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 0.5
July 27th, 2017

This version is confidential, only for FREEWAT Project Partners
FREEWAT User Manual - Volume 1

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

Version 0.5
July 27th, 2017

By G. De Filippis(1), M. Ghetta(1), J. Neumann(2), M. Cardoso(2), M. Cannata(2), I. Borsi(3)
and R. Rossetto(1)

(1) Istituto di Scienze della Vita – Scuola Superiore Sant'Anna, Pisa (IT)
(2) Istituto di Scienze della Terra – SUPSI, Canobbio (CH)
(3) TEA SISTEMI SpA, Pisa (IT)

This project has received funding from the European Union's Horizon 2020 research
and innovation programme under grant agreement No 642224

This project document reflects only the authors' views and the European Union is not
liable for any use that may be made of the information contained therein.
FREEWAT Development has received funding from the following projects:

1. Hydrological part has been developed starting from a former project, named SID&GRID, funded by Regione Toscana through EU POR-FSE 2007-2013 (sidgrid.isti.cnr.it)

2. Porting of SID&GRID under QGis has been performed through funds provided by Regione Toscana to Scuola Superiore S.Anna - Project Evoluzione del sistema open source SID&GRID di elaborazione dei dati geografici vettoriali e raster per il porting negli ambienti QGis e Spatialite in uso presso la Regione Toscana (CIG: ZA50E4058A)

3. Saturated zone solute transport simulation capability has been developed within the EU FP7-ENV-2013-WATER-INNO-DEMO MARSOL. MARSOL project receives funding from the European Union's Seventh Framework Programme for Research, Technological Development and Demonstration under grant agreement n. 619120 (www.marsol.eu)

4. 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)

Suggested citation:


License:

FREEWAT documentation is licensed as Creative Commons Attribution – Share Alike (CC BY-SA, https://creativecommons.org/licenses/by-sa/3.0/).
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 iii

1 FREEWAT Installation & Requirements 1
  1.1 Installing QGIS ........................................... 1
  1.2 Installing the FREEWAT plugin .......................... 1
  1.3 Starting FREEWAT ....................................... 3
  1.4 Manual installation procedure .......................... 6

2 FREEWAT Hydrological Model 9
  2.1 Simulated processes .................................... 9
  2.2 Workflow of the FREEWAT plugin ....................... 10
  2.3 Limitations ............................................. 12

3 Creating a new hydrological model and geodatabase 13
  3.1 Importing a DB ......................................... 18

4 Space and time discretization 22
  4.1 Creating the finite-difference grid .................... 22
     4.1.1 Rotated grid ....................................... 27
  4.2 Defining model layers .................................. 33
  4.3 Time discretization .................................... 38

5 Tools for model layers parameterization 40
  5.1 Manual editing with selection tools ................. 40
  5.2 Copy from vector layer ................................ 44
  5.3 Copy from raster layer ................................ 47

6 Implementing processes to be simulated: boundary conditions and source/sink terms 49
  6.1 Time Variant Specified Head - CHD ................. 50
  6.2 Well - WEL (specified-flux) .......................... 53
  6.3 Multi-Node Well - MNW (head-dependent flux) .... 56
     6.3.1 Limitations ....................................... 60
  6.4 Recharge - RCH (specified-flux) ...................... 60
  6.5 River - RIV (head-dependent flux) .................... 63
  6.6 Lake - LAK (head-dependent flux) .................... 71
     6.6.1 Limitations ....................................... 80
  6.7 Drain - DRN (head-dependent flux) ................... 81
  6.8 General-Head Boundary - GHB (head-dependent flux) 88
  6.9 Evapotranspiration - EVT (head-dependent flux) .... 95
  6.10 Unsaturated-Zone Flow Package - UZF ............... 99
     6.10.1 Creating the uzf MDO ............................ 100
     6.10.2 Creating the Surface Model Layer MDO ............ 103
     6.10.3 Limitations ....................................... 106
Abstract

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

The 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 cells. Flow associated with external stresses, such as wells, areal recharge, evapotranspiration, drains, and rivers, 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 (Hanson et al., 2014).

MODFLOW-OWHM is a free code developed by the U.S. Geological Survey aimed at simulating the whole hydrological cycle. It is the latest and most complete version, to date, of the MODFLOW family of hydrological simulators and it is an evolution of the previous version. The need to properly manage the conjunctive use of ground- and surface-water required extending MODFLOW-2005 to a fully-coupled, integrated hydrological model 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 integrating the Farm Process within MODFLOW-2005. Farm Process module 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 install and to activate the FREEWAT plugin (Chapter 1), and it contains 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 through the UZF Package. Among the new groundwater flow simulation capabilities embedded in MODFLOW and implemented within the FREEWAT platform, it is worth mentioning the inclusion of the latest version of the Multi-Node Well Package (MNW2; Konikow et al., 2009), used also to simulate farm wells in Farm Process (refer to Volume 3), and the Lake Package (LAK; Merrit and Konikow, 2000) for the simulation of lake-aquifer interaction.

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

FREEWAT has been tested so far within the following QGIS versions:

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

**Note:** Please, notice that some Users are experiencing problems when installing FREEWAT under QGIS 2.18.6 or later. In order to avoid any drawback, we warmly recommend to downgrade to one of the previous QGIS versions (the LTR version 2.14 or 2.16).

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. Furthermore, having QGIS and ArcGIS jointly installed on the same pc is strongly discouraged for the same reason.

1.2 Installing the FREEWAT plugin

In all the Operative Systems, 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 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) 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.

• **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`;
  - `xlsx`.

![Install missing dependencies window](image)

**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.

1.3 Starting 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 -> Manage and Install Plugins... type **FREEWAT** in the Search bar and click on the checkbox to activate the plugin, as shown in the picture below:
The *FREEWAT* platform can now be used by following the logical workflow presented in the following Chapters.

**Note:** It can happen that, even if all the needed dependencies have been correctly installed (and *FREEWAT* appears in the toolbar of the *QGIS* GUI), installation procedure starts each time you re-run *QGIS*. If this happens, a txt file 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`. 
1.4 Manual installation procedure

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

- Close QGIS if it is open:
• From the START button search OSGeo4W Shell -> right click on it and **open as administrator**;

• Type the following instructions one by one (each time you click Enter 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

• 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 -> Manage and Install Plugins...**, type **FREEWAT** in the **Search** bar and click on the checkbox to activate the plugin.
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.

2.1 Simulated processes

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

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

- **Basic Packages:**
  - Basic (BAS)
  - Discretization (DIS)
  - Layer Property Flow (LPF)

- **Hydrogeological processes:**
  - specified-head boundaries
    * Time-Variant Specified Head (CHD)
  - specified-flux boundaries
    * Recharge (RCH)
    * Well (WEL)
  - head-dependent flux
    * Unsaturated Zone Flow (UZF)
2.2 Workflow of the FREEWAT plugin

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

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

The FREEWAT terminology is the following:

- **GIS layer** - it indicates a generic geographic informative layer, not still processed for the modelling scenario;
- **model layer** - the discrete domain is divided in $n$ layers (model layers) corresponding to the hydrostratigraphic units identified in the conceptual model;
- **Model Data Object (MDO)** - it is the GIS layer processed according to the model properties and containing at least the information on both spatial (row and column) and temporal (Stress Period - SP) discretization;
- **model file** - is a text file generated from an MDO and required to run the simulation.
The User has to organize all the GIS data (vector and raster) referring to the study area. This means importing or creating each layer in QGIS in a proper Coordinate Reference System (CRS), eventually clipping it according to the extent of the study area.

Furthermore, model layers and MDOs are permanently stored within a SpatiaLite geodatabase.

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

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

Finally, once selected all the Packages which have to be activated for the aims of the simulation, all of the model layers and MDOs are translated in MODFLOW input files and the model can be run, as described in Chapter 7.

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

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

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

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

Anyway, these limitations concern only the GUI. The advanced User can eventually edit the MODFLOW input files created and set there flags and parameters as needed.
CHAPTER 3

Creating a new hydrological model and geodatabase

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

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

FREEWAT -> Model Setup -> Create Model

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

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

---

**Note:** There should not be spaces and/or special characters in the path of the *Working Folder*.

Once the new model is created, the corresponding model DB is created as *model_name.sqlite* and an *Information* window appears reporting that the model DB has been stored within the selected *Working Folder*.

The model DB can be consulted by using *QGIS* tools. For example, with the *DB Manager* plugin each MDO stored within the model DB can be simply renamed, deleted or added to the Map Canvas as needed.

Three tables named *modeltable_model_name*, *timetable_model_name* and *prg_locations_model_name* are loaded in the Layers Panel and stored within the model DB.
The model table contains the following fields:

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

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) or through the menu **FREEWAT -> Model Setup -> Update Working Directory** (see details in section **Importing a DB**).

The time table contains the following fields:

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

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

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

A path for the needed executables can be set using the browse button which appears at each cell of the field *executable*. The following executables are needed, according to the processes to be simulated (the folder *executables* is available, containing all the executables 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 coupled flow and transport modeling in the saturated zone with *SEAWAT* (Langevin et al., 2007);
- **UCODE** for sensitivity analysis and parameter estimation with *UCODE* (Poeter et al., 2014);
- **ZONE** to explicit the water budget for different zones of the active domain with *ZONE BUDGET* (Harbaugh, 1990);
- **MODPATH** for particle-tracking post-processing model with *MODPATH* (Pollock, 2016).
Note: Once loaded all the executables needed through the browse button, it is necessary to click wherever out of the last cell edited, so that the paths of the executables are 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 just need to be loaded in the prg_locations_model_name table.

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

FREEWAT -> Program Locations.
3.1 Importing a DB

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

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

To import the DB, in the QGIS GUI, the User must use the button Add SpatiaLite Layer.

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 loaded in advance, the User must previously delete the old one.

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

Once the DB is connected, some layers with MULTIPLYYGON geometry type should be displayed, corresponding to the MDO stored within the DB itself. The User must select all these MDOs and click on Add to add them to the Layers Panel.
As some tables are also needed, the User must check the *Also list tables with no geometry* checkbox (at the lower left corner of the *Add Spatialite Layer(s)* window), select the tables needed and click on *Add* to add them to the Layers Panel.

The following tables are **mandatory**:  
- *model table*;  
- *time table*;  
- *lpf table*;  
- *program locations*.

Furthermore, if the SFR Package is implemented, the related table must be loaded (further details will be provided in Chapter 6).
Once all the needed MDOs and tables are loaded in the Layers Panel, the path of the Working Directory in the model table must be updated through the following menu:

**FREEWAT -> Model Setup -> Update Working Directory**

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

- **Model Name**: name of the new hydrological model;
- **Working Directory**: folder within which the .sqlite file has been saved and where the MODFLOW input files and the output files will be stored (it must be selected through the **Browse** button).
The path for all the needed executables must be updated as well editing the fields *executable* in the table of program locations.
Once the input geographical files are ready and the conceptual model defined, it is necessary to set up the 3D geometry of the aquifer system (i.e., the finite-difference horizontal grid and the vertical discretization) and the time discretization of the simulation. It is so required defining:

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

### 4.1 Creating the finite-difference grid

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

To create the finite-difference grid, the extent of the study area must be known. For this purpose, a polygon shapefile, which limits 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 size is 100 m, each border can extend for 1000 m, but not for 1025 m). Alternatively, a background map cut to the study area extent can be used.

To create the grid, 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:**
  - the polygon shapefile previously created (if any), containing the extent of the domain, 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. There are three options to specify them:
    * they can be loaded from a polygon shapefile containing the extent of the domain, 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 entered 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;

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

**Note:** The extension `_grid` must not be changed in the Layers Panel and neither in the DB, as the grid MDO will be filtered in each dialog according to such extension.
The Attribute Table of such MDO may contain several records, according to the number of grid cells, and the following fields:

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

It is also possible to build a model based on a rotated grid.

The steps which need to be performed to get a 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 inland 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 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).
**Step 5** Be sure that the grid MDO is selected in the Layers Panel (it must be highlighted in blue in the Layers Panel) and activate the *Toggle Editing* mode.
Step 6 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 7 Save your edits, deactivate the Toggle Editing mode and deselect all cells.
4.2 Defining model layers

Once defined the model grid, the user can create the model layers corresponding to the hydrostratigraphic units identified in the conceptual model. Each model layer will be stored within the model DB as 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 current model layer;

• **TOP**: height of the top surface of the model layer [L] with respect to a reference plan;

• **BOTTOM**: height of the bottom surface of the model layer [L] with respect to a reference plan;

• **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 MDOs are limited by flat horizontal surfaces. These fields can be edited later.

A new MDO is created, stored within the model DB and loaded in the Layers Panel for each model layer created.
The Attribute Tables of such MDOs may contain several records, according to the number of grid cells, and the following fields:

- **PKUID**: database primary key (it must not be modified);
- **ID**: database primary key (it must not be modified);
- **ROW**: row number of a grid cell;
- **COL**: column number of a grid cell;
- **BORDER**: integer value which allows to distinguish between a border cell (i.e., a cell along the border of the
domain - \textit{BORDER}=1) and an internal one (\textit{BORDER}=0);

- \textit{ACTIVE}: integer value corresponding to the \textit{IBOUND} flag in \textit{MODFLOW} (Harbaugh, 2005), which allows to distinguish among active variable-head cells (i.e., where the hydraulic head will be computed at each iteration - \textit{ACTIVE}=1), non-active cells (i.e., where the groundwater flow equation is not solved - \textit{ACTIVE}=0) and active specified-head cells (i.e., where the hydraulic head is specified and does not vary throughout the simulation - \textit{ACTIVE}=-1);

- \textit{TOP}: height of the top surface of the model layer at each cell [L];

- \textit{BOTTOM}: height of the bottom surface of the model layer at each cell [L];

- \textit{THICKNESS}: thickness of the model layer, calculated as \textit{TOP} minus \textit{BOTTOM} at each cell [L];

- \textit{STRT}: hydraulic head assigned at each cell at the beginning of the simulation (initial condition) [L];

- \textit{KX}: hydraulic conductivity along the x direction [L/T];

- \textit{KY}: hydraulic conductivity along the y direction [L/T];

- \textit{KZ}: hydraulic conductivity along the z direction [L/T];

- \textit{SS}: specific storage [L$^{-1}$];

- \textit{SY}: specific yield;

- \textit{NT}: total porosity;

- \textit{NE}: effective porosity;

- \textit{WETDRY}: flag indicating if the cell can be re-wetted thanks to water exchange with the cell below it (\textit{WETDRY}<0), or with the cell below it and the four horizontally adjacent cells (\textit{WETDRY}>0). \textit{WETDRY} is 0 if the cell cannot be re-wetted.

\begin{itemize}
\item \textbf{Note:} All the dimension quantities must be expressed in model units and elevations are referred to a reference datum.
\item \textbf{Note:} top and bottom surfaces cannot intersect. As such, \textit{THICKNESS} values cannot be negative.
\item \textbf{Note:} \textit{STRT} should be at least above the \textit{BOTTOM} surface of the model layer to avoid that cells are dry at the beginning of the simulation.
\item \textbf{Note:} \textit{NT} and \textit{NE} are not used in groundwater flow simulations, but will be used in solute transport simulations (Volume 2).
\end{itemize}
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 MDO. 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 MDO is created, a table named *lpf_model_name* is created, stored within the model DB and loaded in the Layers Panel. It updates as soon as a new model layer MDO is created.

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

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

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

**Note:** If the User wishes to rename a model layer in the Layers Panel, its name must be modified within 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 MDOs must be deleted from the Layers Panel and the model DB and created again in the correct order.
4.3 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), during which the solution is calculated within each cell of the active domain.

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 a Stress Period window:

- **Time Table**: name of the time table created (see Chapter 3);

- in the Add parameters section:
  - **SP Length**: length of the current SP [T];
  - **Time Steps**: number of TSs within the current SP;
  - **Multiplier**: multiplier to calculate the length [T] of each TS within the current SP;
  - **State**: two options are available for the current SP (Steady State or Transient);

- in the Load parameters from CSV section, the path of a CSV file containing parameters for the SPs to be defined must be entered in the Load table from 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 the MODFLOW-2005 manual (Harbaugh, 2005).

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

Note: In the CSV file required to load SPs parameters, the User must specify:
- \textit{length}: length of each SP \([T]\);
- \textit{ts}: number of TSs within each SP;
- \textit{multiplier}: multiplier to calculate the length of each TS within each SP;
- \textit{state}: two options are available for each SP (SS for Steady State or TR for Transient).

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

```
1 length, ts, multiplier, state
2 10, 1, 1.0, SS
3 60, 15, 1.3, TR
4 180, 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 \textit{Toggle editing mode} (refer to Chapter 5).
CHAPTER 5

Tools for model layers parameterization

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

The Attribute Table of each model layer MDO 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).

5.1 Manual editing with selection tools

This editing methodology may use 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 MDO. Such procedure can be applied to any parameter defined in the Attribute Table of the model layer MDO. Hereinafter, we describe how to edit the ACTIVE field to distinguish between active, inactive and specified-head cells.

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

*View -> Select.*

- The Select Feature(s) tool allows to select cells one by one, eventually using the Ctrl button of the keyboard;
- the Select Features by Polygon tool allows to select cells intersected by a polygon, whose border is a polyline;
- the Select Features by Freehand tool allows to select cells intersected by a polygon, whose border is a curved line;
- the Select Features by Radius tool allows to select cells intersected by a circle;
- the Select Features By Expression... tool allows to select cells for which particular conditions occur: a condition is described by an expression typed in the Expression bar by using mathematical, logical, conditional operators and/or values from other fields within the Attribute Table of the MDO involved in the selection;
- the Select Features By Value... tool, which is similar Select Features By Expression..., but the User can only act on numeric fields (e.g., no logical or conditional operators are available);
- the Select All Features tool allows to select all cells within the Attribute Table.

The following tools are further available:

- Deselect Features from All Layers;
- Invert Feature Selection, if a selection is already active for an MDO listed in the Layers Panel.
**Note:** Using one of the available selection tools requires 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) and the *ACTIVE* values of such cells can be edited, by activating the *Toggle editing mode* and using the expression bar or the *Field calculator*. 
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 MDO 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 MDO 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 allows to:

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

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

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

### 5.2 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 $K_X$, $K_Y$ and $K_Z$ values at each cell of the model layer MDO, using the *Copy from Vector layer* tool integrated in *FREEWAT*. The algorithm checks for a correspondence between each node of the grid cells and the polygons defined within the shapefile: if a node is inside a certain polygon, hydraulic conductivity values along $x$, $y$ and $z$ directions of that polygon are assigned to $K_X$, $K_Y$ and $K_Z$ 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 must be checked on the left side of the interface.

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., grid or model layers), 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.
5.3 Copy from raster layer

If a raster file, e.g., the Digital Elevation Model (DEM) is available, it can be used to assign TOP values at each cell of the model layer MDO, using the Copy from Raster layer tool integrated in FREEWAT. The origin raster layer must have at least the same extension as 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, calculated involving raster cells matching a single grid cell, is assigned at each node of the coarse scale grid. On the other hand, if the model grid has a finer space discretization than the origin raster layer, the same value will be assigned at grid cells matching a single raster cell.

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 (MDO);
  - Target field: the target field to be updated.

Hereinafter, an example about how to assign values to the TOP field, 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.
Implementing processes to be simulated: boundary conditions and source/sink terms

Once defined the geometry of the domain and the hydrodynamic parameterization of each model layer, boundary conditions and source/sink terms must be set, according to the conceptual model. This means expressing, with proper mathematical formalism, processes involved in the hydrological cycle. For the conceptualization of most of these processes, the reader can refer to the MODFLOW-2005 online guide, section Ground-Water Flow Processes -> Boundary Condition Packages.

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

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

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

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

*Boundary Condition Packages* can be activated through the following menu:

**FREEWAT -> MODFLOW Boundary Conditions**
Note: Each MDO through one of these sub-menus will be saved 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.

6.1 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. To achieve this purpose, the QGIS selection tools presented in Chapter 5 can be used.

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

FREEWAT -> MODFLOW Boundary Conditions -> Create CHD Layer
The following data are required in the **Create a layer for CHD package** window:

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

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

**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 may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- **PKUID**: database primary key (it must not be modified);
- **ID**: database primary key (it must not be modified);
- **ROW**: row number of a grid cell;
- **COL**: column number of a grid cell;
- **from_lay**: number of the uppermost layer where the boundary condition must be assigned;
- **to_lay**: number of the deepest layer where the boundary condition must be assigned;
- the following fields are repeated according to the number of SPs implemented (n refers to the number of a SP):
  - **n_shead**: specified head [L] at the beginning of the n-th SP;
  - **n_ehead**: specified head [L] at the end of the n-th SP.

The fields from_lay, to_lay, n_shead and n_ehead are filled with default values, which can be modified using QGIS selection and editing tools described in Chapter 5.
Note: \( n_{\text{shead}} \) and \( n_{\text{ehead}} \) values must be expressed in model units and referred to a reference datum.

Note: Please notice that the MODFLOW CHD Package cannot be applied if more than about 200 grid cells are selected. As such, if you need to apply it 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)).

Note: Once the chd MDO is successfully created, the selected grid cells automatically deselect.

### 6.2 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 individual cells.

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

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

**FREEWAT -> MODFLOW Boundary Conditions -> Create WEL Layer**
The following data are required in the **Create a layer for WEL package** window:

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

A new MDO, renamed *wel_layer_well*, is created, stored within 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 may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- **PKUID**: database primary key (it must not be modified);
- **ID**: database primary key (it must not be modified);
- **ROW**: row number of a grid cell;
- **COL**: column number of a grid cell;
- **from_lay**: number of the uppermost layer where the boundary condition must be assigned;
- **to_lay**: number of the deepest layer where the boundary condition must be assigned;
- **active**: integer flag to activate \((active=1)\) or not \((active=0)\) the corresponding well during the simulation (not yet implemented in the current version);
- **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 positive/negative flux \([L^3/T]\) during the \(n\)-th SP.

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

**Note**: **sp_n** values must be expressed in model units.
Note: If the recharge/pumping flow is assigned to more than one model layer, the specified flux is equally distributed among the model layers involved.

Note: Once the well MDO is successfully created, the selected grid cells automatically deselect.

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

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

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

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

FREEWAT -> MODFLOW Boundary Conditions -> Create MNW Layer

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

- Model Name: name of the hydrological model;
- in the Create a Multi Node Layer (Model Data Object) section:
  - Grid Layer: grid MDO;
  - Name of new layer: name of the mnw MDO which has to be created.
A new MDO, renamed `mnw_layer_mnw`, is created, stored within 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 may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

- **PKUID:** database primary key (it must not be modified);
- **ID:** database primary key (it must not be modified);
- **ROW:** row number of a grid cell;
- **COL:** column number of a grid cell;
• **WELLID**: name assigned to each multi-node well;

• the following field is repeated according to the number of SPs implemented (n refers to the number of a SP):
  
  – **Qw_n**: actual volumetric pumping rate (negative for withdrawal or positive for injection) at each well \([L^3/T]\) during the n-th SP.

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

![](image.png)

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

**Note:** Once the mnw MDO is successfully created, the selected grid cells automatically deselect.

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

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

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

• **MNW Model Data Object**: name of the mnw MDO created;

• for each multi-node well:
  
  – the **WELLID** must be selected from the drop-down menu near to **Select Well Name**;

  – the number of model layer(s) to which the multi-node well is screened must be checked in the drop-down 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 assigned in the `WELLID` when creating the mnw MDO;
- `layer`: number of the model layer(s) to which the multi-node well is screened; if the multi-node well is screened to more than one model layer, multiple lines are repeated for the same `well_id`;
- `Rw`: radius of the multi-node well as assigned in the `Well Radius (Rw)` field when editing the `Create or Update Table for Well Properties` section;
- `B`, `C` and `P` as defined when editing the `Create or Update Table for Well Properties` section.

**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.
6.3.1 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: \( h_{WEL} = h_n + AQ_n + BQ_n + CQ_n^P \) (for details the reader is referred to the MNW2 User manual; Konikow et al., 2009).

6.4 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 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

![Create RCH Layer](image)

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 within 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 may contain several records, according to the number of grid cells, and the following fields:

- **PKUID**: database primary key (it must not be modified);
- **ID**: database primary key (it must not be modified);
- **ROW**: row number of a grid cell;
- **COL**: column number of a grid cell;
- the following fields are repeated according to the number of SPs implemented (n refers to the number of a SP):
  - **sp_n_rech**: specified flux [L/T] during the n-th SP;
  - **sp_n_irch**: number of the model layer 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.
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 recharge is usually used to simulate rainfall infiltration and rainfall is expressed as a rate \([L/T]\). Such specified rate is then automatically multiplied by the area of the grid cell \([L^2]\) to get a specified flux \([L^3/T]\).

Note: To deactivate recharge at some cells during SP \( n \), it is necessary to select the involved cells and set \( sp_n\_rech \) to 0.

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

### 6.5 River - RIV (head-dependent flux)

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

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

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

\textit{FREEWAT} \rightarrow \textit{MODFLOW Boundary Conditions} \rightarrow \textit{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 the river profile only and the required properties must be assigned by the User at each cell once the riv MDO is created.

Anyway, the option *Single Segment* may still be applied even if the river develops over more than one segment. In this case, the multi-line shapefile must be splitted into several single segments 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 is loaded in the Layers Panel.

**Note:** Parameters required when creating the riv MDO are related to the geometry and hydraulic conductivity of the river bed sediments and must be assigned at the upstream and downstream cells of the river segment and for each SP:
- $sp$: SP number;
- $rs_{in}$: river stage [L] at the upstream cell of the river segment;
- $rs_{out}$: river stage [L] at the downstream cell of the river segment;
- $bt_{in}$: height [L] of the river bed bottom at the upstream cell of the river segment;
- $bt_{out}$: height [L] of the river bed bottom at the downstream cell of the river segment;
- $hc_{in}$: hydraulic conductivity [L/T] of the river bed sediments at the upstream cell of the river segment;
- $hc_{out}$: hydraulic conductivity [L/T] of the river bed sediments at the downstream cell of the river segment;
- $thick_{in}$: thickness [L] of the river bed sediments at the upstream cell of the river segment;
- $thick_{out}$: thickness [L] of the river bed sediments at the downstream cell of the river segment.

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`):

A new MDO, renamed `riv_layer_riv`, is created, stored within 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 may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:
- **PKUID**: database primary key (it must not be modified);
- **ID**: database primary key (it must not be modified);
- **ROW**: row number of a grid cell;
- **COL**: column number of a grid cell;
- **layer**: number of the model layer to which the river is in contact;
- **segment**: number of the river segment;
- **length**: length [L] of the river segment within a grid cell;
- the following fields are repeated according to the number of SPs implemented (n refers to the number of a SP):
  - **stage_n**: river stage [L] during the n-th SP;
  - **rbot_n**: height of the river bottom [L] during the n-th SP;
  - **cond_n**: conductance of the river bed sediments [L^2/T] during the n-th SP.

The fields **layer**, **segment**, **stage_n**, **rbot_n** and **cond_n** are filled with values assigned by the User when the riv_layer_riv MDO is created.

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

Furthermore, **cond_n** is automatically calculated depending on the river bed geometry and its hydraulic conductivity (for details the reader is referred to the MODFLOW-2005 User manual; Harbaugh, 2005).

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 listed above.

**Note:** If the river 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 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:
• 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 during the Run procedure.

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.

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

- **Model Name**: name of the hydrological model;
- **Grid Layer**: grid MDO;
- **Line Layer (river segment)**: line shapefile containing the profile of the multi river segment;
- **Name of new layer**: name of the riv MDO which has to be created.
A new MDO, renamed `riv_layer_riv`, is created, stored within the model DB and loaded in the Layers Panel.

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

- **PKUID**: database primary key (it must not be modified);
• **ID**: database primary key (it must not be modified);
• **ROW**: row number of a grid cell;
• **COL**: column number of a grid cell;
• **layer**: number of the model layer to which the river is in contact;
• **xyz**: number of the river segment;
• **length**: length [L] of the river segment within a grid cell;
• the following fields are repeated according to the number of SPs implemented (n refers to the number of a SP):
  - **stage_n**: river stage [L] during the n-th SP;
  - **rbot_n**: height of the river bottom [L] during the n-th SP;
  - **cond_n**: conductance of the river bed sediments [L²/T] during the n-th SP.

The fields **layer**, **stage_n**, **rbot_n** and **cond_n** are filled with default values.

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

The field **xyz** is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.

### 6.6 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 solution for lake stage is solved implicitly \((THETA=*1)\), semi-implicitly \((0.0<*THETA*<1)\) or explicitly \((THETA=*0)\);
- **NSSITR**: maximum number of iterations for Newton’s method 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.

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` layer for each model layer previously created, as described in Chapter 4.

The `_lak` layers are also loaded in the model DB and they will be used to define the location of lakes.

Once the `_lak` layers 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` layer, 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` layer may contain several records, according to the number of grid cells, and the following fields:

- **PKUID**: database primary key (it must not be modified);
- **ID**: database primary key (it must not be modified);
- **ROW**: row number of a grid cell;
- **COL**: column number of a grid cell;
- **LAYER**: number of the model layer which the `_lak` layer represents;
- **LAKE**: the lake ID to identify which lake is located at a certain grid cell;
- **LEAKANCE**: the leakance term at a certain grid cell.
To specify the location of a lake within the *FREEWAT* model, the *LAKE* field must be edited using a non-null, integer value.

**Note:** The 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 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 within the model DB, along with the *_lak* layers:

- *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` just set (see figure below);
• `laksp_model_name` (at this stage, it is empty and will be filled with some lake properties).

![Image of a QGIS database manager plugin]

**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 layers 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 lakebed sediments. Values are assumed to represent the combined leakances of the lakebed material and the aquifer material between the lake and the centers of the underlying grid cells;
- **lake id**: lake identifier. It must be unique for each lake that is to be created 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 [L/T];
  - **EVAPLK**: evaporation flux [L/T];
  - **RNF**: surface runoff [$L^3/T$];
  - **WTHDRW**: direct withdrawal from the lake [$L^2/T$].

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):

<table>
<thead>
<tr>
<th></th>
<th>SP, PRCP, EVAP, RN, WTHDR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 0.00435, 0.00123, 0.000456, 0</td>
</tr>
<tr>
<td>2</td>
<td>2, 0.00436, 0.00122, 0.000421, 0</td>
</tr>
<tr>
<td>3</td>
<td>3, 0.00437, 0.00121, 0.000416, 0</td>
</tr>
</tbody>
</table>

Once the fields SURFDEP, STAGES, SSMN, SSMX and LEAKANCE have been filled out 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 functions, 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).

6.6.1 Limitations

The LAK Package has the following limitations, which can be overcome only by editing the lak MODFLOW input file and running the model independently of the FREEWAT platform (for details 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 for central and sub-lakes, as well as sills between lakes, for the separation and coalescence of lakes is not yet implemented in FREEWAT;
- MOC3D for solute concentrations in lakes is not implemented in FREEWAT, but will be replaced by MT3DMS.
6.7 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 is loaded in the Layers Panel, to activate the *DRN Package* the following menu must be used:

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

![Create DRN Layer Menu](image)

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 the drain profile only and the required properties must be assigned by the User at each cell once the dmn MDO is created.

Anyway, the option **Single Segment** may still be applied even if the drain develops over more than one segment. In this case, the multi-line shapefile must be splitted into several single segments 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 dmn MDOs through the **Single Segment** option. All these MDOs will then be merged using the *Merge SpatiaLite layers* tool.

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

- **Model Name**: name of the hydrological model;
- **Grid Layer**: grid MDO;
- **Line Layer (drain segment)**: line shapefile containing the profile of the single drain segment;
• **Name of new layer**: name of the drn MDO which has to be created;
• **Drain segment (xyz)**: number of the single drain segment;
• **Width**: width [L] of the drain;
• **Layer number**: number of the model layer to which the drain is in contact;
• if **Enter drain parameters** is checked, the User can fill manually the table with all the necessary parameters to be assigned to grid cells where the drain is located;
• if **Load drain parameters from CSV** is checked, the User can load a csv file containing parameters to be assigned to grid cells where the drain is located, using the **Browse...** button (field **CSV Parameters Table**). In this case, the User must define the **Decimal separator** and **Column separator** used in the csv file loaded;
• if **Add the table to the Legend** is checked, a table containing the drain parameters assigned is loaded in the Layers Panel.
Note: Parameters required when creating the drn MDO are related to the geometry and hydraulic conductivity of the drain bed sediments and must be assigned at the upstream and downstream cells of the drain segment and for each SP:

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

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`):

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>SP, ELEV_I, ELEV_E, HC_IN, HC_OUT, THICK_IN, THICK_OUT</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1, 5.5000, 3.0000, 8.640000, 8.640000, 0.500, 0.500</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2, 5.5000, 3.0000, 8.640000, 8.640000, 0.500, 0.500</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>3, 5.5000, 3.0000, 8.640000, 8.640000, 0.500, 0.500</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A new MDO, renamed `drn_layer_drn`, is created, stored within 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 may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

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

The fields *layer*, *xyz*, *elev_n* and *cond_n* are filled with values assigned by the User when the *drn_layer_drn* MDO is created.

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

Furthermore, *cond_n* is automatically calculated depending on the drain bed geometry and its hydraulic conductivity (for details the reader is referred to the *MODFLOW-2005* User manual; Harbaugh, 2005).

![Image](image1.png)

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 listed above.

![Image](image2.png)

**Note:** If the drain 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 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:

• 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 during the Run procedure.

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

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

A new MDO, renamed `drn_layer_drn`, is created, stored within the model DB and loaded in the Layers Panel.
The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

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

The fields **layer**, **elev_n** and **cond_n** are filled with default values.

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

The field **xyz** is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.
6.8 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 is 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 grid cell), as required in
the MODFLOW GHB Package. On the contrary, the option Multi Segment allows to define the general-head boundary profile only and the required properties must be assigned by the User at each cell once the ghb MDO is created.

Anyway, the option Single Segment may still be applied even if the general-head boundary develops over more than one segment. In this case, the multi-line shapefile must be splitted into several single segments 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 in loaded in the Layers Panel.
Parameters required when creating the ghb MDO are related to the geometry and hydraulic conductivity of sediments between the external source and the grid cell and must be assigned for each SP:

- sp: SP number;
- bhe_in: head assigned to the external source [L];
- hc_in: hydraulic conductivity [L/T] between the external source and the grid cell;
- thick_in: thickness [L] of the sediments between the external source and the grid cell.
General-head boundary properties are assigned at each grid cell intersected by the general-head boundary profile.

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`):

![ ghb_parameters.csv](image)

<table>
<thead>
<tr>
<th></th>
<th>SP, BHE_I, HC_IN, THICK_IN</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 6.00, 38.00, 35.00</td>
</tr>
<tr>
<td>2</td>
<td>2, 6.00, 38.00, 35.00</td>
</tr>
<tr>
<td>3</td>
<td>3, 6.00, 38.00, 35.00</td>
</tr>
</tbody>
</table>

A new MDO, renamed `ghb_layer_ghb`, is created, stored within 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 may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

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

The fields from_lay, to_lay, xyz, bhead_n and cond_n are filled with values assigned by the User when the ghb_layer_ghb MDO is created.

The value of cond_n is automatically calculated depending on the cells geometry, their distance from the external source and the hydraulic conductivity between the external source and the grid cells (for details the reader is referred to the MODFLOW-2005 User manual; Harbaugh, 2005).

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 listed above.

**Note:** If the general-head boundary 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 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:

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

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

A new MDO, renamed *ghb_layer_ghb*, is created, stored within the model DB and loaded in the Layers Panel.
The Attribute Table of such MDO may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

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

The fields **from_lay**, **to_lay**, **elev_n** and **cond_n** are filled with default values.

The field **xyz** is automatically filled with progressive integer values to identify each segment which composes the multi-line shapefile.
6.9 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 be applied to all grid cells and it is possible to deactivate evapotranspiration at some grid cells, by using QGIS selection and editing tools described in Chapter 5.

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

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

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

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

• if **Enter evt parameters** is checked, the User can fill manually the table with all the parameters necessary to activate this Package;

• if **Load evt parameters from CSV** is checked, the User can load a csv file containing parameters necessary to activate this Package, using the **Browse...** button (field **CSV Parameters Table**). In this case, the User must define the **Decimal separator** and **Column separator** used in the csv file loaded;

• if **Add the table to the Legend** is checked, a table containing the evt parameters assigned in loaded in the Layers Panel.
Note: Parameters required when creating the evt MDO must be assigned for each SP:

- \( sp \): SP number;
- \( surf \): elevation [L] of the evapotranspiration surface;
- \( evtr \): maximum evapotranspiration flux [L/T];
- \( exdp \): evapotranspiration extinction 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`):

```
1 SP, surf, evtr, exdp
2 1, 10.0, 0.002, 0.5
3 2, 10.0, 0.002, 0.5
4 3, 10.0, 0.002, 0.5
```

A new MDO, renamed `evt_layer_evt`, is created, stored within 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 may contain several records, according to the number of grid cells, and the following fields:

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

The fields **surf$_n$**, **evtr$_n$**, **exdp$_n$** and **ievt$_n$** are filled with values assigned by the User when the **evt_layer_evt** MDO is created.
Note: evtr_n is actually a specified rate, rather than a flux. Such specified rate is then automatically multiplied by the area of the grid cell \([L^2]\) to get a specified flux \([L^3/T]\).

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

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

A table 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 listed above.

### 6.10 Unsaturated-Zone Flow Package - UZF

The MODFLOW UZF Package allows to simulate vertical flow of water through the unsaturated zone, by estimating the evapotranspiration and effective infiltration to groundwater, using the land surface precipitation. 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 be applied to all grid cells and it is possible to deactivate evapotranspiration and recharge at some grid cells, by using QGIS selection and editing tools described in Chapter 5.

6.10.1 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 within 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 may contain several records, according to the number of grid cells, and the following fields:

- **PKUID**: database primary key (it must not be modified);
- **ID**: database primary key (it must not be modified);
- **ROW**: row number of a grid cell;
- **COL**: column number of a grid cell;
- **iuzfbnd**: integer value used to define the 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**: infiltration rate [L/T] at land surface during the n-th SP;
– petₙ: ET demand rate \([L/T]\) within the ET extinction depth interval during the \(n\)-th SP;
– extdpₙ: ET extinction depth \([L]\) during the \(n\)-th SP;
– extwcₙ: extinction water content, below which ET cannot be removed from the unsaturated zone, defined during the \(n\)-th SP.

The fields \(iuzfbnd, eps, thts, thti, finfₙ, petₙ, extdpₙ\) and \(extwcₙ\) are filled with default values, which can be modified using QGIS selection and editing tools described in Chapter 5.

Note: \(finfₙ\) and \(petₙ\) values must be expressed in model units.

Note: \(finfₙ\) and \(petₙ\) are actually specified rates, rather than fluxes. Such specified rates are then automatically multiplied by the area of the grid cell \([L^2]\) to get specified fluxes \([L^3/T]\).

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

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

6.10.2 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 is not implemented, no runoff will be relocated to the SFR segments.

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

FREEWAT -> MODFLOW Boundary Conditions -> Create Surface Model Layer
The following data are required in the **Create Surface Model Layer** window:

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

A new MDO, renamed `surf_layer_sml`, is created, stored within 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 may contain several records, according to the number of grid cells, and the following fields:

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

The field **irunbnd** is filled with default values, which can be modified using QGIS selection and editing tools described in Chapter 5.
6.10.3 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 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.

6.11 Streamflow-Routing Package - SFR

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

FREEWAT -> MODFLOW Boundary Conditions -> Create SFR Layer
The following data are required in the **Create a layer for SFR package** window:

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

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

• **flow**: inflow \([L^3/T]\) at the upstream reach of the current stream segment;

• **runoff**: incoming runoff \([L^3/T]\) at each reach of the current stream segment;

• **etsw**: volumetric rate per unit area of water removed by evapotranspiration directly from the stream channel \([L/T]\) (positive value);

• **pptsw**: volumetric rate per unit area of water added by precipitation directly on the stream channel \([L/T]\);

• **roughch**: Manning’s roughness coefficient;

• **hcond1**: hydraulic conductivity \([L/T]\) of the streambed at the upstream reach of the current segment;

• **thickm1**: thickness \([L]\) of streambed material at the upstream reach of the current segment;

• **elevup**: elevation \([L]\) of the top of the streambed at the upstream reach of the current segment;

• **width1**: average width \([L]\) of the stream channel at the upstream reach of the current segment;

• **thts1**: saturated volumetric water content in the unsaturated zone beneath the upstream reach of the current segment;

• **thti1**: initial volumetric water content beneath the upstream reach of the current segment;

• **eps1**: Brooks-Corey exponent used in the relation between water content and hydraulic conductivity within the unsaturated zone beneath the upstream reach of the current segment;

• **hcond2**: hydraulic conductivity \([L/T]\) of the streambed at the downstream reach of the current segment;

• **thickm2**: thickness \([L]\) of streambed material at the downstream reach of the current segment;

• **elevdn**: elevation \([L]\) of the top of the streambed at the downstream reach of the current segment;

• **width2**: average width \([L]\) of the stream channel at the downstream reach of the current segment;

• **thts2**: saturated volumetric water content in the unsaturated zone beneath the downstream reach of the current segment;

• **thti2**: initial volumetric water content beneath the downstream reach of the current segment;

• **eps2**: Brooks-Corey exponent used in the relation between water content and hydraulic conductivity within the unsaturated zone beneath the downstream reach of the current segment.

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](image)

A new MDO, renamed **sfr_layer_sfr**, is created, stored within 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 may contain several records, according to the number of grid cells where this boundary condition is assigned, and the following fields:

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

The fields **layer** and **seg_id**, are filled with values assigned by the User when the sfr_layer_sfr MDO is created.

The field **ireach** is automatically filled. 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).

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

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:

- 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 SpatialLite layers tool must be used to get a single MDO. The latter will then be used during the Run procedure.

### 6.11.1 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):

- stream depth is calculated using Manning’s equation and assuming a wide rectangular channel (MODFLOW flag $ICALC=1$);
• the number of trailing waves used to define the water-content profile following a decrease in the infiltration rate (MODFLOW variable NSTRAIL) is set to 10 as a default value;

• the number of wave sets used to simulate multiple infiltration periods (MODFLOW variable NSFRSETS) is set to 30 as a default value;

• transient streamflow routing is simulated using the kinematic-wave equation (MODFLOW flag IRTFLG>0);

• if the flow in the unsaturated zone beneath stream is not simulated, streambed elevation, thickness and hydraulic conductivity must be defined at each SP (MODFLOW flag ISFROPT=0);

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

6.12 Zone Budget - ZONBUD

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

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

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

FREEWAT -&gt; MODFLOW Boundary Conditions -&gt; 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 within the model DB and loaded in the Layers Panel. The Attribute Table of such MDO may contain several records, according to the number of grid cells, and the following fields:

- **PKUID**: database primary key (it must not be modified);
- **ID**: database primary key (it must not be modified);
- **ROW**: row number of a grid cell;
- **COL**: column number of a grid cell;
- the following field is repeated according to the number of model layers implemented ($n$ refers to the number of a model layer; 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.
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 model files which can be read by the numerical codes is necessary. In FREEWAT, such procedure is automatically performed when the simulation is run.

Hereinafter, a quick list of the MODFLOW input files which can be generated is provided. For further details the reader is suggested to refer to 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 information stored in the table timetable_model_name about time discretization;
- **Layer Property Flow (.LPF) file**: it reports information stored in the table lpf_model_name about hydraulic parameters of each model layer and the wetting capability options;
- **Preconditioned Conjugate Gradient (.PCG) file**: it contains flag options related to the numerical solver;
- **Output Control (.OC) file**: it contains flag options related to the output results to be saved.

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

- **Time-Variant Specified Head (.CHD) file**: it is required if the CHD Package is activated to define specified-head cells;
- **Well (.WEL) file**: it is required if the WEL Package is activated to define recharge or pumping wells;
- **Multi-Node Well (.MNW) file**: it is required if the MNW Package is activated to simulate screened wells;
- **Recharge (.RCH) file**: it is required if the RCH Package is activated to simulate areally-distributed recharge;
- **River (.RIV) file**: it is required if the RIV Package is activated to simulate river-groundwater interaction;
- **Lake (.LAK) file**: it is required if the LAK package is activated to simulate lake-groundwater interaction;
- **Drain (.DRN) file**: it is required if the DRN Package is activated to simulate the effects of features, such as agricultural drains;
- **General-Head Boundary (.GHB) file**: it is required if the GHB Package is activated to simulate inflow to or outflow from the groundwater system, due to the presence of an external source;
- **Evapotranspiration (.EVT) file**: it is required if the EVT Package is activated to simulate the effects of plant transpiration and direct evaporation from the soil;
• **Unsaturated-Zone Flow (.UZF) file**: it is required if the *UZF Package* is activated to simulate vertical flow through the unsaturated zone;

• **Stream Flow Routing (.SFR) file**: it is required if the *SFR Package* is activated to simulate routed runoff within surface streams.

The model run can be performed through the following menu:

*FREEWAT -> Run Model*

The processes which can be simulated are the following:

• **Groundwater Flow**;

• **Solute Transport** (see Volume 2);

• **Water Management and Crop Modeling** (see Volume 3);

• **Model Calibration** (see Volume 4).

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

• according to which among the boundary conditions Packages listed above are activated, the corresponding box must be checked and the related MDO must be selected;

• in the *UZF (Unsaturated Zone)* section (if used) the following data are required:
  
  – *UZF Layer*: name of the uzf MDO;

  – *Surface Layer*: name of the sml MDO (only required if the SFR Package is activated);

  – *Recharge Option*: three options are available to define in which cell of a vertical column recharge and discharge are simulated, *To/From Only Top Model Layer, To/From layer specified in iuzfbnd, To/From Highest Active Cell (NUZTOP flag in MODFLOW; Harbaugh, 2005)*;

  – the box *Simulate Evapotranspiration* must be checked if evapotranspiration has to be simulated;

  – the box *Use SFR Package* must be checked if the SFR Package is used;

• in the **SFR2 (Stream Flow Routing)** section (if used) the following data are required:
  
  – *SFR Layer*: name of the sfr MDO;

  – *SFR Table*: *sfr_layer_sfr_table* containing information about time discretization of the stream parameters;
– the option **Simulate Unsaturated Zone** must be checked if the unsaturated flow beneath streams has to be simulated;

– **Conversion Factor (CONSTANT)**: conversion factor used to calculate stream depth for stream reach (**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** is required, so the box **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 box must be checked and the related MDOs 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;

  – **RCLOSE** is the residual criterion for convergence;

  – **RELAX** is the relaxation parameter to be defined if the **Modified Incomplete Cholesky** method is used;

  – **MUTPCG** is a flag that controls printing of convergence information from the solver: four options are available (**Print maximum head change and residual**, **Print only total number of iterations**, **No printing**, **Print only if convergence fails**);

  – **IPRPCG** is the printout interval;

  – **DAMP** is the damping factor.
Note: If the box corresponding to the RCH and/or EVT Packages is checked, a further option must be selected (Rch Option and/or Evt Option) to properly assign the boundary condition to a specific cell along the vertical column. For the RCH Package, three options are available: Recharge to top grid, Recharge layer defined in irch and Recharge to highest active cell. Similarly, three options are available for the EVT Package as well: ET to top grid, ET layer defined in ievt, ET to highest active cell. For both Packages, through the first option the boundary condition is applied to model layer 1; through the second one the boundary condition is applied to a certain model layer as specified in the fields irch and/or ievt in the Attribute Table of the rch and/or evt MDOs; through the third option the boundary condition is applied to the uppermost active cell in the vertical column.

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

Note: If the aim is to create only 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.

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

The following Information window appears:
Once clicked 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).

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 Packages are created as well.
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 open with any text editor or using the Open Report button in the Groundwater Flow tab of the Run Model window.

### 8.1 Displaying 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 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 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 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 vector file, containing one field for each model layer with output 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, especially if the Select Stress Period section is used, an output layer will be loaded in the Layers Panel for each TS within each selected SP and for each model layer. This procedure could take a long time, according to the complexity of the model implemented.

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

If Vector format is selected, one polygon vector layer is created for all model layers and for each TS selected within a certain SP. Such polygon vector layer is saved in the model DB loaded in the Layers Panel with a default name assigned. For example, the vector layer containing the simulated 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, indeed, the same fields contained within the Attribute Table of the grid MDO, 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.
Note: *Vector format must* be used for rotated model grids or if rectangular grid cells are used.

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.

### 8.2 Displaying 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 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 a drop-down menu);
  - *Time Step*: TS number, within the selected SP, for which the cross section will be drawn;
  - the *Vertical exageration*. 

---

123
**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 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, especially if the *Select Stress Period* section is used, an output layer will be loaded in the Layers Panel for each TS within each selected SP and for each model layer. This procedure could take a long time, according to the complexity of the model implemented.

Hereinafter, the solute concentration simulated at the end of TS 1 within SP 3 was 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.

8.3 Displaying 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 **OK** is clicked, the information window Saving Volumetric Budget appears reporting 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.

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.
8.4 Run ZONE BUDGET

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

FREEWAT -> Post-processing -> Run Zone Budget

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

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

Once the run of the Zone Budget is successfully completed, an information window appears, stating that a CSV file containing water balance for zones has been saved in the working directory.
Such a CSV file, named `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 Time Step.

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

<table>
<thead>
<tr>
<th>totim</th>
<th>time_step</th>
<th>stress_period</th>
<th>name</th>
<th>ZONE_1</th>
<th>ZONE_2</th>
<th>ZONE_3</th>
<th>ZONE_4</th>
</tr>
</thead>
<tbody>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>STORAGE_IN</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>CONSTANT.Head_IN</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>ZONE_1_IN</td>
<td>0</td>
<td>7401.26</td>
<td>23938.9</td>
<td>44470.2</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>ZONE_2_IN</td>
<td>53722.5</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>ZONE_3_IN</td>
<td>22087.9</td>
<td>46321.2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>ZONE_4_IN</td>
<td>0</td>
<td>0</td>
<td>44470.2</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>TOTAL_IN</td>
<td>75810.4</td>
<td>53722.5</td>
<td>68409.1</td>
<td>44470.2</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>STORAGE.OUT</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>CONSTANT.Head.OUT</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>ZONE_1_OUT</td>
<td>0</td>
<td>53722.5</td>
<td>22087.9</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>ZONE_2_OUT</td>
<td>7401.26</td>
<td>0</td>
<td>46321.2</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>ZONE_3_OUT</td>
<td>23938.9</td>
<td>0</td>
<td>0</td>
<td>44470.2</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>ZONE_4_OUT</td>
<td>44470.2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>TOTAL.OUT</td>
<td>75810.4</td>
<td>53722.5</td>
<td>68409.1</td>
<td>44470.2</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>IN-OUT</td>
<td>0</td>
<td>0.007813</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>365</td>
<td>0</td>
<td>0</td>
<td>PERCENT_DISCREPANCY</td>
<td>0</td>
<td>1.45E-05</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

In this example budget for Zones 1 to 4 is reported for Stress Period 1 Time Step 1. Notice that in this file Stress Periods and Time Steps are numbered starting from 0. Furthermore, `totim` value refers to the length of the cumulative time of simulation.

In particular, the figure above highlights water exchanges 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 model run must have been successfully completed and cell-by-cell flow terms saved.

### 8.5 Plot Model Fit

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

**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:

![Plot Observed vs Simulated](image-url)
The scatter plot shows observed vs. simulated values at the SP indicated in the combo box close to Select the stress period. The bisector line, 95% and 90% 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.

### 8.6 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.

### 8.7 Plot Budgets for Water Units

A further post-processing tool allows to plot water units-related budget terms for the analysis of conjunctive use of ground- and surface-water.

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.

### 8.8 Run MODPATH

If the MODPATH executable has been loaded (Version 6.0.01 is needed; see Chapter 3), *Modpath* can be run through the following menu:

`FREEWAT -> Post-processing -> Create Particle Tracking`
The following data are required in the **Particle Tracking (MODPATH)** window:

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

Once the **Particle tracking options** are set, **Modpath** can be run clicking the **Run** button.
Note: To run Modpath, the model run must have been successfully completed and cell-by-cell flow terms saved.

Note: Once the Well (WEL) or Recharge (RCH) option is selected as a Package, the particle tracking will be applied to all the cells contained in WEL or RCH MDO, 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 of WEL or RCH on which 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 shape file with another name, but being sure to save only selected features). Furthermore, it is important to recall to save this new MDO with a name ending with _wel (or _rch).
- Fill again the Run window (see Chapter 7), selecting this new WEL (or RCH) MDO for the WEL (or RCH) Package.
- Check the box 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 selection procedure, the User is referred to the Particle Tracking Tutorial, available on FREEWAT website.

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

- .mpn contains the list of MODFLOW/MODPATH files needed for the simulation;
- .mpbas consists of a combination of data contained in the MODFLOW BAS Package data file and the MODFLOW
\textit{LPF Package} data file (see Chapter 2), plus additional data, such as porosity;

- .mps\textit{sim} contains information about the simulation options set above;
- .mp\textit{strt} contains information about particle starting location.

An output file is saved as well (.mpl\textit{st}). 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 \textit{Load} button is clicked, all the available line shapefiles (model\_name\_pathlines\_lay\_1.shp, model\_name\_pathlines\_lay\_2.shp, ..., model\_name\_pathlines\_lay\_n.shp) are loaded in the combo box. The User must choose the line shapefile to which a style will be applied and click on \textit{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.

\textbf{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.


10.1 Installation

Q: General problems with the pip python package installation.

S: python-pip can be installed in several different ways:

1. For Windows users:
   - go on the official website
   - download the get-pip.py file by right clicking on it and choosing Save link as
   - open the OSGeo Shell AS ADMINISTRATOR
   - within the shell use the cd command to go in the folder where you saved the get-pip.py file. We strongly suggest to use the TAB key in order to autocomplete the computer folder paths. Here an example of the command:
     cd C:UsersDownload
   - type python get-pip.py in order to run the script and install python-pip

   Note: an alternative solution is to install pip via the OSGEO Setup installer. In order to install it, go on the QGIS download page <http://qgis.org/en/site/forusers/download.html> and select OSGeo4W Network Installer. Save and run it. In the appearing dialog window, type Advanced install and go further till you arrive to the page where to choose the package to be installed. In the filter above type pip and hit Next.

2. For Linux users, open a terminal and type:
   
   sudo apt-get install python-pip

Q: FREEWAT plugin broken and the error message is: no module name flopy.modflow or no module name modflow

S: you don’t have successfully installed flopy. Please be sure you have followed the installation guide.

Q: You have many python versions installed (conflicts between ArcGIS and QGIS installations, affects only Windows users):

S: QGIS has its own Python envirnoment and you should not have any problem with the default ArcGIS Python. But if you have made some hacks and if you have touched the python environmental variables some conflicts during the python
libraries uploading are possible. The best solution is to uninstall **QGIS** and reinstall it with the **OSGEO4W installer**. With the **OSGEO4W** installer. In this way, **python** will be installed in the C:\OSGeo4W\app\Python27 folder and it will be independent from the ArcGIS python version so you don’t need to add python in your environmental variables.

**Q:** ImportError: No module named pyparsing

**S:** The **pyparsing** library is missing. In most of the cases you don’t have a correct **matplotlib** installed because it depends on **pyparsing**. You can install **pyparsing** via **pip**:

1. For Windows users:
   - be sure to have **python-pip** utility installed
   - open the **OSGEO4W Shell** and type:
     - just run the downloaded file and follow the installation wizard

2. For Linux users, open a terminal and type:
   - `sudo apt-get install ???`

**Q:** ImportError: No module named xlrd

**S:** The **python-xlrd** library is missing.

1. For Windows users:
   - download the xlrd-version_number.win32.exe from [here](#)
   - just run the downloaded file and follow the installation wizard

   **OR**
   - open the OSGeoShell as Administrator and type `pip install xlrd`

2. For Linux users, open a terminal and type:
   - `sudo apt-get install python-xlrd`

**Q:** ImportError: No module named cycler.

**S:** The **cycler** library is missing. In most of the cases you don’t have a correct **matplotlib** installed because it depends on **cycler**.

1. For Windows users:
   - download the cycler_version_number.whl file from [here](#)
   - copy the file in the python **QGIS** installation folder (likely C:\OSGeo4w64\apps\Python27\lib)

**Q:** ImportError: No module named matplotlib

**S:** The **matplotlib** library is missing.

1. For Windows users:
   - download the zip file from [here](#)
   - extract the zip file in the python **QGIS** installation folder (likely C:\OSGeo4w64\apps\Python27\)

   **OR BETTER**
   - open the OSGeoShell as Administrator and type `pip install matplotlib`

2. For Linux users, open a terminal and type:
   - `sudo apt-get install python-matplotlib`
**Q:** Python libraries and package installation with a **firewall**.

**S:** if you have an active firewall or proxy on your computer you have to change the normal command line of the python, pip and related libraries by adding the user and the server port:

```bash
# example for the *get-pip.py* installation
python get-pip.py --proxy="[user:password]proxy.server:port"
```

```bash
# example for *flopy* library
pip install flopy==3.2.3 --proxy="[user:password]proxy.server:port"
```

.. note:: if your proxy does not have any user and password just get rid of that part in the script, e.g. python get-pip.py --proxy="proxy.server:port" (--proxy="proxy.regione.toscana.it:8080")

**Q:** Problem with the **Run Model** under Unix like systems.

**S:** You have to be sure to have correctly compiled MODFLOW with some parameters:

- download and extract the MODFLOW zip file
- in the src directory change:
  - makefile, look for line 10, F90=f90 and change it to F90=gfortran
  - openspec.inc, uncomment the line DATA FORM/'UNFORMATTED'/ and comment the line DATA FORM/'BINARY'/

now you should be able to use correctly Run Model

**Q:** During the installation of flopy the process fails and the error is **ImportError**: No module named Tkinter.

**S:** the module Tkinter is missing. It could be quite tricky to solve this issue.

1. try to install the module python-tcltk with the OsGEO Network Installer by filtering this name in the advanced installation choice. Try again to install flopy

2. the other trivial solution is to uninstall completely QGIS and reinstall it with the OsGEO Netwrok Installer.
   Then the module Tkinter should be installed and flopy is also installable.
Release history

19/11/2015 release of version alpha 1.0
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)
3/05/2017 release of version 0.4.1
   (new section in Chapter 1, describing the manual installation procedure; minor changes in the text)
7/27/2017 release of version 0.5
   (minor changes in Chapter 8, post-processing)