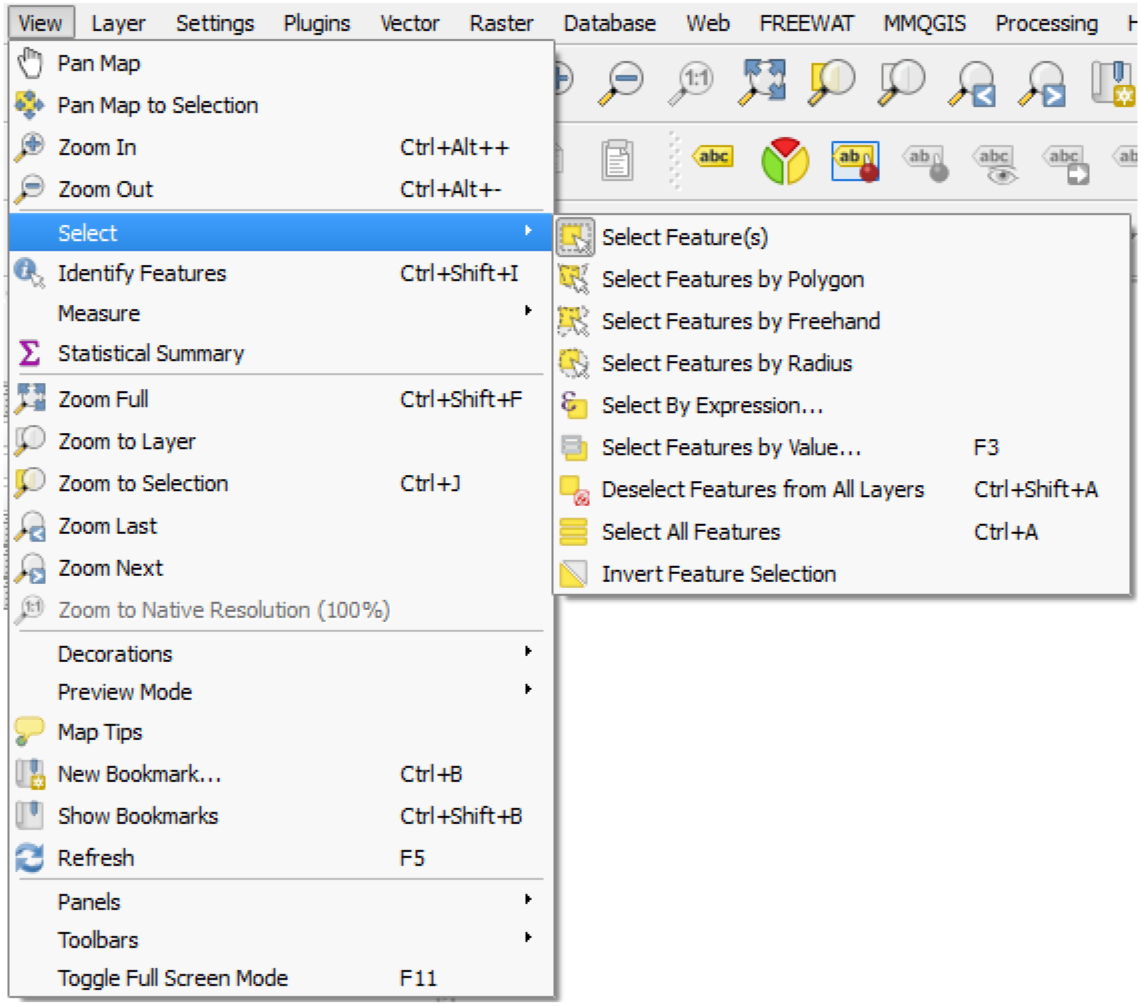
Once the model layer has been created, *1* is assigned at each grid cell as a default value for the *ACTIVE* field. This means that all cells of the model grid are active. To edit such value, so defining inactive cells (*ACTIVE=0*) or specified-head cells (*ACTIVE=-1*), several *QGIS* selection tools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

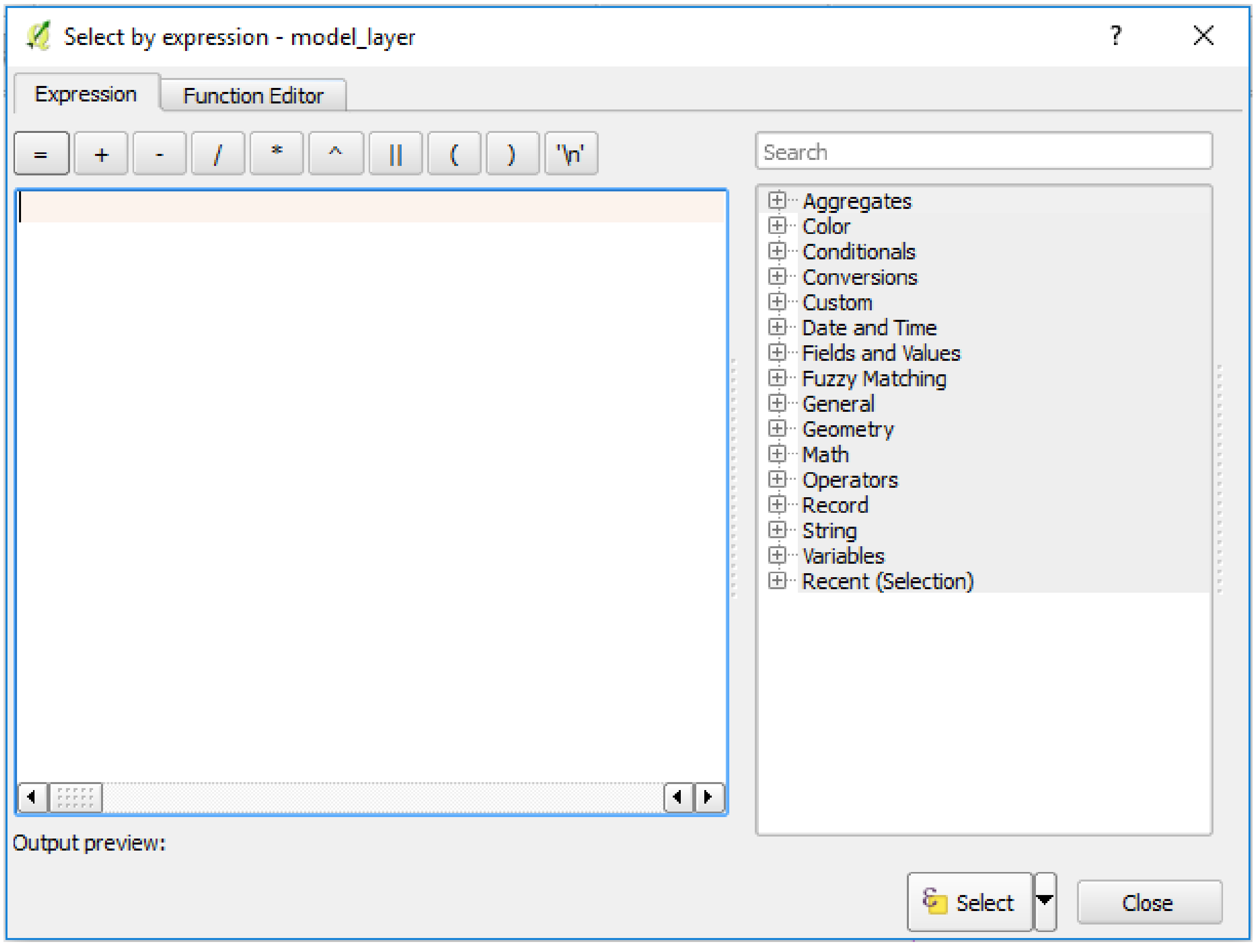
View -> Select.

- The *Select Feature(s)* tool allows to select cells manually, 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 drawn by the User, whose border is a polyline;
- the *Select Features by Freehand* tool allows to select cells intersected by a polygon drawn by the User, whose border is a curved line;
- the *Select Features by Radius* tool allows to select cells intersected by a circle drawn by the User;
- 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* tab by using mathematical, logical, conditional operators and/or values from other fields within the Attribute Table of the model layer/MDO involved in the selection;
- the *Select Features By Value...* tool, which is similar *Select Features By Expression...*, but the User can only act on numerical fields (no logical or conditional operators can be used);
- the *Select All Features* tool allows to select all cells.

The following tools are further available:

- *Deselect Features from All Layers*;
- *Invert Feature Selection*, if a selection is already active for a model layer/MDO listed in the Layers Panel.

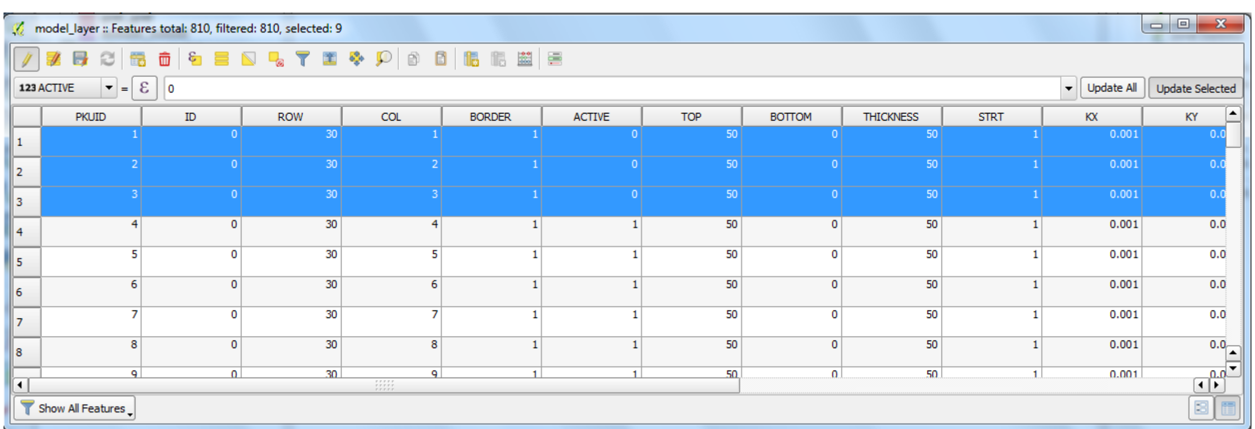


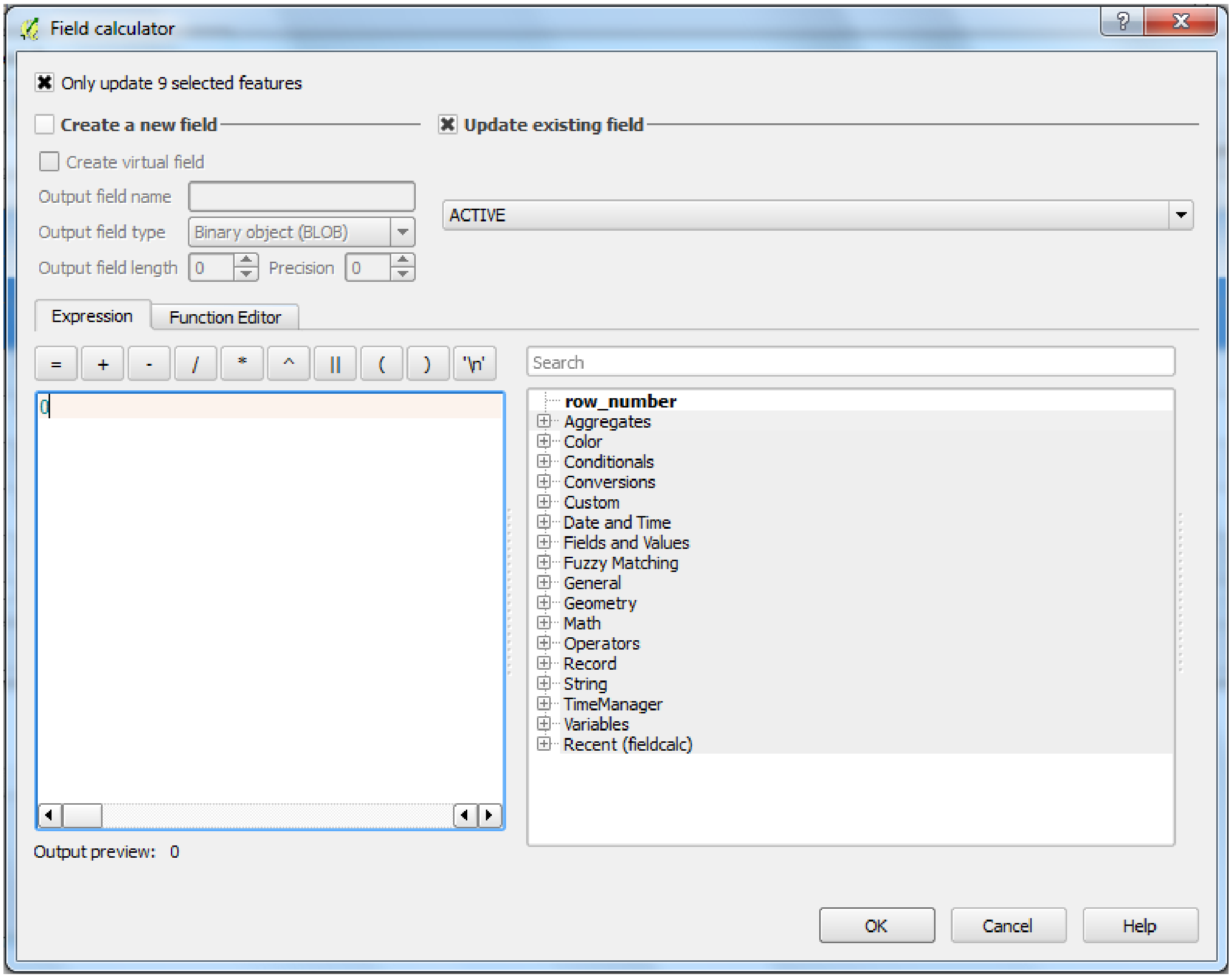


Note: Using one of the available selection tools requires prior selecting, in the Layers Panel, the model layer/MDO which is the object of the selection.

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).

For the aim of our example, at this stage the *ACTIVE* values of the selected cells can be edited, by activating the *Toggle editing mode* and using the expression bar and the *Update Selected* button, or the *Field calculator*.





Among the *QGIS* selection tools, it is worth mentioning also the *Select by location* tool. It can be accessed through the *QGIS Processing Toolbox*.

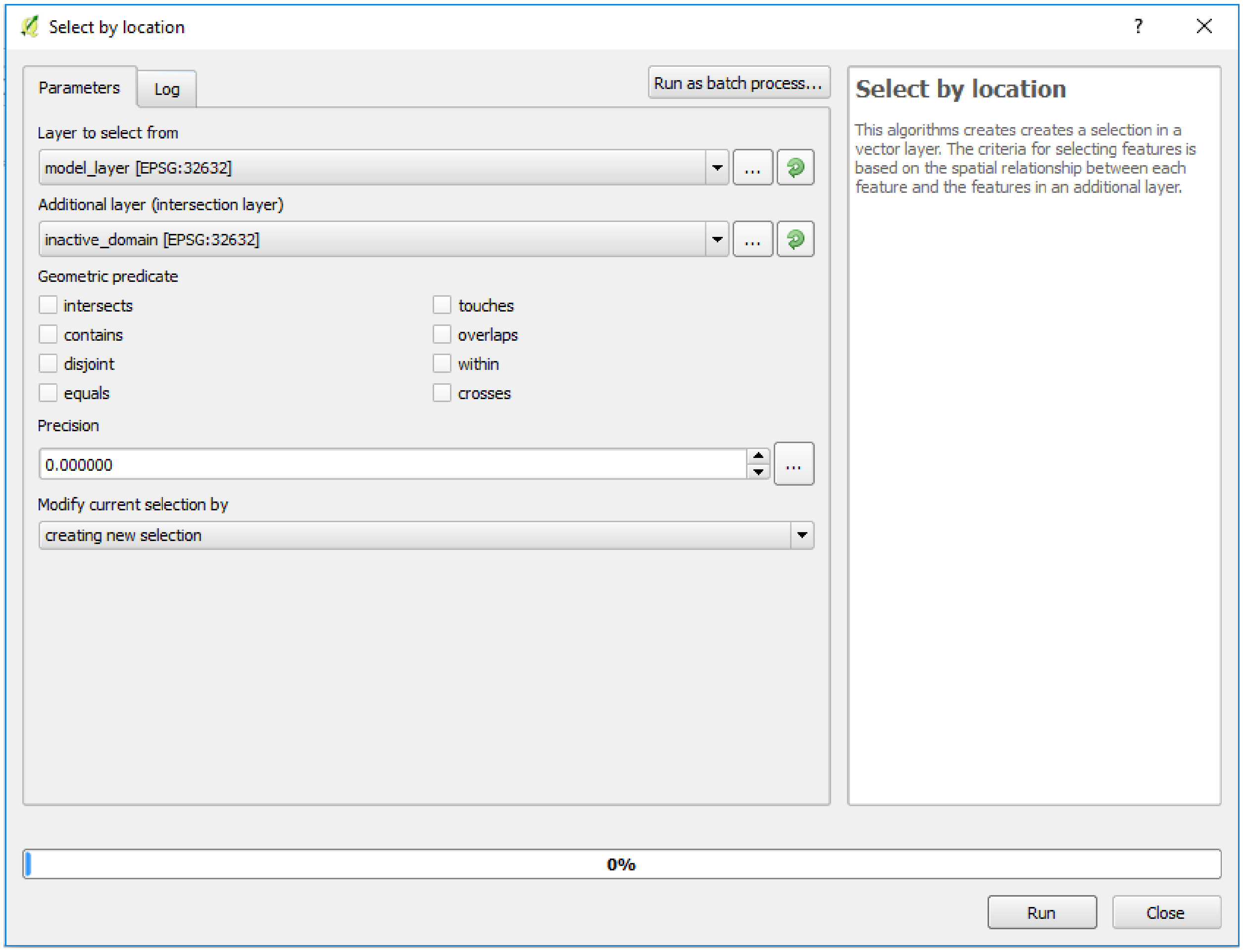
As an example, if a polygon shapefile with the extent of the inactive domain is available, it would be useful to select all grid cells of a model layer which are intersected by this polygon, in order to edit their *ACTIVE* values. In this case, the target of selection (*Layer to select from*) is the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

- *intersects*;
- *contains*;
- *disjoint*;
- *equals*;
- *touches*;
- *overlaps*;
- *within*;
- *crosses*.

The drop-down menu at the bottom of this interface allows to:

- create a new selection (*creating new selection*);

- add a new selection to any current active selection (*adding to current selection*);
- remove a selection from any current active selection (*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.

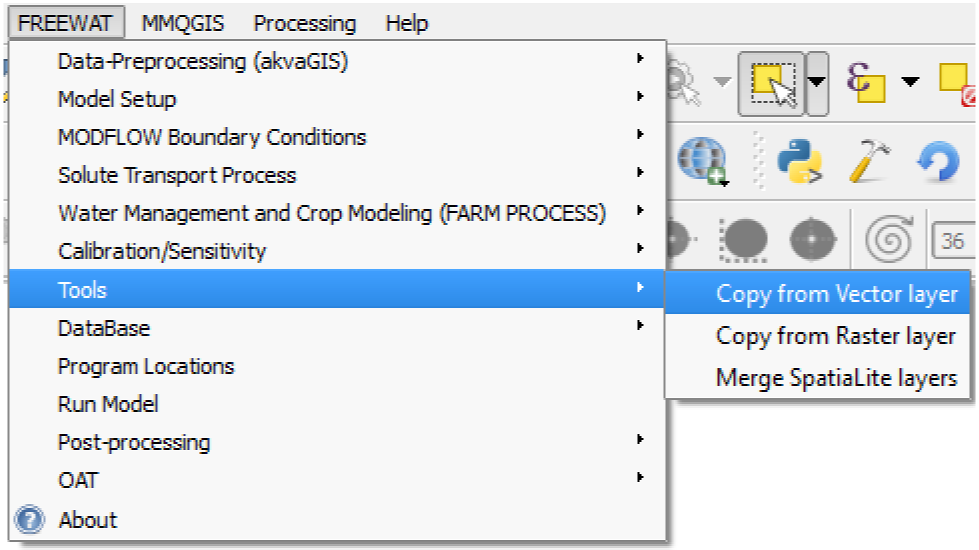
Note: Once the editing is completed, remember to deactivate the *Toggle editing mode* and to use the *Deselect Features from All Layers* tool.

Copy from vector layer

If a polygon shapefile containing, e.g., the values of the hydraulic conductivity along each Cartesian direction is available, such shapefile can be used to assign *KX*, *KY* and *KZ* values at each cell of the model layer, using the *Copy from Vector layer* tool integrated in *FREEWAT*. The algorithm behind this tool 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 copied to *KX*, *KY* and *KZ* fields within the corresponding cell.

To activate the *Copy from Vector layer* tool, the following menu must be used:

FREEWAT -> Tools -> Copy from Vector layer

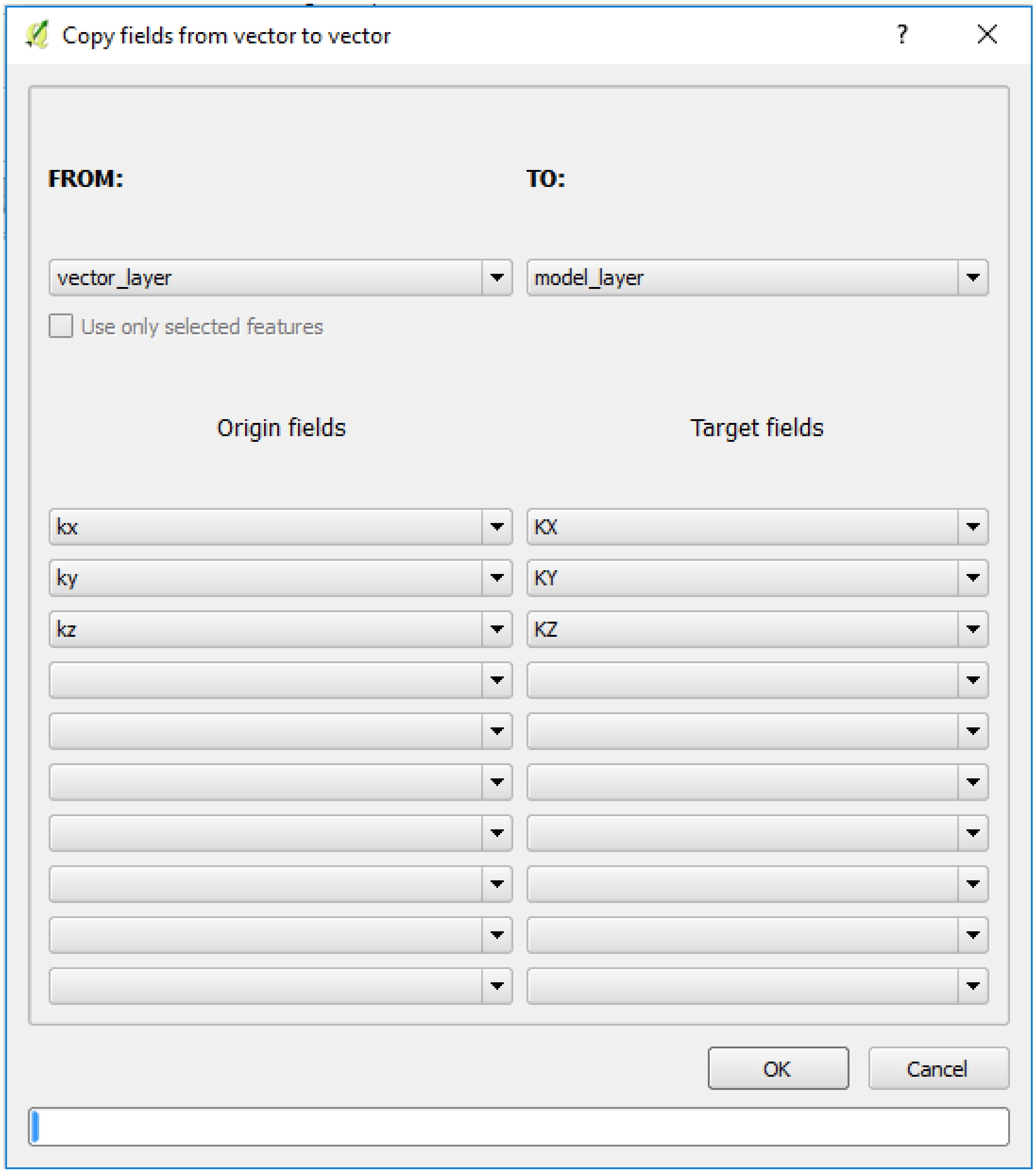


The following data are required in the **Copy fields from vector to vector** window:

- in the **FROM:** section, the origin vector layer and the *Origin fields* involved in the copy procedure must be selected;
- in the **TO:** section, the target vector layer and the *Target fields* involved in the copy procedure must be selected.

Note: It is possible to apply this tools on selected grid cells only. In this case the *Use only selected features* checkbox on the left side of the interface must be checked.

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



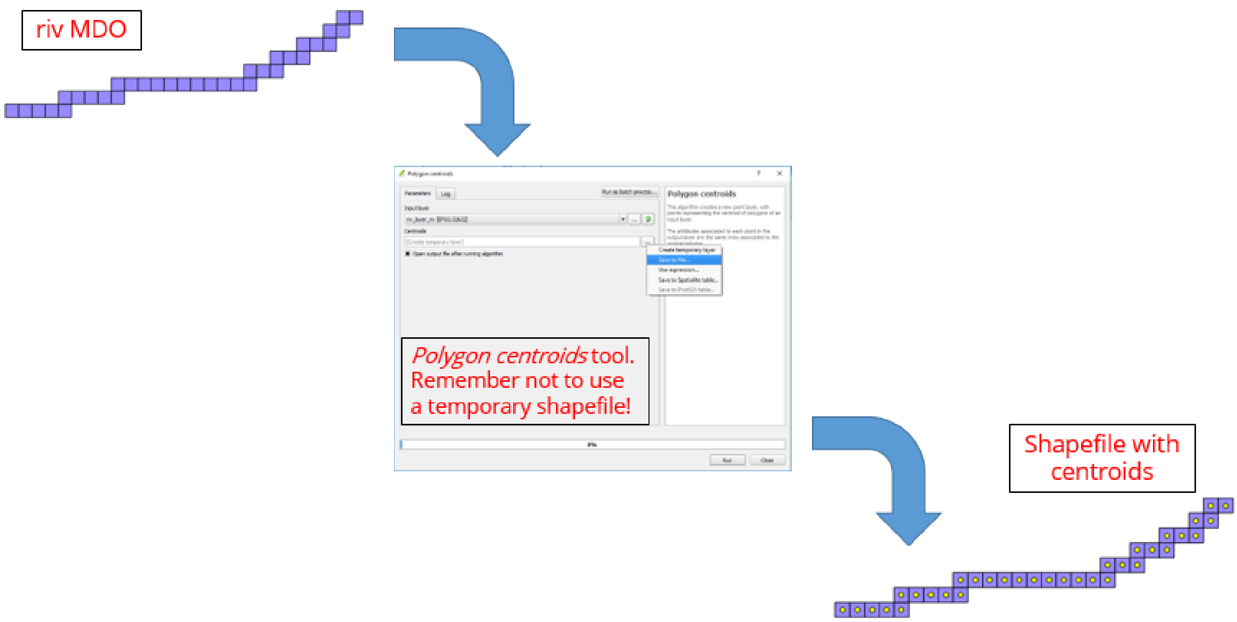
Note: It is possible to copy a maximum of ten parameters at once.

Note: Please notice that this tool may take several minutes when copying values from a vector layer to a grid-based MDO (i.e., an MDO which is made of as many cells as the grid MDO, such as a model layer), especially in models with a large number of grid cells. For example, it may take up to 20 minutes in a model with about 200000 cells.

Note: When using this tool, please be sure that the vector layers involved in the copying procedure are not grouped in the Layers Panel.

Note: This tool cannot be used if the origin vector layer is a temporary shapefile. Should this be the case, the User has to permanently save the temporary shapefile first. Similarly, this tool cannot be used if the origin vector layer is an MDO stored in another DB. Also in such case, the User has to save this MDO as a shapefile first.

Let's suppose now that you created a riv MDO (details in section 6.5) representing a river and that you somehow processed the elevation of the river bed bottom (variable *rbot_n*, where *n* refers to the *n*-th SP, details in section 6.5). Let's suppose that you need to copy *rbot_n* values to the *BOTTOM* field of the uppermost model layer, so that the river is completely contained within the uppermost hydrostratigraphic unit at the corresponding grid cells. For this scope, the *Copy from Vector layer* tool cannot be directly used, as the involved vector layers (i.e., the riv MDO and the uppermost model layer) do not have the same number of grid cells. As such, the riv MDO must be saved in advance as a shapefile. Please notice that some Users reported inconsistencies related to the copied values, when the origin vector layer (a shapefile saved from a riv MDO in our case) is a polygon shapefile with two polygons sharing a vertex. Should this be the case, we suggest to save the riv MDO as a point shapefile, containing a point completely within a grid cell and with no overlaps between neighbouring features, by using the *QGIS* tool *Polygon centroids*, which can be retrieved through the *QGIS* toolbox.

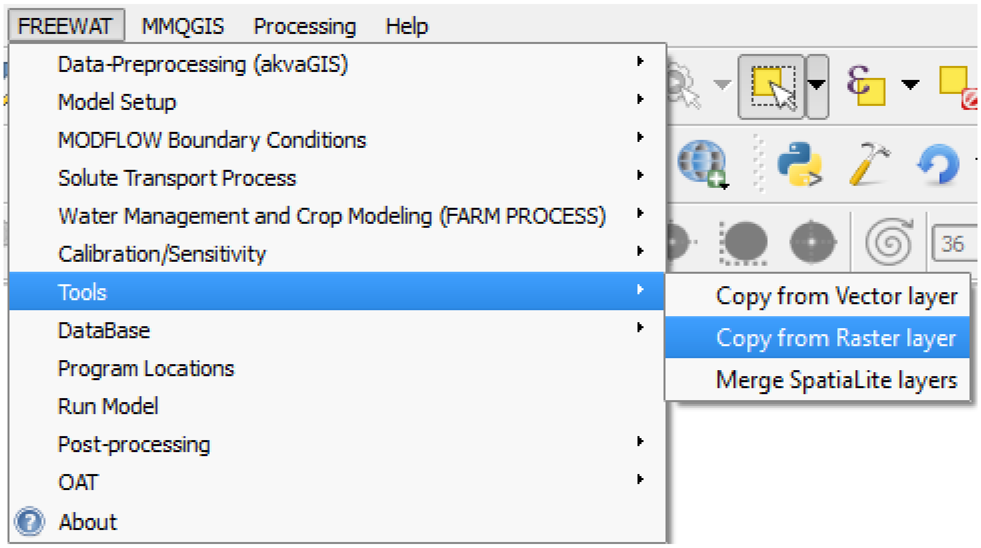


Copy from raster layer

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, using the *Copy from Raster layer* tool integrated in *FREEWAT*. The origin raster layer must have at least the same extension of the model grid, in order to assign features at each node of the grid itself. Furthermore, if the origin raster layer has a finer space discretization than the model grid, the average value of a certain parameter, calculated involving raster pixels 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 space discretization than the origin raster layer, the same value will be assigned at grid cells matching a single raster pixel.

To activate the *Copy from Raster layer* tool, the following menu must be used:

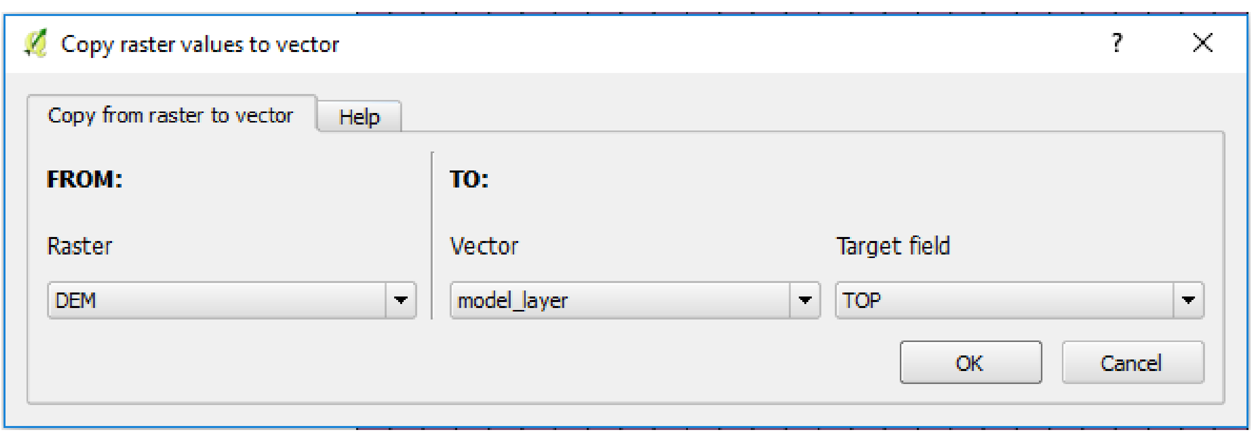
FREEWAT -> Tools -> Copy from Raster layer



The following data are required in the **Copy raster values to vector** window:

- in the **FROM:** section:
  - *Raster*: the origin raster file;
- in the **TO:** section:
  - *Vector*: the target vector layer (i.e., a model layer/MDO);
  - *Target field*: the target field to be updated (i.e., one among the fields contained in the Attribute Table of the vector layer above).

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



Note: When using this tool, please be sure that the layers involved in the copying procedure are not grouped in the Layers Panel.

CHAPTER 6

Implement 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-2005 online guide, section *Ground-Water Flow Processes -> Boundary Condition Packages*.

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

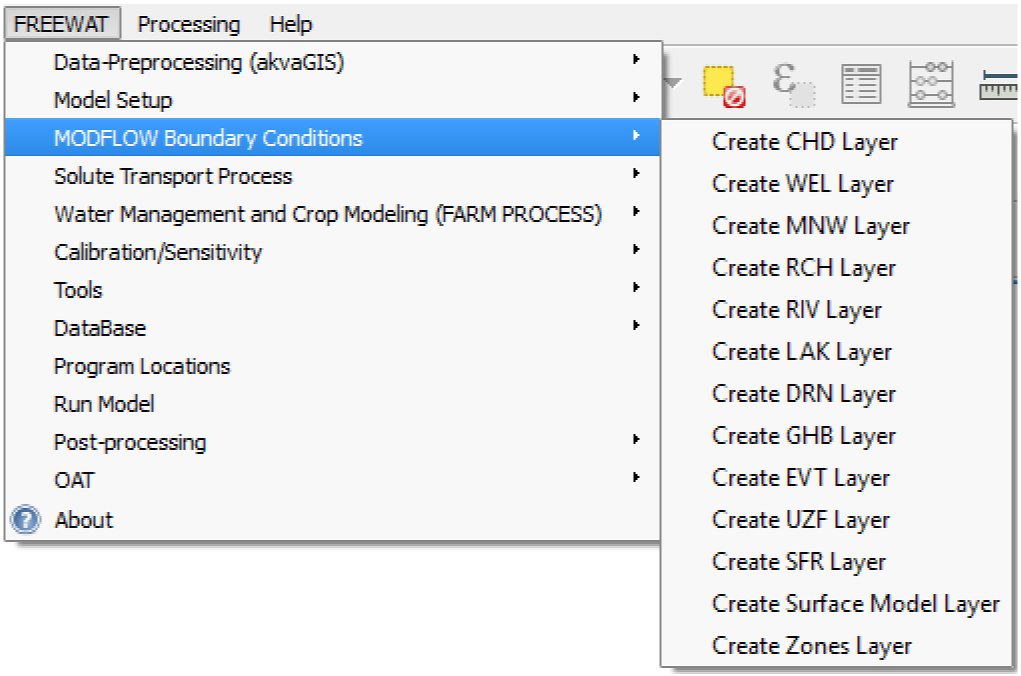
As stated in Chapter 2, in *FREEWAT* implementing each process requires translating a GIS layer into an MDO and then into a *MODFLOW* input file. Such procedure includes at least two of the following steps:

1. loading the GIS layer in the Layers Panel;
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 created.

MODFLOW Packages for defining boundary conditions and source/sink terms can be activated through the following menu:

FREEWAT -> MODFLOW Boundary Conditions



Note: Each MDO created through one of these sub-menus will be stored in the model DB and loaded in the Layers Panel with a specific extension (e.g., *_chd* for an MDO related to the CHD Package). Such extension must not be changed in the Layers Panel and neither in the model DB, as the related MDO will be filtered in the **Run Model** window according to such extension.

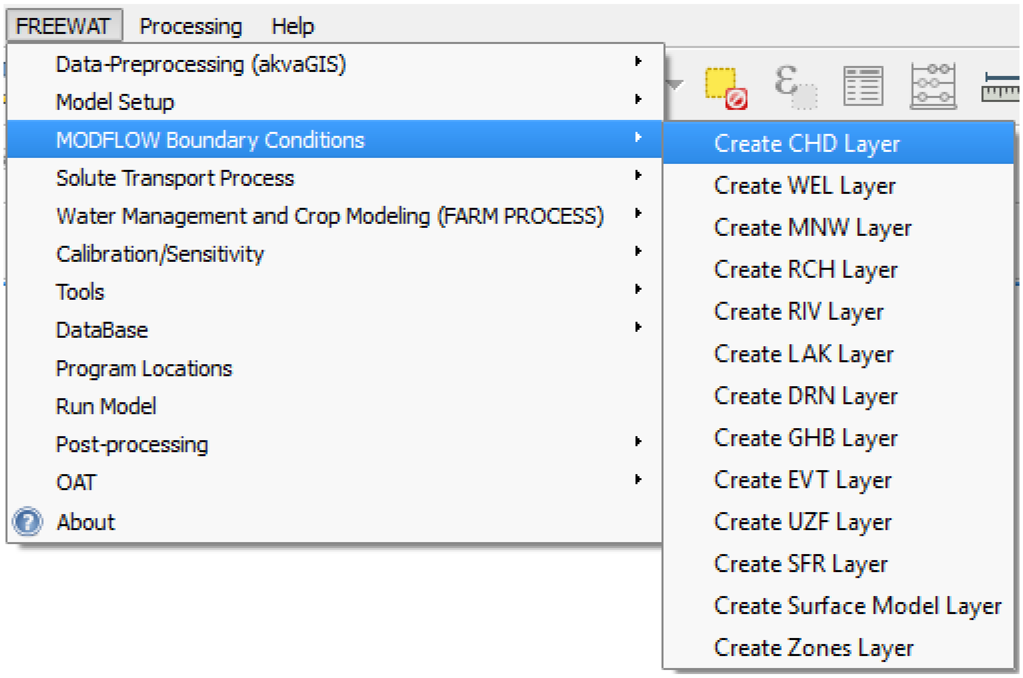
Time-Variant Specified Head - CHD

The *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, or prior processing of a line shapefile intersecting grid cells where such boundary condition has to be assigned.

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

FREEWAT -> MODFLOW Boundary Conditions -> Create CHD Layer

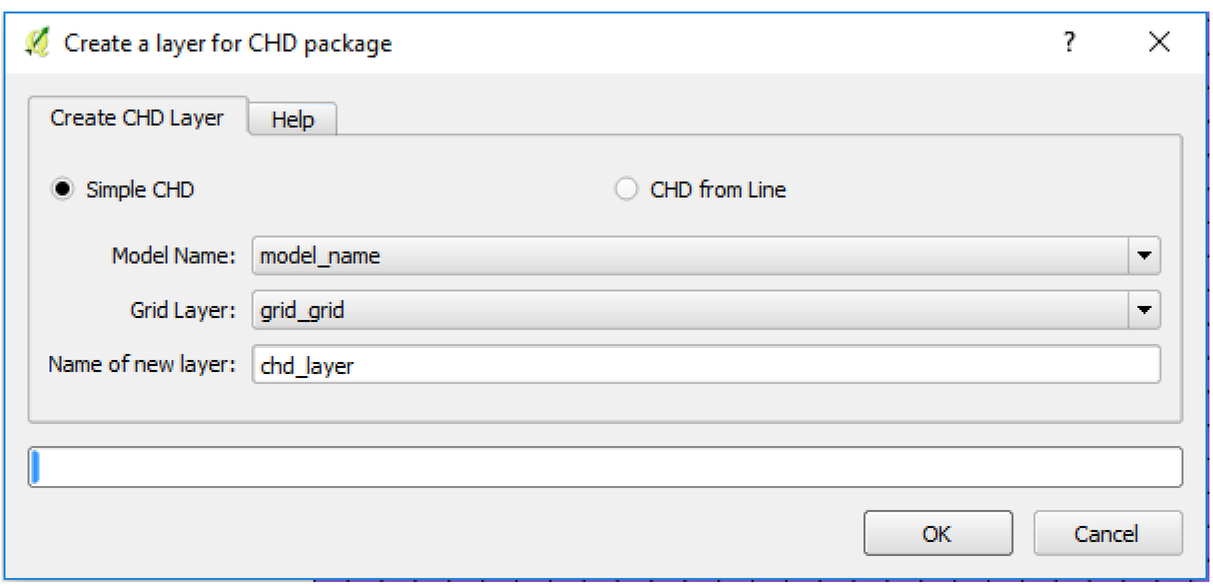


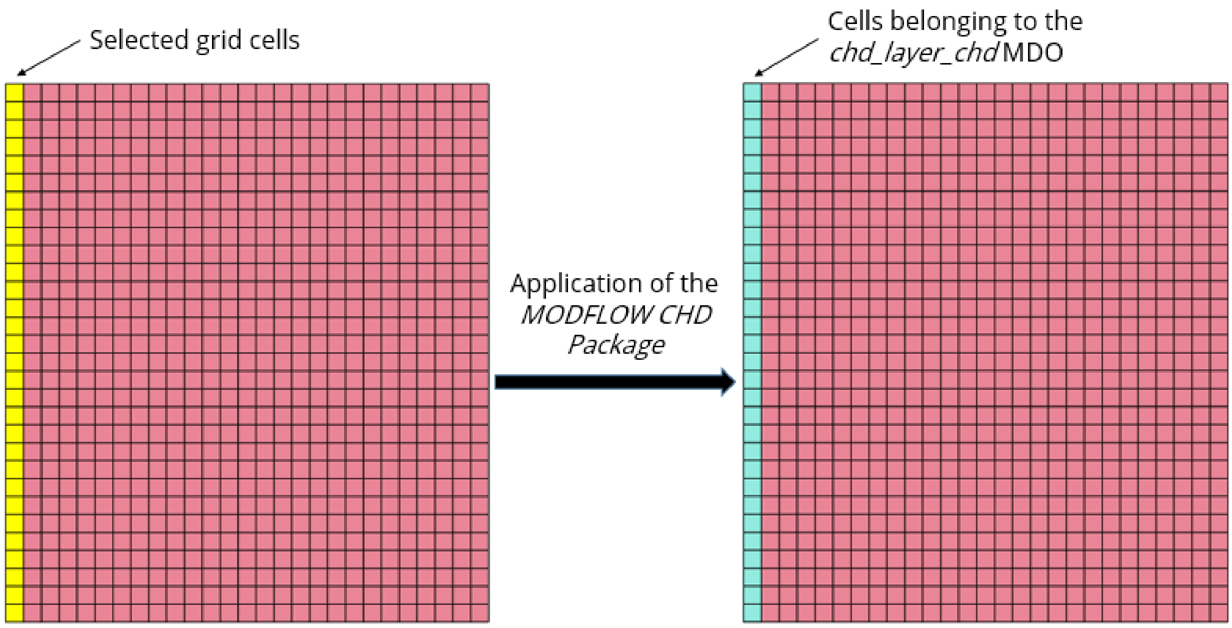
In the **Create a layer for CHD package** window, two alternative options are available:

- *Simple CHD*, if the grid cells, where the specified-head boundary condition has to be assigned, have previously been selected manually, using the *QGIS* selection tools presented in Chapter 5;
- *CHD from Line*, if a line shapefile, intersecting grid cells where the specified-head boundary condition has to be assigned, has previously been processed.

If the *Simple CHD* option is checked, the following data are required in the **Create a layer for CHD package** window:

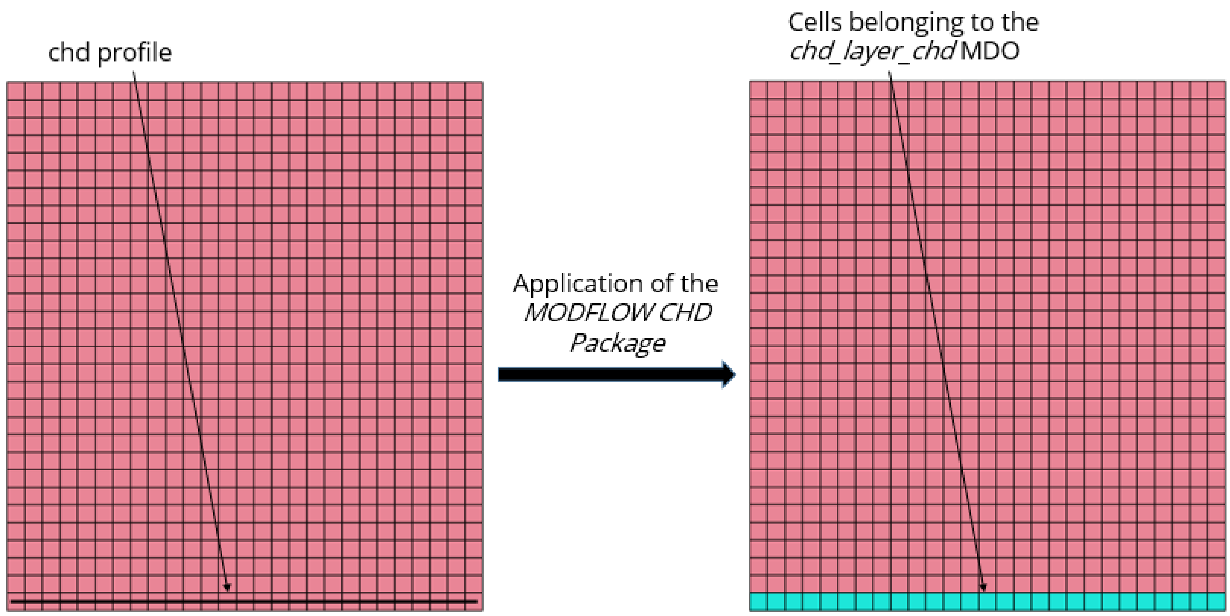
- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Name of new layer*: name of the chd MDO which has to be created.

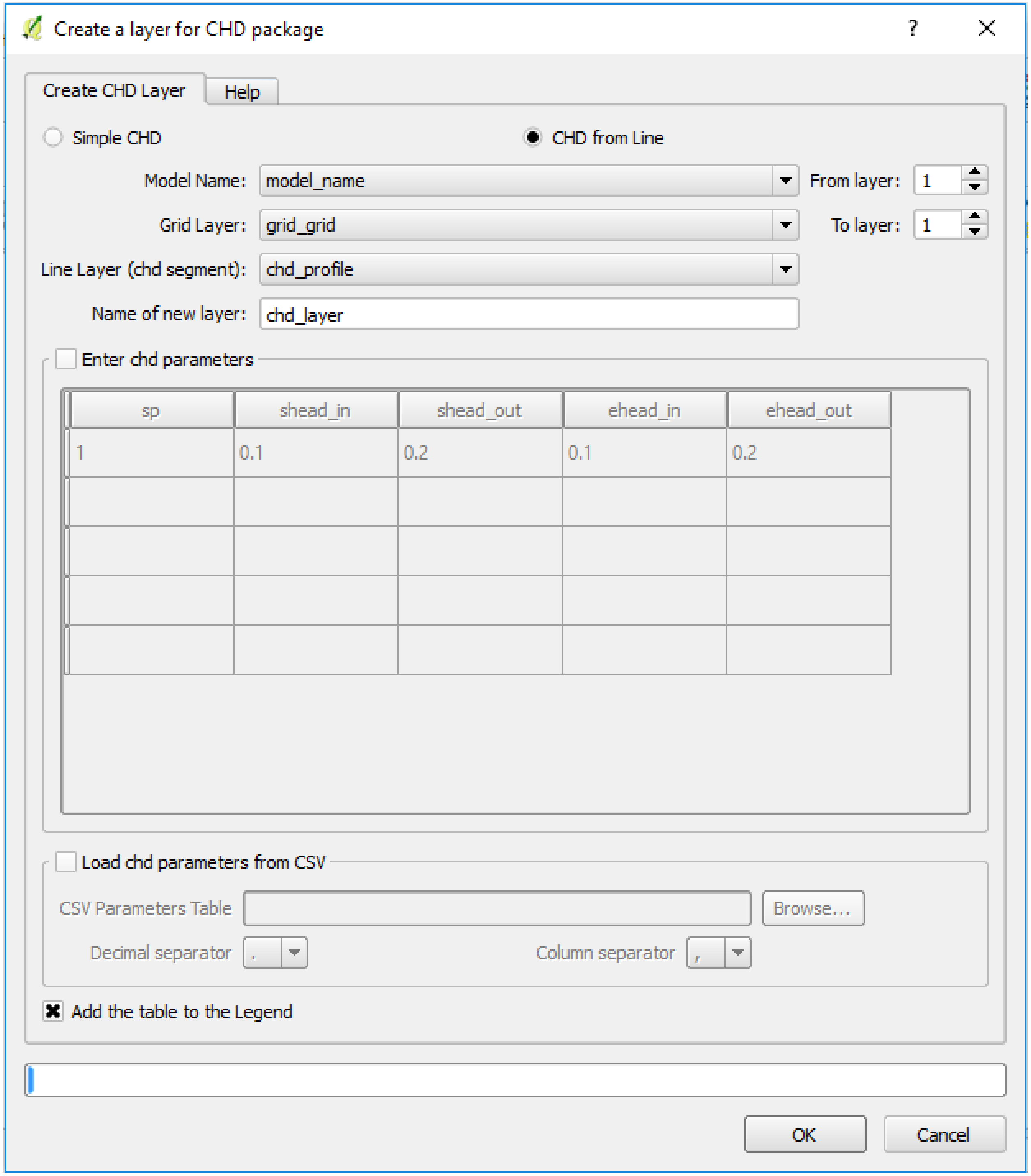




If the *CHD from Line* option is checked, the following data are required in the **Create a layer for CHD package** window:

- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer*: line shapefile intersecting the grid cells where the specified-head boundary condition has to be assigned;
- *Name of new layer*: name of the chd MDO which has to be created;
- *From layer*: number of the uppermost model layer where the specified-head boundary condition has to be assigned;
- *To layer*: number of the deepest model layer where the specified-head boundary condition has to be assigned;
- if *Enter chd parameters* is checked, the User can fill manually the table with all the necessary parameters to be assigned to grid cells where the specified-head boundary condition has to be assigned;
- if *Load chd parameters from CSV* is checked, the User can load a csv file containing parameters to be assigned to grid cells where the specified-head boundary condition has to be assigned, 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 chd parameters assigned through the csv file will be loaded in the Layers Panel and stored in the model DB.


chd profile
Application of the *MODFLOW CHD Package*
Cells belonging to the *chd_layer_chd* MDO



Note: Parameters required when creating the chd MDO with the *CHD from Line* option are related to the specified head values at the beginning and at the end of each SP and must be assigned at the upstream and downstream cells of the chd segment:

- *sp*: SP number;
- *shead_in*: specified head [L], with respect to a reference datum, at the upstream cell of the chd segment and at the beginning of the SP;

- *shead_out*: specified head [L], with respect to a reference datum, at the downstream cell of the chd segment and at the beginning of the SP;
- *ehead_in*: specified head [L], with respect to a reference datum, at the upstream cell of the chd segment and at the end of the SP;
- *ehead_out*: specified head [L], with respect to a reference datum, at the downstream cell of the chd segment and at the end of the SP.

Such values are assigned at the upstream and downstream cells of the chd segment. Linear interpolation is automatically performed at the remaining cells.

If used, the csv file must have the following scheme (the template file *chd_parameters.csv* is provided within the *FREEWAT* plugin folder `freewat\csv_templates\chd`):

chd_parameters.csv

```
SP,SHEAD_IN,SHEAD_OUT,EHEAD_IN,EHEAD_OUT
1,0.00,5.00,0.00,5.00
2,0.50,5.50,0.50,5.50
3,0.70,5.70,0.70,5.70
```

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

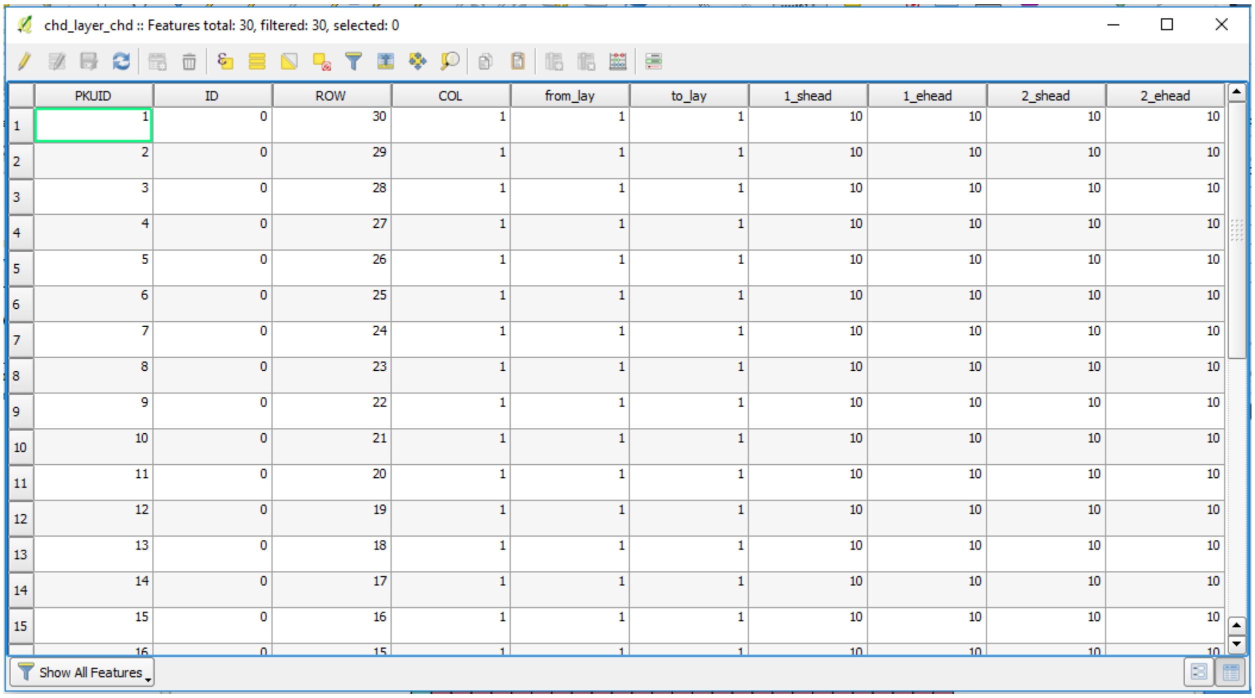
Note: If the *Simple CHD* option has been used, once the chd MDO has been successfully created, the selected grid cells automatically deselect.

Note: The extension *_chd* must not be changed in the Layers Panel and neither in the DB, as the chd MDO will be filtered in the **Run Model** window according to such extension.

The Attribute Table of such MDO contains several records, according to the number of grid cells where this Package is applied, and the following fields:

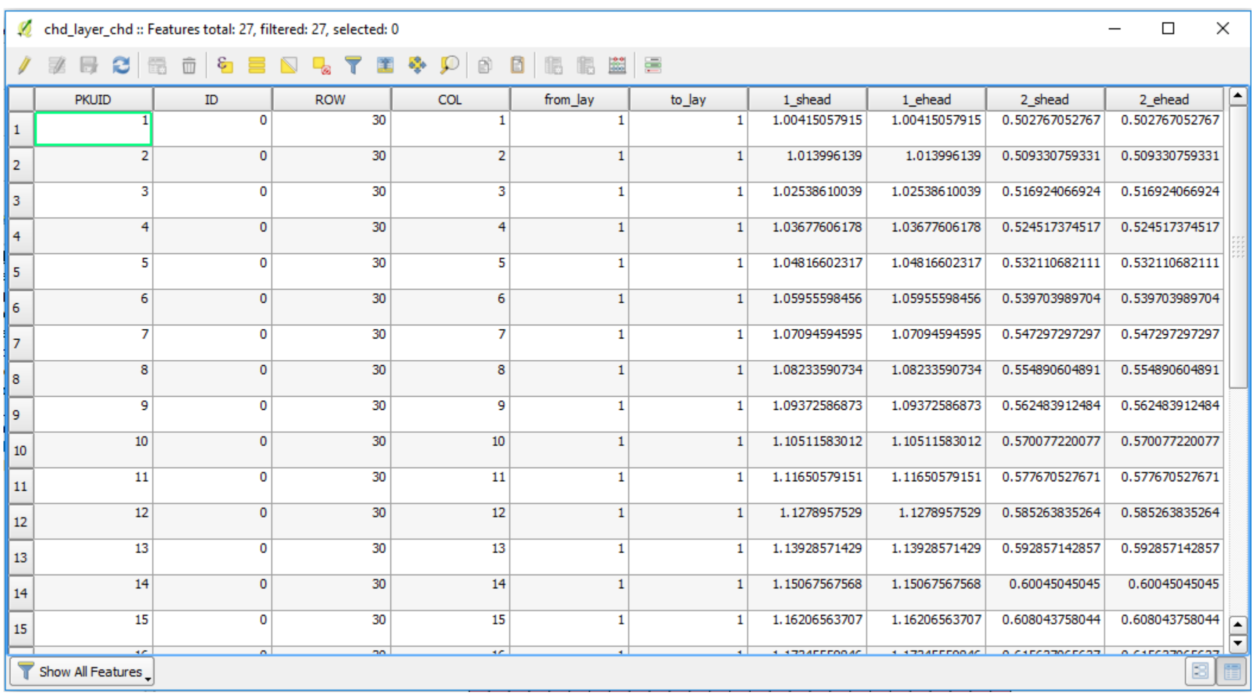
- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row index of a grid cell;
- *COL*: column index number of a grid cell;
- *from_lay*: number of the uppermost model layer where the specified-head boundary condition must be assigned;
- *to_lay*: number of the deepest model layer where the specified-head 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], with respect to a reference datum, at the beginning of the *n*-th SP;
  - *n_ehead*: specified head [L], with respect to a reference datum, at the end of the *n*-th SP.

If the *Simple CHD* option has been used, 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.



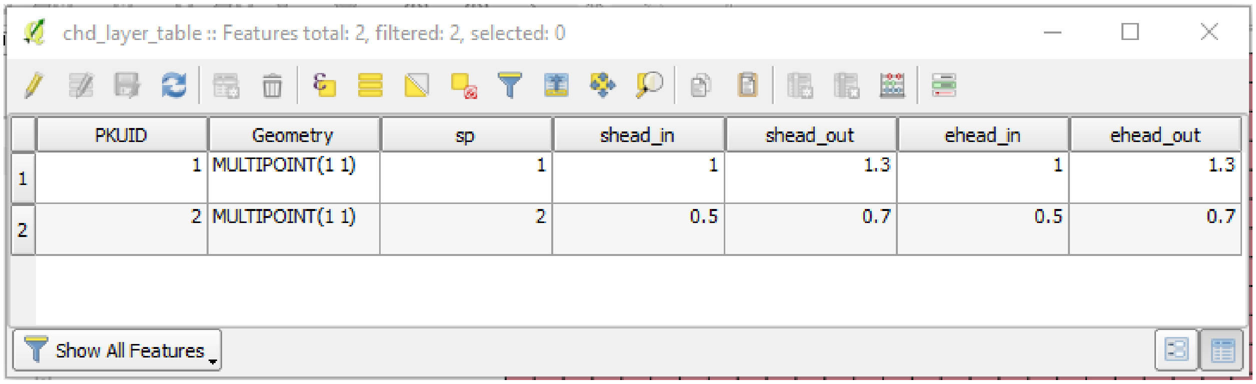
	PKUID	ID	ROW	COL	from_lay	to_lay	1_shead	1_ehead	2_shead	2_ehead
1	1	0	30	1	1	1	10	10	10	10
2	2	0	29	1	1	1	10	10	10	10
3	3	0	28	1	1	1	10	10	10	10
4	4	0	27	1	1	1	10	10	10	10
5	5	0	26	1	1	1	10	10	10	10
6	6	0	25	1	1	1	10	10	10	10
7	7	0	24	1	1	1	10	10	10	10
8	8	0	23	1	1	1	10	10	10	10
9	9	0	22	1	1	1	10	10	10	10
10	10	0	21	1	1	1	10	10	10	10
11	11	0	20	1	1	1	10	10	10	10
12	12	0	19	1	1	1	10	10	10	10
13	13	0	18	1	1	1	10	10	10	10
14	14	0	17	1	1	1	10	10	10	10
15	15	0	16	1	1	1	10	10	10	10

If the *CHD from Line* option has been used, the fields *from_lay*, *to_lay*, *n_shead* and *n_ehead* are filled with values assigned by the User through the csv file.



	PKUID	ID	ROW	COL	from_lay	to_lay	1_shead	1_ehead	2_shead	2_ehead
1	1	0	30	1	1	1	1.00415057915	1.00415057915	0.502767052767	0.502767052767
2	2	0	30	2	1	1	1.013996139	1.013996139	0.509330759331	0.509330759331
3	3	0	30	3	1	1	1.02538610039	1.02538610039	0.516924066924	0.516924066924
4	4	0	30	4	1	1	1.03677606178	1.03677606178	0.524517374517	0.524517374517
5	5	0	30	5	1	1	1.04816602317	1.04816602317	0.532110682111	0.532110682111
6	6	0	30	6	1	1	1.05955598456	1.05955598456	0.539703989704	0.539703989704
7	7	0	30	7	1	1	1.07094594595	1.07094594595	0.547297297297	0.547297297297
8	8	0	30	8	1	1	1.08233590734	1.08233590734	0.554890604891	0.554890604891
9	9	0	30	9	1	1	1.09372586873	1.09372586873	0.562483912484	0.562483912484
10	10	0	30	10	1	1	1.10511583012	1.10511583012	0.570077220077	0.570077220077
11	11	0	30	11	1	1	1.11650579151	1.11650579151	0.577670527671	0.577670527671
12	12	0	30	12	1	1	1.1278957529	1.1278957529	0.585263835264	0.585263835264
13	13	0	30	13	1	1	1.13928571429	1.13928571429	0.592857142857	0.592857142857
14	14	0	30	14	1	1	1.15067567568	1.15067567568	0.60045045045	0.60045045045
15	15	0	30	15	1	1	1.16206563707	1.16206563707	0.608043758044	0.608043758044

If the *CHD from Line* option has been used, a table renamed *chd_layer_table* is created with the chd MDO, stored in the model DB and eventually loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters defined in the csv file.



	PKUID	Geometry	sp	shead_in	shead_out	ehead_in	ehead_out
1	1	MULTIPOINT(1 1)	1	1	1.3	1	1.3
2	2	MULTIPOINT(1 1)	2	0.5	0.7	0.5	0.7

Note: *n_shead* and *n_ehead* values must be expressed in model units and referred to a reference datum.

Note: Please notice that some Users experienced problems when creating a chd MDO over more than 200 grid cells. As such, if you need to apply the *MODFLOW CHD Package* at more cells, several selections must be made and more than one chd MDO must be created. The tool *Merge SpatiaLite layers* can then be used (further details in section *River - RIV (head-dependent flux)*).

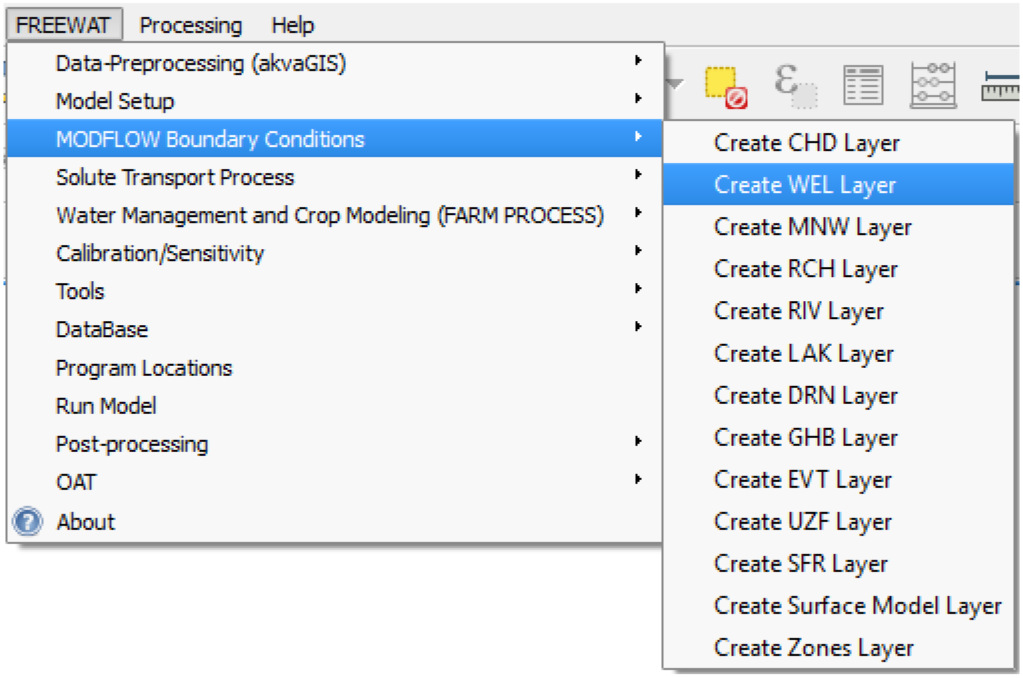
Well - WEL (specified-flux)

The *MODFLOW WEL Package* allows to simulate recharge to the aquifer or extraction of groundwater, defining a specified positive or negative flux, respectively, to grid cells where this condition has to be applied.

Activating this Package requires selecting cells from the grid MDO to which such Package has to be assigned, or prior processing of a point shapefile containing the location of recharge/pumping wells within the study area.

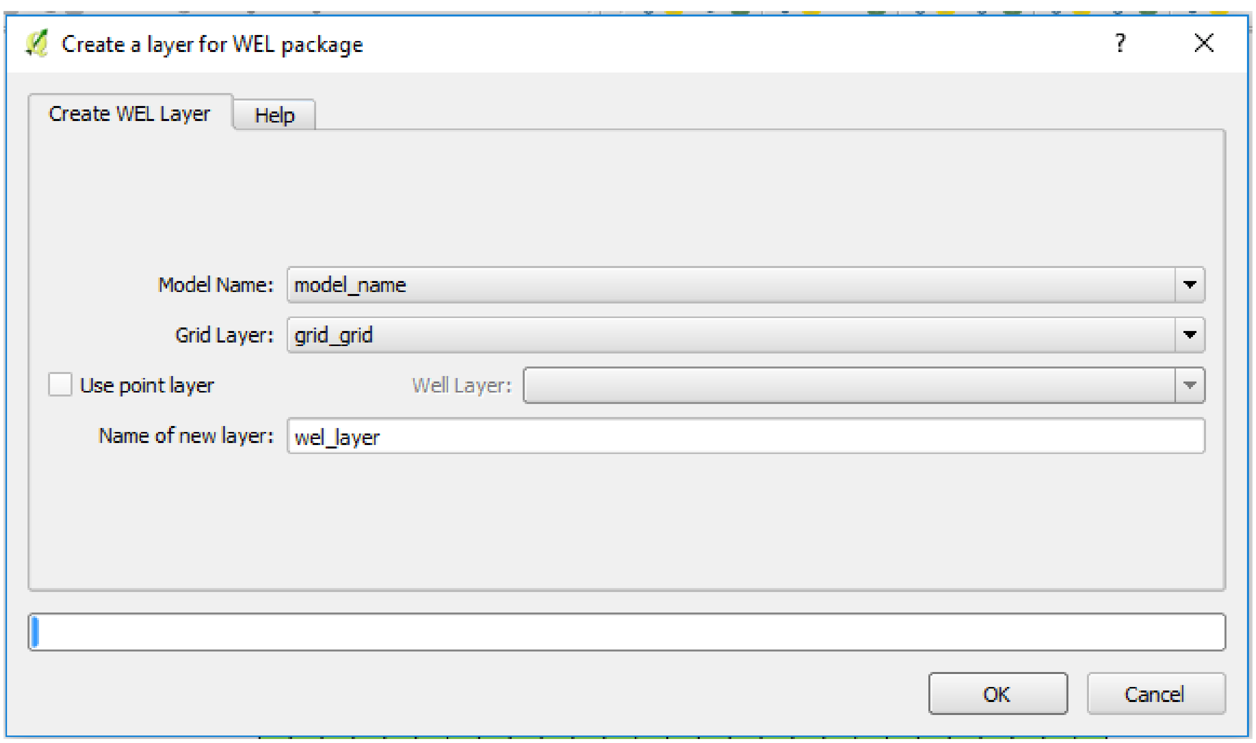
To activate the *WEL Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create WEL Layer



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

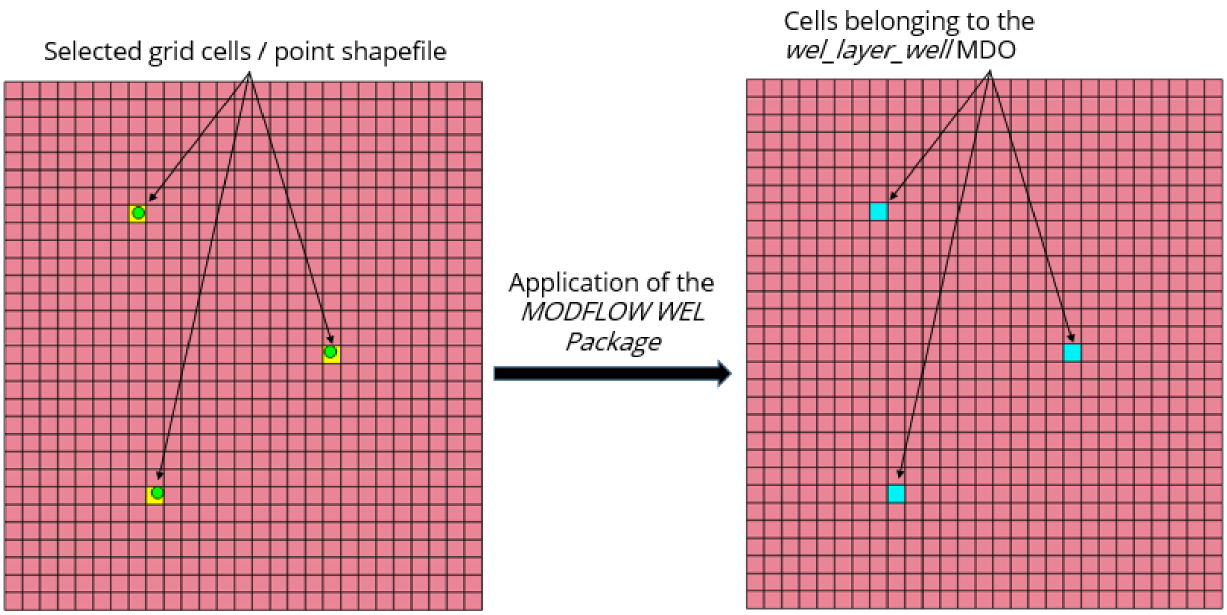
- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- if *Use point layer* is checked:
  - *Well Layer*: point shapefile containing the location of recharge/pumping wells within the study area;
- *Name of new layer*: name of the well MDO which has to be created.



Note: If *Use point layer* is NOT checked, manual selection of cells from the grid MDO must be previously performed, using the *QGIS* selection tools presented in Chapter 5. In such case, once the well MDO has been successfully created, the selected grid cells automatically deselect. Viceversa, checking *Use point layer* requires having a point shapefile containing the location of recharge/pumping wells in the Layers Panel.

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

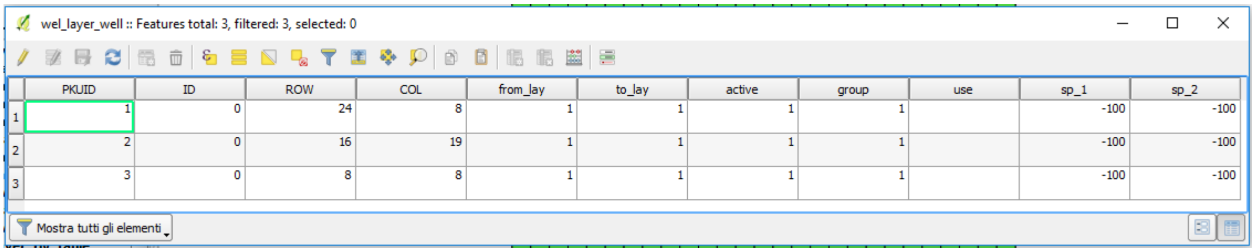
Note: The extension *_well* must not be changed in the Layers Panel and neither in the DB, as the well MDO will be filtered in the **Run Model** window according to such extension.



The Attribute Table of such MDO contains several records, according to the number of grid cells where this Package is applied, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row index of a grid cell;
- *COL*: column index of a grid cell;
- *from_lay*: number of the uppermost model layer where the recharge/pumping wells must be assigned;
- *to_lay*: number of the deepest model layer where the recharge/pumping wells 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);
- *group*: integer value which can be used as a label to distinguish different subsets of wells;
- *use*: text field which can be used to distinguish different subsets of wells according to their use (e.g., wells for drinking, irrigation, domestic, industrial use);
- the following field is repeated according to the number of SPs implemented (n refers to the number of a SP):
  - *sp_n*: specified recharge/pumping flow rate $[L^3/T]$ during the n-th SP.

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


wel_layer_well :: Features total: 3, filtered: 3, selected: 0

	PKUID	ID	ROW	COL	from_lay	to_lay	active	group	use	sp_1	sp_2
1	1	0	24	8	1	1	1	1		-100	-100
2	2	0	16	19	1	1	1	1		-100	-100
3	3	0	8	8	1	1	1	1		-100	-100

Mostra tutti gli elementi

Note: *sp_n* values must be expressed in model units. Positive values are required for recharge wells, negative values are required for pumping wells.

Note: If the recharge/pumping rate is assigned to more than one model layer, the specified flux will be equally distributed by *MODFLOW* at each of the model layers involved. As such, the User has to calculate externally the rate which has to be assigned at each model layer, i.e., by equally dividing the whole rate by the number of the involved model layers.

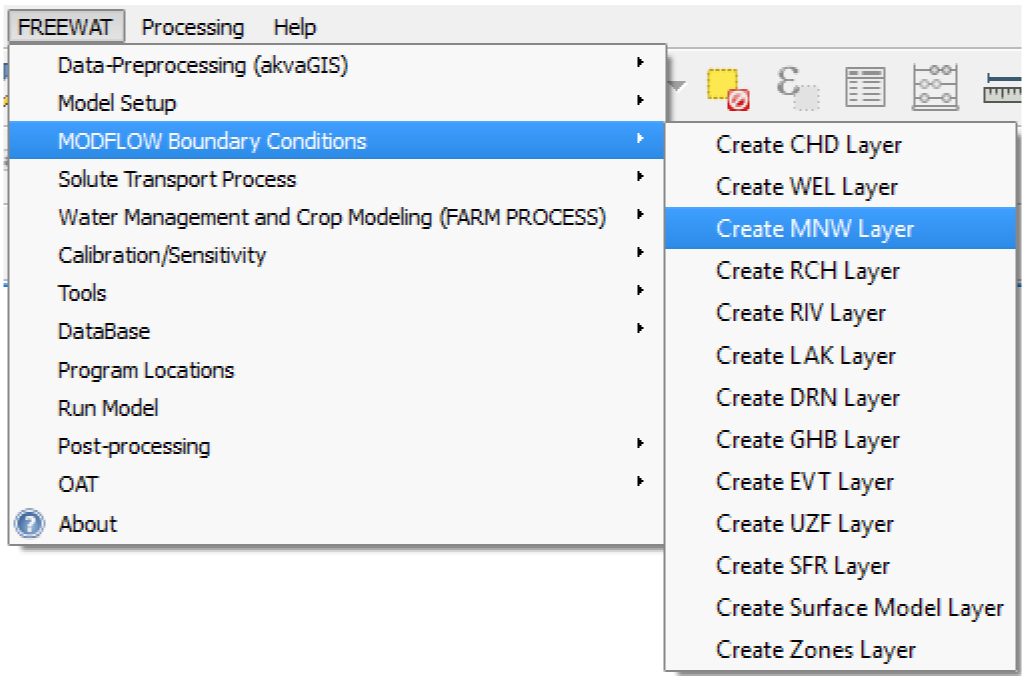
Multi-Node Well - MNW (head-dependent flux)

The *MODFLOW MNW Package* allows to simulate screened wells 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 has been 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.

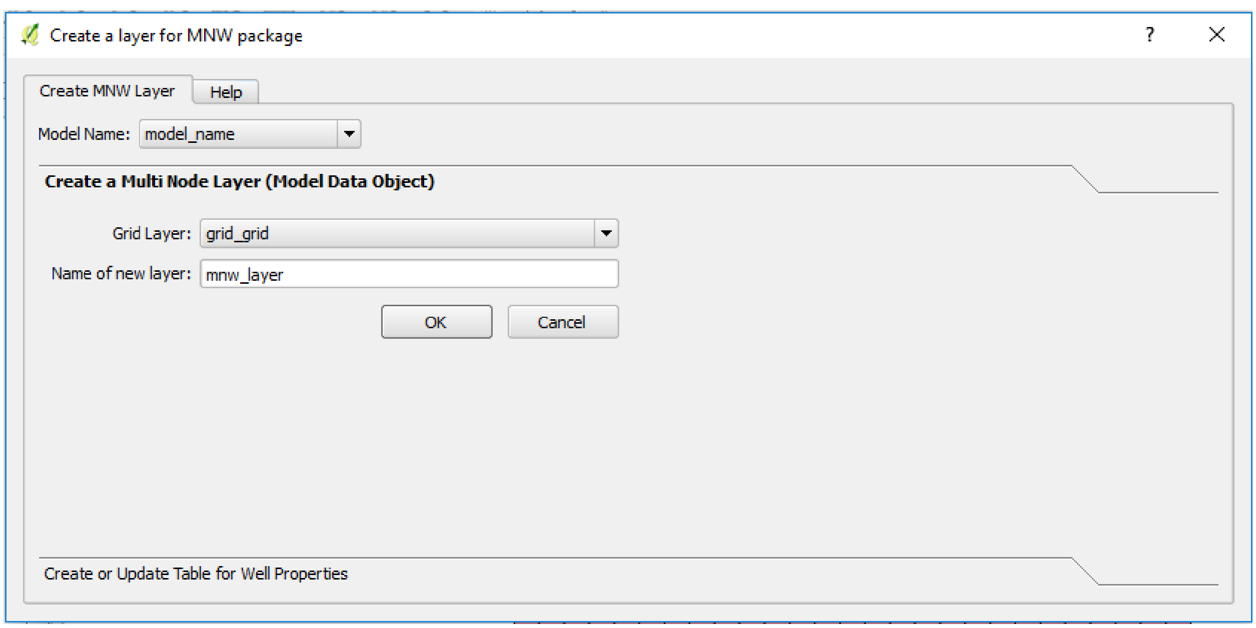
To activate the *MNW Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create MNW Layer



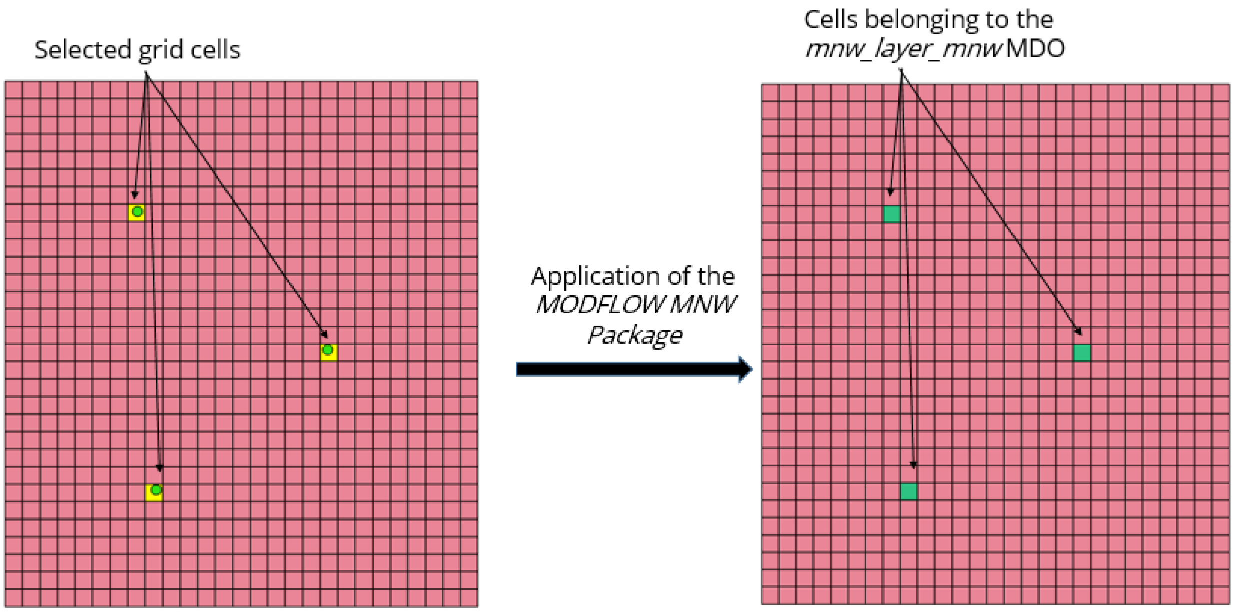
The following data are required in the **Create a layer for MNW package** window:

- *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, renamed *mnw_layer_mnw*, is created, stored in the model DB and loaded in the Layers Panel.

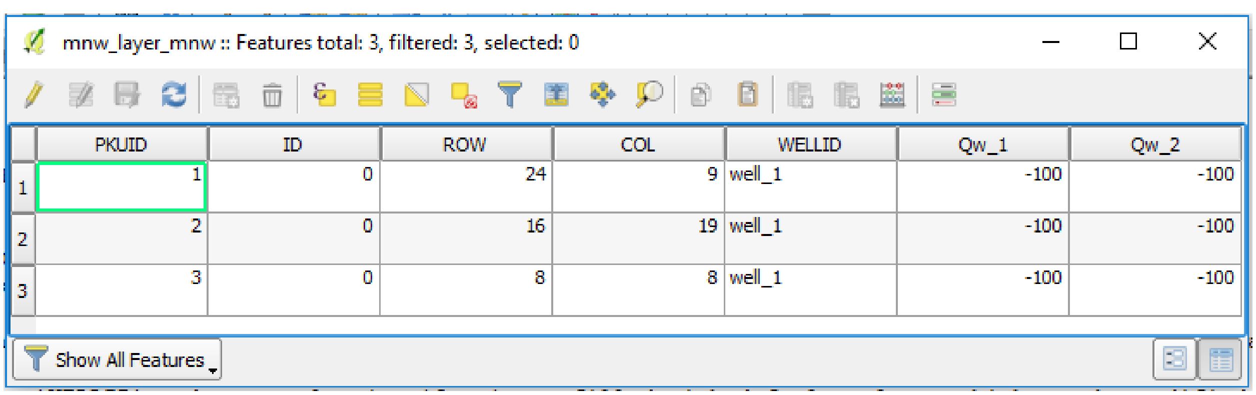
Note: The extension *_mnw* must not be changed in the Layers Panel and neither in the DB, as the mnw MDO will be filtered in the **Run Model** window according to such extension.



The Attribute Table of such MDO contains several records, according to the number of grid cells where this Package is applied, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row index of a grid cell;
- *COL*: column index 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	Qw_2
1	1	0	24	9	well_1	-100	-100
2	2	0	16	19	well_1	-100	-100
3	3	0	8	8	well_1	-100	-100

Note: *Qw_n* values must be expressed in model units.

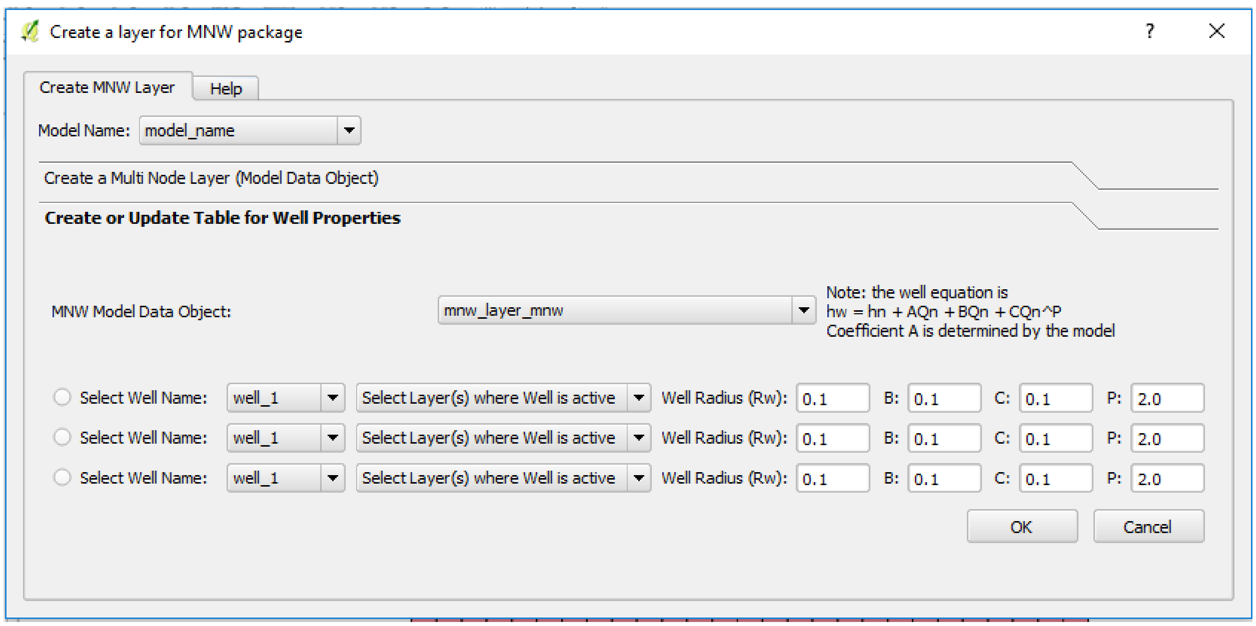
Note: Once the mnw MDO has been successfully created, the selected grid cells automatically deselect.

Once the mnw MDO has been successfully 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:

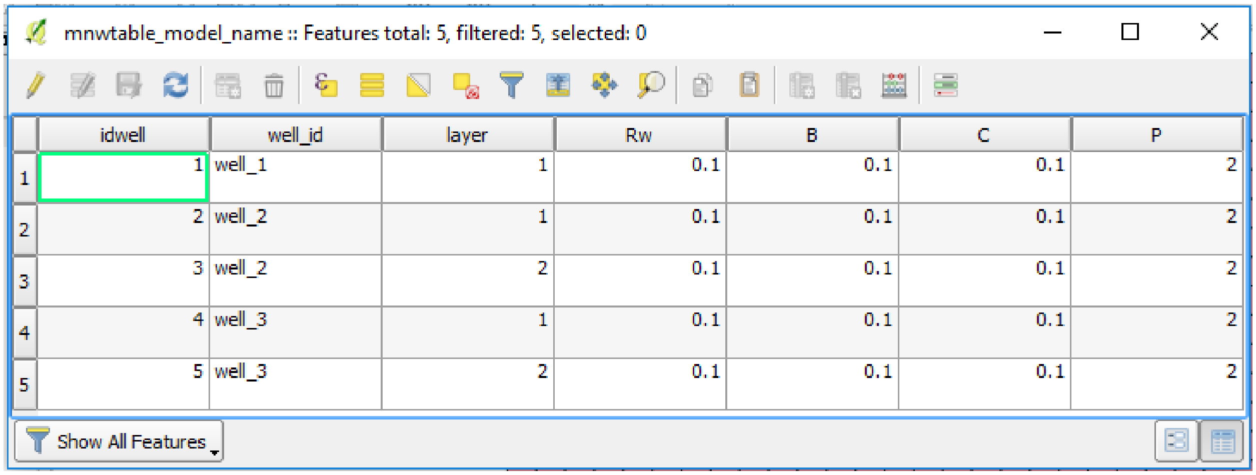
- *MNW Model Data Object*: name of the mnw MDO created;
- for each multi-node well:
  - the *WELLID* must be selected from the drop-dowm menu near to *Select Well Name* (this requires prior editing of the *WELLID* field in the Attribute Table of the mnw MDO);
  - the number of model layer(s) to which 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* User manual; Konikow et al., 2009).



A table renamed *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 specified 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 defined in the *Well Radius (Rw)* field when editing the *Create or Update Table for Well Properties* section;
- *B*, *C* and *P* coefficients as defined when editing the *Create or Update Table for Well Properties* section.



	idwell	well_id	layer	Rw	B	C	P
1	1	well_1	1	0.1	0.1	0.1	2
2	2	well_2	1	0.1	0.1	0.1	2
3	3	well_2	2	0.1	0.1	0.1	2
4	4	well_3	1	0.1	0.1	0.1	2
5	5	well_3	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, to define parameters for more than three multi-node wells, the *Create or Update Table for Well Properties* section can be used again and the *mnwtable_model_name* automatically updates.

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* User manual; Konikow et al., 2009).

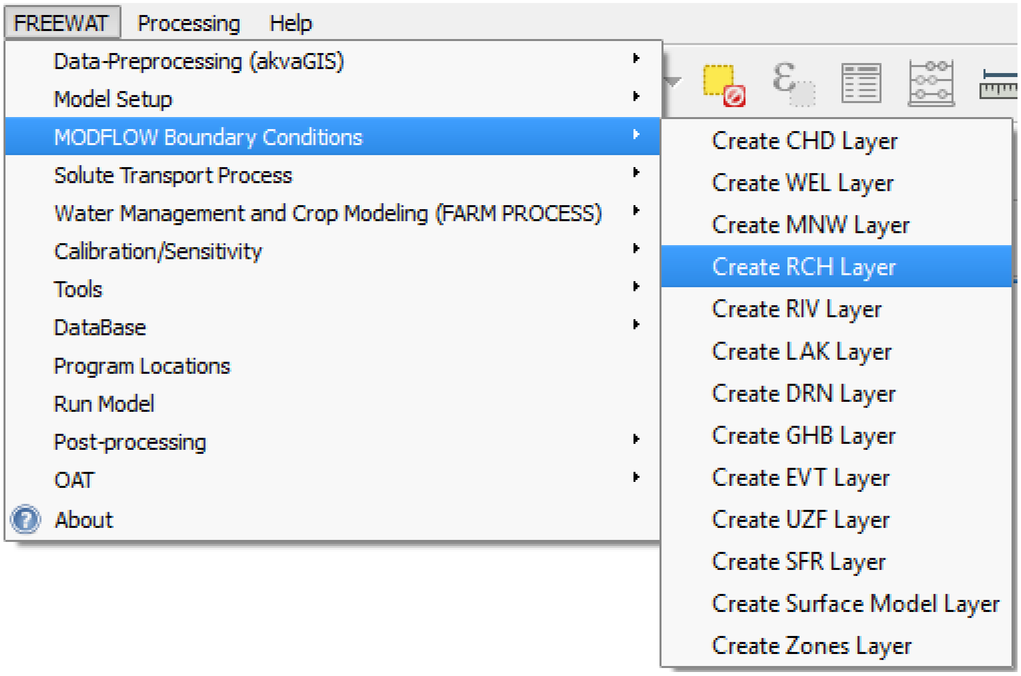
Recharge - RCH (specified-flux)

The *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 potentially 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.

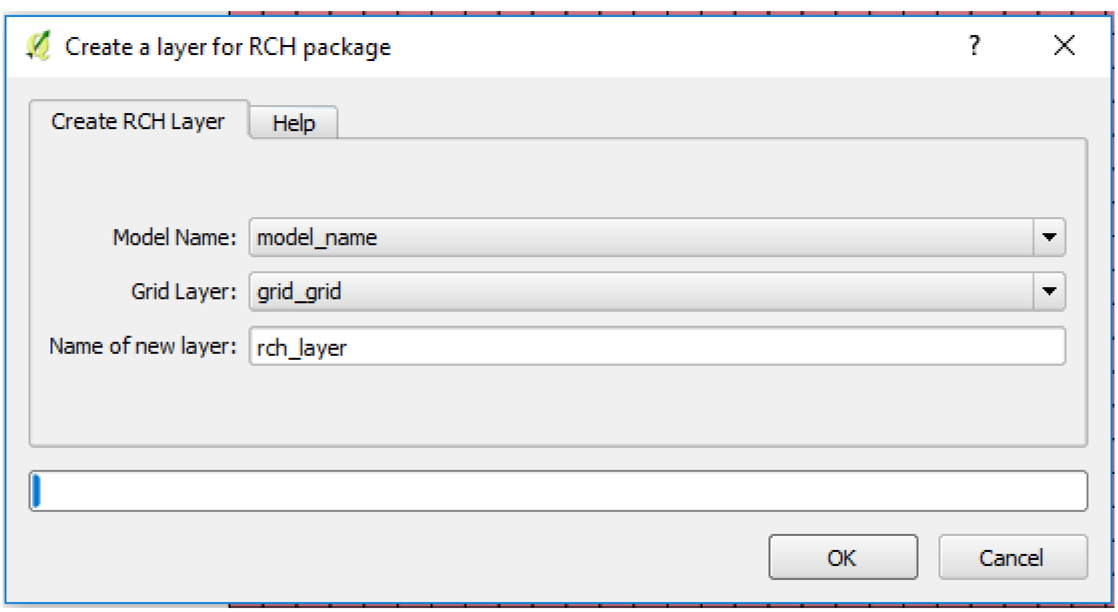
To activate the *RCH Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create RCH Layer



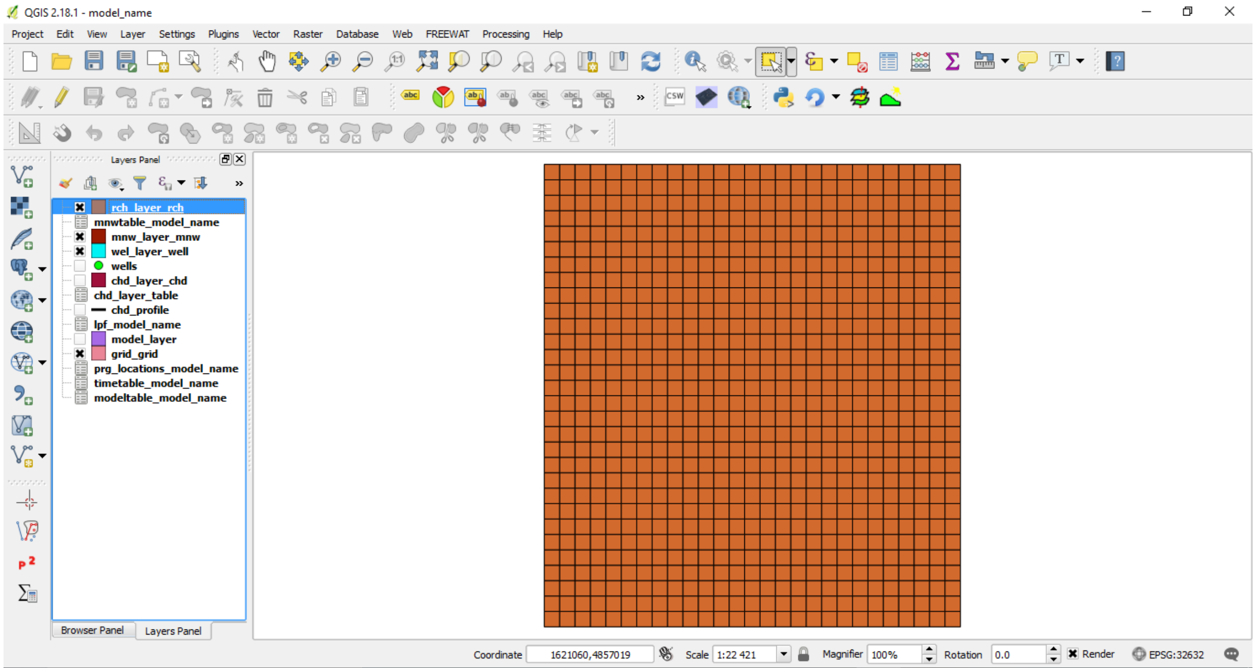
The following data are required in the **Create a layer for RCH package** window:

- *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, renamed *rch_layer_rch*, is created, stored in the model DB and loaded in the Layers Panel.

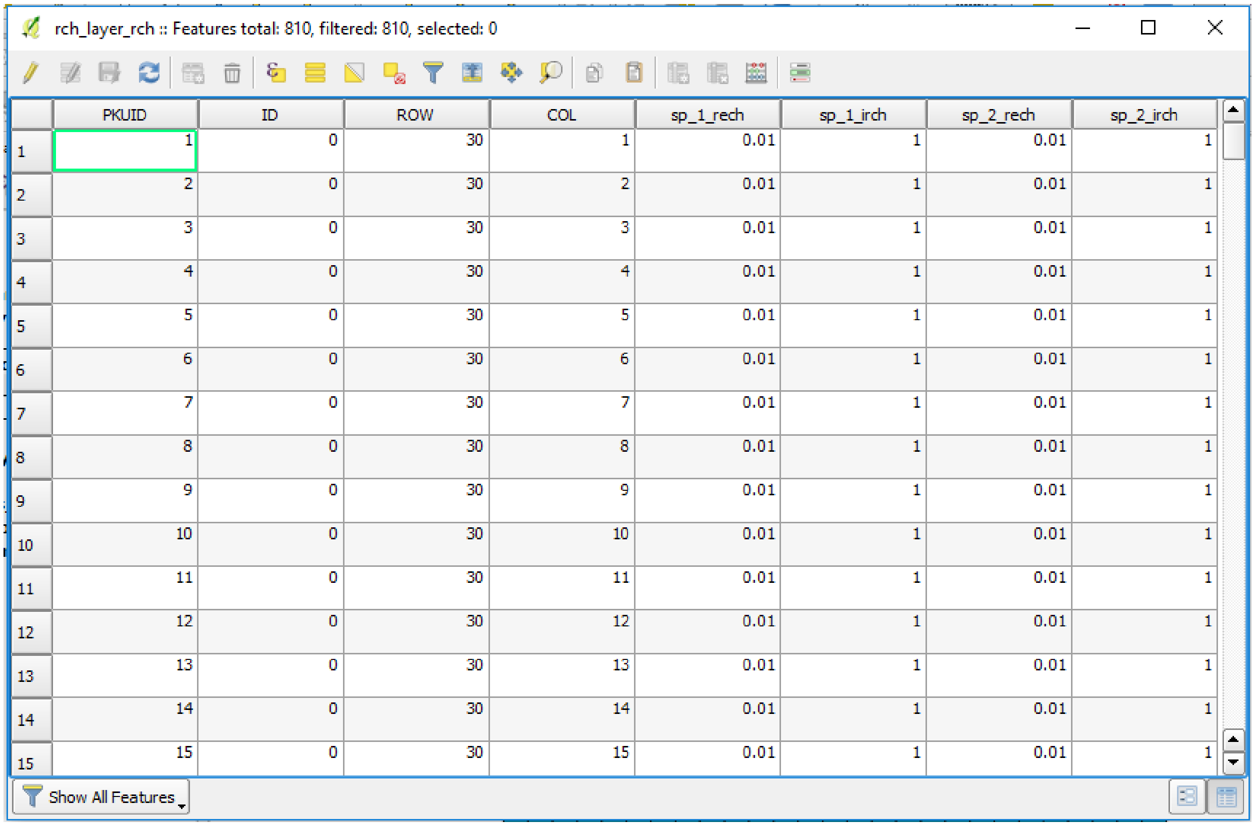
Note: The extension *_rch* must not be changed in the Layers Panel and neither in the DB, as the rch MDO will be filtered in the **Run Model** window according to such extension.



The Attribute Table of such MDO contains 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 index of a grid cell;
- *COL*: column index 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 recharge flux [L/T] during the *n*-th SP;
  - *sp_n_irch*: number of the model layer to which 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.


rch_layer_rch :: Features total: 810, filtered: 810, selected: 0

	PKUID	ID	ROW	COL	sp_1_rech	sp_1_irch	sp_2_rech	sp_2_irch
1	1	0	30	1	0.01	1	0.01	1
2	2	0	30	2	0.01	1	0.01	1
3	3	0	30	3	0.01	1	0.01	1
4	4	0	30	4	0.01	1	0.01	1
5	5	0	30	5	0.01	1	0.01	1
6	6	0	30	6	0.01	1	0.01	1
7	7	0	30	7	0.01	1	0.01	1
8	8	0	30	8	0.01	1	0.01	1
9	9	0	30	9	0.01	1	0.01	1
10	10	0	30	10	0.01	1	0.01	1
11	11	0	30	11	0.01	1	0.01	1
12	12	0	30	12	0.01	1	0.01	1
13	13	0	30	13	0.01	1	0.01	1
14	14	0	30	14	0.01	1	0.01	1
15	15	0	30	15	0.01	1	0.01	1

Note: *sp_n_rech* values must be expressed in model units.

Note: *sp_n_rech* is actually a specified rate, rather than a flux. This is because this Package is usually used to simulate rainfall infiltration and rainfall is expressed as a rate [L/T]. Such specified rate will then be 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.

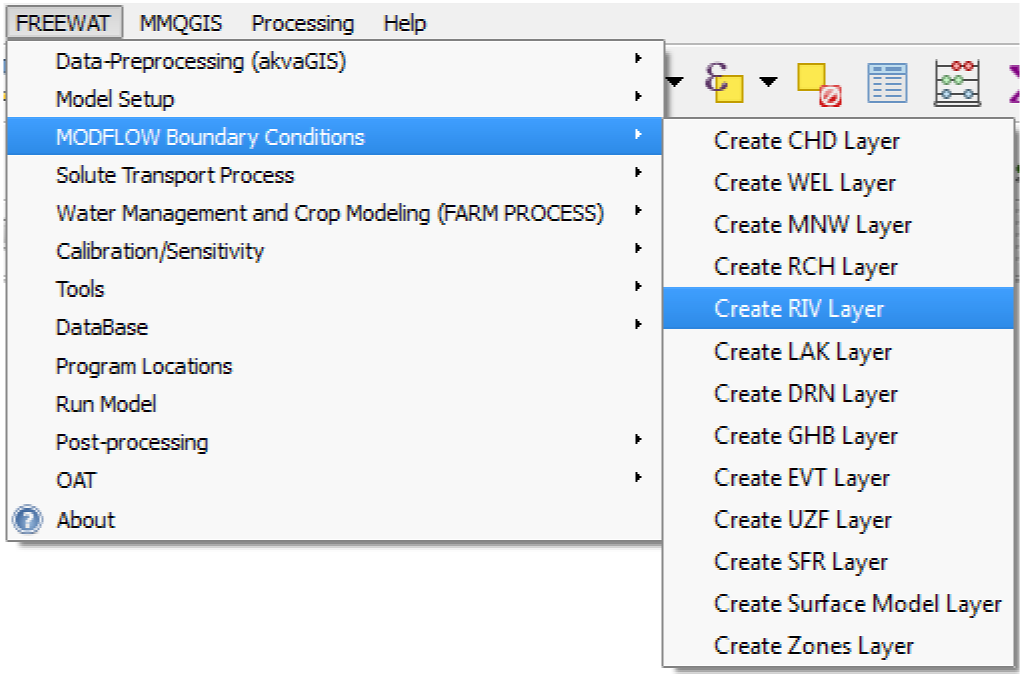
River - RIV (head-dependent flux)

The *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 has been loaded in the Layers Panel, to activate the *RIV Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create RIV Layer



In the **Create a layer for RIV package** window, 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.

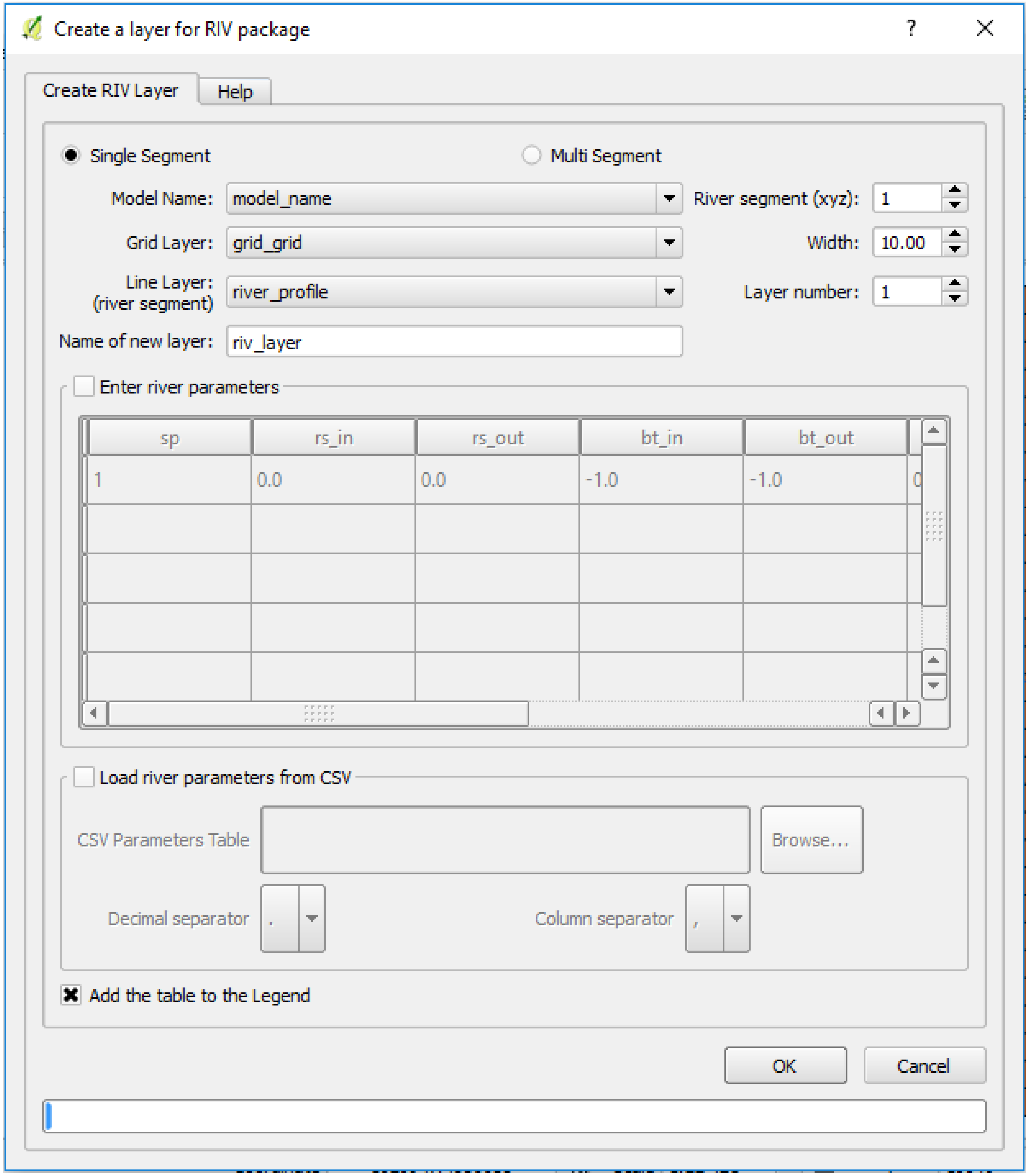
Note: The option *Single Segment* allows the User to assign river properties (i.e., river stage, river width, river bed bottom and thickness, hydraulic conductivity of the river bed sediments), as required in the *MODFLOW RIV Package*. On the contrary, the option *Multi Segment* allows to define only at which grid cells the river is located and the required properties must be assigned by the User at each cell once the riv MDO has been successfully created.

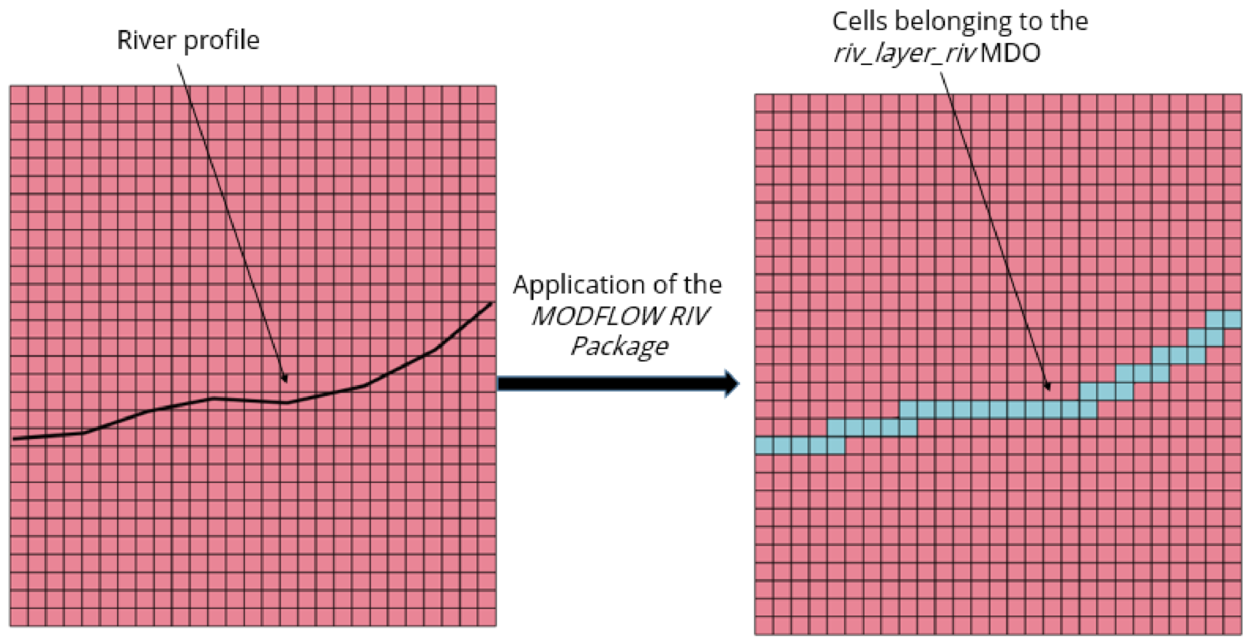
Anyway, the option *Single Segment* may still be applied, even if the river develops over more than one segment. In this case, the multi-line shapefile must be splitted into several single segments and the User should avoid editing the downstream vertex of a segment and the upstream one of the following segment in the same grid cell. These single segments 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;

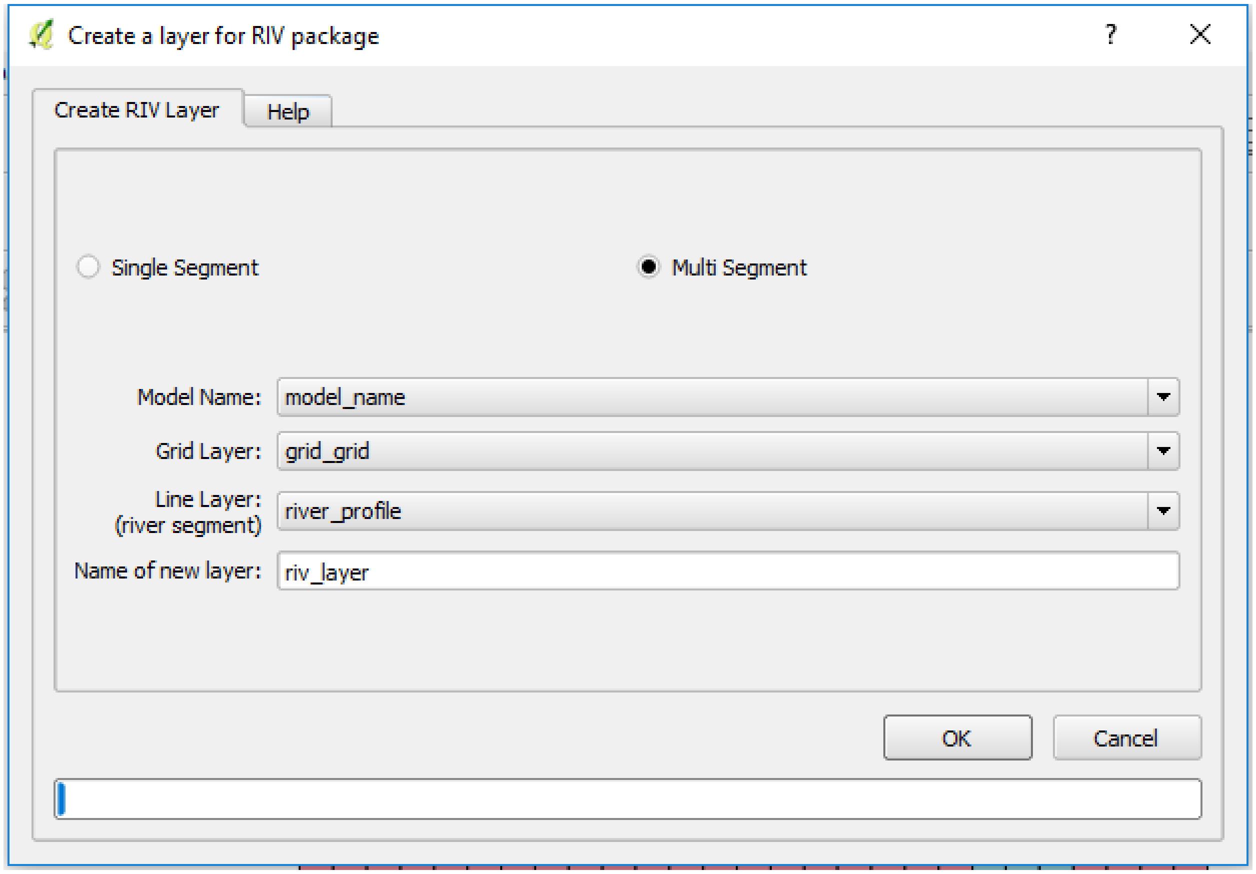
- *Layer number*: number of the model layer to which the river is in contact;
- if *Enter river parameters* is checked, the User can fill manually the table with all the necessary parameters to be assigned to grid cells where the river is located;
- if *Load river parameters from CSV* is checked, the 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 through the csv file will be loaded in the Layers Panel and stored in the model DB.

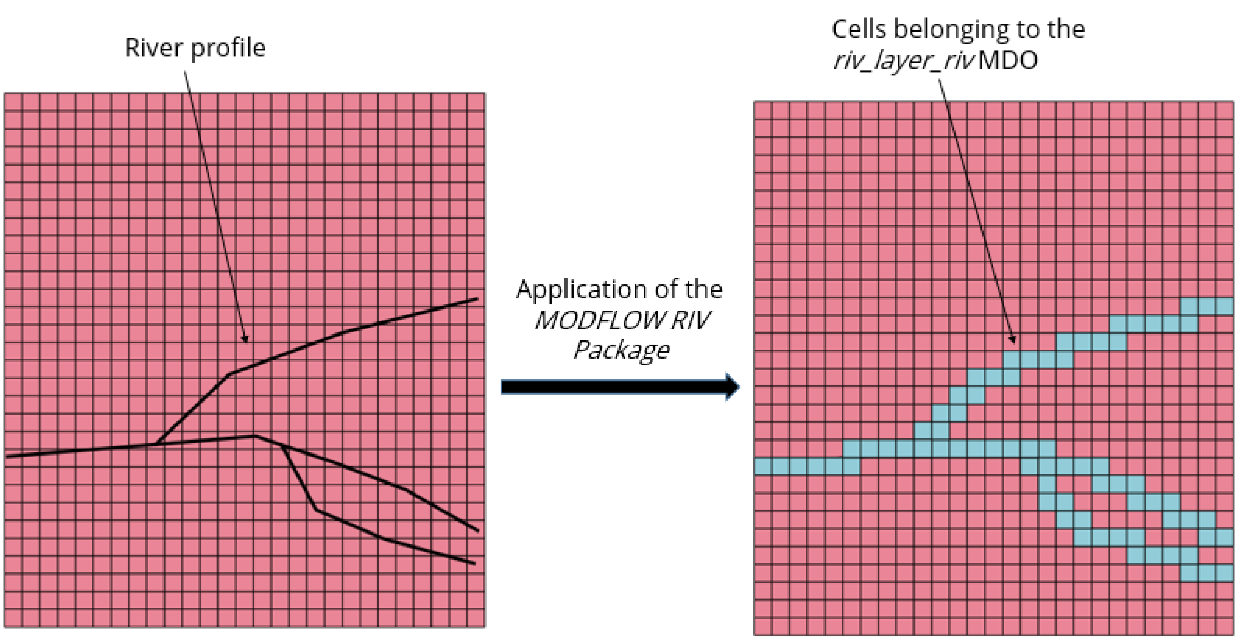

Create a layer for RIV package
Create RIV Layer
Help
Single Segment
Multi Segment
Model Name:
model_name
River segment (xyz):
1
Grid Layer:
grid_grid
Width:
10.00
Line Layer:
(river segment)
river_profile
Layer number:
1
Name of new layer:
riv_layer
Enter river parameters
sp
rs_in
rs_out
bt_in
bt_out
1
0.0
0.0
-1.0
-1.0
Load river parameters from CSV
CSV Parameters Table
Browse...
Decimal separator
Column separator
Add the table to the Legend
OK
Cancel



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.





Note: Parameters required when creating the riv MDO with the *Single Segment* option 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], with respect to a reference datum, at the upstream cell of the river segment;
- *rs_out*: river stage [L], with respect to a reference datum, at the downstream cell of the river segment;
- *bt_in*: height [L], with respect to a reference datum, of the river bed bottom at the upstream cell of the river segment;
- *bt_out*: height [L], with respect to a reference datum, 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.

River properties are assigned at the upstream and downstream cells of the river segment. Linear interpolation is automatically performed at the remaining cells.

If used, the csv file must have the following scheme (the template file *river_parameters.csv* is provided within the *FREEWAT* plugin folder `freewat\csv_templates\river`):

river_parameters.csv

```
SP,RS_I,RS_E,BT_IN,BT_OUT,HC_IN,HC_OUT,THICK_IN,THICK_OUT
1,0.00,0.00,-5.00,-5.00,1e-6,1e-6,1.50,1.50
2,0.00,0.00,-5.00,-5.00,1e-6,1e-6,1.50,1.50
3,0.00,0.00,-5.00,-5.00,1e-6,1e-6,1.50,1.50
```

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

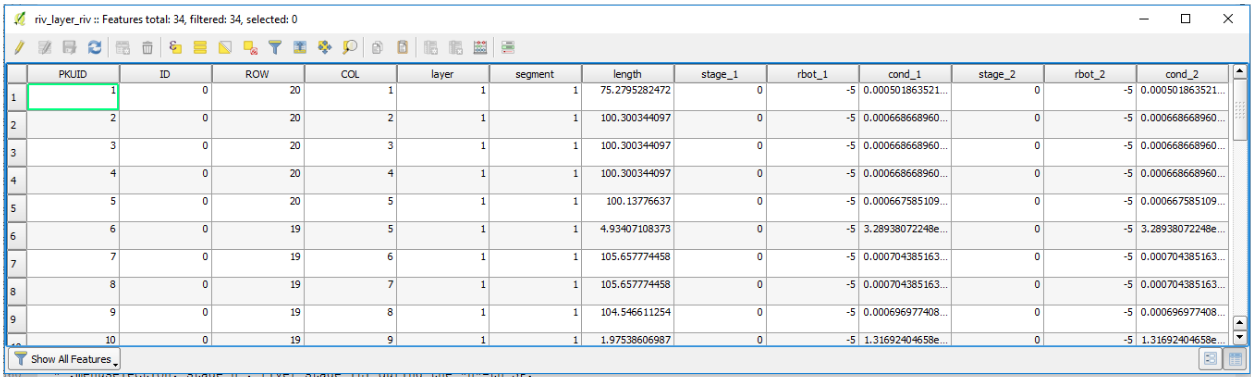
Note: The extension *_riv* must not be changed in the Layers Panel and neither in the DB, as the riv MDO will be filtered in the **Run Model** window according to such extension.

The Attribute Table of such MDO contains several records, according to the number of grid cells where this Package is applied, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row index of a grid cell;
- *COL*: column index of a grid cell;
- *layer*: number of the model layer to which the river is in contact;
- *segment* (if the *Single Segment* option has been used) or *xyz* (if the *Multi Segment* option has been used): 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], with respect to a reference datum, during the *n*-th SP;
  - *rbot_n*: height [L], with respect to a reference datum, of the river bottom during the *n*-th SP;
  - *cond_n*: conductance of the rever bed sediments $[L^2/T]$ during the *n*-th SP.

The values of *length* within each grid cell are automatically calculated according to the portion of the river segment which intersects a grid cell.

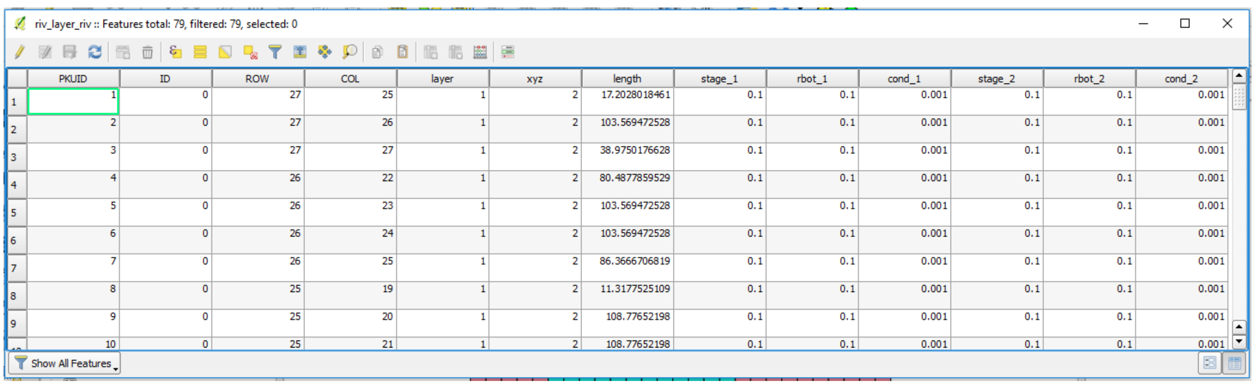
If the *Single Segment* option has been used, the fields *layer*, *segment*, *stage_n* and *rbot_n* are filled with values assigned by the User (manually or through the csv file) when the *riv_layer_riv* MDO is created. Furthermore, *cond_n* is automatically calculated depending on the river bed geometry and its hydraulic conductivity, as defined by the User (manually or through the csv file; for details the reader is referred to the *MODFLOW-2005* User manual; Harbaugh, 2005).


riv_layer_riv :: Features total: 34, filtered: 34, selected: 0

	PKUID	ID	ROW	COL	layer	segment	length	stage_1	rbot_1	cond_1	stage_2	rbot_2	cond_2
1	1	0	20	1	1	1	75.2795282472	0	-5	0.000501863521...	0	-5	0.000501863521...
2	2	0	20	2	1	1	100.300344097	0	-5	0.000668668960...	0	-5	0.000668668960...
3	3	0	20	3	1	1	100.300344097	0	-5	0.000668668960...	0	-5	0.000668668960...
4	4	0	20	4	1	1	100.300344097	0	-5	0.000668668960...	0	-5	0.000668668960...
5	5	0	20	5	1	1	100.13776637	0	-5	0.000667585109...	0	-5	0.000667585109...
6	6	0	19	5	1	1	4.93407108373	0	-5	3.28938072248e...	0	-5	3.28938072248e...
7	7	0	19	6	1	1	105.657774458	0	-5	0.000704385163...	0	-5	0.000704385163...
8	8	0	19	7	1	1	105.657774458	0	-5	0.000704385163...	0	-5	0.000704385163...
9	9	0	19	8	1	1	104.546611254	0	-5	0.000696977408...	0	-5	0.000696977408...
	10	0	19	9	1	1	1.97538606987	0	-5	1.31692404658e...	0	-5	1.31692404658e...

Show All Features

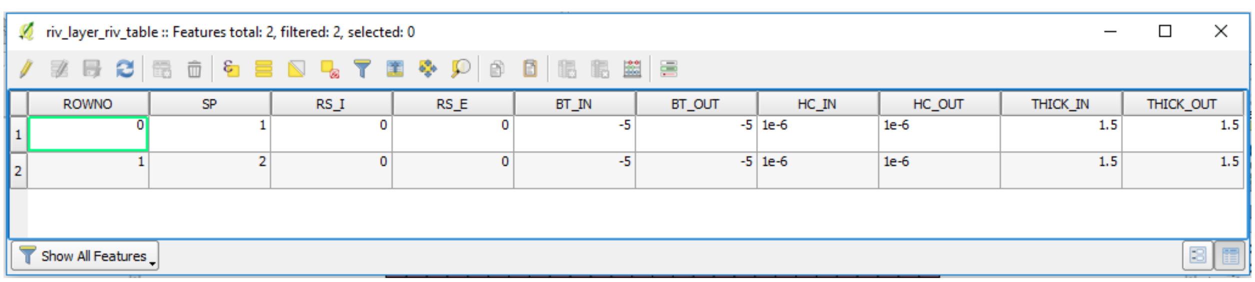
If the *Multi Segment* option has been used, the fields *layer*, *stage_n*, *rbot_n* and *cond_n* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5. Furthermore, the field *xyz* is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.


riv_layer_riv :: Features total: 79, filtered: 79, selected: 0

	PKUID	ID	ROW	COL	layer	xyz	length	stage_1	rbot_1	cond_1	stage_2	rbot_2	cond_2
1	1	0	27	25	1	2	17.2028018461	0.1	0.1	0.001	0.1	0.1	0.001
2	2	0	27	26	1	2	103.569472528	0.1	0.1	0.001	0.1	0.1	0.001
3	3	0	27	27	1	2	38.9750176628	0.1	0.1	0.001	0.1	0.1	0.001
4	4	0	26	22	1	2	80.4877859529	0.1	0.1	0.001	0.1	0.1	0.001
5	5	0	26	23	1	2	103.569472528	0.1	0.1	0.001	0.1	0.1	0.001
6	6	0	26	24	1	2	103.569472528	0.1	0.1	0.001	0.1	0.1	0.001
7	7	0	26	25	1	2	86.3666706819	0.1	0.1	0.001	0.1	0.1	0.001
8	8	0	25	19	1	2	11.3177525109	0.1	0.1	0.001	0.1	0.1	0.001
9	9	0	25	20	1	2	108.77652198	0.1	0.1	0.001	0.1	0.1	0.001
	10	0	25	21	1	2	108.77652198	0.1	0.1	0.001	0.1	0.1	0.001

Show All Features

A table renamed *riv_layer_riv_table* is created with the riv MDO, stored in the model DB and eventually loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters defined in the csv file.


riv_layer_riv_table :: Features total: 2, filtered: 2, selected: 0

	ROWNO	SP	RS_I	RS_E	BT_IN	BT_OUT	HC_IN	HC_OUT	THICK_IN	THICK_OUT
1	0	1	0	0	-5	-5	1e-6	1e-6	1.5	1.5
2	1	2	0	0	-5	-5	1e-6	1e-6	1.5	1.5

Show All Features

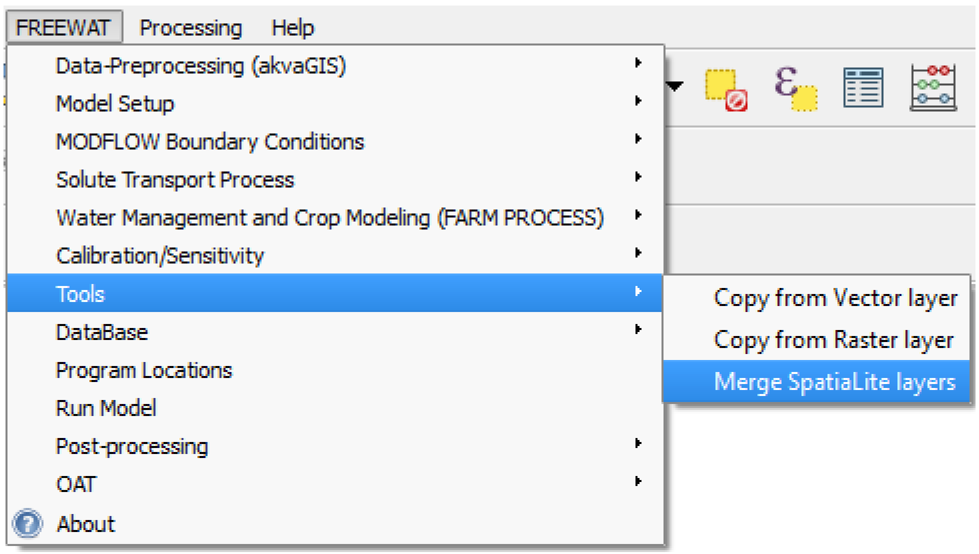
Note: If the river develops over more than one segment, the *Single Segment* option can be used for each segment. This requires editing as many line shapefiles as many river segments. In this case, the User should avoid editing the downstream vertex of a segment and the upstream one of the following segment in the same grid cell.

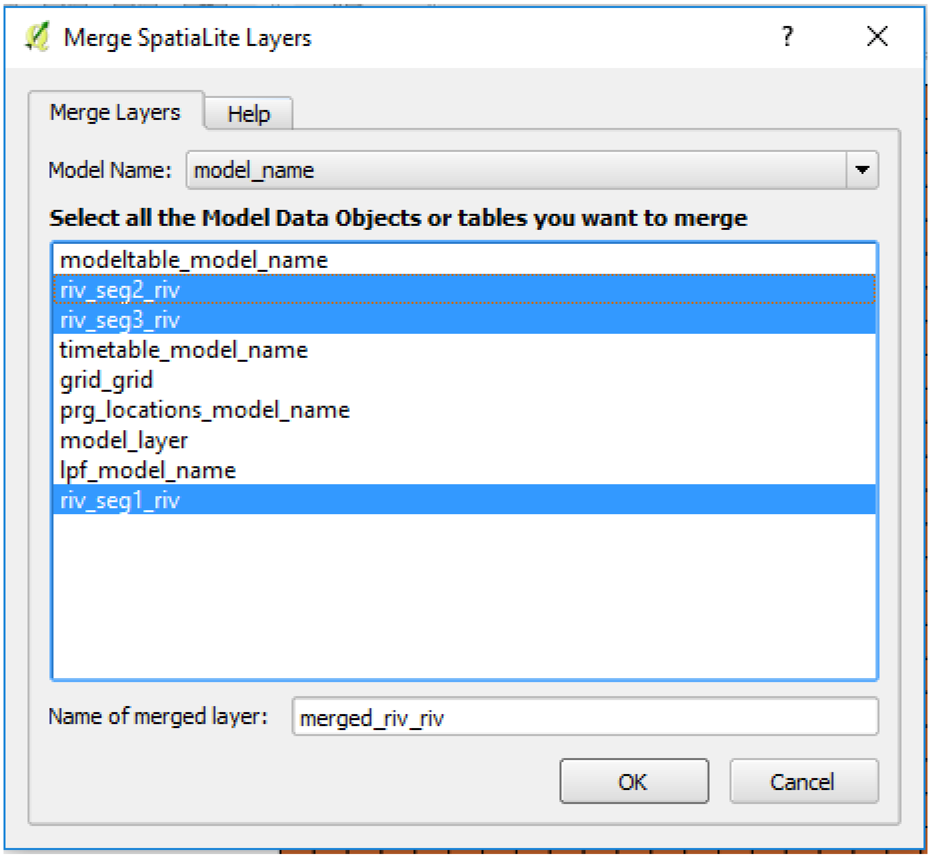
Furthermore, the User must pay attention to the following. In the **Create a layer for RIV package** window:

- different names must be assigned in the *Name of new layer* field;
- the correct line shapefile must be selected in the *Line Layer (river segment)* field;
- progressive segment numbers must be used 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 in the **Run Model** window.

The following figures refer to an application of the *Merge SpatiaLite layers* tool for two riv MDOs. In the **Merge Layers** window, the User must simply select the MDOs which have to be merged and a new name (with the *_riv* extension) must be assigned 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.





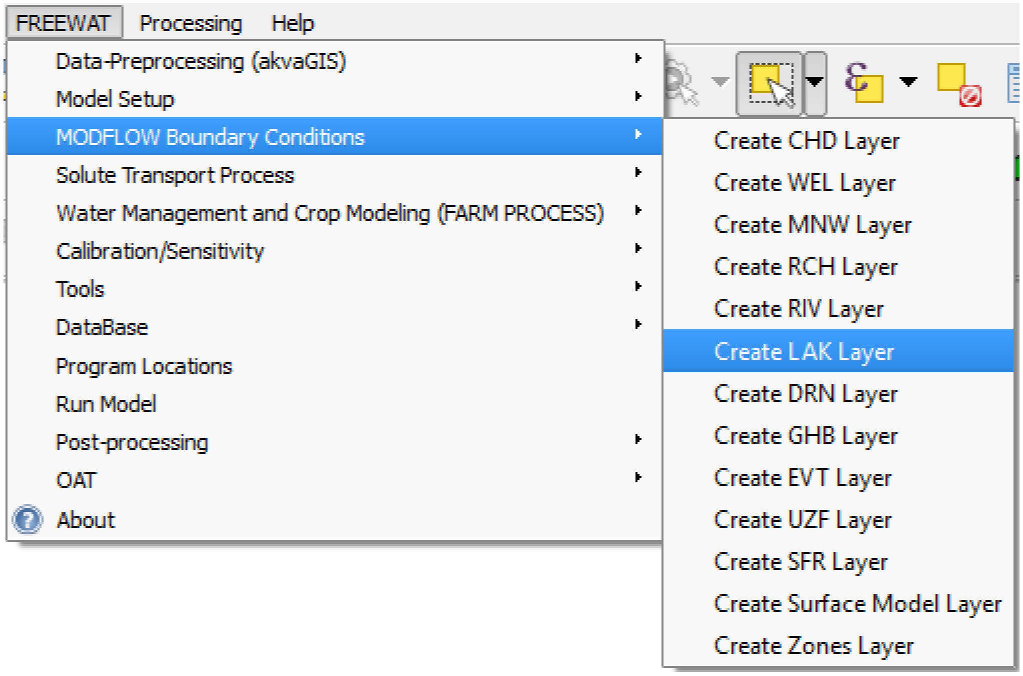
Note: When two or more MDOs are merged, the User must not forget to assign the proper extension (e.g., *_riv*, *_chd*, *_wel*, etc.) to the merged MDO.

Lake - LAK (head-dependent flux)

The *MODFLOW LAK Package* allows to simulate lake/aquifer seepage, depending on the head gradient between the lake and the groundwater system.

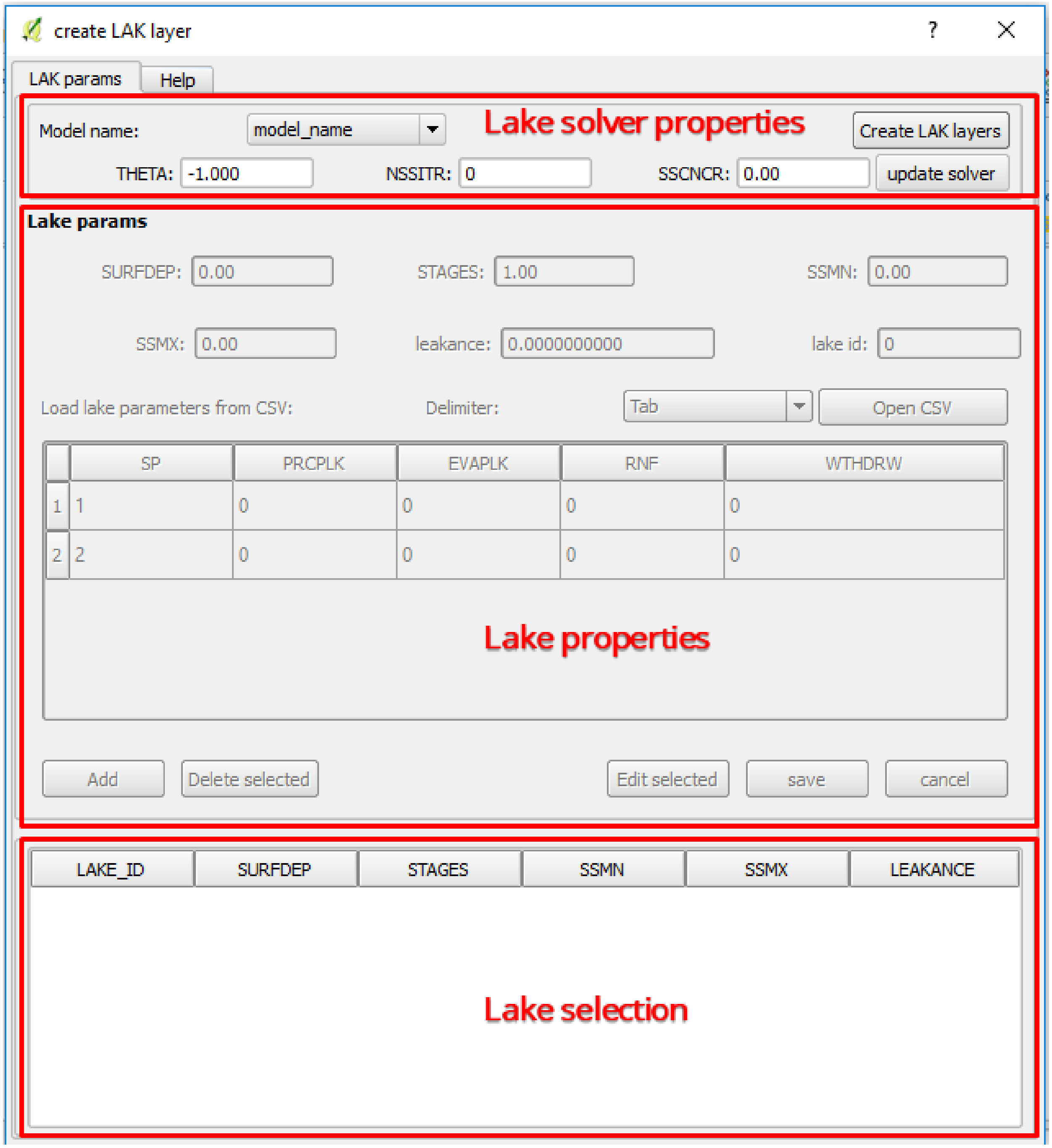
To activate the *LAK Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create LAK Layer



The **Create Lak Layer** window is composed by 3 sections:

- the *Lake solver properties* section contains options for the solver of the lake budget;
- the *Lake properties* section allows to input specific properties for each lake;
- the *Lake selection* section contains a summary for the created lakes.

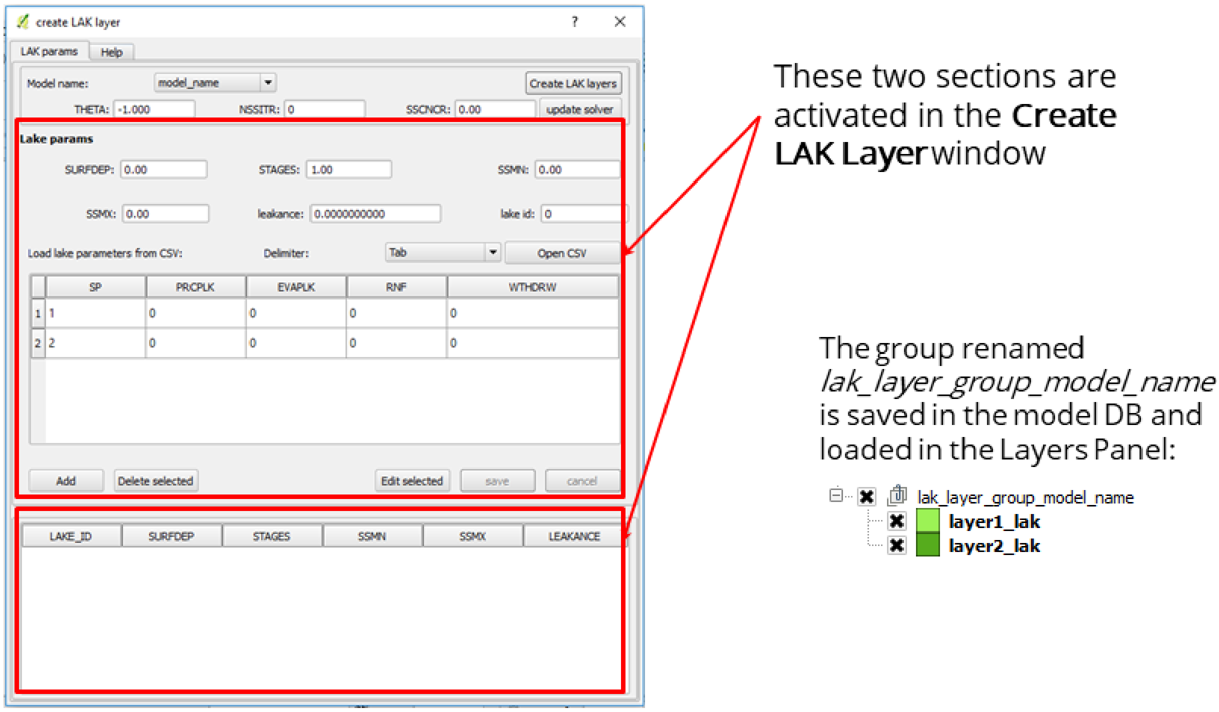


The following data are required in the *Lake solver properties* section:

- *Model Name*: name of the hydrological model;
- *THETA*: integer value which determines whether the equation for lake stage is solved implicitly (*THETA=1*), semi-implicity (*0<THETA<1*) or explicitly (*THETA=0*);
- *NSSITR*: maximum number of iterations for Newton's method of solution for equilibrium lake stages in each *MODFLOW* iteration for steady-state aquifer head solution;
- *SSCNCR*: convergence criterion for equilibrium lake stage solution by Newton's method.

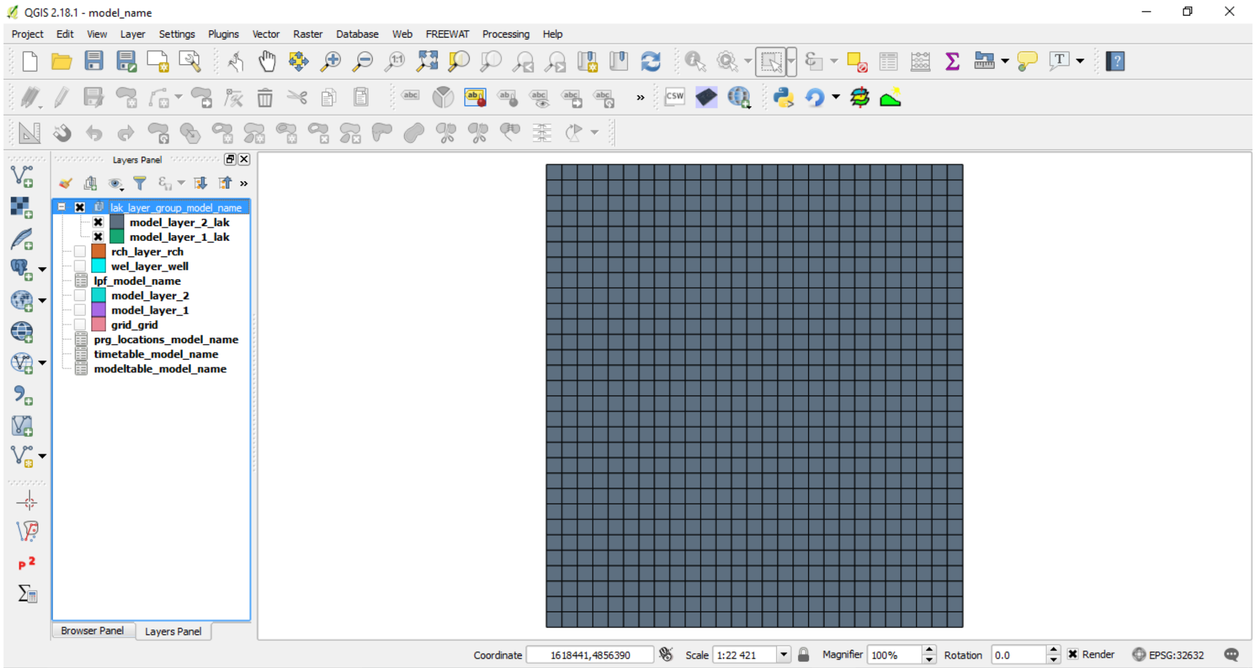
Note: A negative *THETA* value is used as a flag for additional options in the *LAK Package* for transient calculations. *MODFLOW* will automatically convert it to a positive value for calculations of the lake stage (for details the reader is referred to the *LAK* User manual; Merritt and Konikow, 2000).

Once the *Lake solver properties* have been set, pressing the *Create LAK layers* button will activate the *Lake properties* and the *Lake selection* sections in the **Create Lak Layer** window and will create a new MDO group in the Layers Panel, renamed *lak_layer_group_model_name*.



The *lak_layer_group_model_name* group loaded in the Layers Panel contains one lak MDO for each model layer.

The lak MDOs are also stored in the model DB and they will be used to define the location of lakes.

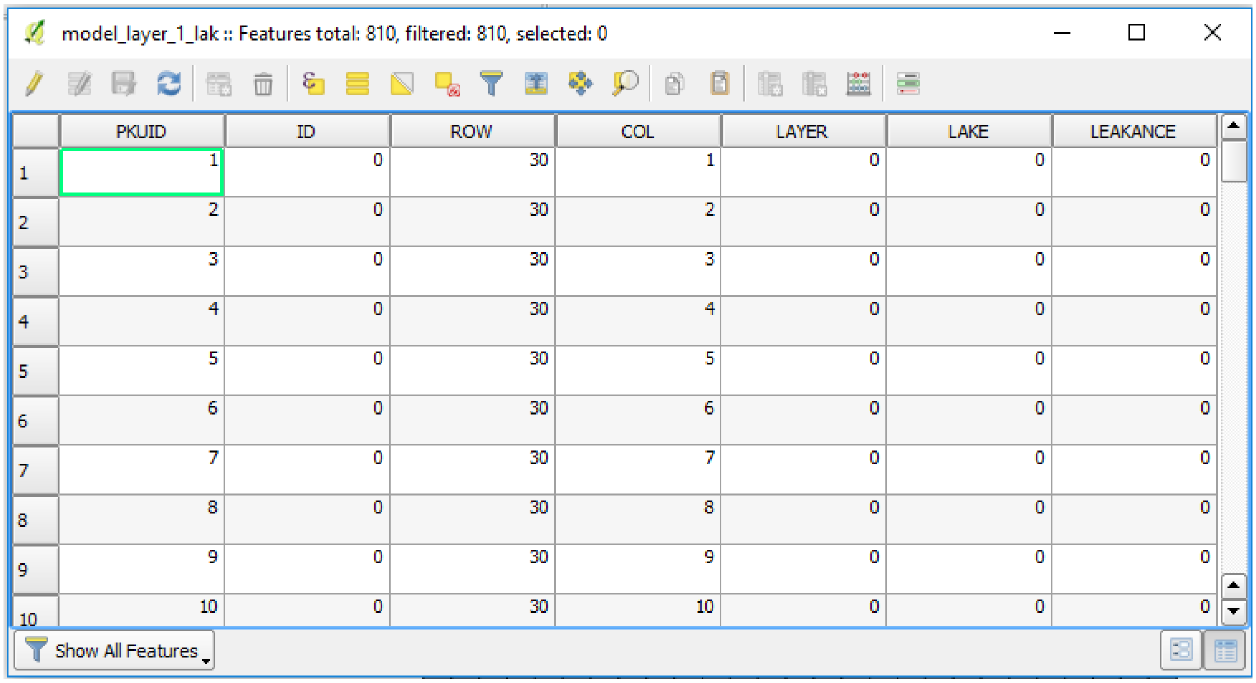


Once the lak MDOs have been created, the *update solver* button in the **Create Lak Layer** window can be used to update the lake budget solver criteria.

Note: The name of the *lak_layer_group_model_name* group, and the extension *_lak* of each lak MDO, must not be changed in the Layers Panel and neither in the DB, as they will be filtered in the **Run Model** window according to such name and extension.

The Attribute Table of each lak MDO contains 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 index of a grid cell;
- *COL*: column index of a grid cell;
- *LAYER*: number of the model layer which the lak MDO represents;
- *LAKE*: lake ID to identify which lake is located at a certain grid cell;
- *LEAKANCE*: leakance term at a certain grid cell.

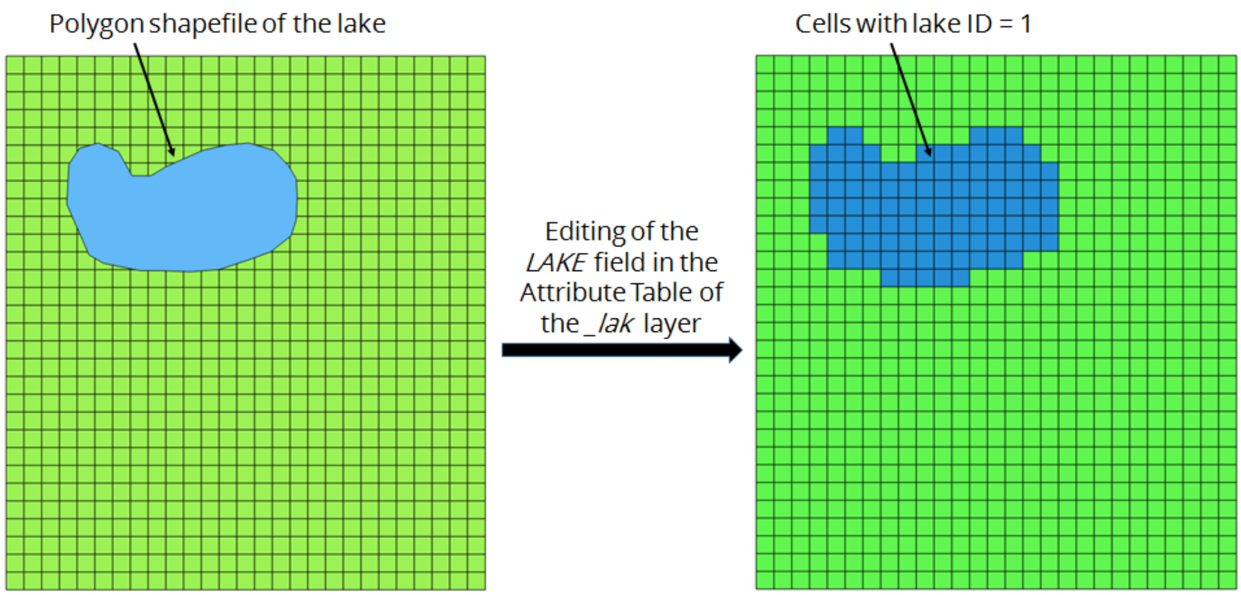


model_layer_1_lak :: Features total: 810, filtered: 810, selected: 0

	PKUID	ID	ROW	COL	LAYER	LAKE	LEAKANCE
1	1	0	30	1	0	0	0
2	2	0	30	2	0	0	0
3	3	0	30	3	0	0	0
4	4	0	30	4	0	0	0
5	5	0	30	5	0	0	0
6	6	0	30	6	0	0	0
7	7	0	30	7	0	0	0
8	8	0	30	8	0	0	0
9	9	0	30	9	0	0	0
10	10	0	30	10	0	0	0

Show All Features

To specify the location of a lake within the study area, the *LAKE* field must be edited using a non-null, integer value.



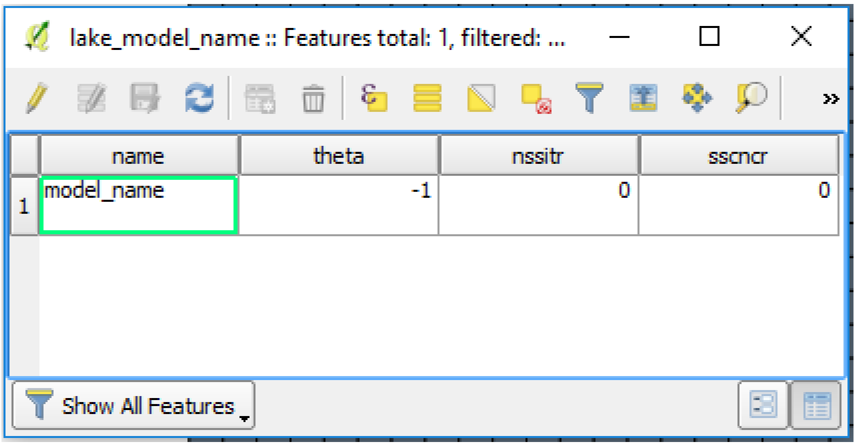
Note: The *MODFLOW LAK Package* calculates a separate water budget for those cells where a non-null value is set for *LAKE*, removing them from the solution of the groundwater equation and setting them as inactive. As such, any cell in which a lake is located must be set to inactive, by editing the *ACTIVE* field (*ACTIVE = 0*) in the Attribute Table of the model layer to which that lake is in contact.

Any model layer hydraulically connected to one or more lakes must also be set to *convertible* in the *lpf_model_name* table and the *laywet* option must be active (*laywet=Yes*).

The following tables are further created in the model DB, along with the lak MDOs:

- *lak_model_name* (at this stage, it is empty and will be filled with some lake properties);

- *lake_model_name*, containing information about the *THETA*, *NSSITR* and *SSCNCR* values just set (see figure below);
- *laksp_model_name* (at this stage, it is empty and will be filled with some lake properties).



Note: By default, the three tables listed above are not loaded in the Layers Panel, but they can be added to the Layers Panel using the *QGIS* Database Manager plugin.

Note: If the *update solver* button in the **Create Lak Layer** window is used later to update the lake budget solver criteria, the corresponding fields in the *lake_model_name* table are automatically updated.

Once the lak MDOs have been created, the *Lake properties* can be assigned to each lake individually through the **Create LAK Layers** window, which must be open again.

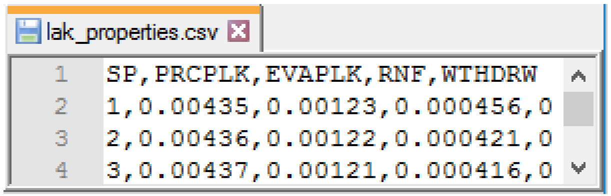
The following data are required in the *Lake properties* section:

- *SURFDEP*: lake bottom elevation undulations. It 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 for each lake at the beginning of the iteration procedure;
- *SSMN*: minimum lake stage for steady-state simulations;
- *SSMX*: maximum lake stage for steady-state simulations;
- *leakance*: leakance term representing the lake bed sediments. This value is assumed to represent the combined leakances of the lake bed material and the aquifer material between the lake and the centers of the underlying grid cells;
- *lake id*: lake identifier. It must be unique for each lake that is to be simulated and it must have a non-null, integer value;
- the following fields must be filled for each lake and for each SP:
  - *PRCPLK*: precipitation flux at the lake surface [L/T];
  - *EVAPLK*: evaporation from the lake surface flux [L/T];
  - *RNF*: surface runoff $[L^3/T]$;
  - *WTHDRW*: direct withdrawal from the lake surface $[L^3/T]$.

The fields *SURFDEP*, *STAGES*, *SSMN*, *SSMX* and *LEAKANCE* are time-constant properties.

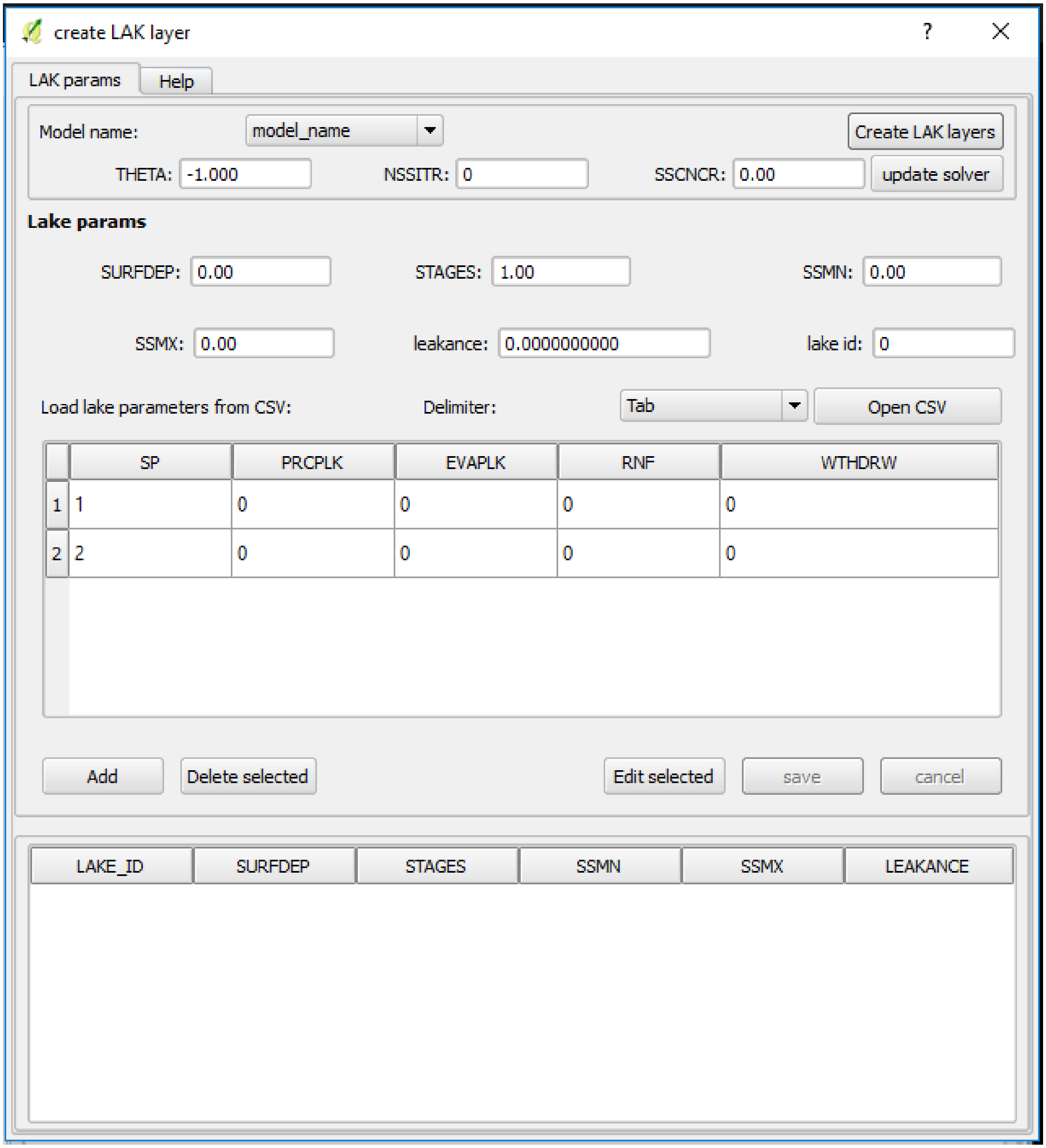
On the other hand, the fields *PRCPLK*, *EVAPLK*, *RNF* and *WTHDRW* must be filled for each SP. This can be done manually or loading a csv file through the *Open CSV* button. It such case, the User must define the *Delimiter* used in the csv file loaded.

Note: If used, the csv file must have the following scheme (the template file *lak_properties.csv* is provided within the *FREEWAT* plugin folder `freewat\csv_templates\lake`):


lak_properties.csv

```
SP,PRCPLK,EVAPLK,RNF,WTHDRW
1,0.00435,0.00123,0.000456,0
2,0.00436,0.00122,0.000421,0
3,0.00437,0.00121,0.000416,0
```

Once the fields *SURFDEP*, *STAGES*, *SSMN*, *SSMX* and *LEAKANCE* have been filled out manually for **one** lake, pressing the *Add* button allows to add such properties for that lake (identified through a unique non-null ID) to the *Lake selection* frame, which displays a summary of the time-constant properties.

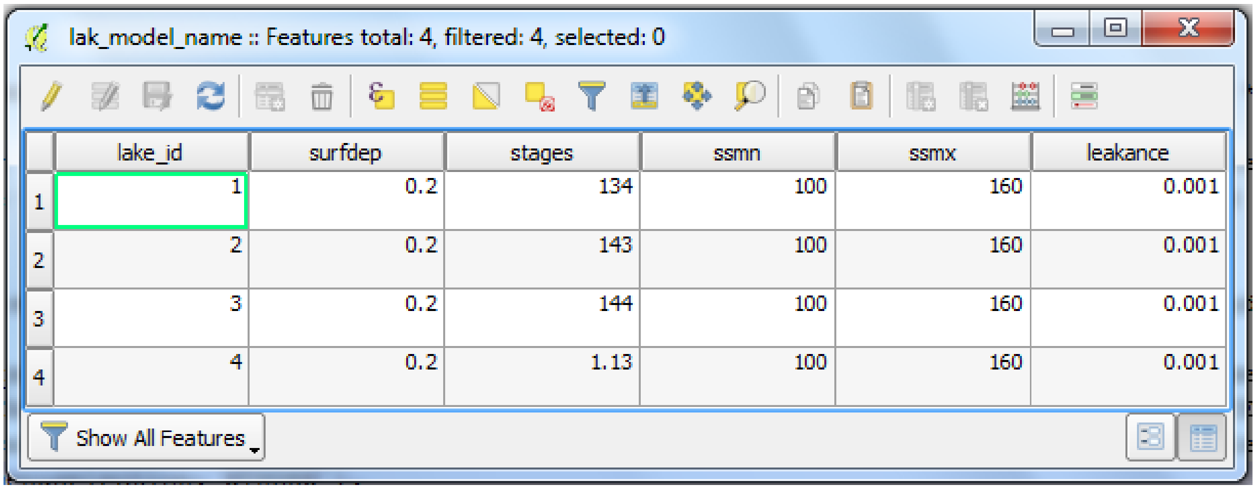


Once one or more rows have been added to the *Lake selection* frame, they can be deleted by selecting the corresponding row in the *Lake selection* frame and using the *Delete selected* button.

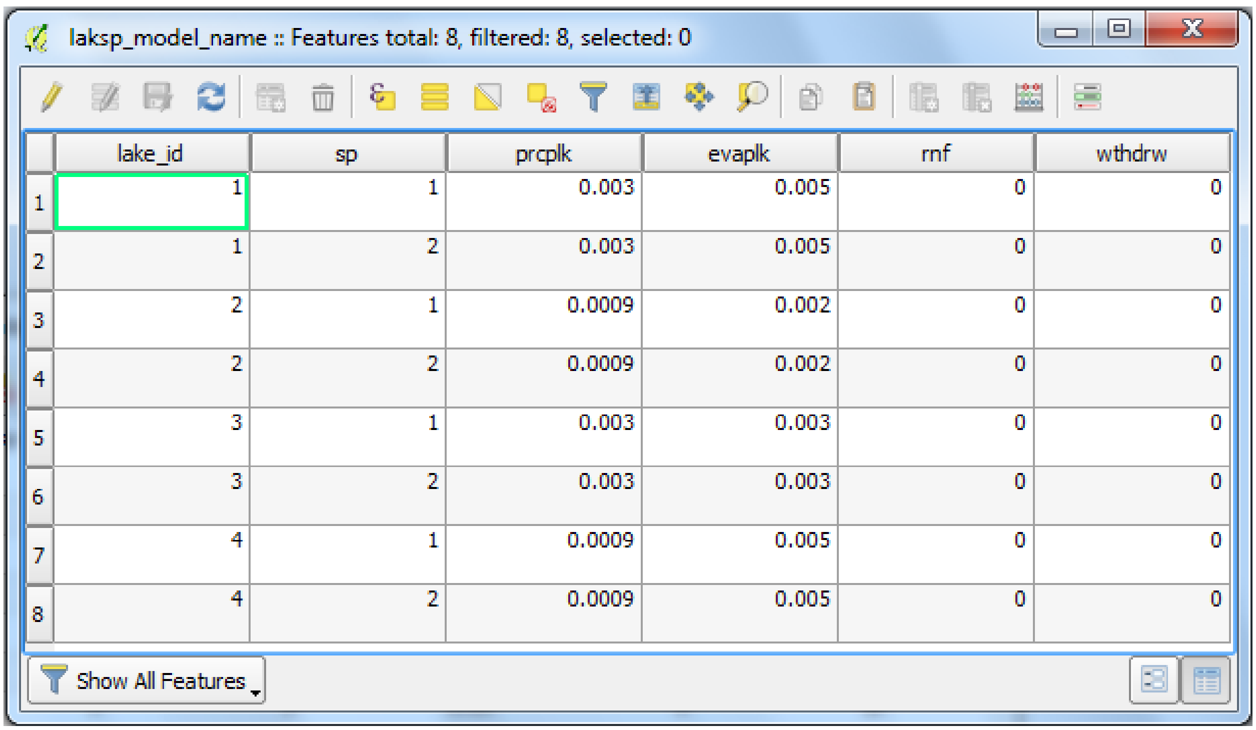
Lakes properties can be edited as well, by selecting the corresponding row in the *Lake selection* frame and using the *Edit selected* button. This will re-load the properties of the selected lake into the *Lake properties* frame. Any change can be applied using the *save* button, or discarded using the *cancel* button.

Note: During the editing, the *Add* and *Delete selected* buttons are locked. To use these funtions, the editing must be concluded, by saving or cancelling.

Once the lakes properties have been input, the *lak_model_name* table will be automatically updated with values assigned to the time-constant properties (fields *SURFDEP*, *STAGES*, *SSMN*, *SSMX* and *LEAKANCE* for each *lake id*), while the *laksp_model_name* table will be automatically updated with values assigned to time-dependant properties (fields *PRCPLK*, *EVAPLK*, *RNF* and *WTHDRW*).



	lake_id	surfdep	stages	ssmn	ssmx	leakance
1	1	0.2	134	100	160	0.001
2	2	0.2	143	100	160	0.001
3	3	0.2	144	100	160	0.001
4	4	0.2	1.13	100	160	0.001



	lake_id	sp	prcplk	evaplk	rnf	wthdrw
1	1	1	0.003	0.005	0	0
2	1	2	0.003	0.005	0	0
3	2	1	0.0009	0.002	0	0
4	2	2	0.0009	0.002	0	0
5	3	1	0.003	0.003	0	0
6	3	2	0.003	0.003	0	0
7	4	1	0.0009	0.005	0	0
8	4	2	0.0009	0.005	0	0

Limitations

The *MODFLOW 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 the reader is referred to the *LAK* User manual; Merrit and Konikow, 2000):

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

- *MOC3D* for solute concentrations in lakes is not implemented in the present version of the *FREEWAT* plugin, but it will be replaced by *MT3DMS*.

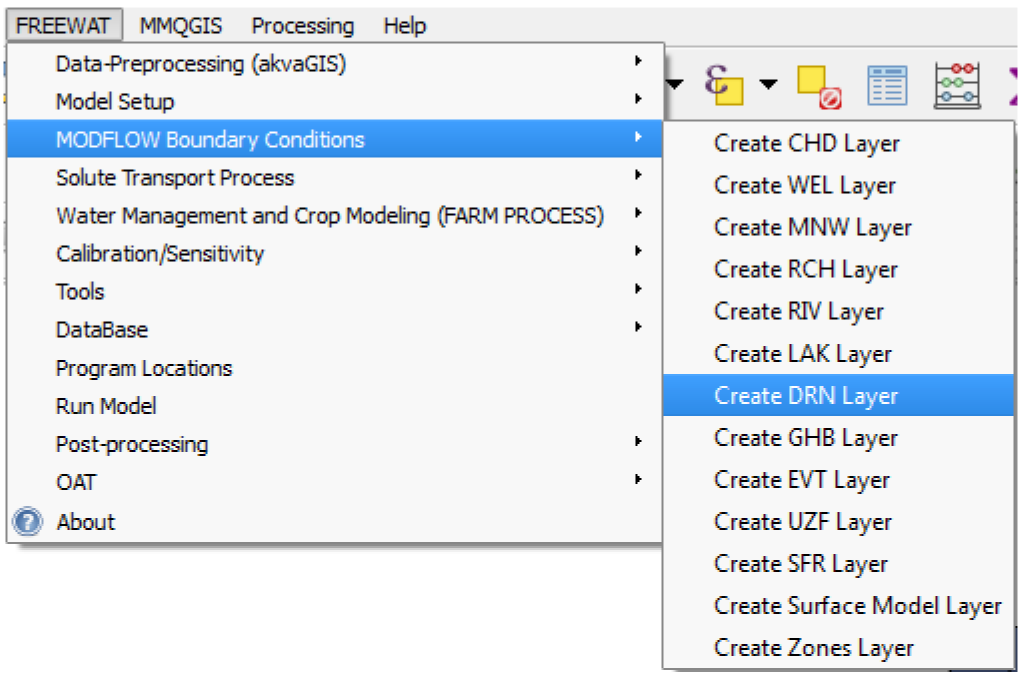
Drain - DRN (head-dependent flux)

The *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 has been loaded in the Layers Panel, to activate the *DRN Package* the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create DRN Layer



In the **Create a layer for DRN package** window, two alternative options are available:

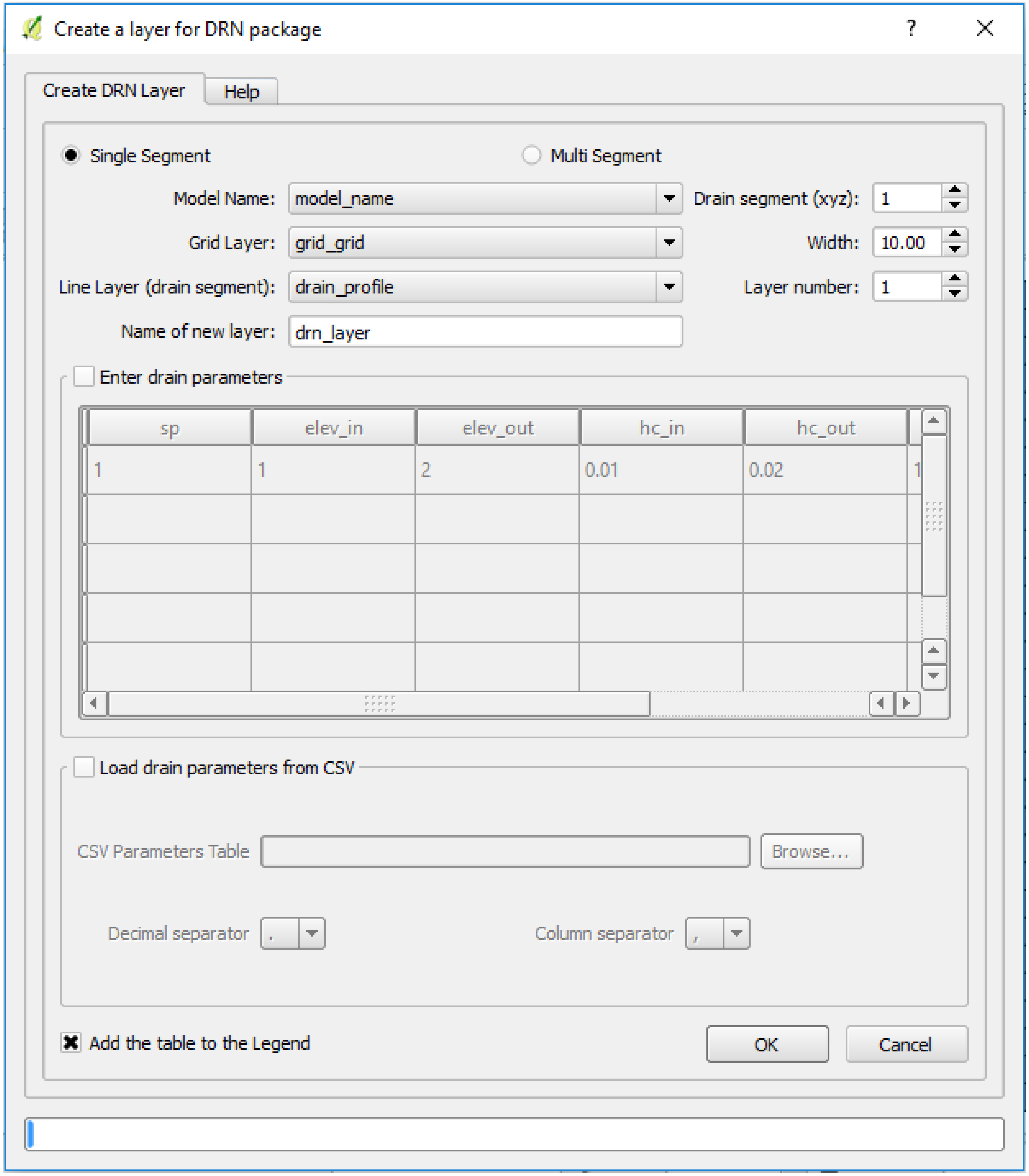
- *Single Segment*, if the drain profile develops over one single line;
- *Multi Segment*, if the drain profile develops over a multi-line.

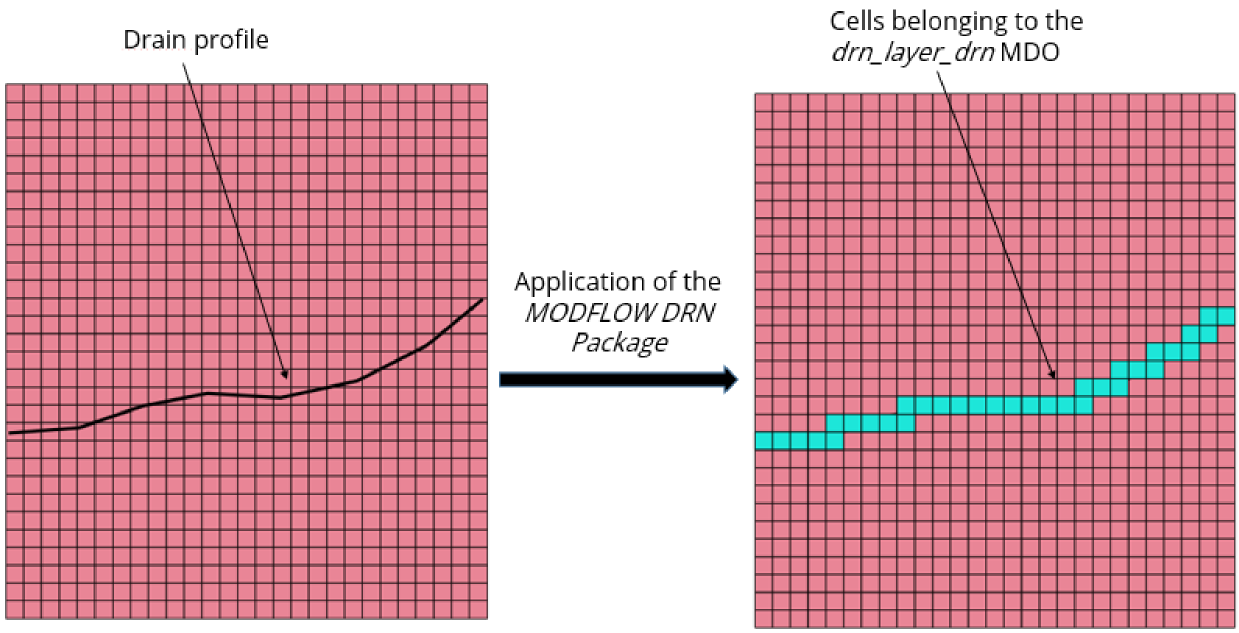
Note: The option *Single Segment* allows the User to assign drain properties (i.e., drain elevation, drain width, drain bed thickness, hydraulic conductivity of the drain bed sediments), as required in the *MODFLOW DRN Package*. On the contrary, the option *Multi Segment* allows to define only at which grid cells the drain is located and the required properties must be assigned by the User at each cell once the drn MDO has been successfully 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 and the User should avoid editing the downstream vertex of a segment and the upstream one of the following segment in the same grid cell. These single segments 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:

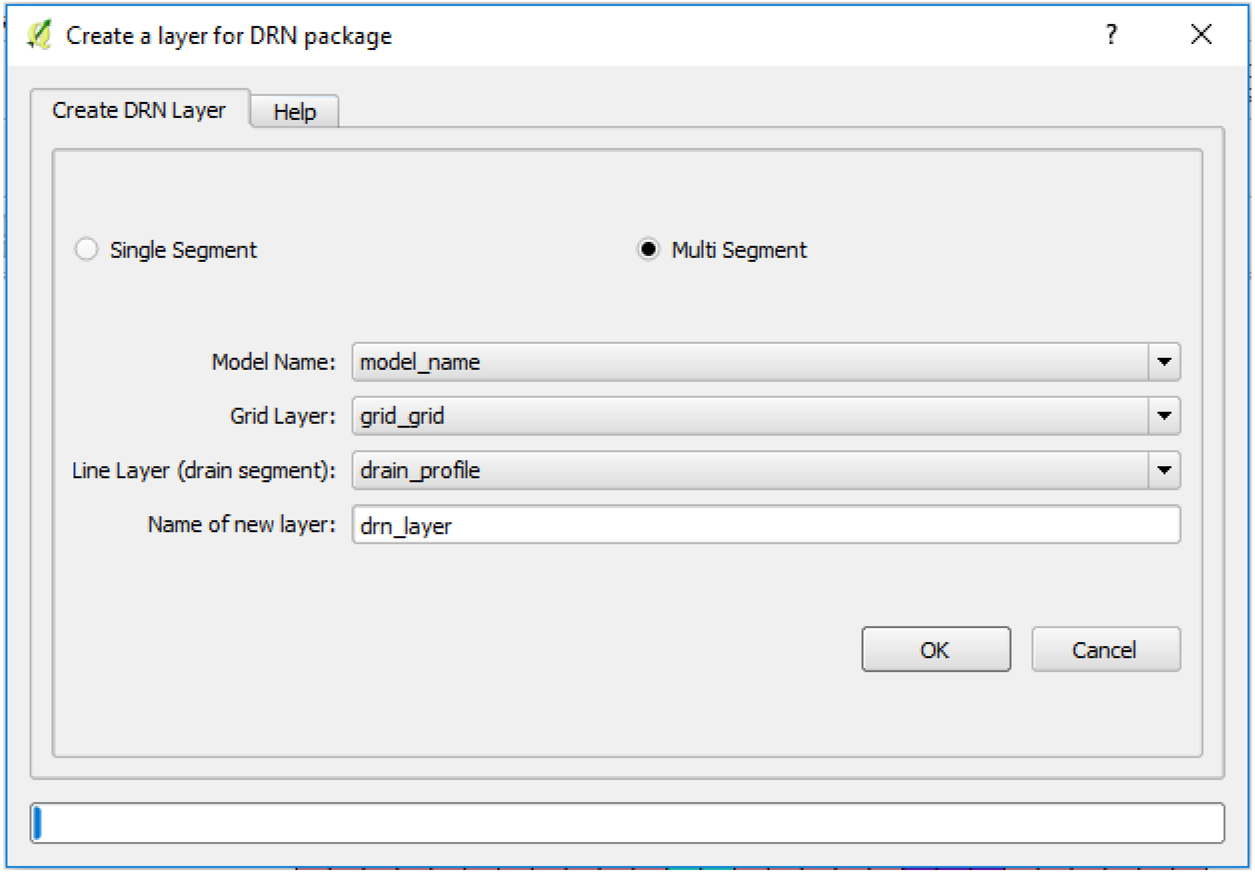
- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer (drain segment)*: line shapefile containing the profile of the single drain segment;
- *Name of new layer*: name of the drn MDO which has to be created;
- *Drain segment (xyz)*: number of the single drain segment;
- *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 through the csv file will be loaded in the Layers Panel and stored in the model DB.

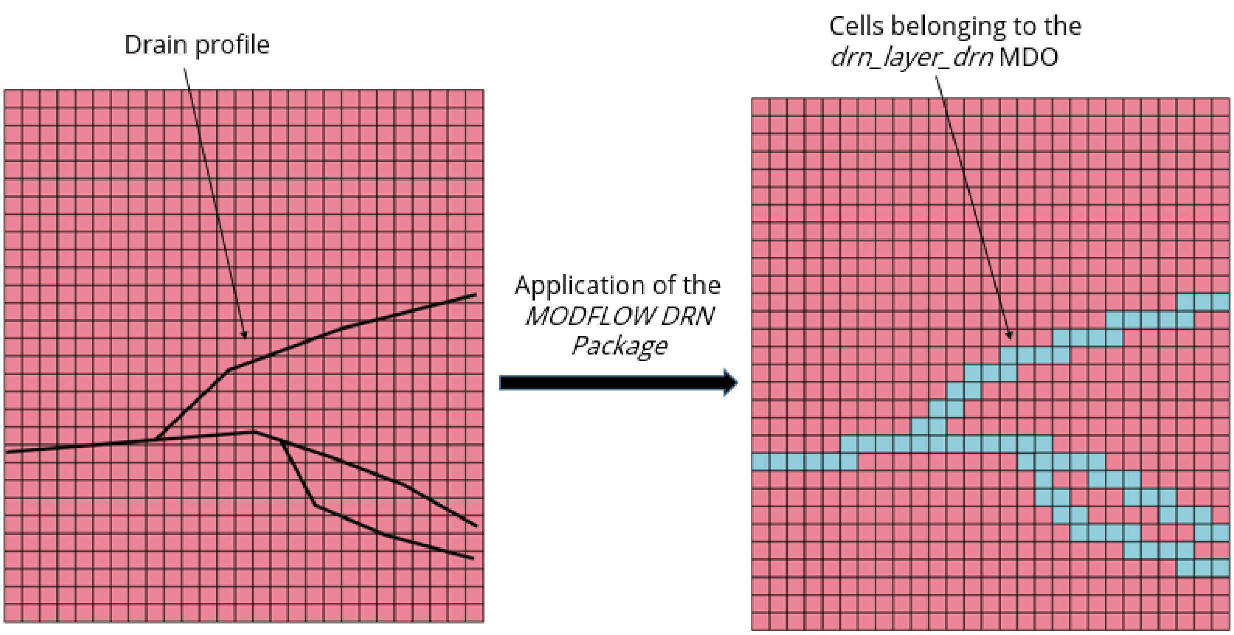

Create a layer for DRN package
Create DRN Layer
Help
Single Segment
Multi Segment
Model Name:
model_name
Drain segment (xyz):
1
Grid Layer:
grid_grid
Width:
10.00
Line Layer (drain segment):
drain_profile
Layer number:
1
Name of new layer:
drn_layer
Enter drain parameters
sp
elev_in
elev_out
hc_in
hc_out
1
1
2
0.01
0.02
Load drain parameters from CSV
CSV Parameters Table
Browse...
Decimal separator
Column separator
Add the table to the Legend
OK
Cancel



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.





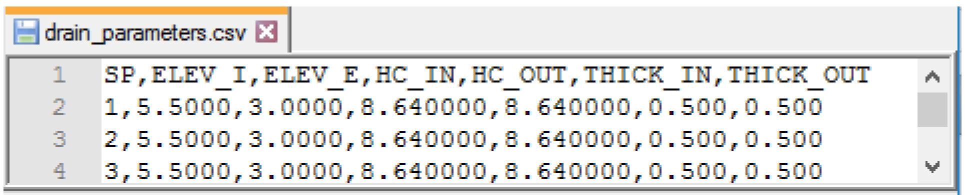
Note: Parameters required when creating the drn MDO with the *Single Segment* option are related to the geometry and hydraulic conductivity of the drain bed sediments and must be assigned at the upstream and downstream cells of the drain segment and for each SP:

- *sp*: SP number;

- *elev_in*: drain elevation [L], with respect to a reference datum, at the upstream cell of the drain segment;
- *elev_out*: drain elevation [L], with respect to a reference datum, 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.

Drain properties are assigned at the upstream and downstream cells of the drain segment. Linear interpolation is automatically performed at the remaining cells.

If used, the csv file must have the following scheme (the template file *drain_parameters.csv* is provided within the *FREEWAT* plugin folder `freewat\csv_templates\drain`):



drain_parameters.csv

```
SP,ELEV_I,ELEV_E,HC_IN,HC_OUT,THICK_IN,THICK_OUT
1,5.5000,3.0000,8.640000,8.640000,0.500,0.500
2,5.5000,3.0000,8.640000,8.640000,0.500,0.500
3,5.5000,3.0000,8.640000,8.640000,0.500,0.500
```

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

Note: The extension *_drn* must not be changed in the Layers Panel and neither in the DB, as the drn MDO will be filtered in the **Run Model** window according to such extension.

The Attribute Table of such MDO contains several records, according to the number of grid cells where this Package is applied, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row index of a grid cell;
- *COL*: column index of a grid cell;
- *layer*: number of the model layer to which the drain is in contact;
- *segment* (if the *Single Segment* option has been used) or *xyz* (if the *Multi Segment* option has been used): 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], with respect to a reference datum, during the n-th SP;
  - *cond_n*: drain conductance $[L^2/T]$ during the n-th SP.

The values of *length* within each grid cell are automatically calculated according to the portion of the drain segment which intersects a grid cell.

If the *Single Segment* option has been used, the fields *layer*, *segment* and *elev_n* are filled with values assigned by the User (manually or through the csv file) when the *drn_layer_drn* MDO is created. Furthermore, *cond_n* is automatically calculated depending on the drain bed geometry and its hydraulic conductivity, as defined by the User (manually or through the csv file; for details the reader is referred to the *MODFLOW-2005* User manual; Harbaugh, 2005).

drn_layer_drn :: Features total: 34, filtered: 34, selected: 0

	PKUID	ID	ROW	COL	layer	segment	length	elev_1	cond_1	elev_2	cond_2
1	1	0	20	1	1	1	75.2795282472	5.46665698046	13008.3024811	5.46665698046	13008.3024811
2	2	0	20	2	1	1	100.300344097	5.38888865154	17331.8994599	5.38888865154	17331.8994599
3	3	0	20	3	1	1	100.300344097	5.30003803278	17331.89946	5.30003803278	17331.89946
4	4	0	20	4	1	1	100.300344097	5.21118741401	17331.89946	5.21118741401	17331.89946
5	5	0	20	5	1	1	100.13776637	5.12341973368	17303.8060287	5.12341973368	17303.8060287
6	6	0	19	5	1	1	4.93407108373	5.07793703725	852.607483268	5.07793703725	852.607483268
7	7	0	19	6	1	1	105.657774458	5.02794245816	18257.6634263	5.02794245816	18257.6634263
8	8	0	19	7	1	1	105.657774458	4.93328996711	18257.6634263	4.93328996711	18257.6634263
9	9	0	19	8	1	1	104.546611254	4.84029993499	18065.6544246	4.84029993499	18065.6544246

Show All Features

If the *Multi Segment* option has been used, the fields *layer*, *elev_n* and *cond_n* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5. Furthermore, the field *xyz* is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.

drn_layer_drn :: Features total: 79, filtered: 79, selected: 0

	PKUID	ID	ROW	COL	layer	xyz	length	elev_1	cond_1	elev_2	cond_2
1	1	0	27	25	1	2	17.2028018461	0.1	0.001	0.1	0.001
2	2	0	27	26	1	2	103.569472528	0.1	0.001	0.1	0.001
3	3	0	27	27	1	2	38.9750176628	0.1	0.001	0.1	0.001
4	4	0	26	22	1	2	80.4877859529	0.1	0.001	0.1	0.001
5	5	0	26	23	1	2	103.569472528	0.1	0.001	0.1	0.001
6	6	0	26	24	1	2	103.569472528	0.1	0.001	0.1	0.001
7	7	0	26	25	1	2	86.3666706819	0.1	0.001	0.1	0.001
8	8	0	25	19	1	2	11.3177525109	0.1	0.001	0.1	0.001
9	9	0	25	20	1	2	108.77652198	0.1	0.001	0.1	0.001

Show All Features

A table renamed *drn_layer_drn_table* is created with the drn MDO, stored in the model DB and eventually loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters defined in the csv file.

drn_layer_drn_table :: Features total: 2, filtered: 2, selected: 0

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

Show All Features

Note: If the drain develops over more than one segment, the *Single Segment* option can be used for each segment. This requires editing as many line shapefiles as many drain segments. In this case, the User should avoid editing the downstream vertex of a segment and the upstream one of the following segment in the same grid cell.

Furthermore, the User must pay attention to the following. In the **Create a layer for DRN package** window:

- different names must be assigned in the *Name of new layer* field;
- the correct line shapefile must be selected in the *Line Layer (drain segment)* field;

- progressive segment numbers must be used 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 in the **Run Model** window.

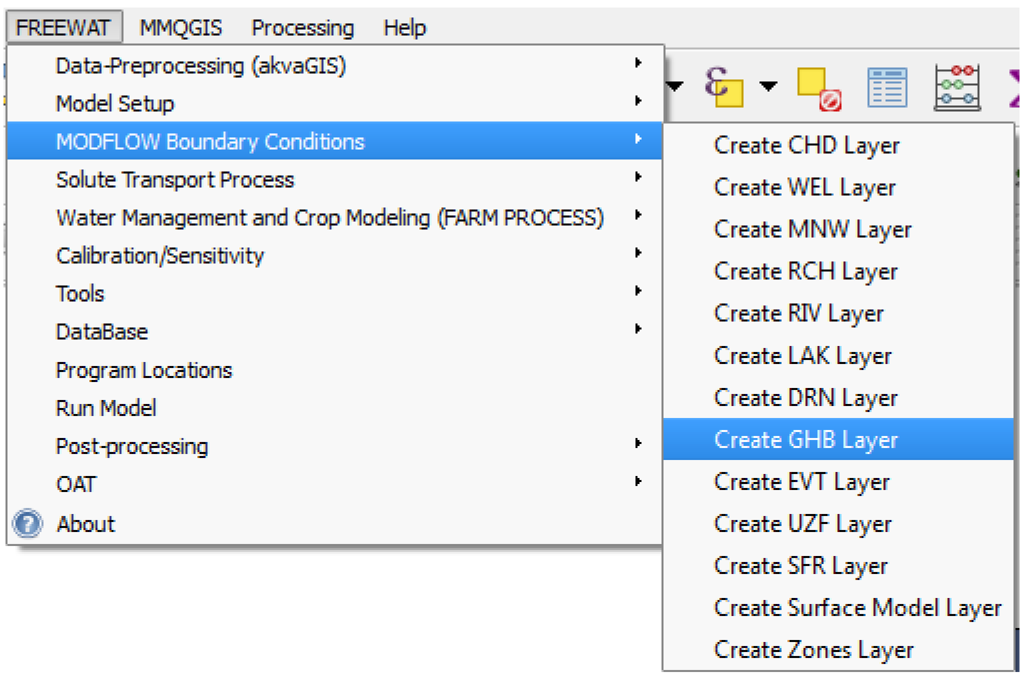
General-Head Boundary - GHB (head-dependent flux)

The *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 has been loaded in the Layers Panel, to activate the *GHB Package* the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create GHB Layer



In the **Create a layer for GHB package** window, 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.

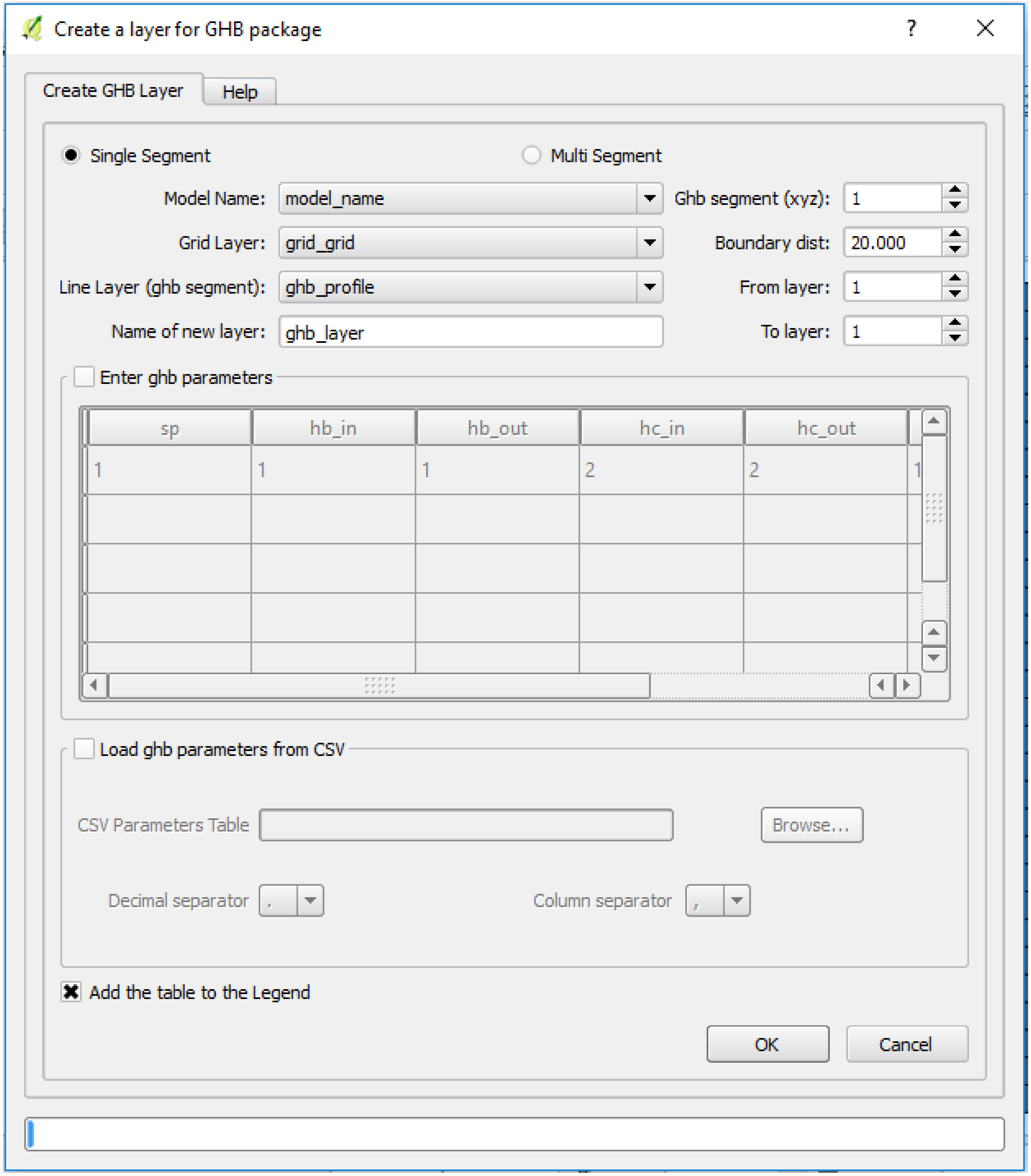
Note: The option *Single Segment* allows the User to assign ghb properties (i.e., head assigned to the external source, hydraulic conductivity and thickness of the sediments between the external source and the border cells), as required in the *MODFLOW GHB Package*. On the contrary, the option *Multi Segment* allows to define only at which grid cells the general-head boundary is located and the required properties must be assigned by the User at each cell once the ghb MDO has been successfully created.

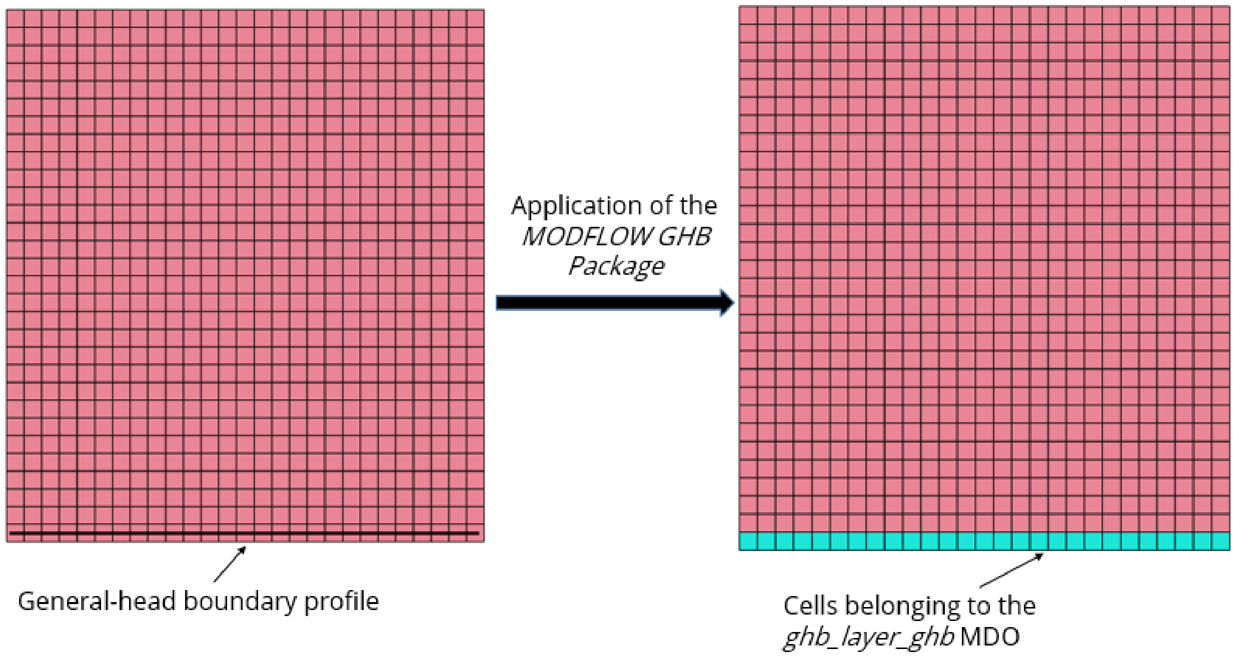
Anyway, the option *Single Segment* may still be applied, even if the general-head boundary develops over more than one segment. In this case, the multi-line shapefile must be splitted into several single segments and the User should avoid editing the downstream vertex of a segment and the upstream one of the following segment in the same grid cell.

These single segments 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:

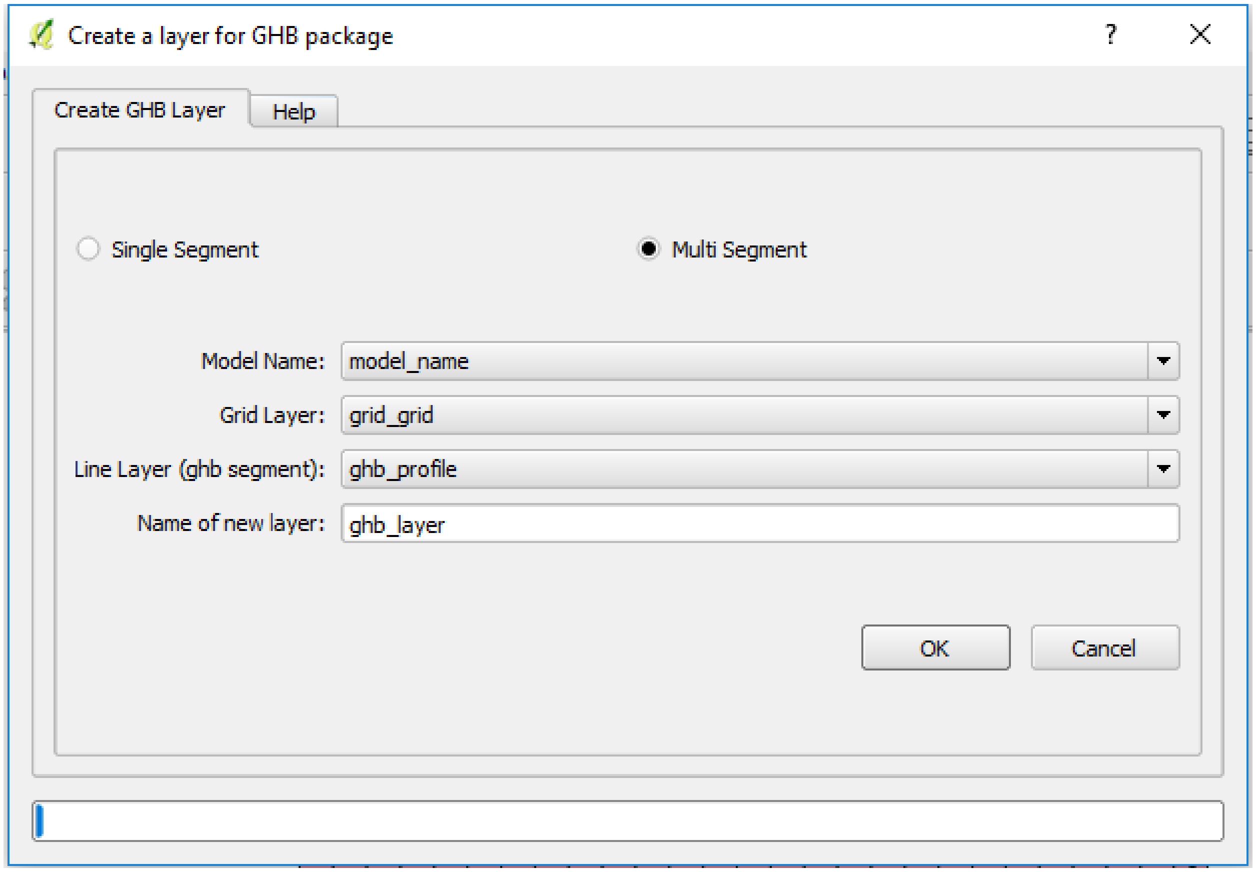
- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;
- *Line Layer (ghb segment)*: line shapefile containing the profile of the single ghb segment;
- *Name of new layer*: name of the ghb MDO which has to be created;
- *Ghb segment (xyz)*: number of the single ghb segment;
- *Boundary 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 through the csv file will be loaded in the Layers Panel and stored in the model DB.

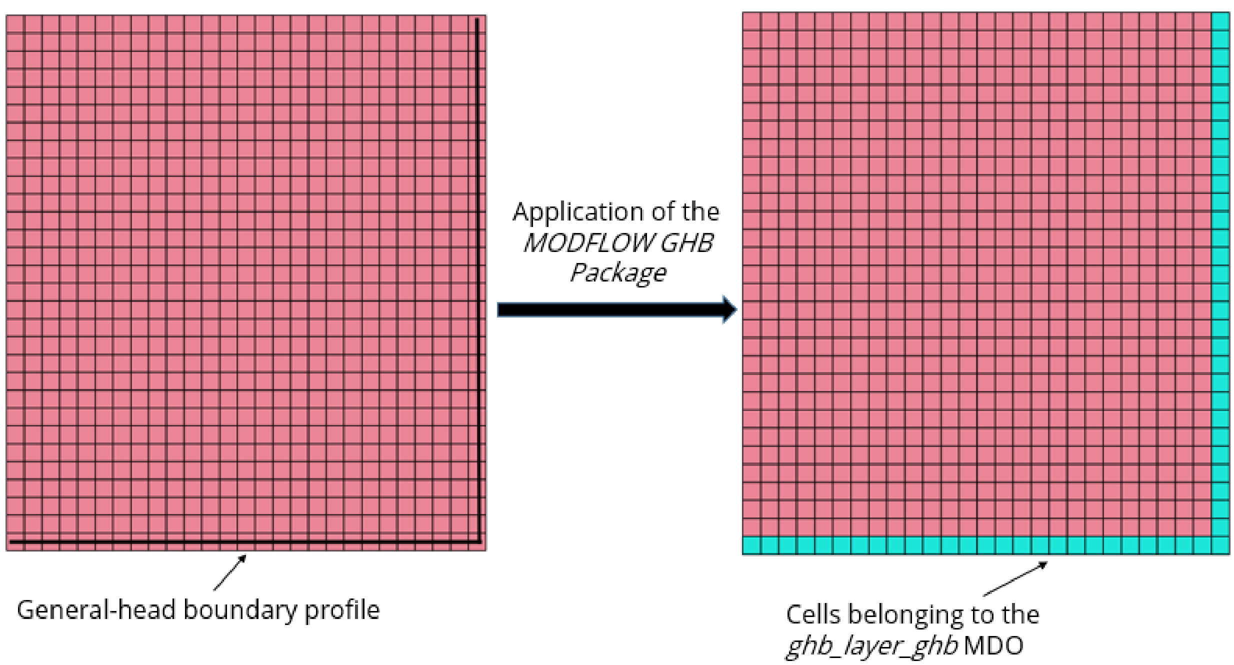

Create a layer for GHB package
Create GHB Layer
Help
Single Segment
Multi Segment
Model Name:
model_name
Ghb segment (xyz):
1
Grid Layer:
grid_grid
Boundary dist:
20.000
Line Layer (ghb segment):
ghb_profile
From layer:
1
Name of new layer:
ghb_layer
To layer:
1
Enter ghb parameters
sp
hb_in
hb_out
hc_in
hc_out
Load ghb parameters from CSV
CSV Parameters Table
Browse...
Decimal separator
Column separator
Add the table to the Legend
OK
Cancel



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.





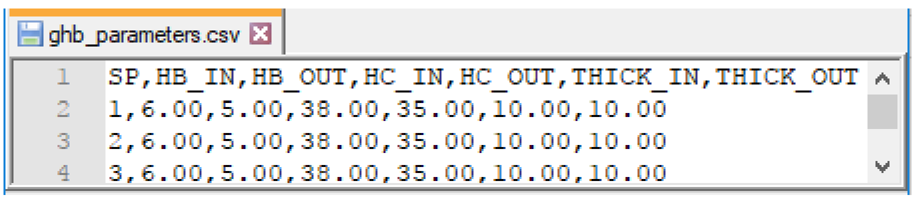
Note: Parameters required when creating the ghb MDO with the *Single Segment* option are related to the geometry and hydraulic conductivity of sediments between the external source and the grid cell and must be assigned for each SP:

- *sp*: SP number;

- *hb_in*: head [L], with respect to a reference datum, assigned to the external source at the upstream cell of the ghb segment;
- *hb_out*: head [L], with respect to a reference datum, assigned to the external source at the downstream cell of the ghb segment;
- *hc_in*: hydraulic conductivity [L/T] of the saturated sediments between the external source and the upstream cell of the ghb segment;
- *hc_out*: hydraulic conductivity [L/T] of the saturated sediments between the external source and the downstream cell of the ghb segment;
- *thick_in*: thickness [L] of the saturated sediments between the external source and the upstream cell of the ghb segment;
- *thick_out*: thickness [L] of the saturated sediments between the external source and the downstream cell of the ghb segment.

General-head boundary properties are assigned at the upstream and downstream cells of the ghb segment. Linear interpolation is automatically performed at the remaining cells.

If used, the csv file must have the following scheme (the template file *ghb_parameters.csv* is provided within the *FREEWAT* plugin folder `freewat\csv_templates\ghb`):




```
SP,HB_IN,HB_OUT,HC_IN,HC_OUT,THICK_IN,THICK_OUT
1,6.00,5.00,38.00,35.00,10.00,10.00
2,6.00,5.00,38.00,35.00,10.00,10.00
3,6.00,5.00,38.00,35.00,10.00,10.00
```

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

Note: The extension *_ghb* must not be changed in the Layers Panel and neither in the DB, as the ghb MDO will be filtered in the **Run Model** window according to such extension.

The Attribute Table of such MDO contains several records, according to the number of grid cells where this Package is applied, and the following fields:

- *PKUID*: database primary key (it must not be modified);
- *ID*: database primary key (it must not be modified);
- *ROW*: row index of a grid cell;
- *COL*: column index of a grid cell;
- *from_lay*: number of the uppermost model layer to which the ghb condition is applied;
- *to_lay*: number of the deepest model layer to which the ghb condition is applied;
- *segment* (if the *Single Segment* option has been used) or *xyz* (if the *Multi Segment* option has been used): 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 [L], with respect to a reference datum, assigned to the external source 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.

If the *Single Segment* option has been used, the fields *from_lay*, *to_lay*, *segment* and *bhead_n* are filled with values assigned by the User (manually or through the csv file) when the *ghb_layer_ghb* MDO is created. Furthermore, *cond_n* is automatically calculated depending on the distance between the boundary cells and the external source and the geometry and the hydraulic conductivity of the saturated sediments between the external source and the boundary cells, as defined by the User (manually or through the csv file; for details the reader is referred to the *MODFLOW-2005* User manual; Harbaugh, 2005).

ghb_layer_ghb :: Features total: 27, filtered: 27, selected: 0

	PKUID	ID	ROW	COL	from_lay	to_lay	segment	bhead_1	cond_1	bhead_2	cond_2
1	1	0	30	1	1	1	1	6	6650	6	6650
2	2	0	30	2	1	1	1	6	6650	6	6650
3	3	0	30	3	1	1	1	6	6650	6	6650
4	4	0	30	4	1	1	1	6	6650	6	6650
5	5	0	30	5	1	1	1	6	6650	6	6650
6	6	0	30	6	1	1	1	6	6650	6	6650
7	7	0	30	7	1	1	1	6	6650	6	6650
8	8	0	30	8	1	1	1	6	6650	6	6650
9	9	0	30	9	1	1	1	6	6650	6	6650

Show All Features

If the *Multi Segment* option has been used, the fields *from_lay*, *to_lay*, *elev_n* and *cond_n* are filled with default values, which can be modified using *QGIS* selection and editing tools described in Chapter 5. Furthermore, the field *xyz* is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.

ghb_layer_ghb :: Features total: 57, filtered: 57, selected: 0

	PKUID	ID	ROW	COL	from_lay	to_lay	xyz	bhead_1	cond_1	bhead_2	cond_2
1	1	0	30	1	0	0	1	0.1	0.001	0.1	0.001
2	2	0	30	2	0	0	1	0.1	0.001	0.1	0.001
3	3	0	30	3	0	0	1	0.1	0.001	0.1	0.001
4	4	0	30	4	0	0	1	0.1	0.001	0.1	0.001
5	5	0	30	5	0	0	1	0.1	0.001	0.1	0.001
6	6	0	30	6	0	0	1	0.1	0.001	0.1	0.001
7	7	0	30	7	0	0	1	0.1	0.001	0.1	0.001
8	8	0	30	8	0	0	1	0.1	0.001	0.1	0.001
9	9	0	30	9	0	0	1	0.1	0.001	0.1	0.001
	10	0	30	10	0	0	1	0.1	0.001	0.1	0.001

Show All Features

A table renamed *ghb_layer_ghb_table* is created with the ghb MDO, stored in the model DB and eventually loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters defined in the csv file.

ghb_layer_ghb_table :: Features total: 2, filtered: 2, selected: 0

	ROWNO	SP	HB_IN	HB_OUT	HC_IN	HC_OUT	THICK_IN	THICK_OUT
1	0	1	6	5	38	35	10	10
2	1	2	6	5	38	35	10	10

Show All Features

Note: If the general-head boundary develops over more than one segment, the *Single Segment* option can be used for each segment. This requires editing as many line shapefiles as many ghb segments. In this case, the User should avoid editing the downstream vertex of a segment and the upstream one of the following segment in the same grid cell.

Furthermore, the User must pay attention to the following. In the **Create a layer for GHB package** window:

- different names must be assigned in the *Name of new layer* field;
- the correct line shapefile must be selected in the *Line Layer (ghb segment)* field;
- progressive segment numbers must be used 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 in the **Run Model** window.

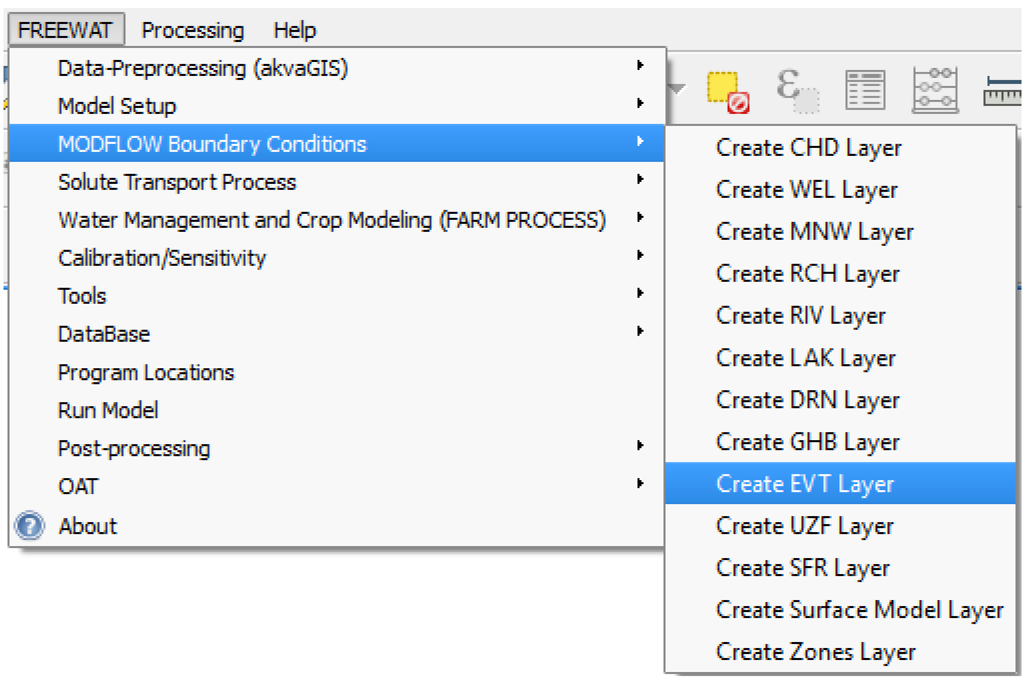
Evapotranspiration - EVT (head-dependent flux)

The *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 potentially 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:

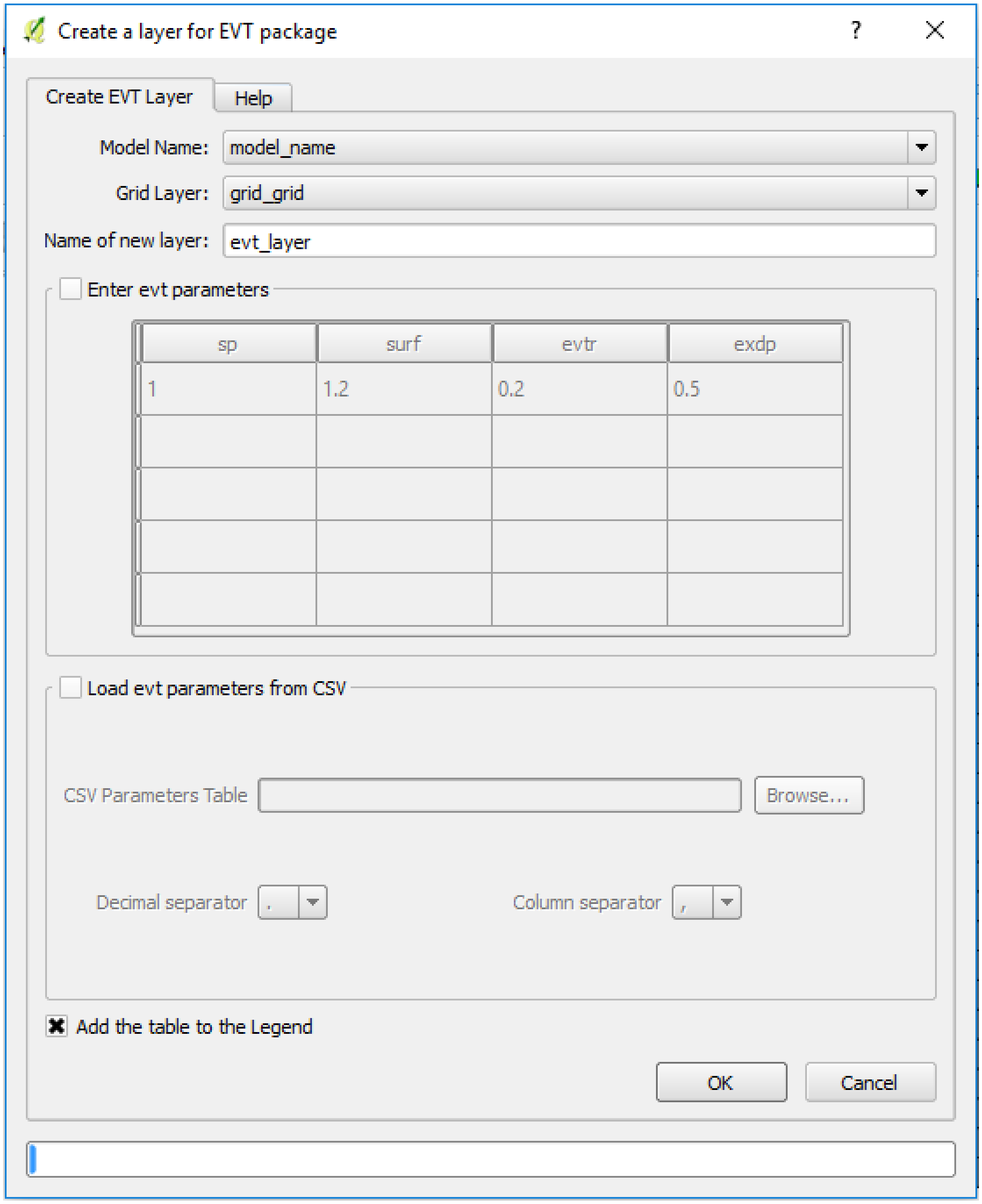
FREEWAT -> MODFLOW Boundary Conditions -> Create EVT Layer



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 through the csv file will be loaded in the Layers Panel and stored in the model DB.



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

- *sp*: SP number;
- *surf*: elevation [L], with respect to a reference datum, of the evapotranspiration surface;
- *evtr*: maximum evapotranspiration flux [L/T];
- *exdp*: evapotranspiration extintion depth [L].

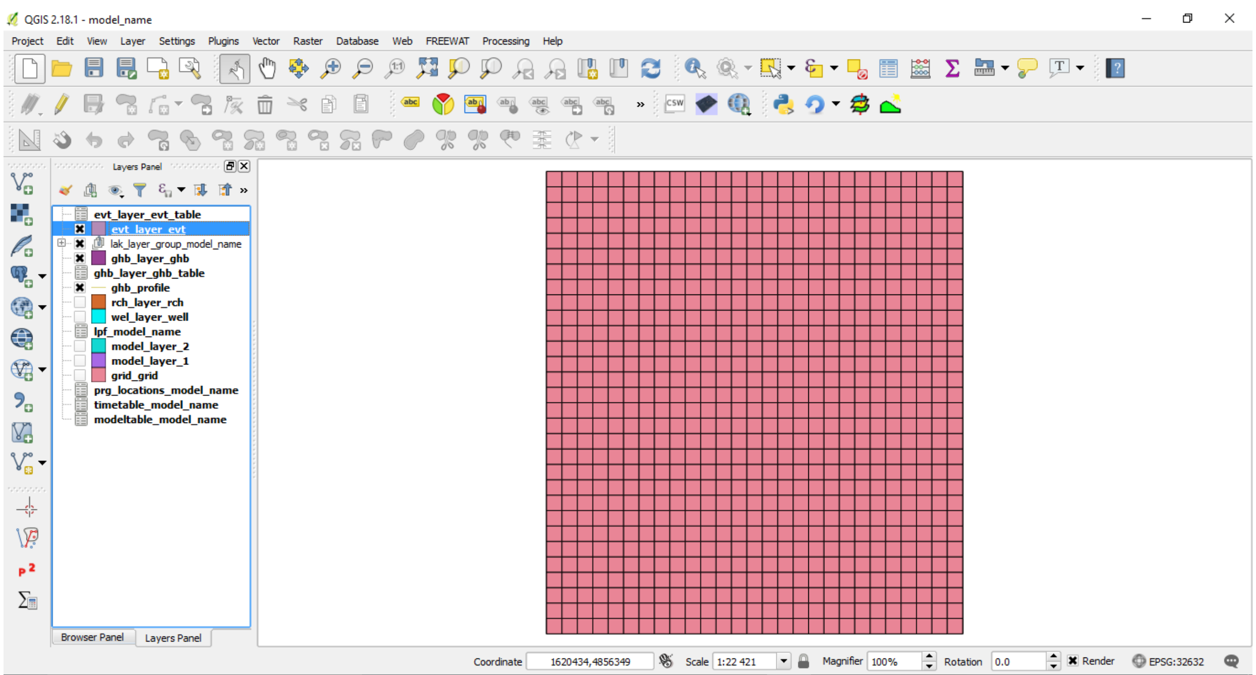
If used, the csv file must have the following scheme (the template file *evt_parameters.csv* is provided within the *FREEWAT* plugin folder `freewat\csv_templates\evt`):

evt_parameters.csv

```
sp,surf,evtr,exdp
1,10.0,0.002,0.5
2,10.0,0.002,0.5
3,10.0,0.002,0.5
```

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

Note: The extension *_evt* must not be changed in the Layers Panel and neither in the DB, as the evt MDO will be filtered in the **Run Model** window according to such extension.



The Attribute Table of such MDO contains 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 index of a grid cell;
- *COL*: column index of a grid cell;
- the following fields are repeated according to the number of SPs implemented (*n* refers to the number of a SP):

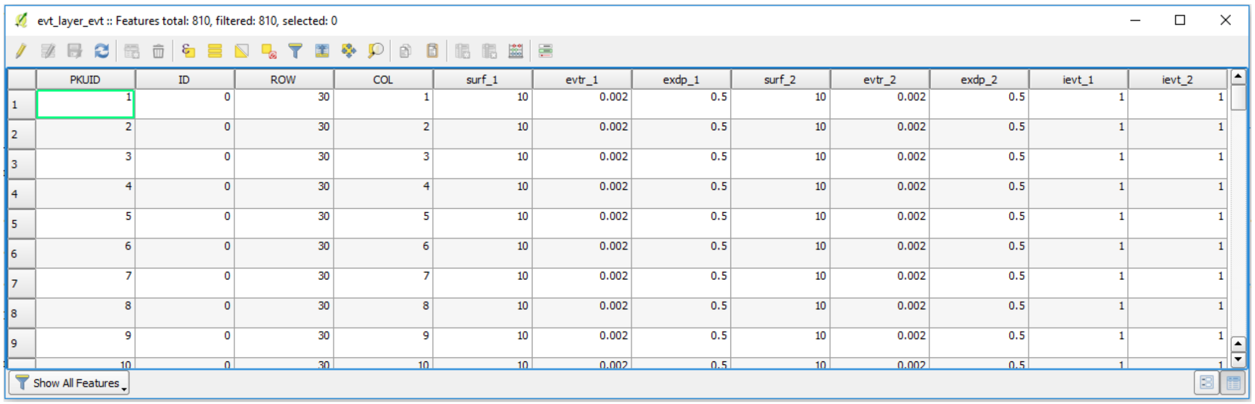
– *surf_n*: elevation [L], with respect to a reference datum, of the evapotranspiration surface during the *n*-th SP;

– *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 (manually or through the csv file) when the *evt_layer_evt* MDO is created.


evt_layer_evt :: Features total: 810, filtered: 810, selected: 0

	PKUID	ID	ROW	COL	surf_1	evtr_1	exdp_1	surf_2	evtr_2	exdp_2	ievt_1	ievt_2
1	1	0	30	1	10	0.002	0.5	10	0.002	0.5	1	1
2	2	0	30	2	10	0.002	0.5	10	0.002	0.5	1	1
3	3	0	30	3	10	0.002	0.5	10	0.002	0.5	1	1
4	4	0	30	4	10	0.002	0.5	10	0.002	0.5	1	1
5	5	0	30	5	10	0.002	0.5	10	0.002	0.5	1	1
6	6	0	30	6	10	0.002	0.5	10	0.002	0.5	1	1
7	7	0	30	7	10	0.002	0.5	10	0.002	0.5	1	1
8	8	0	30	8	10	0.002	0.5	10	0.002	0.5	1	1
9	9	0	30	9	10	0.002	0.5	10	0.002	0.5	1	1
	10	0	30	10	10	0.002	0.5	10	0.002	0.5	1	1

Show All Features

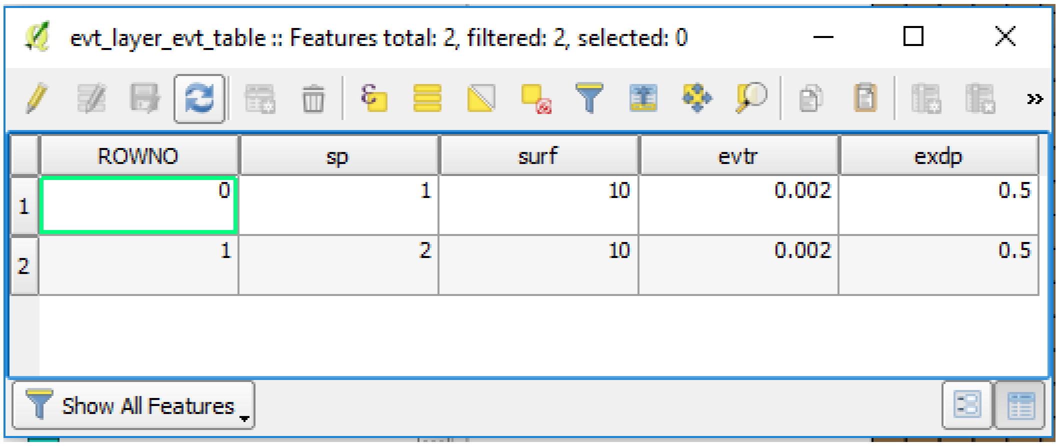
Note: *surf_n*, *evtr_n* and *exdp_n* values must be expressed in model units.

Note: *evtr_n* is actually a specified rate, rather than a flux. Such specified rate will then be 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_n* 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 renamed *evt_layer_evt_table* is created with the evt MDO, stored in the model DB and eventually loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters defined in the csv file.



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

Unsaturated-Zone Flow Package - UZF

The *MODFLOW UZF Package* allows to simulate vertical flow of water through the unsaturated zone, by etimating the evapotransporation and the effective infiltration through the vadose zone. This Package also allows the estimation of direct runoff to surface waterways.

Note: If the *UZF Package* is used, *RCH* and *EVT Packages* should not be activated.

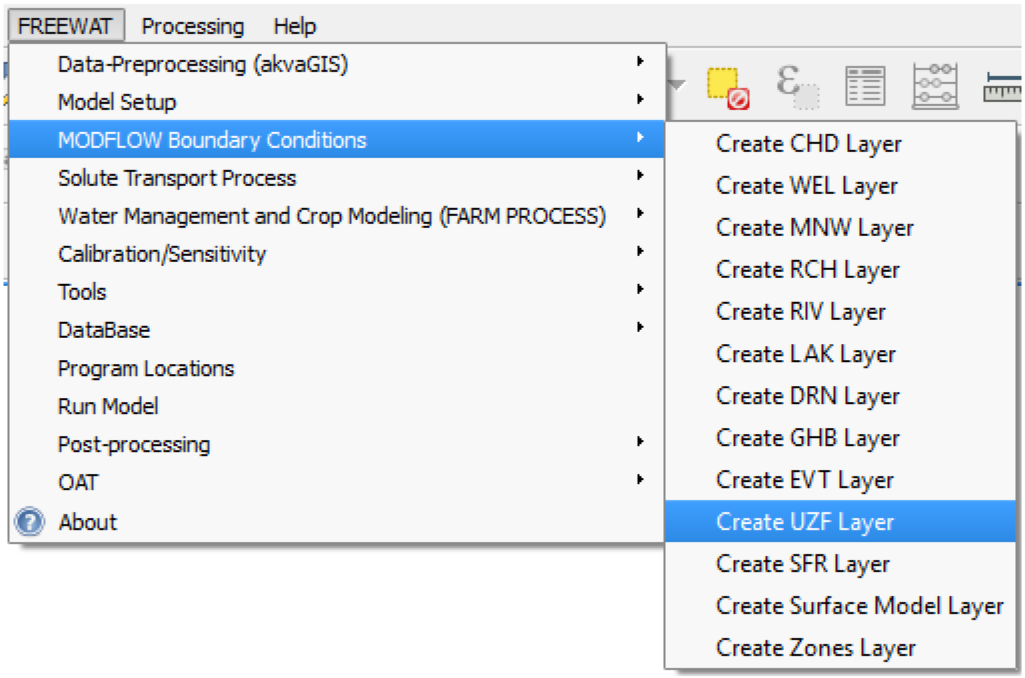
Implementing the *MODFLOW UZF Package* requires creating two MDOs: the uzf and the Surface Model Layer MDOs.

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

Creating the uzf MDO

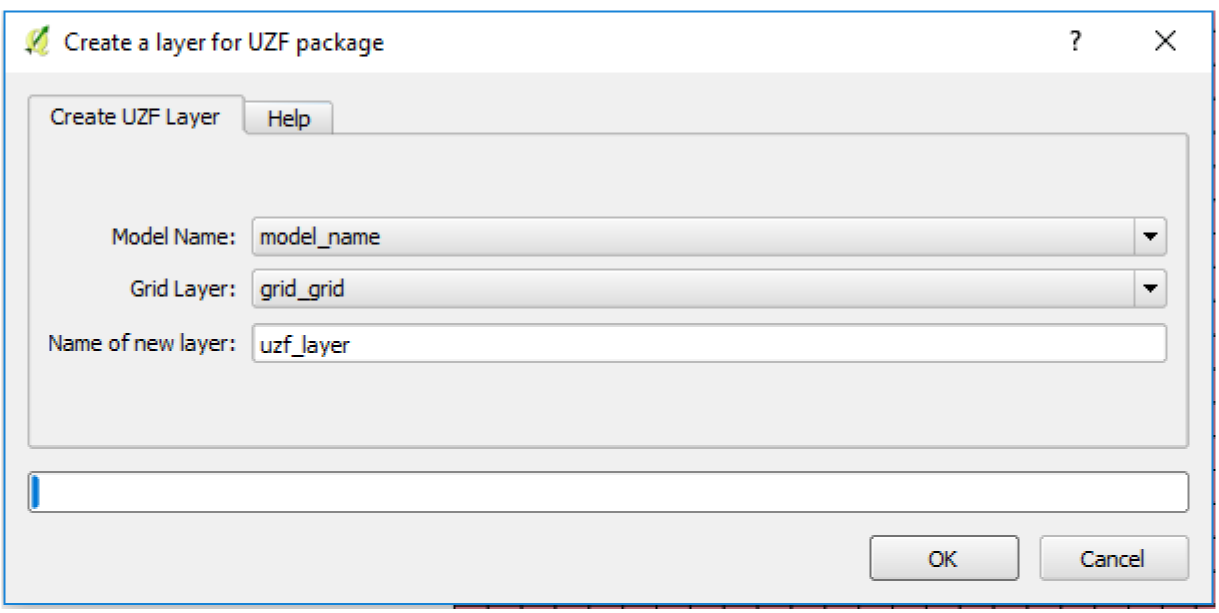
To activate the *UZF Package*, the following menu must be used:

FREEWAT -> MODFLOW Boundary Conditions -> Create UZF Layer



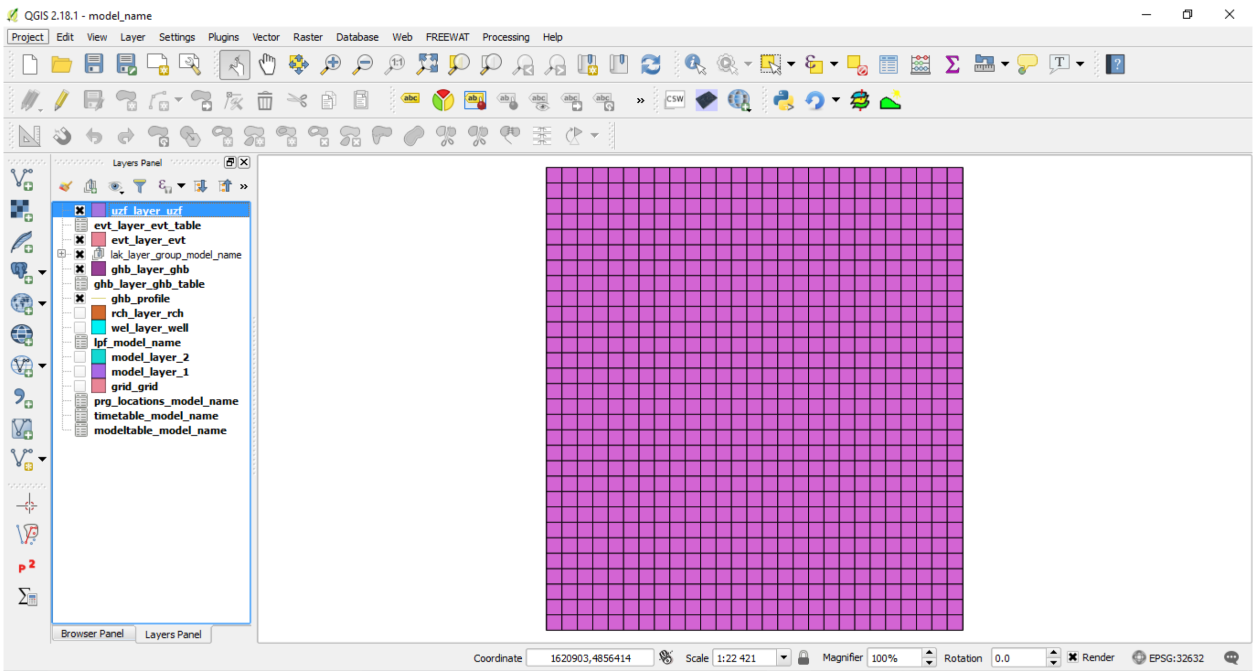
The following data are required in the **Create a layer for UZF package** window:

- *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, renamed *uzf_layer_uzf*, is created, stored in the model DB and loaded in the Layers Panel.

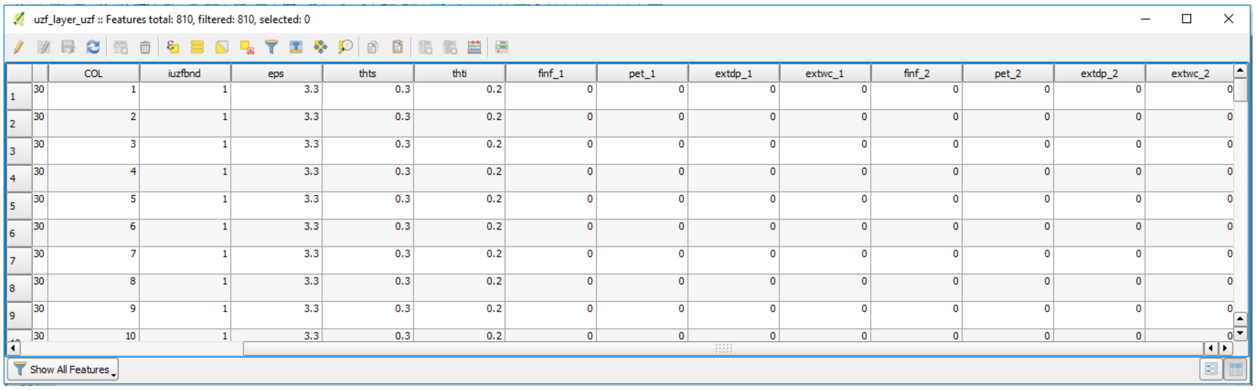
Note: The extension *_uzf* must not be changed in the Layers Panel and neither in the DB, as the uzf MDO will be filtered in the **Run Model** window according to such extension.



The Attribute Table of such MDO contains 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 index of a grid cell;
- *COL*: column index of a grid cell;
- *iuzfbnd*: integer value used to define the extent of the active domain in which recharge and discharge will be simulated (it must be set to *0* in grid cells where recharge and discharge will not be simulated; if a non-null value is used, that value indicates to which model layer recharge and discharge will occur);
- *eps*: Brooks-Corey epsilon parameter of the unsaturated zone, used 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 the 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*: rainfall rate [L/T] at the 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.



uzf_layer_uzf :: Features total: 810, filtered: 810, selected: 0

		COL	iuzfbnd	eps	thts	thti	finf_1	pet_1	extdp_1	extwc_1	finf_2	pet_2	extdp_2	extwc_2
1	30	1	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
2	30	2	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
3	30	3	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
4	30	4	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
5	30	5	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
6	30	6	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
7	30	7	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
8	30	8	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
9	30	9	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0
10	30	10	1	3.3	0.3	0.2	0	0	0	0	0	0	0	0

Show All Features

Note: *finf_n*, *pet_n*, *extdp_n* and *extwc_n* values must be expressed in model units.

Note: *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 recharge and discharge through the unsaturated zone at some cells during SP *n*, it is necessary to select the involved cells and set *iuzfbnd* to *0*.

Note: The *iuzfbnd* field can also be used 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.

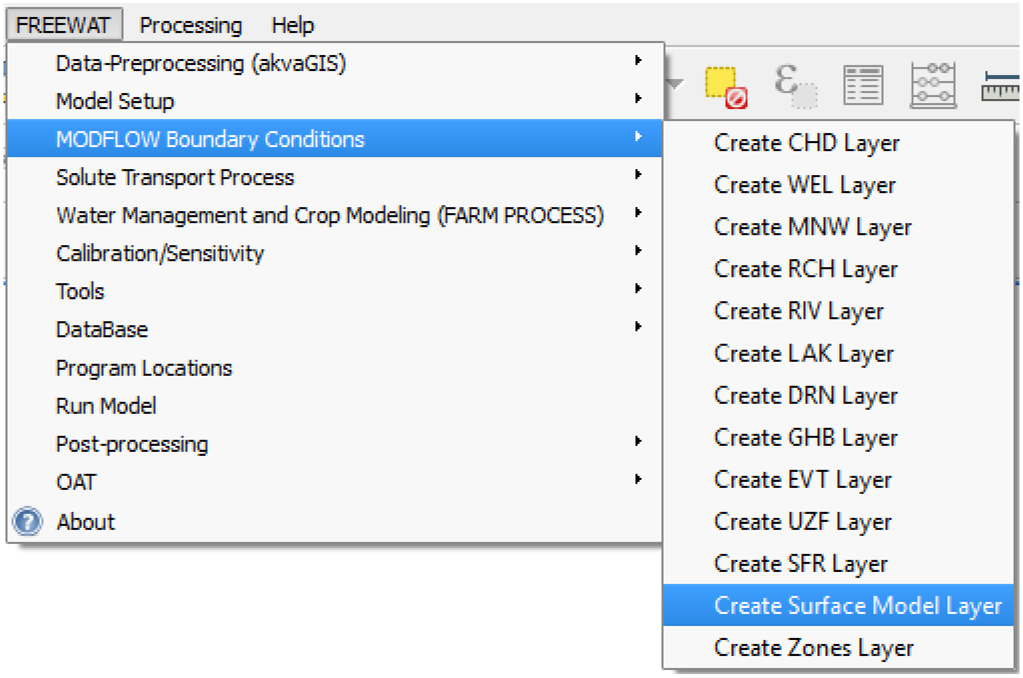
Creating the Surface Model Layer MDO

Creating the *Surface Model Layer (sml)* is necessary **only if** the *UZF Package* has to be coupled with the *SFR Package* to address runoff.

Of course, if the *SFR Package* is activated, but the *Surface Model Layer* has not been created, no runoff will be relocated to any SFR segments.

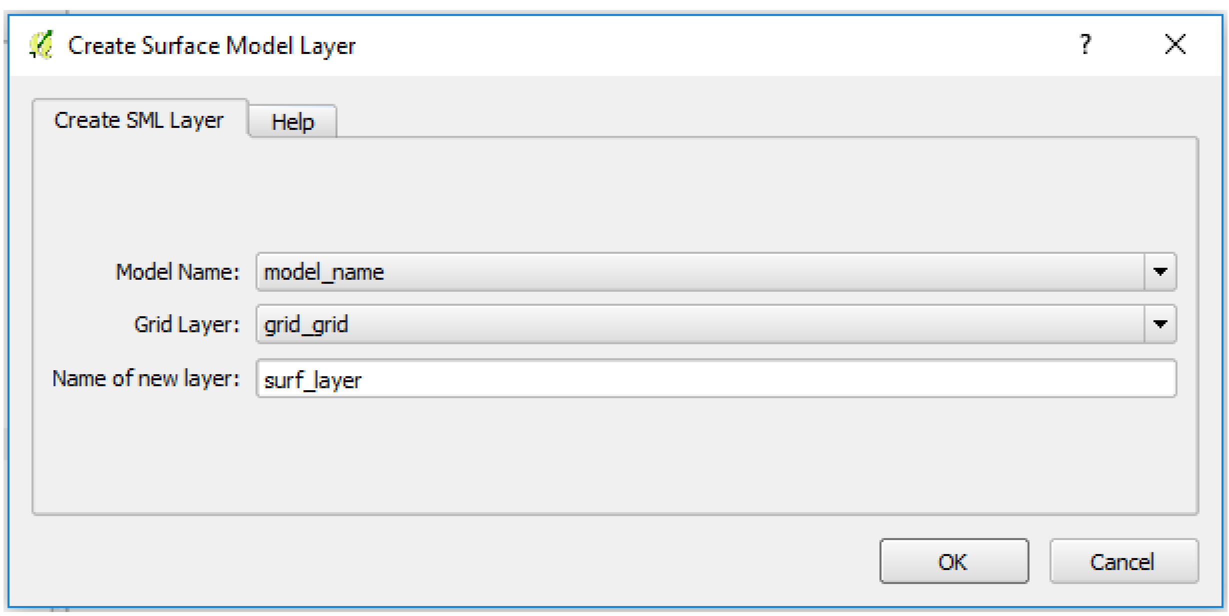
To define the *Surface Model Layer* the following menu must be used:

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



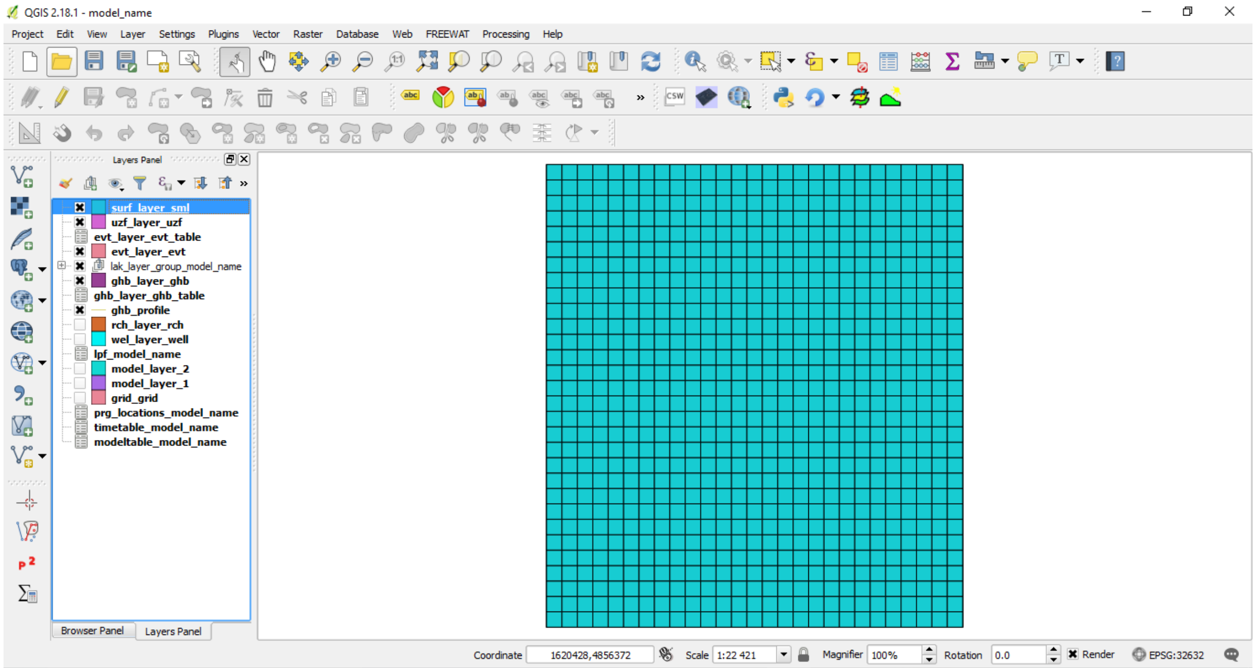
The following data are required in the **Create Surface Model Layer** window:

- *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, renamed *surf_layer_sml*, is created, stored in the model DB and loaded in the Layers Panel.

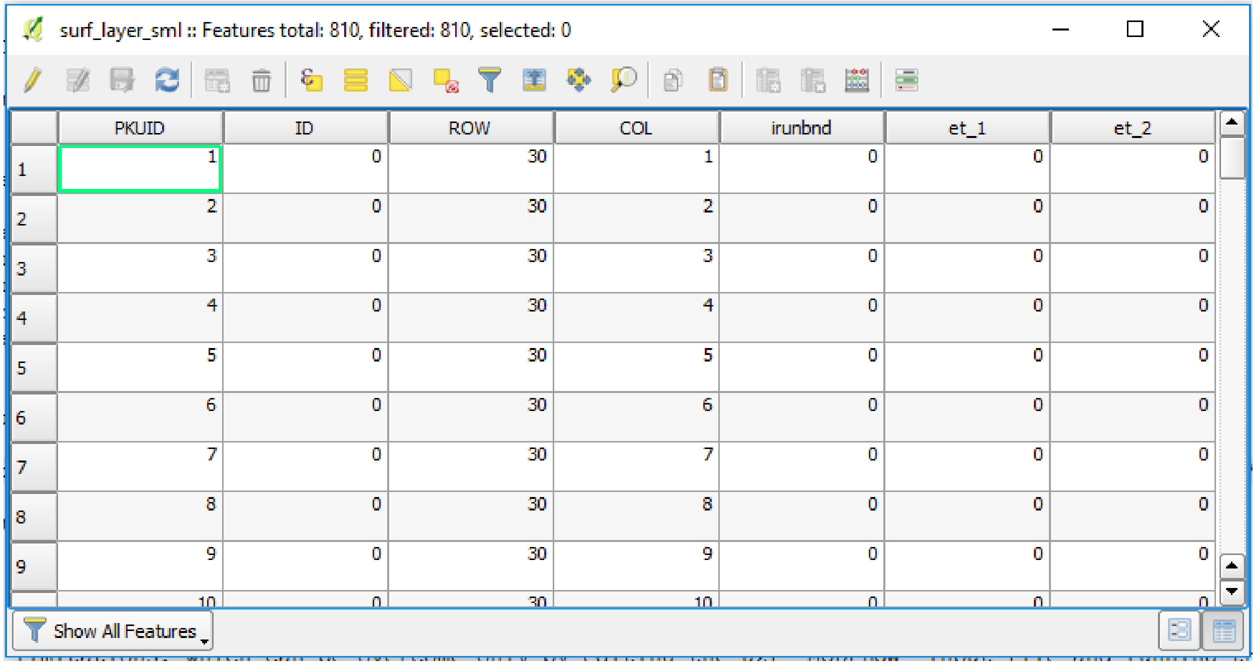
Note: The extension *_sml* must not be changed in the Layers Panel and neither in the DB, as the uzf MDO will be filtered in the **Run Model** window according to such extension.



The Attribute Table of such MDO contains 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 index of a grid cell;
- *COL*: column index of a grid cell;
- *irunbnd*: integer value used to define the stream segment to which run off will be addressed;
- the following field is repeated according to the number of SPs implemented (*n* refers to the number of a SP):
  - *et_n*: these fields are not relevant for the current version of the *FREEWAT* plugin.

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



	PKUID	ID	ROW	COL	irunbnd	et_1	et_2
1	1	0	30	1	0	0	0
2	2	0	30	2	0	0	0
3	3	0	30	3	0	0	0
4	4	0	30	4	0	0	0
5	5	0	30	5	0	0	0
6	6	0	30	6	0	0	0
7	7	0	30	7	0	0	0
8	8	0	30	8	0	0	0
9	9	0	30	9	0	0	0
	10	0	30	10	0	0	0

Limitations

The *MODFLOW 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 the reader is referred to the *UZF1* User manual; Niswonger et al., 2006):

- the vertical hydraulic conductivity of the aquifer is the same as defined in the *KZ* field of the related 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* User 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.

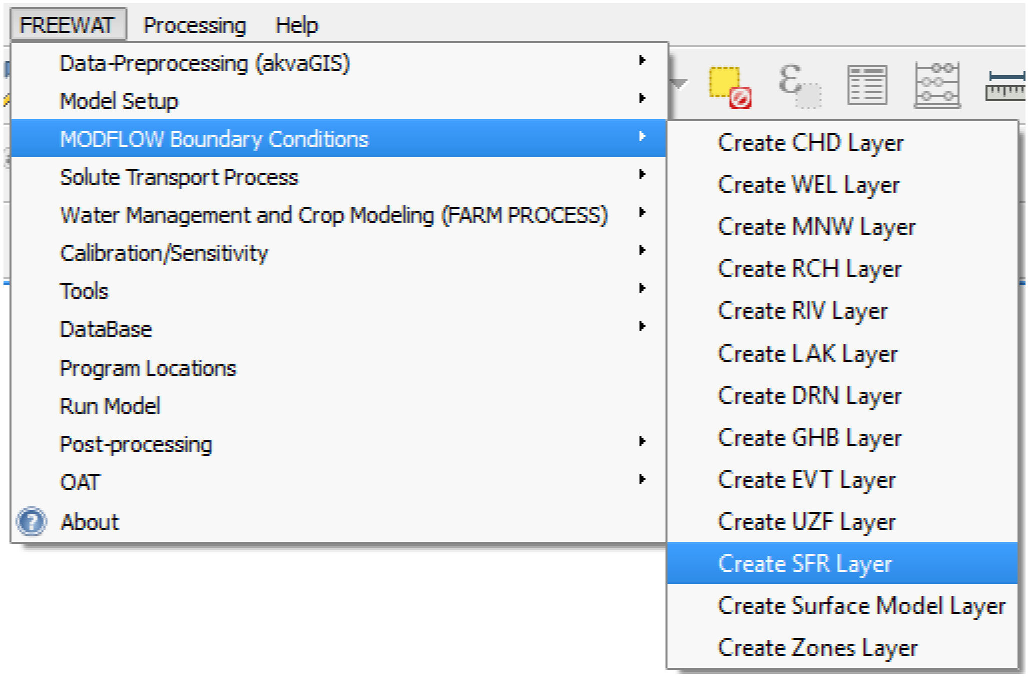
Streamflow-Routing Package - SFR (head-dependent flux)

The *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.

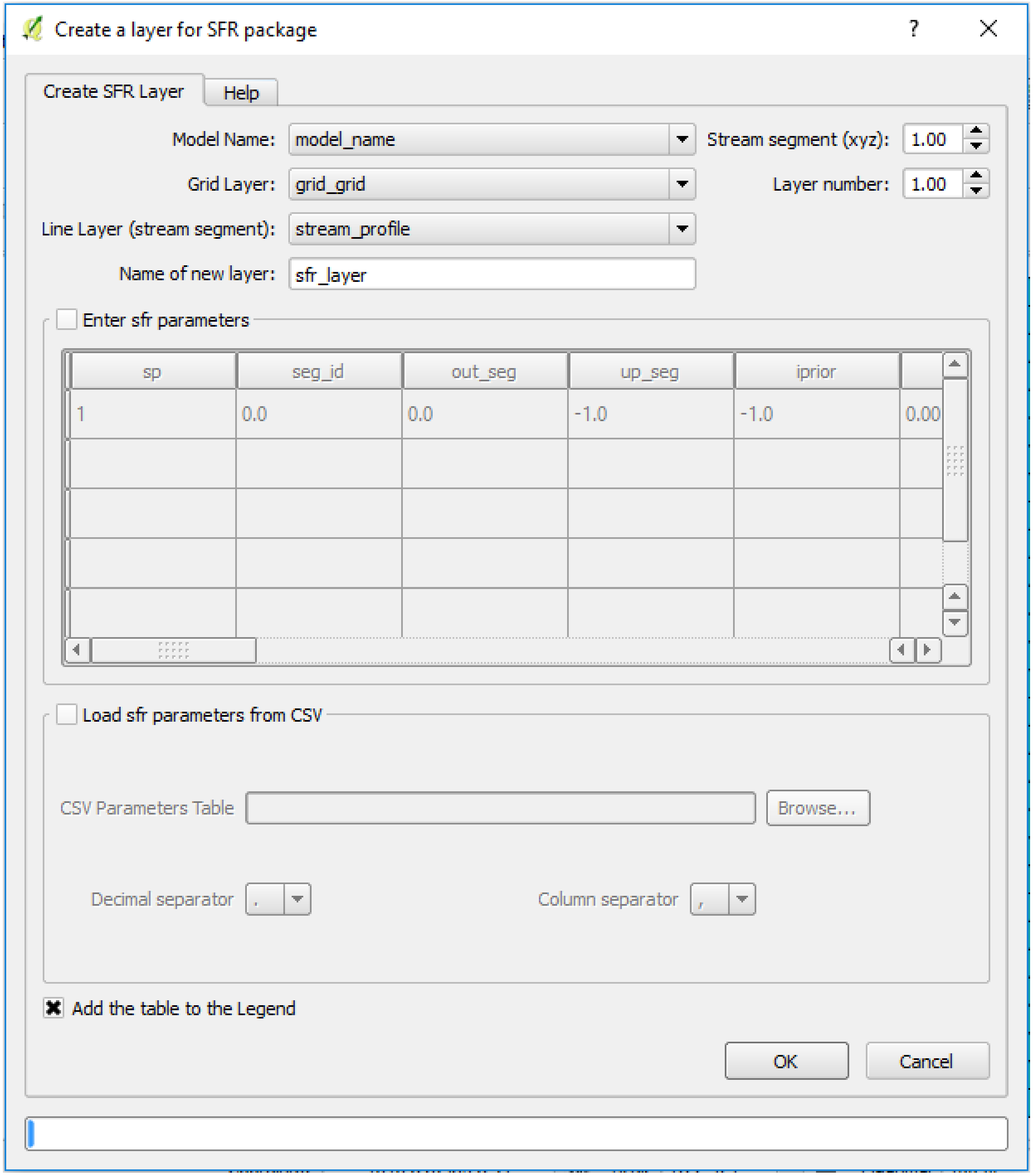
Once the line shapefile has been loaded in the Layers Panel, to activate the *SFR Package* the following menu must be used:

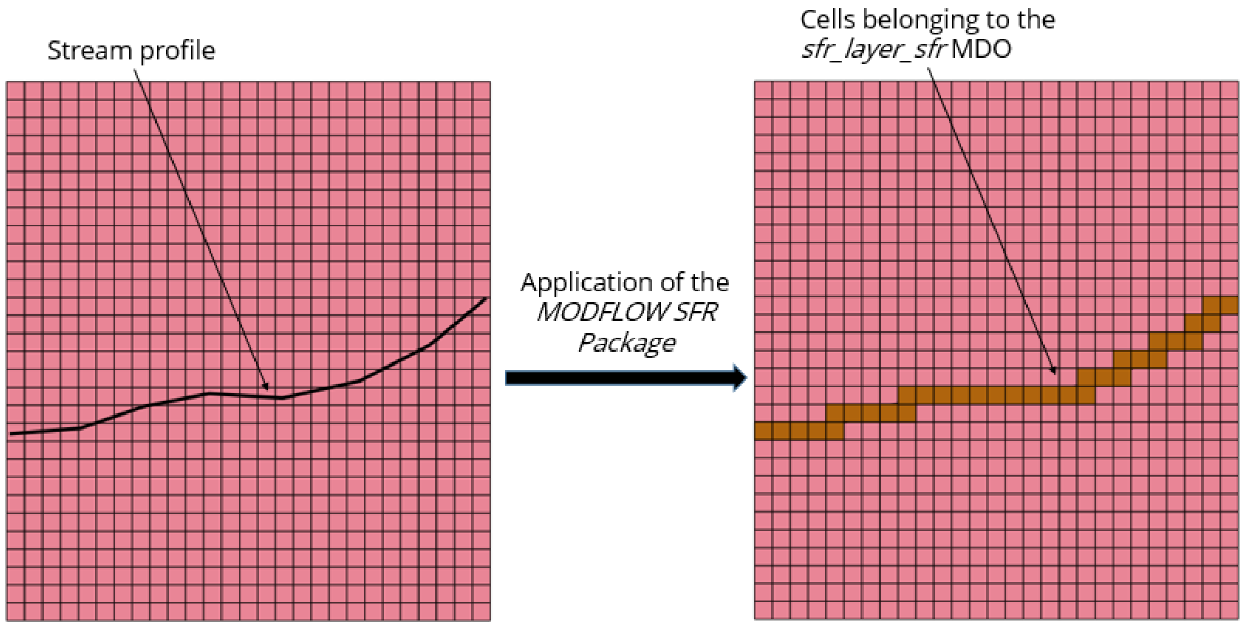
FREEWAT -> MODFLOW Boundary Conditions -> Create SFR Layer



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 the stream is in contact;
- 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 where the stream is located;
- if *Load sfr parameters from CSV* is checked, the User can load a csv file containing parameters to be assigned to grid cells where the stream 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 sfr parameters assigned through the csv file will be loaded in the Layers Panel and stored in the model DB.


Create a layer for SFR package
Create SFR Layer
Help
Model Name:
model_name
Stream segment (xyz):
1.00
Grid Layer:
grid_grid
Layer number:
1.00
Line Layer (stream segment):
stream_profile
Name of new layer:
sfr_layer
Enter sfr parameters
sp
seg_id
out_seg
up_seg
iprior
1
0.0
0.0
-1.0
-1.0
0.00
Load sfr parameters from CSV
CSV Parameters Table
Browse...
Decimal separator
Column separator
Add the table to the Legend
OK
Cancel



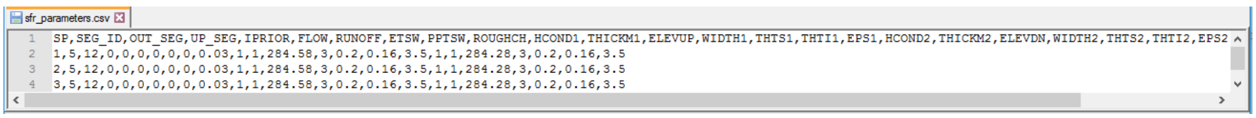
Note: Parameters required when creating the sfr MDO are related to connections among channels of the surface network and to the geometry and hydraulic conductivity of the stream bed sediments and must be assigned at the upstream and downstream cells of the stream segment and for each SP:

- *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], with respect to a reference datum, 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], with respect to a reference datum, 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.

Stream properties are assigned at the upstream and downstream cells of the stream segment. Linear interpolation is automatically performed at the remaining cells.

If used, the csv file must have the following scheme (the template file *sfr_parameters.csv* is provided within the *FREEWAT* plugin folder `freewat\csv_templates\sfr`):


sfr_parameters.csv

```
SP,SEG_ID,OUT_SEG,UP_SEG,IPRIOR,FLOW,RUNOFF,ETSW,PPTSW,ROUGHCH,HCOND1,THICKM1,ELEVUP,WIDTH1,THTS1,THTI1,EPS1,HCOND2,THICKM2,ELEVDN,WIDTH2,THTS2,THTI2,EPS2
1,5,12,0,0,0,0,0,0,0.03,1,1,284.58,3,0.2,0.16,3.5,1,1,284.28,3,0.2,0.16,3.5
2,5,12,0,0,0,0,0,0,0.03,1,1,284.58,3,0.2,0.16,3.5,1,1,284.28,3,0.2,0.16,3.5
3,5,12,0,0,0,0,0,0,0.03,1,1,284.58,3,0.2,0.16,3.5,1,1,284.28,3,0.2,0.16,3.5
```

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

Note: The extension *_sfr* must not be changed in the Layers Panel and neither in the DB, as the sfr MDO will be filtered in the **Run Model** window according to such extension.

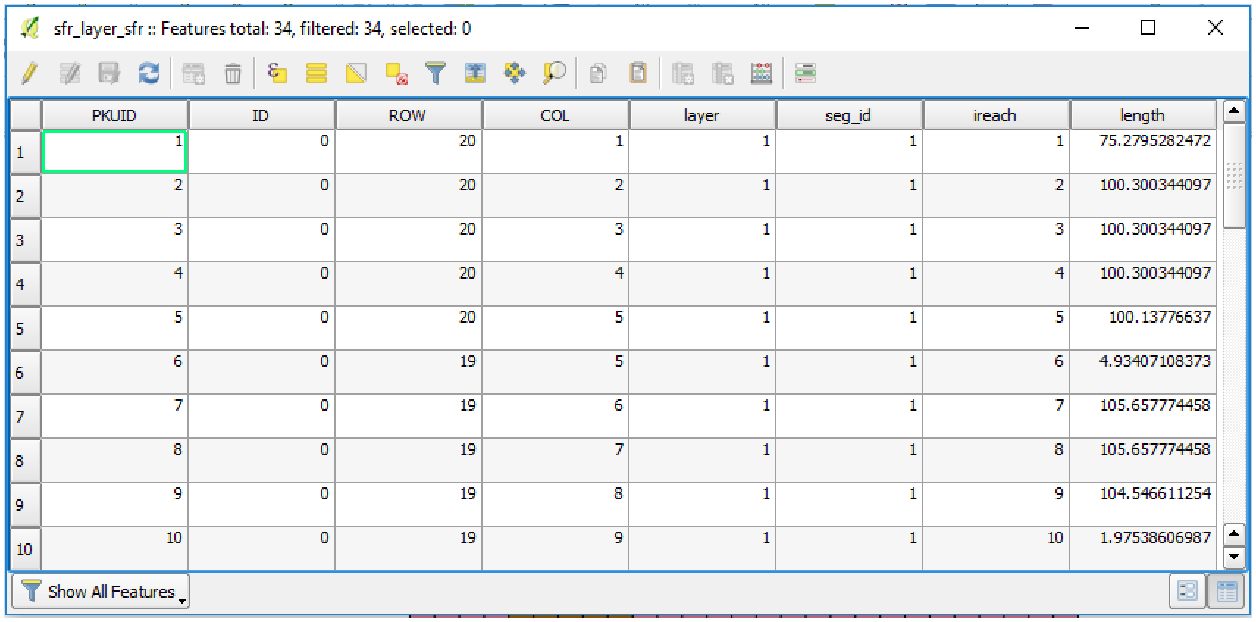
The Attribute Table of such MDO contains several records, according to the number of grid cells where this Package is applied, and the following fields:

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

The values of *length* within each grid cell are automatically calculated according to the portion of the stream segment which intersects a grid cell.

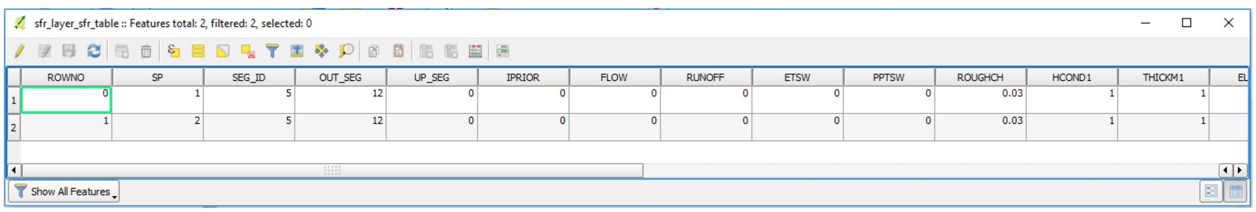
The fields *layer* and *seg_id*, are filled with values assigned by the User (manually or through the csv file) when the *sfr_layer_sfr* MDO is created.

Furthermore, the field *ireach* is automatically filled. Anyway, the User should always double-check that reaches in a segment are sorted according to the stream flow direction (i.e., from the farthest upstream cell until the last downstream one).



	PKUID	ID	ROW	COL	layer	seg_id	ireach	length
1	1	0	20	1	1	1	1	75.2795282472
2	2	0	20	2	1	1	2	100.300344097
3	3	0	20	3	1	1	3	100.300344097
4	4	0	20	4	1	1	4	100.300344097
5	5	0	20	5	1	1	5	100.13776637
6	6	0	19	5	1	1	6	4.93407108373
7	7	0	19	6	1	1	7	105.657774458
8	8	0	19	7	1	1	8	105.657774458
9	9	0	19	8	1	1	9	104.546611254
10	10	0	19	9	1	1	10	1.97538606987

A table renamed *sfr_layer_sfr_table* is created with the sfr MDO, stored in the model DB and eventually loaded in the Layers Panel. It may contain several records, according to the number of SPs, and several fields related to parameters defined in the csv file.



	ROWNO	SP	SEG_ID	OUT_SEG	UP_SEG	IPRIOR	FLOW	RUNOFF	ETSW	PPTSW	ROUGHCH	HCOND1	THICKM1
1	0	1	5	12	0	0	0	0	0	0	0.03	1	1
2	1	2	5	12	0	0	0	0	0	0	0.03	1	1

Note: If the stream develops over more than one segment, the procedure described above must be repeated for each segment. This requires editing as many line shapefiles as many stream segments. In this case, the User should avoid editing the downstream vertex of a segment and the upstream one of the following segment in the same grid cell.

Furthermore, the User must pay attention to the following. In the **Create a layer for SFR package** window:

- different names must be assigned in the *Name of new layer* field;
- the correct line shapefile must be selected in the *Line Layer (stream segment)* field;
- progressive segment numbers must be used 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. The latter will then be used in the **Run Model** window.

Limitations

The *MODFLOW 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 the reader is refer to the *SFR2* User manual; Niswonger and Prudic, 2005):

- the stream is represented as a wide rectangular channel. This results in using Manning's equation to express the relationship between the stage and the flow (*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 for 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 for 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 used.

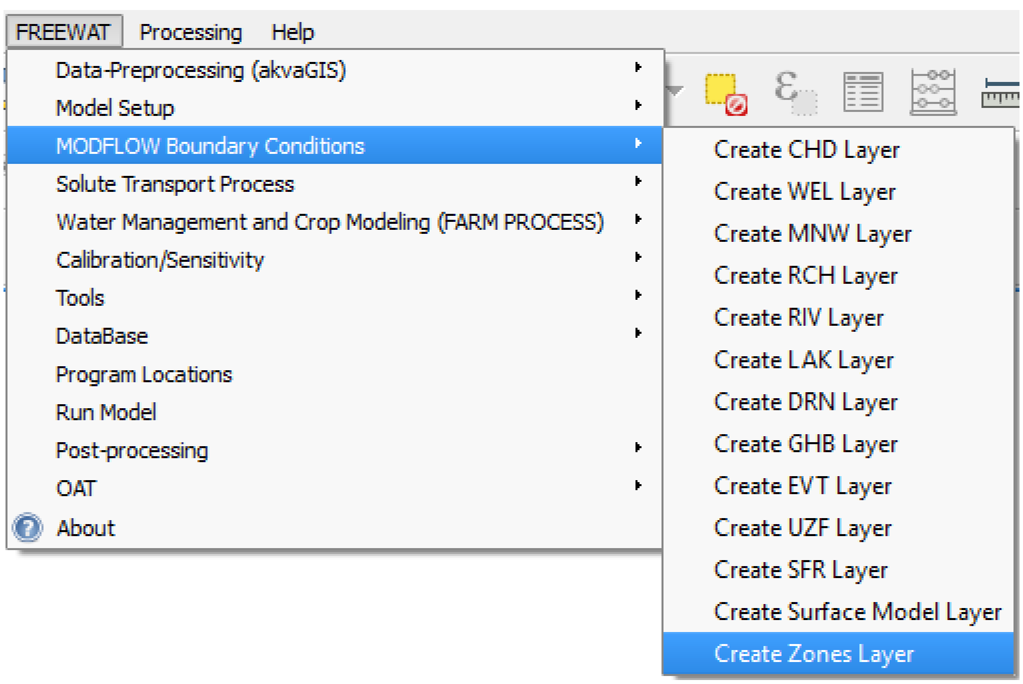
Zone Budget - ZONBUD

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 adjacent zones.

Activating this Package does NOT require prior processing of a polygon shapefile, as this condition can potentially 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:

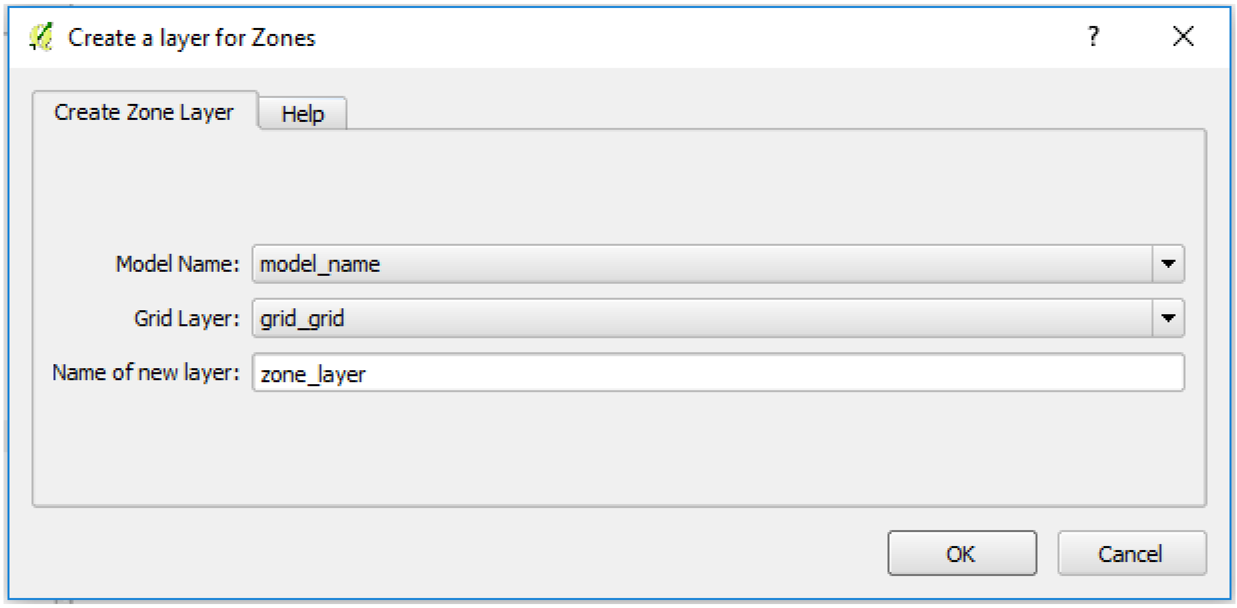
FREEWAT -> MODFLOW Boundary Conditions -> Create Zones Layer.



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

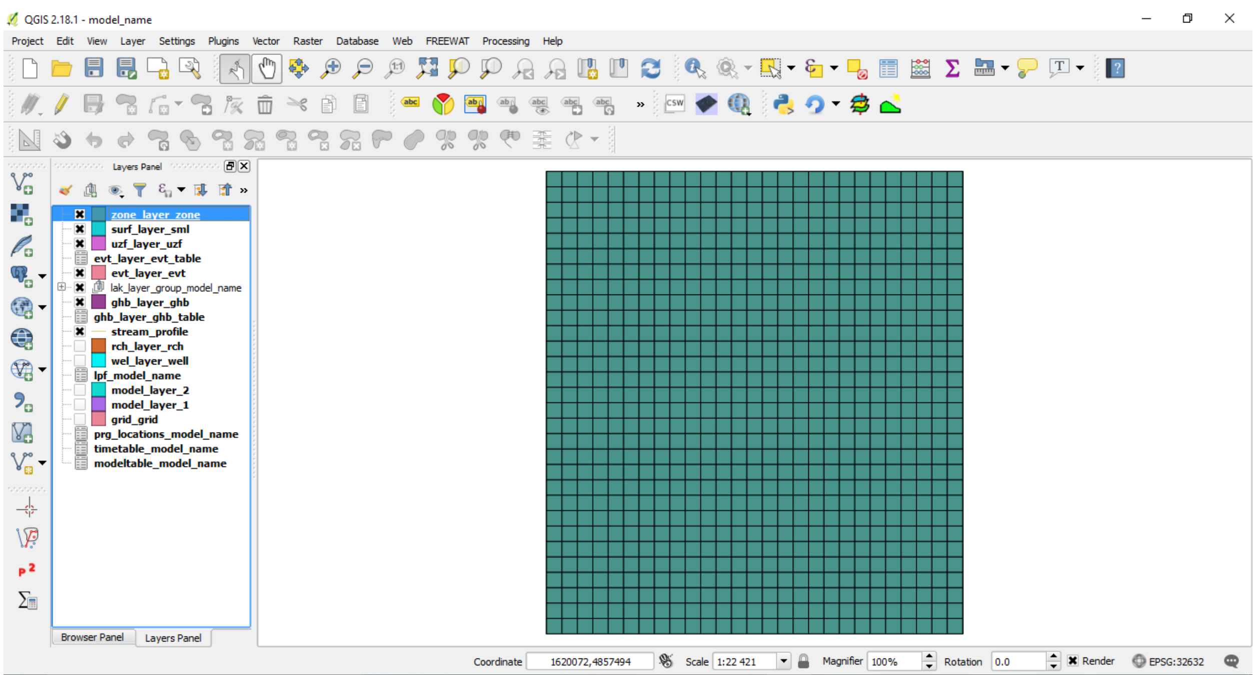
- *Model Name*: name of the hydrological model;
- *Grid Layer*: grid MDO;

- *Name of new layer*: name of the zonbud MDO which has to be created.



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

Note: The extension *_zone* must not be changed in the Layers Panel and neither in the DB, as the zonebud MDO will be filtered in the **Run Zone Budget** window according to such extension.

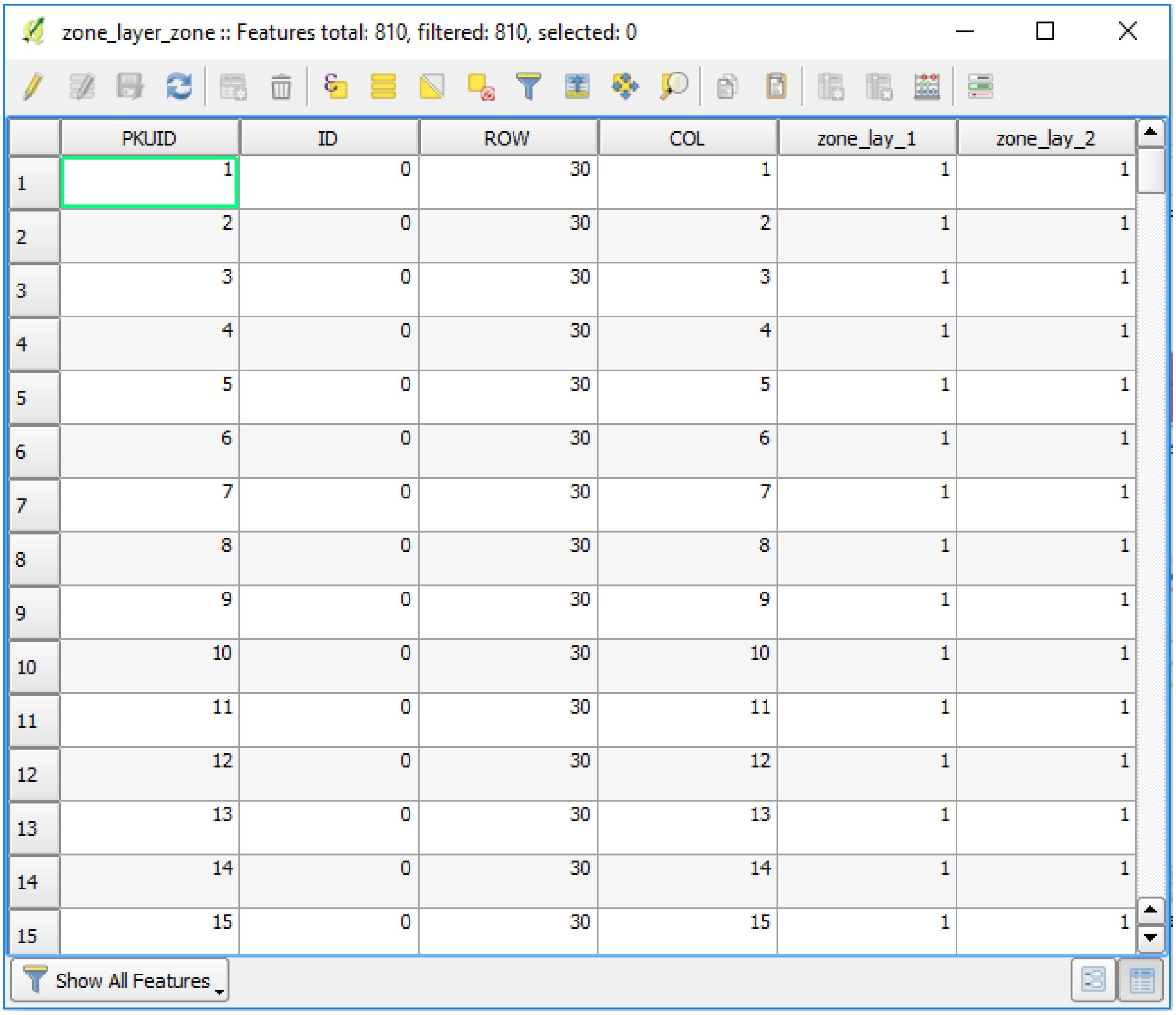


The Attribute Table of such MDO contains several records, according to the number of grid cells, and the following fields:

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

- *ROW*: row index of a grid cell;
- *COL*: column index 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; such number is read through the *lpf_model_name* table):
  - *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
1	1	0	30	1	1	1
2	2	0	30	2	1	1
3	3	0	30	3	1	1
4	4	0	30	4	1	1
5	5	0	30	5	1	1
6	6	0	30	6	1	1
7	7	0	30	7	1	1
8	8	0	30	8	1	1
9	9	0	30	9	1	1
10	10	0	30	10	1	1
11	11	0	30	11	1	1
12	12	0	30	12	1	1
13	13	0	30	13	1	1
14	14	0	30	14	1	1
15	15	0	30	15	1	1

Note: Before setting the **Create a layer for Zones** window, please be sure that the *lpf_model_name* table is present in the Layers Panel.

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

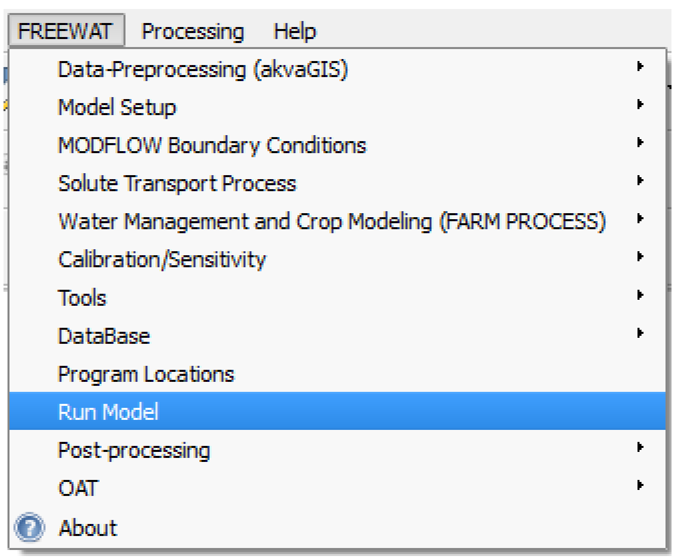
CHAPTER 7

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. As such, before running the model, translating such datasets in files which can be read by the numerical codes is necessay. In *FREEWAT*, such procedure is authomatically performed when the simulation is run.

The model run can be performed through the following menu:

FREEWAT -> Run Model



The processes which can be simulated are the following:

- **Groundwater Flow**;
- **Solute Transport** (see Volume 2);
- **OWHM - FARM PROCESS** (see Volume 3);
- **Model Calibration** (see Volume 4).

The following data are required in the **Groundwater Flow** tab:

- in the upper-left part of the tab, according to which among the *MODFLOW* Packages listed in Chapter 6 have been implemented, the corresponding checkbox 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 at 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* (*NUZTOP* flag in *MODFLOW*; Harbaugh, 2005);
- the checkbox *Simulate Evapotranspiration* must be checked if evapotranspiration has to be simulated;
- the checkbox *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 radiobox *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 (*CONST* variable in *MODFLOW*; Harbaugh, 2005);
  - *Weighting Factor (WEIGHT)*: time weighting factor used to calculate the change in channel storage (*WEIGHT* variable in *MODFLOW*; Harbaugh, 2005);
  - *Tolerance Level (DLEAK)*: closure tolerance for stream depth used to calculate leakage between each stream reach and active model cell (*DLEAK* variable in *MODFLOW*; Harbaugh, 2005);
  - *Num. of Sub-Time Steps (NUMTIM)*: number of sub-time steps used to route streamflow (*NUMTIM* variable in *MODFLOW*; Harbaugh, 2005);
  - *Streamflow Tolerance (FLWTOL)*: streamflow tolerance for convergence of the kinematic wave equation used for transient streamflow routing (*FLWTOL* variable in *MODFLOW*; Harbaugh, 2005);

• if the Solute Transport process has to be simulated, the link between *MODFLOW* and *MT3DMS* or *MT3D-USGS* is required, so the checkbox *Activate Link with MT3DMS (LMT) Package* must be checked. If such capability is activated, the User can specify if *Transport through Unsaturated zone is not simulated* or if *Transport through Unsaturated zone is simulated* (further details are provided in Volume 2);

• in the *OBSERVATIONS* section, according to which among the observation Packages (see Volume 6) are activated, the corresponding checkbox 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 (*WETFCT* variable in *MODFLOW*; Harbaugh, 2005);
  - *IWETIT* is the iteration interval for attempting to re-wet dry cells (*IWETIT* variable in *MODFLOW*; Harbaugh, 2005);
  - *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 (*IHDWET* flag in *MODFLOW*; Harbaugh, 2005);

• in the *PCG Solver parameters* section, the following data are required:
  - the number of *Outer Iterations* (i.e., iterations among which non-linear terms of the groundwater flow equation can change) to be performed;
  - the number of *Inner Iterations* (i.e., iterations among which the accuracy of the solution is improved without changing non-linear terms of the groundwater flow equation) to be performed;
  - the matrix conditioning method to be used (*NPCOND* flag in *MODFLOW*; Harbaugh, 2005): two options are available (*Modified Incomplete Cholesky* or *Polynomial*);

– *HCLOSE* is the head change criterion for convergence [L] (in length units; it represents a threshold for the maximum absolute value of head change at all active grid cells and between consecutive iterations; this must be met along with *RCLOSE*, in order to reach the convergence);

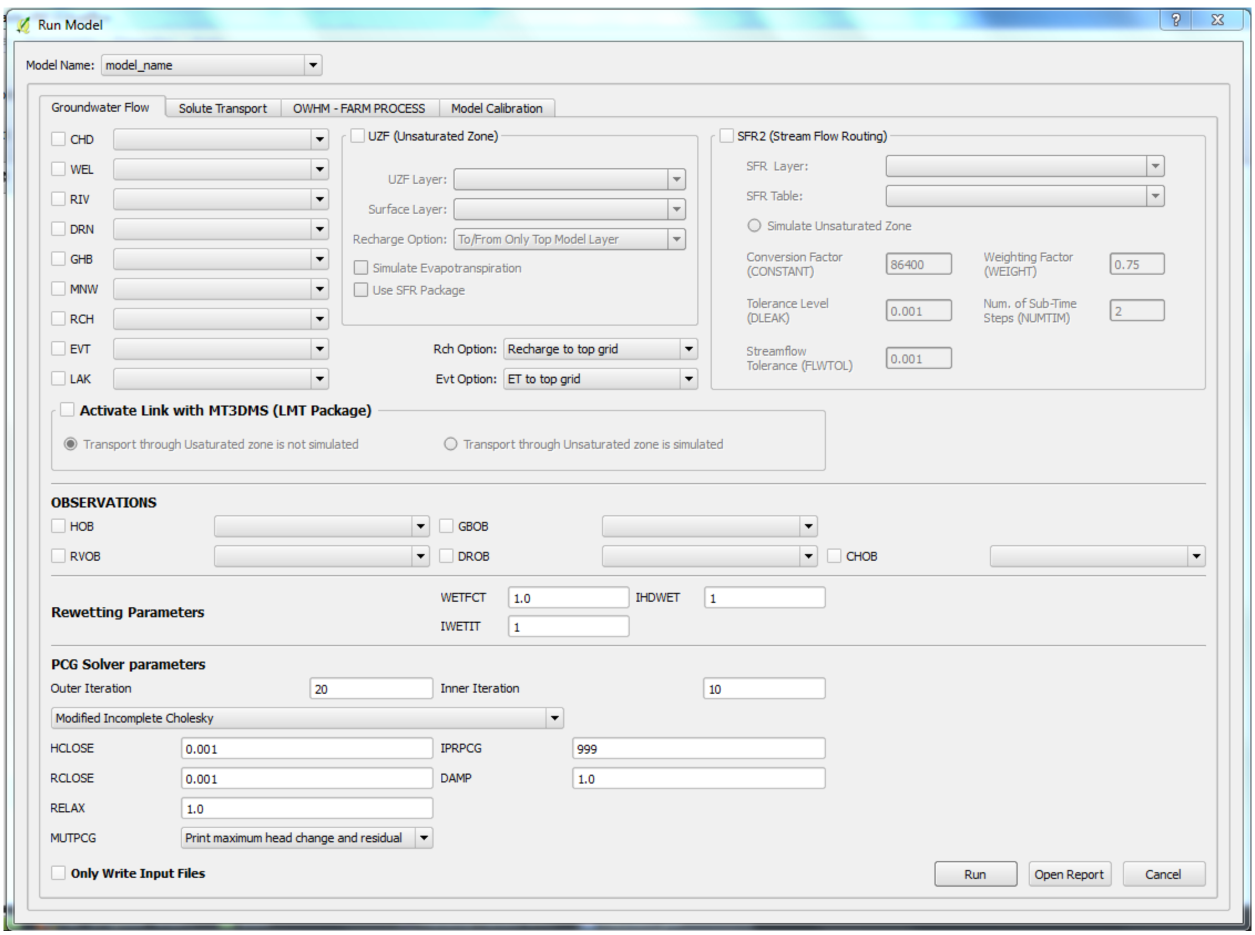
– *RCLOSE* is the residual criterion for convergence $[L^3/T]$ (in length and time units; it represents a threshold for the maximum absolute value of residual change, i.e., the difference between inflow and outflow terms in the groundwater budget, at all active grid cells and between consecutive iterations; this must be met along with *HCLOSE*, in order to reach the 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 for outputs;

– *DAMP* is the damping factor.



Note: If the checkbox 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 source/sink term at 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 source/sink term is applied to model layer 1; through the second one the source/sink term is applied at a certain model layer as specified in the fields *irch* and/or *ievt* in the Attribute Table of the rch and/or evt MDOs; through the third option the source/sink term is applied at the uppermost active cell in the vertical column.

Note: If the aim is to create only *MODFLOW* model files, without running the simulation, in the **Groundwater Flow** tab the checkbox *Only Write Input Files* must be checked before clicking the *Run* button.

Once the required settings are defined, the *Run* button allows to write the *MODFLOW* input files and start the simulation.

Hereinafter, a list of the *MODFLOW* input files which can be generated is provided. For further details the reader is suggested to refer to Harbaugh (2005).

The following are basic model files required for any simulation:

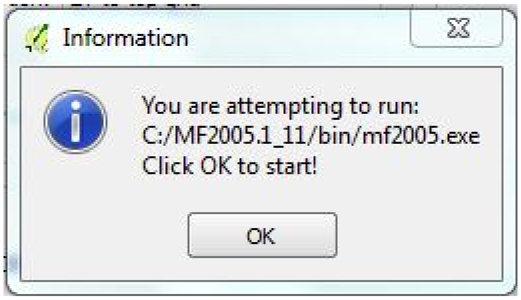
- **Name (.nam) file**: it contains a list of all the input and output files involved in the current simulation;
- **Basic Package (.bas) file**: it reports the fields *ACTIVE* and *STRT* for each model layer;
- **Discretization (.dis) file**: it reports the fields *TOP* and *BOTTOM* for each model layer and information stored in the table *timetable_model_name* about time discretization;
- **Layer Property Flow (.lpf) file**: it reports the fields *KX*, *KY*, *KZ*, *SS* and *SY* for each model layer and information stored in the table *lpf_model_name* about the type for each model layer (convertible or confined) and the wetting capability options;
- **Preconditioned Conjugate Gradient (.pcg) file**: it contains flage and options related to the numerical solver;
- **Output Control (.oc) file**: it contains flags and options related to the output results to be saved.

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

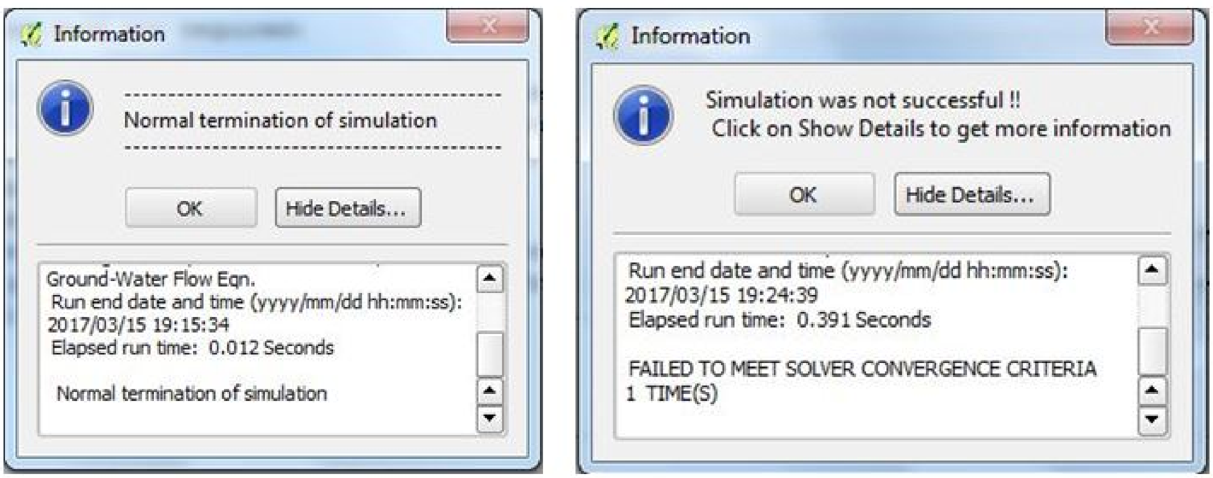
- **Time-Variant Specified Head (.chd) file**: it is created if the *CHD Package* is activated to define specified-head cells;
- **Well (.wel) file**: it is created if the *WEL Package* is activated to define recharge or pumping wells;
- **Multi-Node Well (.mnw) file**: it is created if the *MNW Package* is activated to simulate screened wells;
- **Recharge (.rch) file**: it is created if the *RCH Package* is activated to simulate areally-distributed recharge;
- **River (.riv) file**: it is created if the *RIV Package* is activated to simulate river-groundwater interaction;
- **Lake (.lak) file**: it is created if the *LAK package* is activated to simulate lake-groundwater interaction;
- **Drain (.drn) file**: it is created if the *DRN Package* is activated to simulate the effects of features, such as agricultural drains;
- **General-Head Boundary (.ghb) file**: it is created if the *GHB Package* is activated to simulate inflow to or outflow from the groundwater system, due to the presence of an external source;
- **Evapotranspiration (.evt) file**: it is created 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 created if the *UZF Package* is activated to simulate vertical flow through the unsaturated zone;
- **Stream Flow Routing (.sfr) file**: it is created if the *SFR Package* is activated to simulate streamflow and routed runoff within surface streams.

Note: Writing *MODFLOW* input files may require several minutes, especially for complex models.

Once *MODFLOW* input files have been created within the working folder, the following **Information** window appears, stating that *MODFLOW* executable (whose path is retrieved from the table of program locations) is going to be run:



Once clicking *OK*, the simulation starts and the following **Information** window appears to inform the User if the simulation ran successfully or not. In the second case, clicking on *Show Details...* can help in understanding why the simulation was not successful (i.e., if solver convergence criteria were not met or if something was set incorrectly). **Any problem should occur, information about the error can be found at the bottom of the MODFLOW output .list file (details are provided in Chapter 8)**.



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

CHAPTER 8

Model output and post-processing

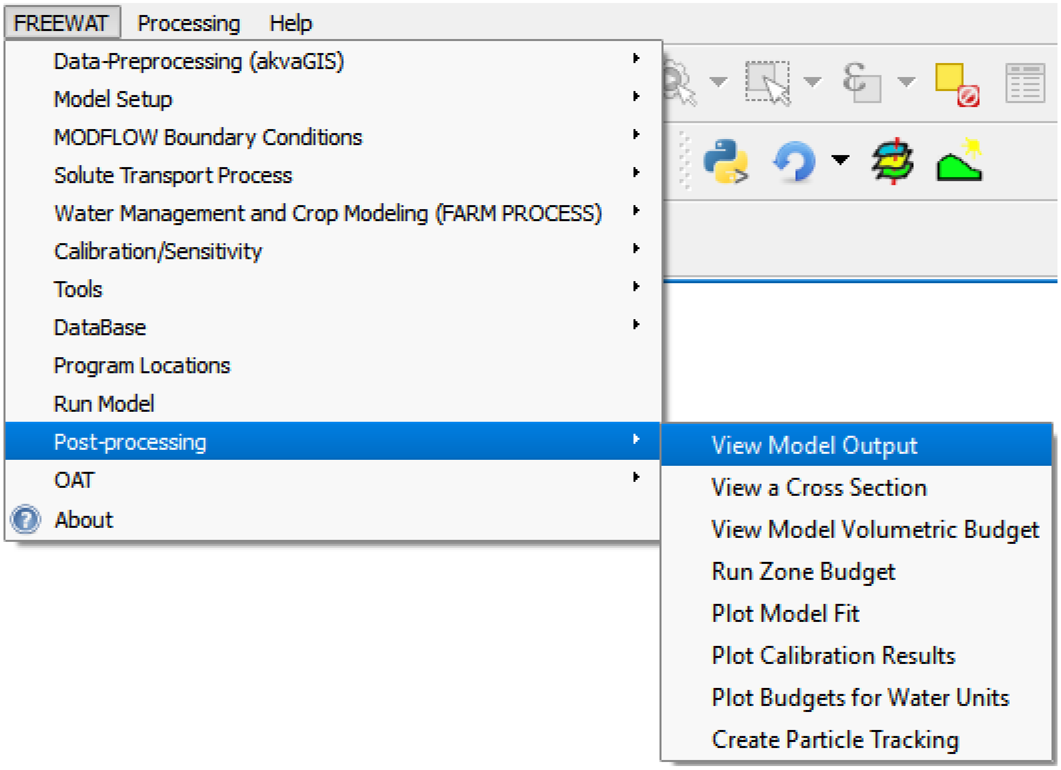
Besides the input files listed in Chapter 7, within the **.nam** file the following output files are also listed:

- **.hds**: binary file containing simulated hydraulic head for each model layer;
- **.ddn**: binary file containing simulated drawdown for each model layer;
- **.cbc**: binary file containing simulated cell-by-cell budget for each model layer;
- **.list**: text file containing several information about the simulation, among which the aquifer budget; it can be opened with any text editor or using the *Open Report* button at the bottom of the **Groundwater Flow** tab of the **Run Model** window.

Display model output

Once the model run has been successfully completed, the hydraulic head simulated for each model layer (or the solute concentration simulated after a solute transport simulation has been successfully completed; further details are provided in Volume 2) can be displayed through the following menu:

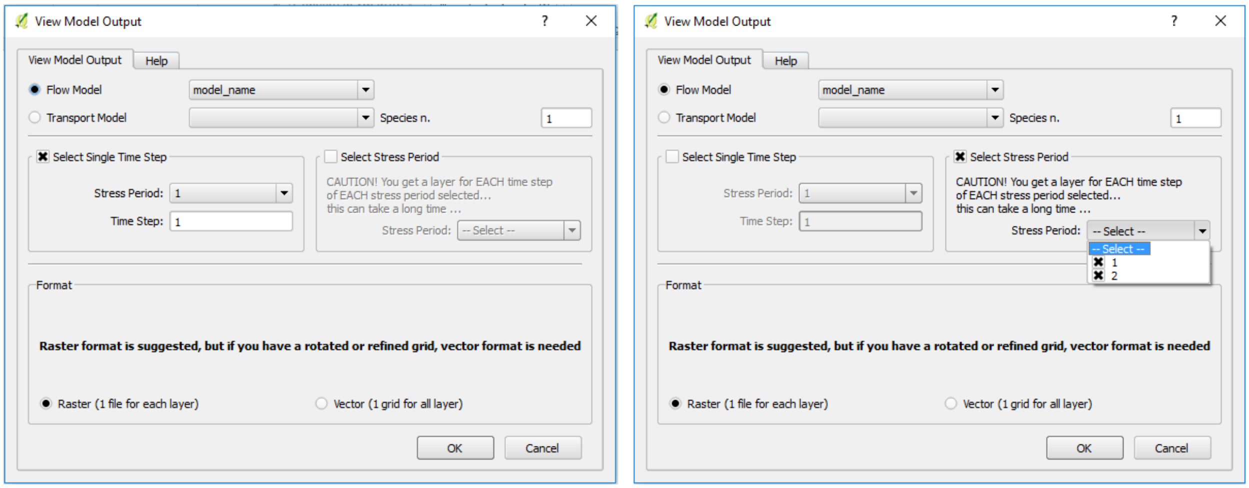
FREEWAT -> Post-processing -> View Model Output



The User has the possibility to load in the Layers Panel the simulated hydraulic head (or solute concentration) distribution for each model layer, at the end of a particular TS within a selected SP, or 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* (the output displayed will be the simulated hydraulic head in the first case, the simulated solute concentration in the second case);
- in the *Select Single Time Step* section (it must be checked if used):
  - *Stress Period*: SP number for which the simulated hydraulic head (or solute concentration) will be loaded for each model layer (it can be selected from a drop-down menu);
  - *Time Step*: TS number, within the selected SP, for which the simulated hydraulic head (or solute concentration) will be loaded for each model layer;
- alternatively, in the *Select Stress Period* section (it must be checked if used):
  - the SP number(s) for which the simulated hydraulic head (or solute concentration) will be loaded for each model layer and for eact TS must be checked from the drop-down menu close to *Stress Period*;
- in the *Format* section:
  - the output format must be selected; two options are available (*Raster (1 file for each layer)*, to get a raster file of the output solution for each model layer, *Vector (1 grid for each layer)*, to get a polygon vector file, containing one field for each model layer with the simulated hydraulic head values, or the simulated solute concentration values, at each grid cell).

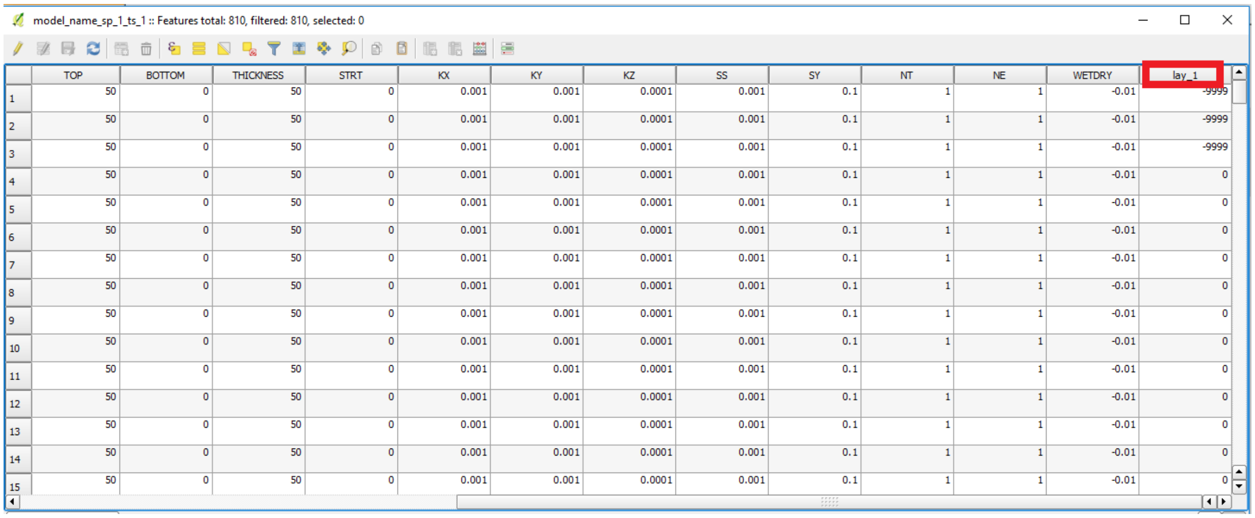


Note: If the User wishes to load the solution of a *Transport Model* simulation (i.e., the simulated concentration of a certain species for each model layer), the species number for which the solution will be displayed must be input in the *Species n.* bar.

Note: In the current version of the *FREEWAT* plugin, there is not the possibility to display output distributions for selected model layer(s). As such, an output (raster or vector) layer will be loaded in the Layers Panel for each model layer. This procedure could take a long time, according to the complexity of the model implemented, especially if the *Select Stress Period* section is used.

If the *Raster* format is selected, raster output files (one for each model layer and, potentially, for each TS within selected SP(s)) are created in the working folder and loaded in the Layers Panel with default names assigned. As an example, the raster file containing the simulated hydraulic head values for model layer 1, at the end of TS 5 within SP 2 will be renamed as *model_name_lay_1_sp_2_ts_5.asc*.

If the *Vector* format is selected, a unique polygon vector layer is created for **all** model layers and, potentially for each TS selected within a certain SP. Such polygon vector layer is saved in the model DB and loaded in the Layers Panel with a default name assigned. As an example, the polygon vector layer containing the simulated hydraulic head values for **all** model layers, at the end of TS 5 within SP 2 will be renamed as *model_name_sp_2_ts_5*. Please, notice that such vector layer is nothing but a clone of the model grid. Its Attribute Table contains the same fields contained within the Attribute Table of a model layer, filled with default values, plus an additional field for each model layer (the headings of such fields are *lay_n*, where *n* in the *n*-th model layer), with the simulated hydraulic head (or solute concentration) at each grid cell.



	TOP	BOTTOM	THICKNESS	STRT	KX	KY	KZ	SS	SY	NT	NE	WETDRY	lay_1
1	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	-9999
2	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	-9999
3	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	-9999
4	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
5	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
6	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
7	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
8	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
9	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
10	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
11	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
12	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
13	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
14	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0
15	50	0	50	0	0.001	0.001	0.0001	0.001	0.1	1	1	-0.01	0

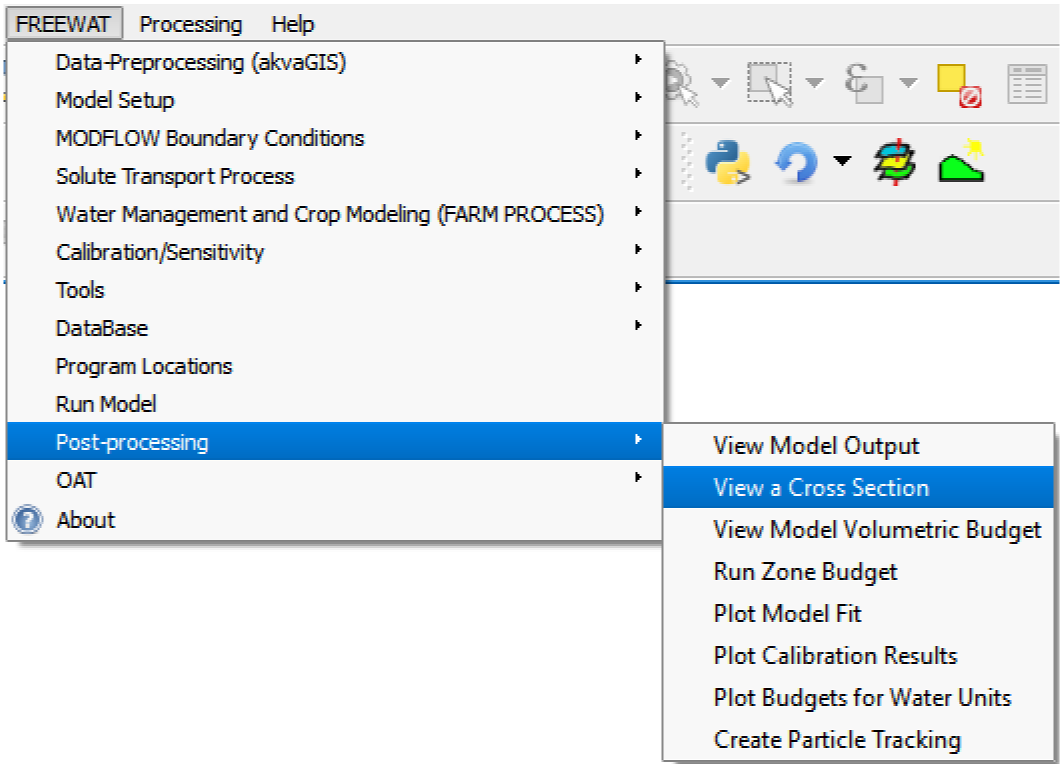
Note: *Vector* format **must** be used for rotated model grids, refined model grids or if rectangular grid cells are used. This because the *Raster* format does not allow to get raster layers with rotated or rectangular pixels.

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* or *SAGA* plugins.

Display output as a cross section

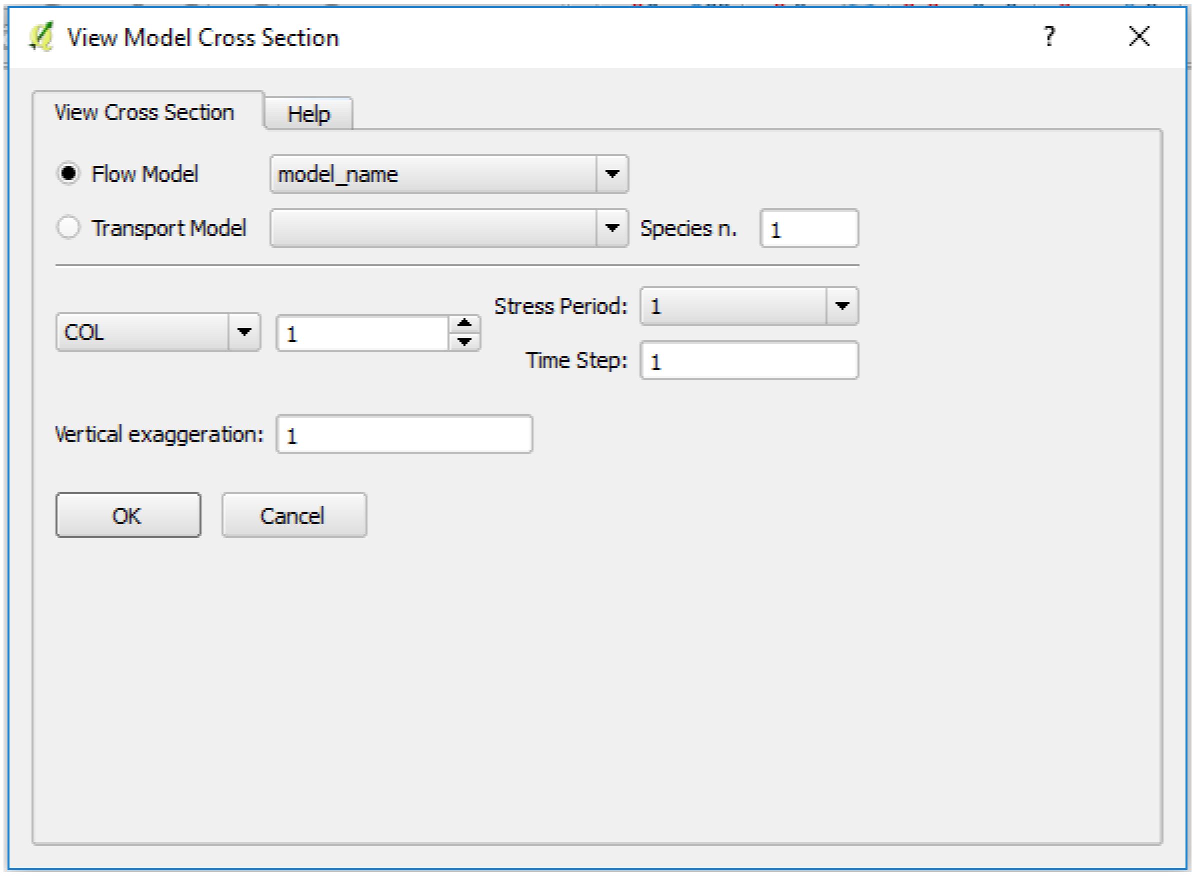
The hydraulic head (or the solute concentration) simulated can be displayed over a cross section through the following menu:

FREEWAT -> Post-processing -> View a Cross Section



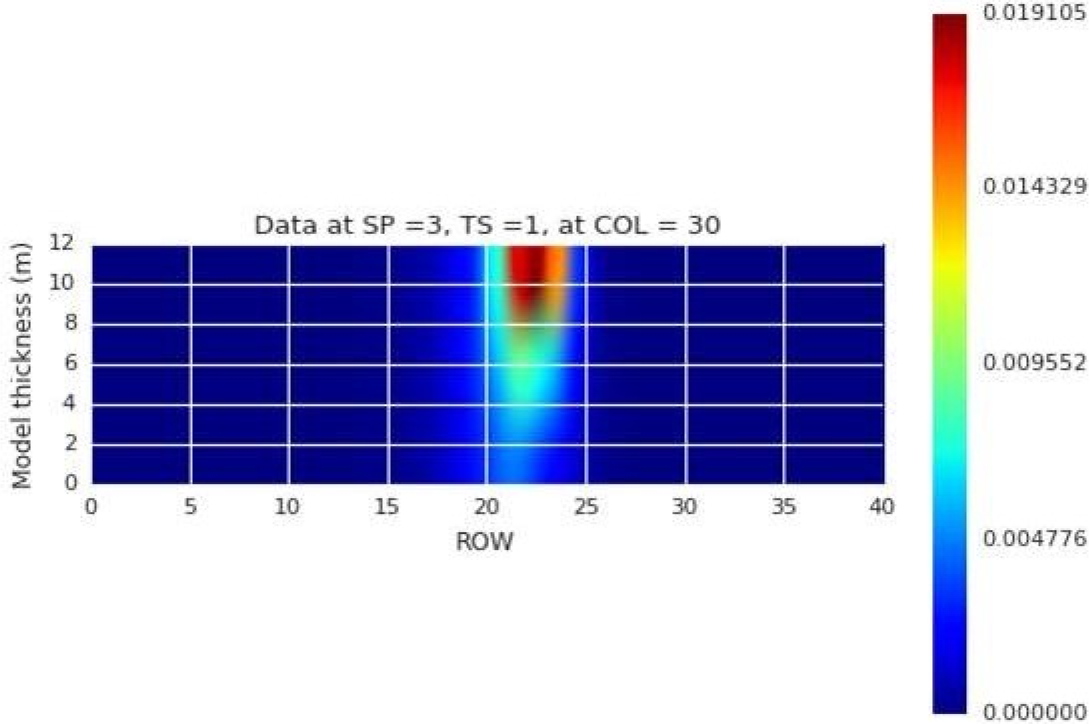
The following data are required in the **View Model Cross Section** window:

- 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* (the output displayed will be the simulated hydraulic head in the first case, the simulated solute concentration in the second case);
- in the second part of the window, the User must choose:
  - if the cross section will be drawn along a column (*COL* must be selected from the drop-down menu) or along a row (*ROW* must be selected from the drop-down menu);
  - the column or row number along which the cross section will be drawn;
  - *Stress Period*, i.e., the SP number for which the cross section will be drawn (it can be selected from the drop-down menu);
  - *Time Step*: TS number, within the selected SP, for which the cross section will be drawn;
  - the *Vertical exageration*.



Note: If the User wishes to load the solution of a *Transport Model* simulation (i.e., the simulated concentration of a certain species), the species number for which the cross section will be drawn must be input in the *Species n.* bar.

Hereinafter, the solute concentration simulated at the end of TS 1 within SP 3 is represented as a cross section along the 30th column of the model grid.

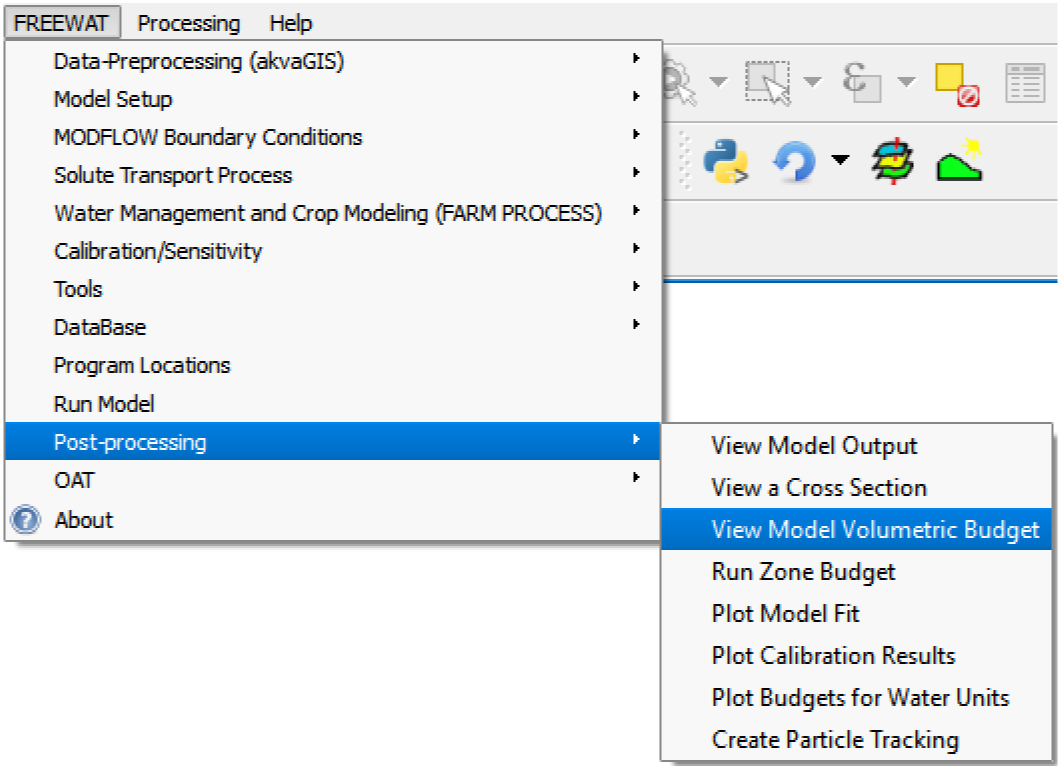


Note: This post-processing tool is still under development. The User will get a reasonable output **only** for model layers with flat top and bottom surfaces and with *ACTIVE = 1* all over the model grid.

Display model budget

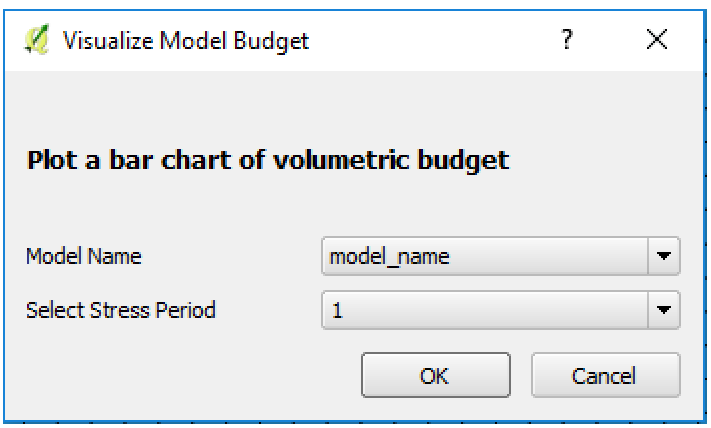
Among the model outputs, the volumetric budget can be displayed as well through the following menu:

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

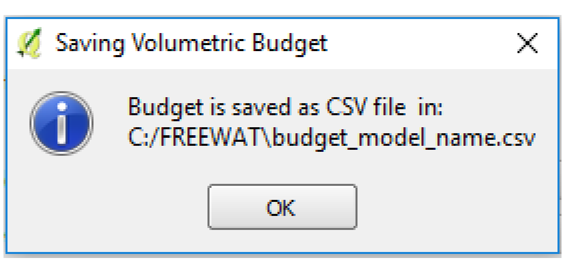


The following data are required in the **Visualize Model Budget** window:

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



Once clicking *OK*, the information window **Saving Volumetric Budget** appears stating that a csv file renamed as *budget_model_name.csv* has been saved in the working folder.

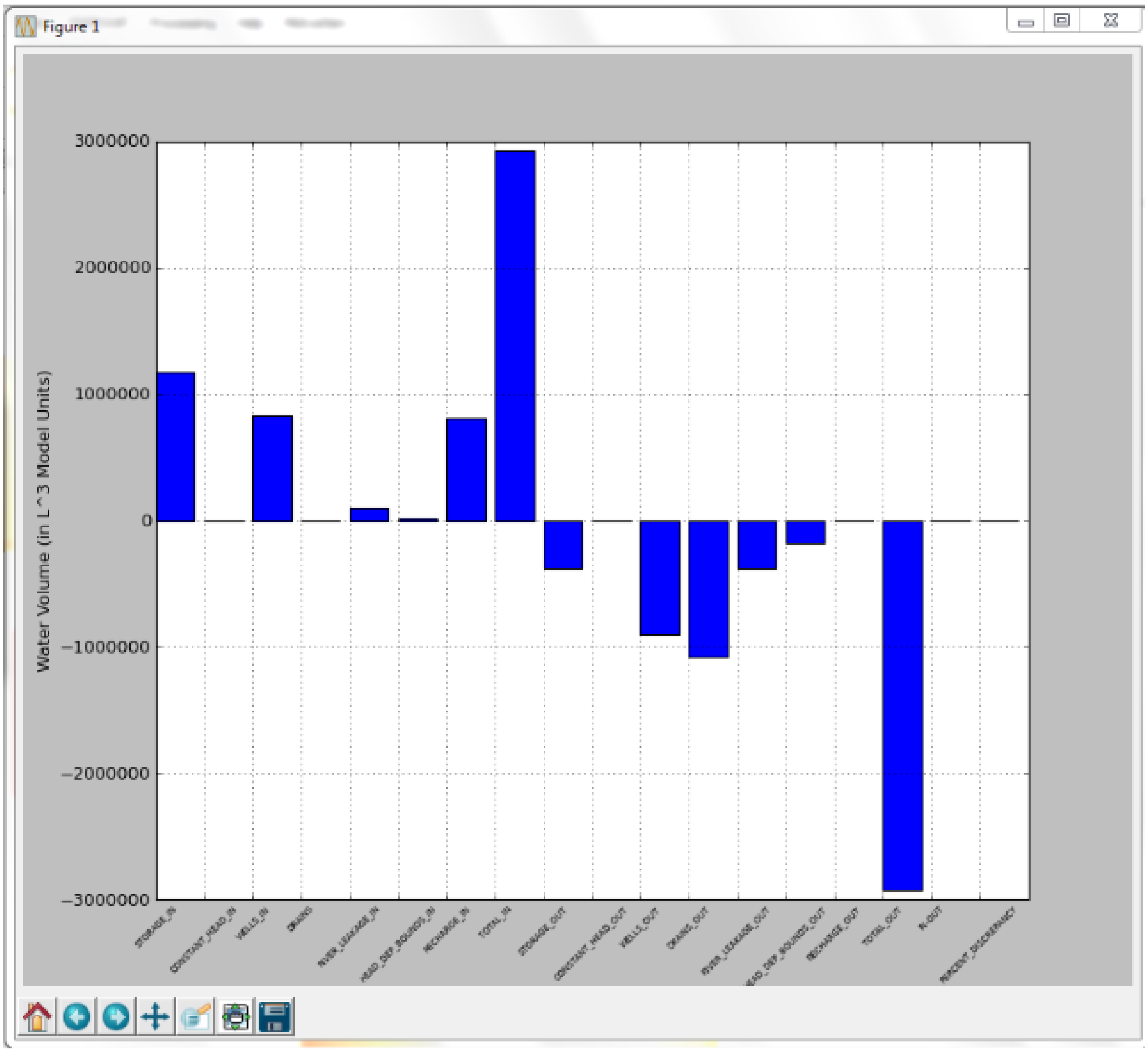


This csv file contains input and output simulated budget terms, in terms of cumulative volumes $[L^3]$ and flow rates $[L^3/T]$, at the end of each SP. As an example, the column *Volume StressPeriod 1* reports cumulative volumes calculated at the end of SP 1, while the column *Rate StressPeriod 1* reports flow rates calculated at the end of SP 1.

budget_model_name.csv

```
VOLUMETRIC BUDGET of MODEL "model_name"
Budget_Term, Volume StressPeriod 1, Rate StressPeriod 1, Volume Stress Period 2, Rate StressPeriod 2
STORAGE_IN ,   0.000000 ,   0.000000,   0.000000 ,   0.000000
CONSTANT_HEAD_IN ,   0.000000 ,   0.000000,   0.000000 ,   0.000000
TOTAL_IN ,   0.000000 ,   0.000000,   0.000000 ,   0.000000
STORAGE_OUT ,  -0.000000 ,  -0.000000,  -0.000000 ,  -0.000000
CONSTANT_HEAD_OUT ,  -0.000000 ,  -0.000000,  -0.000000 ,  -0.000000
TOTAL_OUT ,  -0.000000 ,  -0.000000,  -0.000000 ,  -0.000000
IN-OUT ,   0.000000 ,   0.000000,   0.000000 ,   0.000000
PERCENT_DISCREPANCY ,   0.000000 ,   0.000000,   0.000000 ,   0.000000
```

A bar chart is displayed as well, with cumulative volumes $[L^3]$ along the Y axis and flow terms along the X axis, at the end of the SP selected in the **Visualize Model Budget** window.

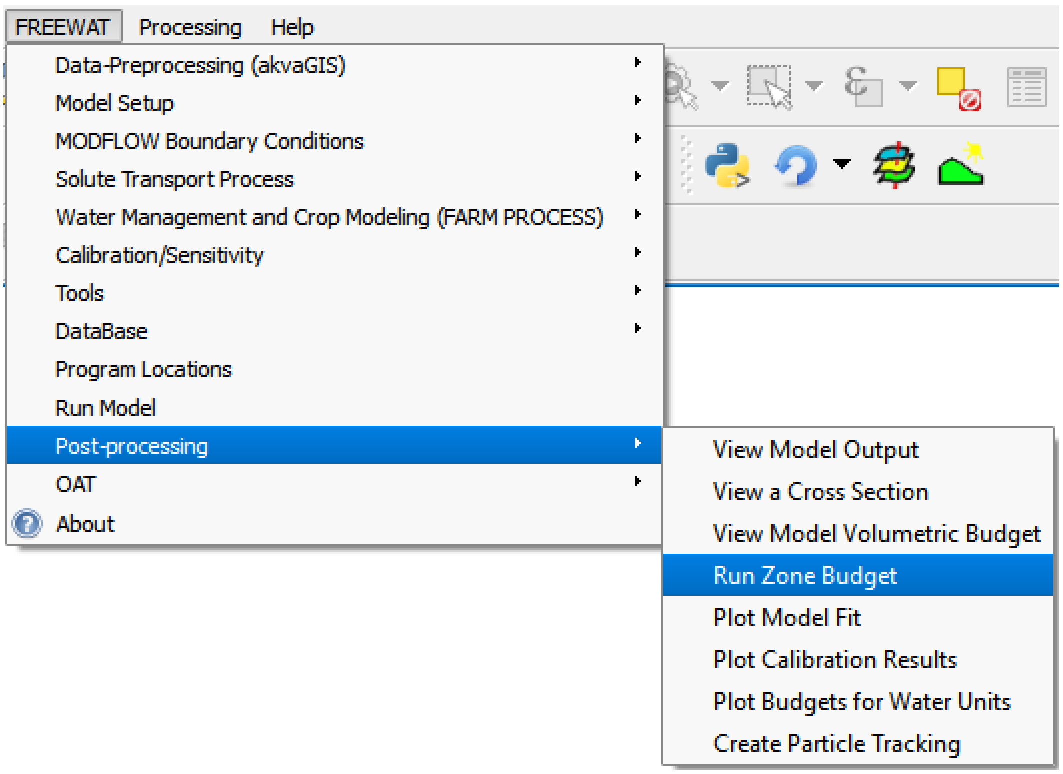


Note: Bar charts can be saved as images with different formats. Saving them as .png images could produce a minidump error.

Run ZONE BUDGET

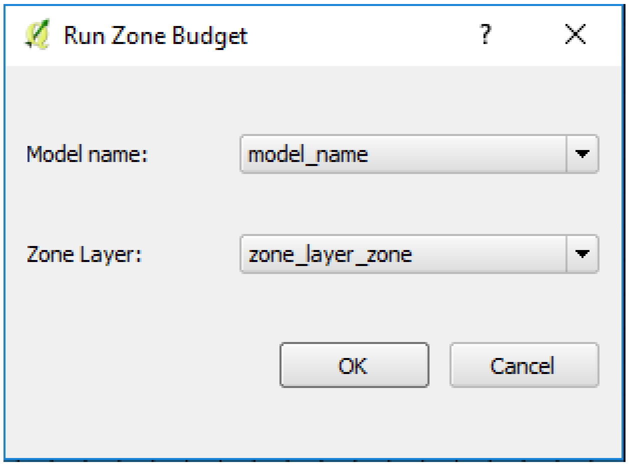
If a zonbud MDO has been created (see Chapter 6) and the path for the *ZONE BUDGET* executable has been defined in the *prg_locations_model_name* table (see Chapter 3), the *ZONE BUDGET* executable can be run through the following menu:

FREEWAT -> Post-processing -> Run Zone Budget

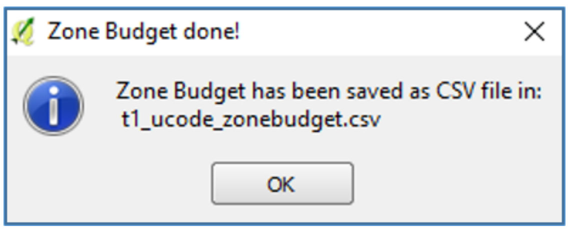


The following data are required in the **Run Zone Budget** window:

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



Once the run of the *ZONE BUDGET* is successfully completed, an information window appears, stating that a csv file containing water balance for different zones defined has been saved in the working directory.



Such a csv file, renamed *model_name_zonebudget.csv*, can be used by the User for additional analysis of the water budget. It reports budgets for each zone at the end of each TS.

Hereinafter, an example on how to analyze the zones budgets reported in the csv file is provided.

totim	time_step	stress_period	name	ZONE_1	ZONE_2	ZONE_3	ZONE_4
365	0	0	STORAGE_IN	0	0	0	0
365	0	0	CONSTANT_HEAD_IN	0	0	0	0
365	0	0	ZONE_1_IN	0	7401.26	23938.9	44470.2
365	0	0	ZONE_2_IN	53722.5	0	0	0
365	0	0	ZONE_3_IN	22087.9	46321.2	0	0
365	0	0	ZONE_4_IN	0	0	44470.2	0
365	0	0	TOTAL_IN	75810.4	53722.5	68409.1	44470.2
365	0	0	STORAGE_OUT	0	0	0	0
365	0	0	CONSTANT_HEAD_OUT	0	0	0	0
365	0	0	ZONE_1_OUT	0	53722.5	22087.9	0
365	0	0	ZONE_2_OUT	7401.26	0	46321.2	0
365	0	0	ZONE_3_OUT	23938.9	0	0	44470.2
365	0	0	ZONE_4_OUT	44470.2	0	0	0
365	0	0	TOTAL_OUT	75810.4	53722.5	68409.1	44470.2
365	0	0	IN-OUT	0	0.007813	0	0
365	0	0	PERCENT_DISCREPANCY	0	1.45E-05	0	0

In this example, budget for Zones 1 to 4 is reported for SP 1 and TS 1. Notice that in this file SPs and TSs are numbered starting from 0. Furthermore, the *totim* value refers to the length of the comulative time of that selected TS (e.g., in this example we are analyzing results at the end of SP 1 and TS 1, whose length is 365 days).

The figure above highlights water exchange between Zone 1 and Zone 2. The term *ZONE_2_IN* indicates the amount of water entering Zone 1 from Zone 2. Conversely, *ZONE_2_OUT* reports water exchange from Zone 1 towards Zone 2.

Note: To run the *ZONE BUDGET*, the run of the groundwater flow model must have been successfully completed.

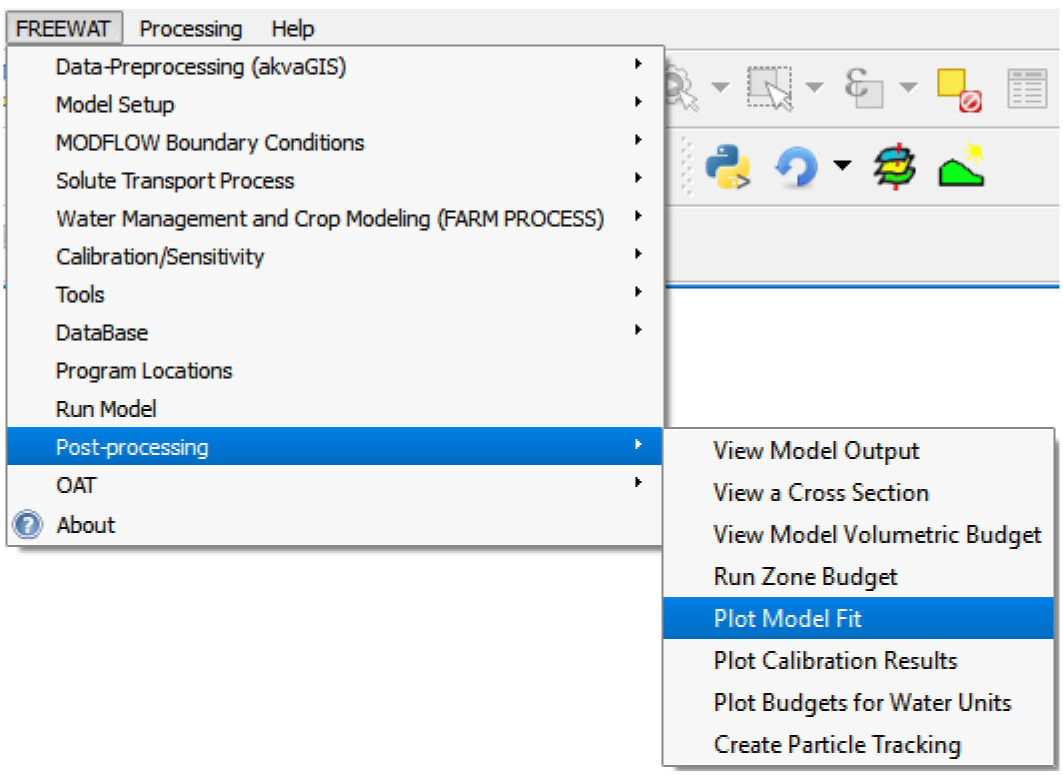
Plot Model Fit

A simple tool to evaluate model fit without running *UCODE* (further details in Volume 6) is also available among the post-processing tools. It allows to compare simulated hydraulic head and observations at a certain SP.

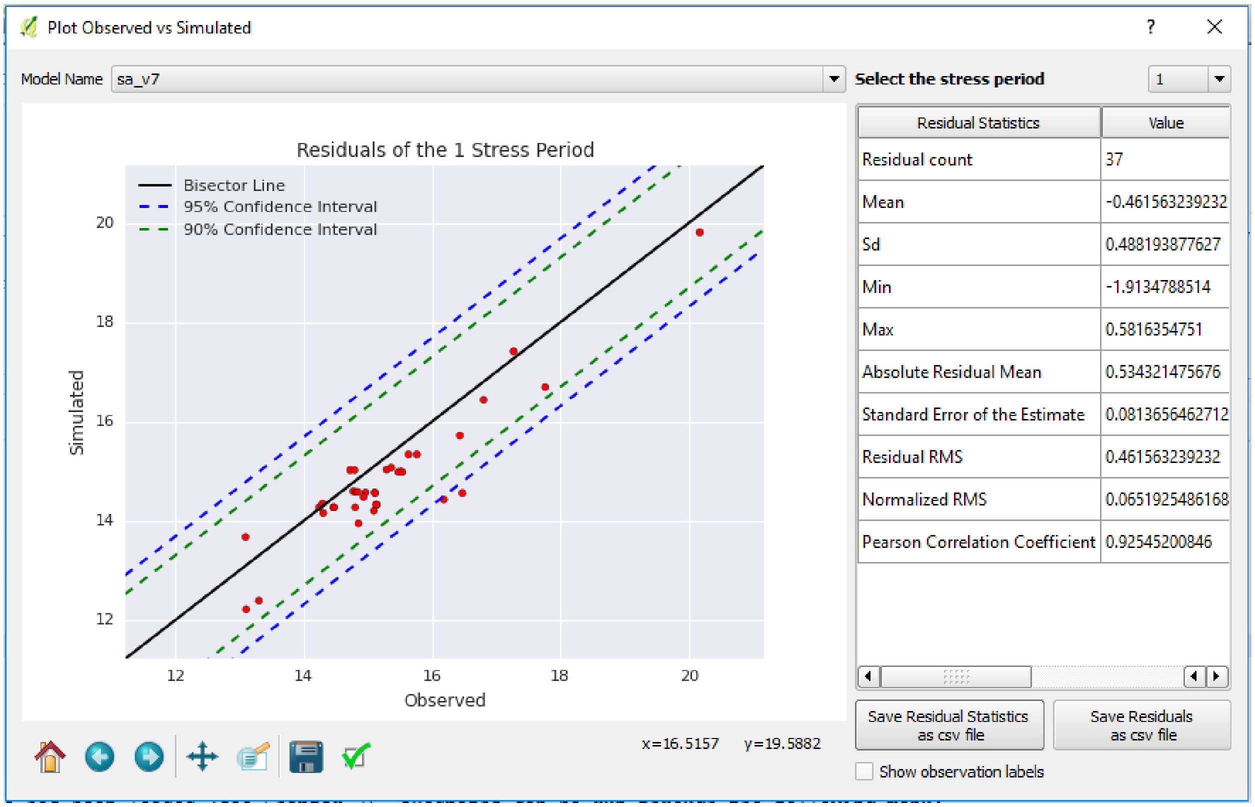
Note: Using the *Plot Model Fit* tool requires a prior, successful run of the *MODFLOW* model **with** the HOB Package checked (see Chapter 7 of this Volume and refer to Volume 6 for creation of an hob MDO).

The *Plot Model Fit* tool can be used through the following menu:

FREEWAT -> Post-processing -> Plot Model Fit



The window **Plot Observed vs Simulated** pops up:



The scatter plot shows observed vs. simulated values at the SP indicated in the drop-down menu close to *Select the stress period*. The bisector line, 90% and 95% confidence intervals are shown as well. Labels with the names of the observation points can be added, by clicking on *Show observation labels* at the lower right corner of the **Plot Observed vs Simulated** window.

Some statistics related to residuals (i.e., simulated minus observed values) are shown as well:

- *Residual count* (i.e., the number of observation points over which residuals are calculated);
- *Mean* (i.e., arithmetic average of residuals);
- *Sd* (i.e., standard deviation);
- *Min* (i.e., minimum residual);
- *Max* (i.e., maximum residual);
- *Absolute Residual Mean*;
- *Standard Error of the Estimate*;
- *Residual RMS*;
- *Normalized RMS*;
- *Pearson Correlation Coefficient*.

Such statistics can be saved in a csv file within the working directory, by clicking on *Save Residual Statistics as csv file* at the lower right corner of the **Plot Observed vs Simulated** window. Such csv file is renamed as *model_name_residuals_statistics_sp_n.csv*, where *n* is the number of the *n*-th SP.

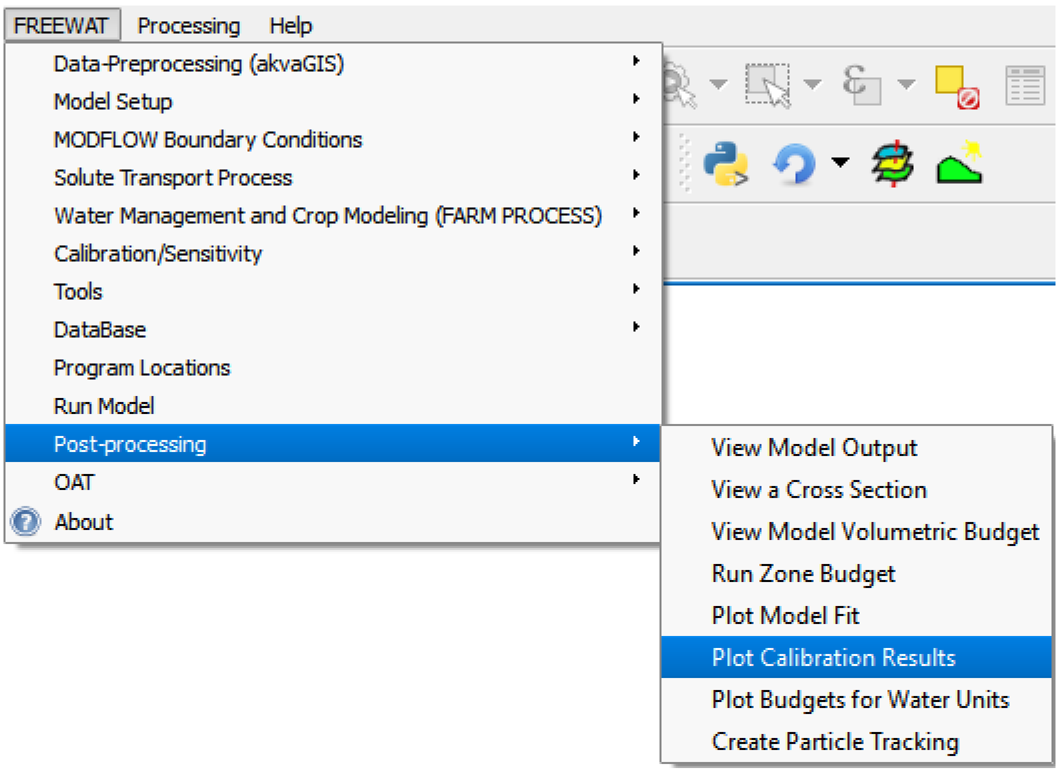
Residuals can be saved as well in a csv file within the working directory, by clicking on *Save Residuals as csv file* at the lower right corner of the **Plot Observed vs Simulated** window. Such csv file is renamed as *model_name_residuals_sp_n.csv*, where *n* is the number of the *n*-th SP, and contains residuals calculated at each observation point, for which the observation name is reported.

Plot Calibration Results

A more advanced tool, to evaluate model fit analyzing sensitivity analysis and parameter estimation results obtained through running *UCODE*, is available as well among the post-processing tools.

The *Plot Calibration Results* tool can be used through the following menu:

FREEWAT -> Post-processing -> Plot Calibration Results



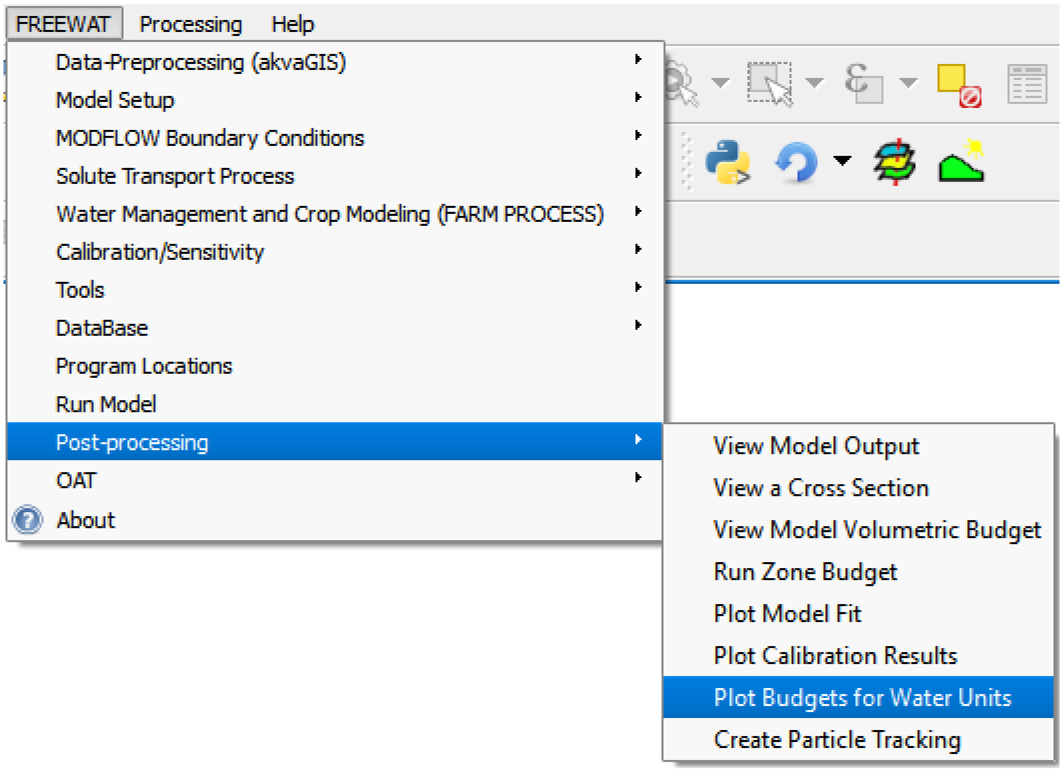
For further details about the *Plot Calibration Results* tool, the reader is referred to Volume 6.

Plot Budgets for Water Units

A further post-processing tool allows to plot budget terms for water units for the analysis of conjunctive use of ground- and surface-water (please, refer to Volume 3).

The *Plot Budgets for Water Units* tool can be used through the following menu:

FREEWAT -> Post-processing -> Plot Budgets for Water Units

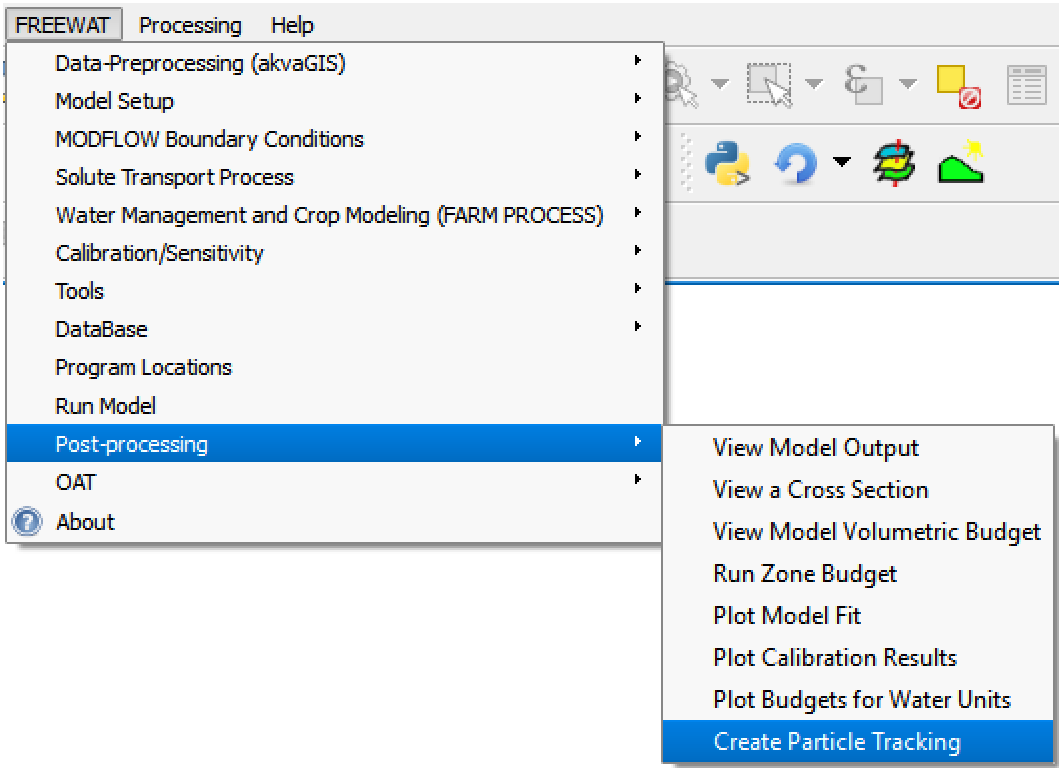


For further details about the *Plot Budgets for Water Units* tool, the reader is referred to Volume 3.

Run MODPATH

If the path for the *MODPATH* executable has been defined in the *prg_locations_model_name* table (Version 6.0.01 is needed; see Chapter 3), the *MODPATH* executable can be run through the following menu:

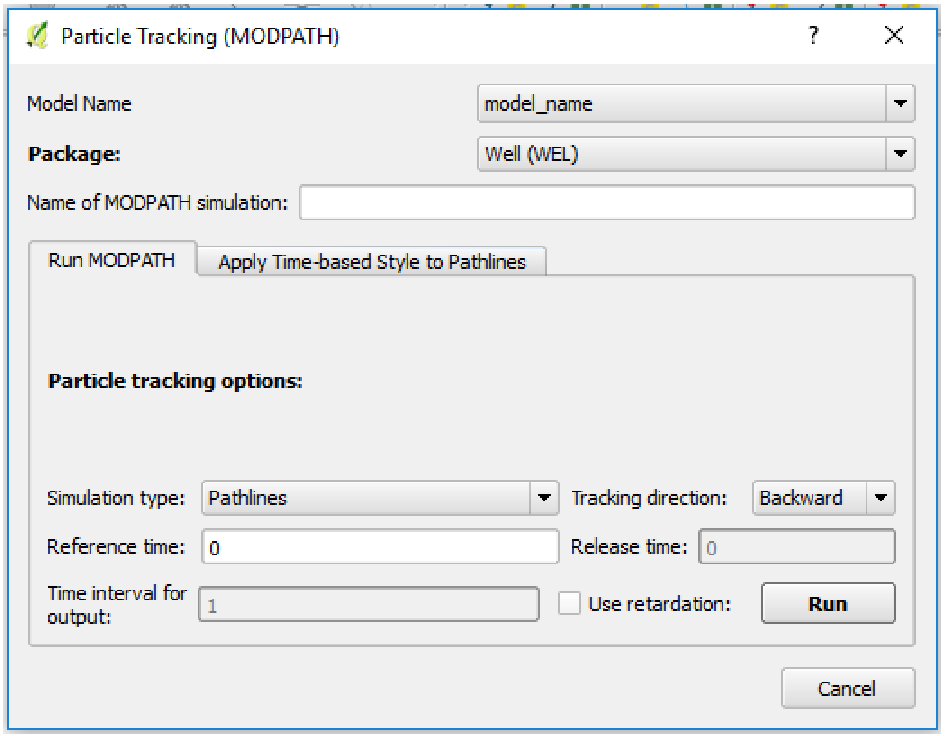
FREEWAT -> Post-processing -> Create Particle Tracking



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

- *Model Name*: name of the hydrological model;
- *Package*: *MODFLOW* Package which will be used to apply particle tracking; two options (*Well (WEL)* and *Recharge (RCH)*) are available in the current version of the *FREEWAT* plugin;
- *Name of MODPATH simulation*: name to assign to the MODPATH simulation;
- 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 User wishes to record the end point only of the path of each particle);
  - *Tracking direction*: two options are available (*Forward*, if the User wishes to track particles in the downstream direction; *Backward*, if the User wishes to track particles 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 [T] (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 run of the groundwater flow model must have been successfully completed.

Note: Once the *Well (WEL)* or *Recharge (RCH)* option is selected as a *Package*, the particle tracking is applied at all the cells contained in the wel or rch MDOs, respectively, that have been used for the model run. This could require a very long time for the *MODPATH* post-processing, especially for models having more than 10000 cells.

However, the User has the possibility to select only cells within the wel or rch MDOs where the application of *MODPATH* is really needed.

To do that, the following steps must be done:

- create a new wel (or rch) MDO containing **only** the wells to which *MODPATH* has to be applied (for instance selecting those cells in the original MDO and then saving the MDO as a shapefile with another name, but being sure to save *only selected features*). Important: this shapefile must be saved with a name ending with *_wel* (or *_rch*);
- fill again the *Run* window (see Chapter 7), selecting this shapefile whose name ends with *_wel* (or *_rch*) for the *WEL* (or *RCH*) Package;
- check the checkbox *Only Write Input Files* and click the *Run* button (only the *MODFLOW* input files will be written, without performing the *MODFLOW* run);
- open and fill again the **Particle Tracking (MODPATH)** window, selecting the *Well (WEL)* (or *Recharge (RCH)*) option as *Package*, and run *MODPATH*.

For a more detailed guideline on this procedure, the User is referred to the *Particle Tracking Tutorial*, available on the *FREEWAT* website.

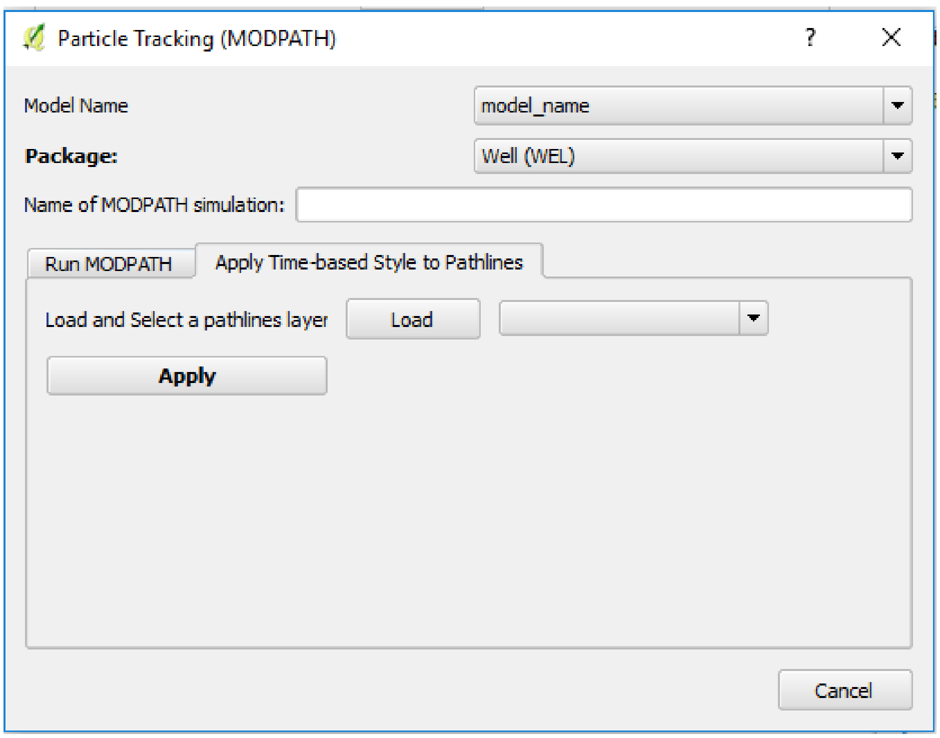
Once the run of *MODPATH* is successfully completed, the following *MODPATH* input files are created and stored in the working folder:

- **.mpn** contains the list of *MODFLOW/MODPATH* files needed for the simulation of particle tracking;
- **.mpbas** consists of a combination of data contained in the *MODFLOW* BAS and LPF files (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.

A *MODPATH* 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 (the point shapefiles are renamed as *modpath_simulation_name_particles_lay_1.shp*, *modpath_simulation_name_particles_lay_2.shp*, ..., *modpath_simulation_name_particles_lay_n.shp*, while the line shapefiles are renamed as *modpath_simulation_name_pathlines_lay_1.shp*, *modpath_simulation_name_pathlines_lay_2.shp*, ..., *modpath_simulation_name_pathlines_lay_n.shp*, where *n* is the maximum number of model layers implemented).

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 drop-down menu. 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 (especially if *MODPATH* has been applied to tens of wells), so it is suggested to use it just for model layers of interest.

CHAPTER 9

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31/01/2016 release of version beta 1.0

(new post-processing tool to visualize model budget; minor changes in the text)

31/07/2016 release of version 0.1

(minor changes in the text)

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

31/01/2017 release of version 0.3.1

(new cover page; description of the *Plot Model Fit* tool; minor changes in the text)

31/03/2017 release of version 0.4

(new FAQ Chapter inserted; minor changes in the text)

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(new section in Chapter 1, describing the manual installation procedure; minor changes in the text)

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(minor changes in Chapter 8 , post-processing)

30/09/2017 release of version 1.0

(major changes in Chapter 6 related to *MODFLOW CHD, WEL* and *GHB Packages*; the FAQ Chapter has been removed; minor changes in the text)

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(section Telescopic Mesh Refinement added; minor changes in the text)