

FREEWAT

Free and Open Source Software Tools for Water Resource Management

EU HORIZON 2020 Project

FREE and Open Source Software Tools for WATer Resource Management

FREEWAT User Manual

Volume 6

MODFLOW OBServation process

by ***Laura Foglia[(1)], Anja Toegl[(1)] and Steffen Mehl[(2)]***

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This version is confidential, only for FREEWAT Project Partners



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FOREWORD

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

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

FREEWAT Development has received funding from the following projects:

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

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

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Abstract

The **Calibration/Sensitivity Analysis Module** combines the capabilities of the MODFLOW Observation Process Package (OBS) with those of UCODE_2014. A brief theory and detailed instructions for implementation in FREEWAT of each part are presented in this manual.

The **OBServation process** provides the capability to compare model-calculated heads, flows and water quality information to observed data. The OBS process represents the first step toward the implementation of the sensitivity analysis and calibration capabilities for FREEWAT. The types of observations supported include hydraulic heads; changes in hydraulic head over time; flows to or from surface-water bodies represented using the General-Head Boundary (GHB), Drain (DRN), River (RIV), or Streamflow Routing (STR) Packages; and flow to or from Constant-Head Boundary (CHD) cells.

The **Sensitivity Analysis** is a method, based on several statistics, to evaluate model construction and select parameters for calibration, while **Calibration** refers to optimizing the value of selected model parameters by fitting the simulated values of a dependent variable to the observed values based on a regression using a sum of squared weighted residuals objective function.

CHAPTER 1

OBSERVATION PROCESS: Theory

MODFLOW-2005 (Harbaugh, 2005) provides the capability to compare model-calculated heads and flows to observed data. This capability is called the Observation Process (OBS), and OBS in MODFLOW-2005 is derived from OBS in MODFLOW-2000 (Hill and others, 2000, Chapter 4). The OBS capability as implemented in MODFLOW-2005 does not contain any features related to the weighting of observations, this is implemented in UCODE_2014 (see this manual Chapter 3 and 4). The OBS process represents the first step toward the implementation of the sensitivity analysis and calibration capabilities for FREEWAT. The types of observations supported include hydraulic heads; changes in hydraulic head over time; flows to or from surface-water bodies represented using the General-Head Boundary (GHB), Drain (DRN), River (RIV), or Streamflow Routing (STR) Packages; and flow to or from constant-head cells. Before discussing each type of observation, the overarching issue of observation times is discussed.

Time of observations

The discussion about how to define the time of the observations is common to all the observation types which will be presented later in this manual. It is extrapolated almost completely from the MODFLOW-OBS manual and adapted for the future use in FREEWAT (Hill et al., 2000, Chapter 4). The user identifies the time of an observation by a stress period number (referred to as the reference stress period, IREFSP) and a time offset (TOFFSET). The time of the observation is the time at the beginning of the reference stress period plus the time offset. The time offset may exceed the length of the reference stress period as long as the resulting observation time is not later than the end of the final stress period. This method of specifying observation time can facilitate construction and maintenance of input files for Observation-Process Packages because it allows the number and length of stress periods and time steps to be changed without changing the observation time definition. For example, consider a flow system simulated with one steady-state stress period (stress period 1) followed by several transient stress periods (stress periods 2, 3, 4). In an observation input file, the user can specify a reference stress period of 2 (the first transient stress period) for all transient observations and define time offsets to identify observation times as the time since the beginning of the transient simulation. In this circumstance, the number and length of transient stress periods and time steps in the Discretization File can be changed without changing the OBS input files, as long as the total simulation time is sufficient to include all specified observation times. The time unit in the Discretization File need not be the time unit used for TOFFSET. A multiplier (TOMULT) for TOFFSET is provided as a conversion factor for time units. For example, a value of 86400 for TOMULT allows the observation times to be defined in days even though the simulation time is in seconds. TOMULT can be specified as 1.0 if the observation times are specified in the same time units used in the Discretization File. When an observation time falls within a transient time step, linear interpolation between the beginning and end of the time step is used to calculate the simulated value. If the first stress period of the simulation is transient, the conditions at the beginning of the first time step are the initial conditions. Head observations at the very beginning of such a time step are not allowed. In this situation, the simulated equivalents would equal the initial conditions and would not change as a result of any model stresses or hydraulic input data. There would be no point in attempting to compute a simulated equivalent for this situation. If this situation is detected, the simulation is stopped. Similarly, flow observations within the first time step of the simulation are not allowed if the first time step is transient. In this situation, the observation would depend on the flow for the initial condition, which is not specifically defined in MODFLOW. When this situation is detected,

the flow observation is moved to the end of the first time step. When the observation time for a head-dependent flow boundary is before the end of the first time step in the first stress period in which the boundary becomes active, a zero-conductance boundary needs to be specified in the same cell in the stress period preceding the stress period in which the boundary becomes active. The zero-conductance boundary is required to provide a flow value (equal to zero) for the end of the preceding stress period, which will be used in temporal interpolation. This requirement applies whether the boundary is specified as part of a parameter or is non-parameterized, and it applies to observations specified in any of the head-dependent flow packages (DRN, GHB, and RIV). Note, however, that in most cases, performing a temporal interpolation between zero flow at the time when a head-dependent flow boundary becomes active and a nonzero flow at the end of the first time step after it becomes active will result in a value that is not a good estimate of the true flow. In general, a better solution would be to revise the time-step discretization to ensure that the end of the first time step is no later than the observation time. When an observation falls within a steady-state time step, the observation time is moved to the end of the time step rather than using time interpolation. This convention avoids making a meaningless interpolation because the steady-state flow equation provides no definition for how heads and flows change within a steady-state time step.

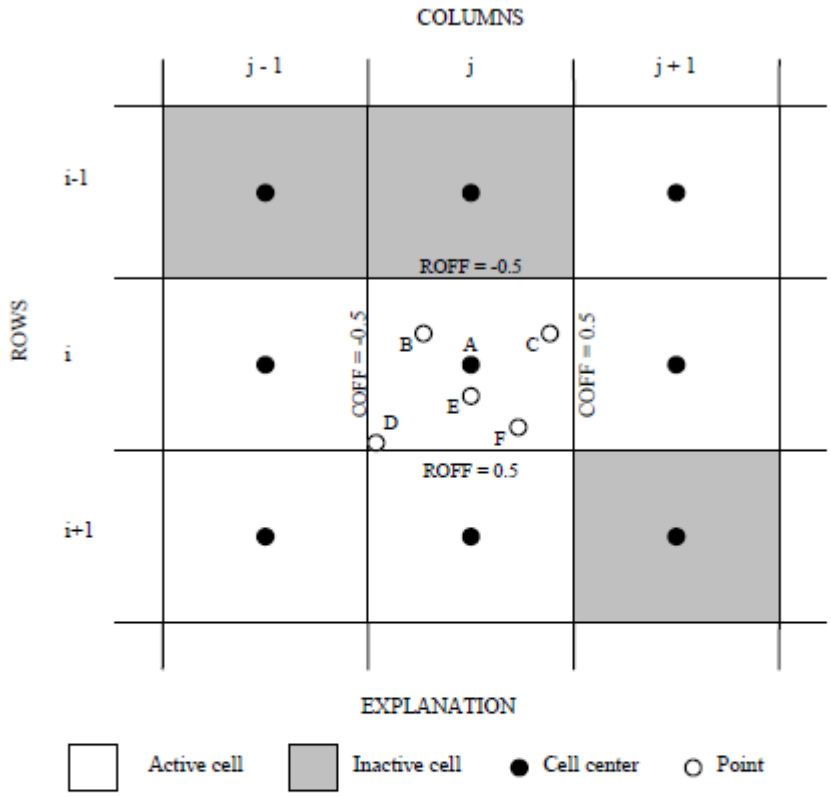
HOB: Head-observations package

The Head-OBservation (HOB) package allows the definition of head observations to be used for the comparison with heads simulated by the model. Hydraulic heads can be defined at any location and time. Spatial interpolation is applied when an observation does not correspond directly to a node. The spatial interpolation can apply horizontally and vertically. Temporal interpolation as been described above

Horizontal interpolation

The horizontal interpolation plays an important role in the definition of the hydraulic head observation. We report here some of the discussion provided in the MODFLOW-OBS manual (Hill et., 2000, Chapter 4). The finite-difference method calculates hydraulic heads at the center of each variable-head (IBOUND>0) finite-difference cell. If an observation is located at a cell center, then the simulated equivalent is equal to the model-calculated head. Observation wells, however, rarely are located at cell centers and might not be screened throughout the entire thickness represented by the model layer. To account for observation wells located horizontally away from cell centers, simulated hydraulic heads at observation locations need to be calculated by interpolating within the two-dimensional plane of a single layer. Six locations (A-F) for which hydraulic heads might need to be horizontally interpolated are shown in figure 1. Exact interpolation of hydraulic heads, in which the interpolated hydraulic heads would correspond to the hydraulic heads simulated using a locally very fine numerical grid, is not generally possible for block-centered finite-difference methods. Geometric interpolation methods that ignore the variations in hydraulic conductivity, however, are available. In this report, geometric interpolation based on linear, finite-element basis functions is used.

A linear one-dimensional basis function (equivalent to linear interpolation) is used for locations that are adjacent to two inactive (no flow or constant head) cells, such as location B in figure 1. A linear basis function is also used for locations that are exactly between adjoining cell centers, such as location E. Triangular basis functions are used for locations that are within a triangle formed by the centers of three neighboring cells because the fourth neighboring cell is inactive (locations C and F in figure 1). Quadrilateral basis functions are used for locations such as D in figure 1, which are within a rectangle formed by the centers of four active cells. All basis functions are calculated using local coordinates that are specified by the user and define the observation location within a cell relative to the cell center. These local coordinates are a row offset, ROFF, and a column offset, COFF, that range in value from -0.5 to +0.5, with 0.0 indicating that there is no offset. Use of ROFF and COFF is illustrated in figure 1. Note that ROFF is negative in the direction of decreasing row numbers, and COFF is negative in the direction of decreasing column numbers. The figure below shows how to locate points within a finite-difference cell using ROFF and COFF (from Hill et al., 2000, chapter 4).



POINT	ROFF	COFF
A (Cell center)	0.0	0.0
B	-0.25	-0.25
C	-0.2	0.4
D	0.45	-0.45
E	0.25	0.0
F	0.4	0.25

Similarly to the Head-OBservation packages, flow observation packages for other types of observations can be implemented. These include

- DROB - Drain OBservation package
- RVOB - River Observation package
- GBOB - General head Boundary Observation package
- CHOB - Constant Head Observation Package

CHAPTER 2

OBSERVATION PROCESS: Implementation

Observations are independent values of equivalent simulated dependent variable values, which usually have been measured in the field or derived by calculations (for further details refer to Chapter 1).

Note: Before starting to implement observations, a running MODFLOW groundwater flow model is needed (see FREEWAT manual Volume I).

To implement any observations, the location of the observation needs to be prepared as a shapefile (point, line or polygon depending on type of observation). Further comma-separated-value-files (csv-files) are needed which contain information of date and time of the individual observations, the observation value, as well as statistical weighting method and weighting value. Alternatively HOB can be created from sensor data using the FREEWAT OAT tool.

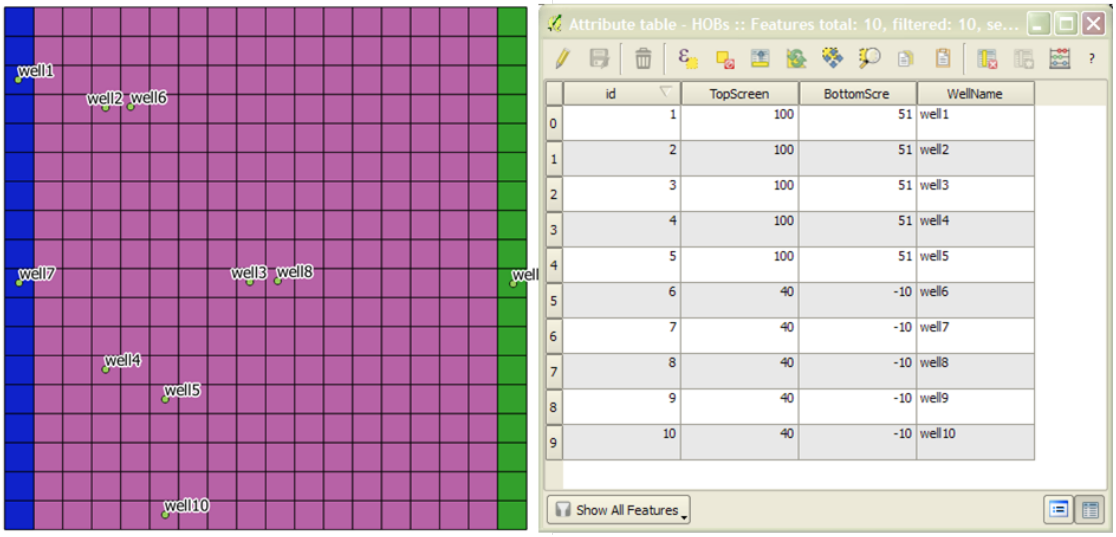
Important: The naming of the individual observation locations e.g. *WellName* need to be consistent with the created observation time series file (csv-file).

Implementing head observations (MODFLOW HOB package)

Head observations are groundwater table measurements usually in an observation well.

Prepare shapefile

To implement head observations into your FREEWAT groundwater model prepare a point shapefile, referenced to the geographic coordinate system of your model project. For each location of head observation add a point in the shapefile and add the information on a unique identifier name for the observation location (e.g. *WellName*), top elevation of the filter screen of the well (e.g. *TopScreen*) and bottom elevation of the filter screen of the well (e.g. *BottomScre*), see example from figure. If the screen top and bottom span over more than one layer, automatically the multi-layer option is activated and the HOB is interpolated vertically in proportion to the layer contribution. Elevations need to be given in the same unit and reference as model layers.



Prepare csv-files

The actual observation information is saved in comma-separated-value files (csv-files). Such a csv-file needs to be given the same name as the observation identifier name (e.g. *WellName*) in the shapefile and contain the following columns: time, data, obsname, weight and statistics. A csv-file can contain only one row, if the observation is only at one point in time, or multiple rows representing several observations in time at this specific location (see figure).

Attribute table - well1 :: Features total: 1, filtered: 1, selected: 0

	time	data	obsname	weight	statistics
0	2016-01-03 00:00:00	128	well1_1	1.05	SD

Attribute table - SPAGu :: Features total: 9, filtered: 9, selected: 0

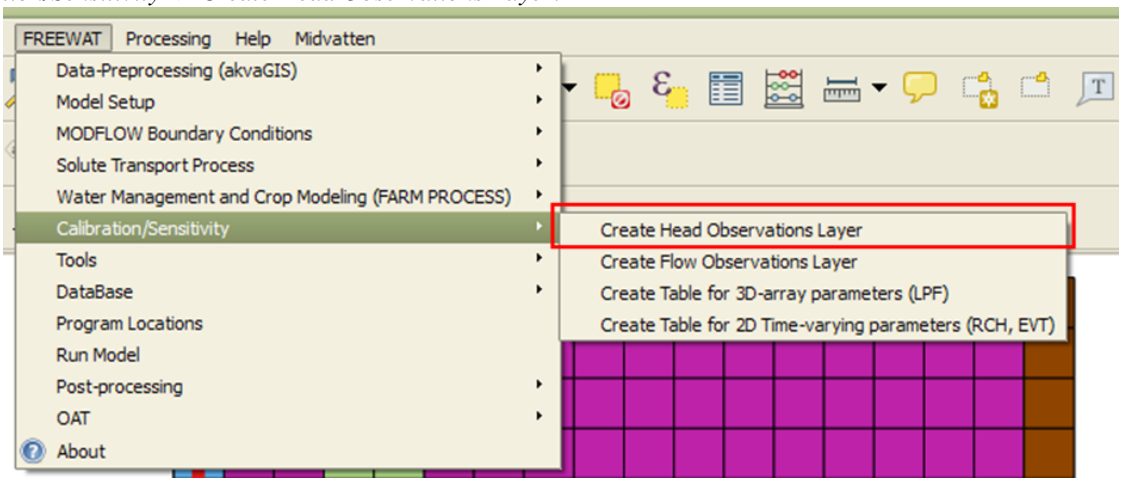
	time	data	obsname	weight	statistics
0	2010-07-06 01:00:00	-1.1	SPA_21	1.05	VAR
1	2010-07-16 01:00:00	-1.62	SPA_22	1.05	VAR
2	2010-07-26 01:00:00	-1.91	SPA_23	1.05	VAR
3	2010-08-05 01:00:00	-1.61	SPA_24	1.05	VAR
4	2010-08-15 01:00:00	-0.79	SPA_25	1.05	VAR
5	2010-08-25 01:00:00	-1.52	SPA_26	1.05	VAR
6	2010-09-04 01:00:00	-2.11	SPA_27	1.05	VAR
7	2010-09-14 01:00:00	-2.41	SPA_28	1.05	VAR
8	2010-09-24 01:00:00	-2.11	SPA_29	1.05	VAR

Show All Features

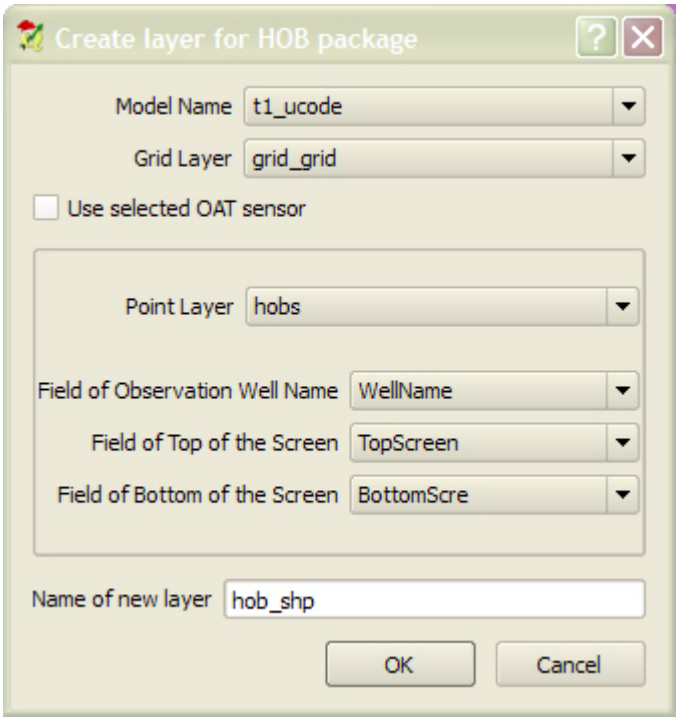
time:	Date and time at which the specific observation is recorded, important the format has to be `YYYY-MM-DD hh:mm:ss` e.g. for the 3rd of January 2016 at Midnight `2016-01-03 00:00:00` (Note: It is needed for the Time Offset calculation (TOFFSET) with respect initial date and time of simulation)
data:	Observed water level in length unit of model
obsname:	Identifier name of time specific head observation, the name needs to start with a letter (e.g. well1_1, well1_2, or HOB1_20160301, HOB1_20160501)
weight:	Weighting value of the specific observation
statistic:	Statistical method for the calculation of the observation weighting, the available methods are either variance (VAR), standard deviation (SD) or coefficient of variation (CV)

Creating the Head Observations Layer

The head observations layer, which is read as input for the FREEWAT model is created under *FREEWAT -> Calibration/Sensitivity -> Create Head Observations Layer*.



The following window opens:

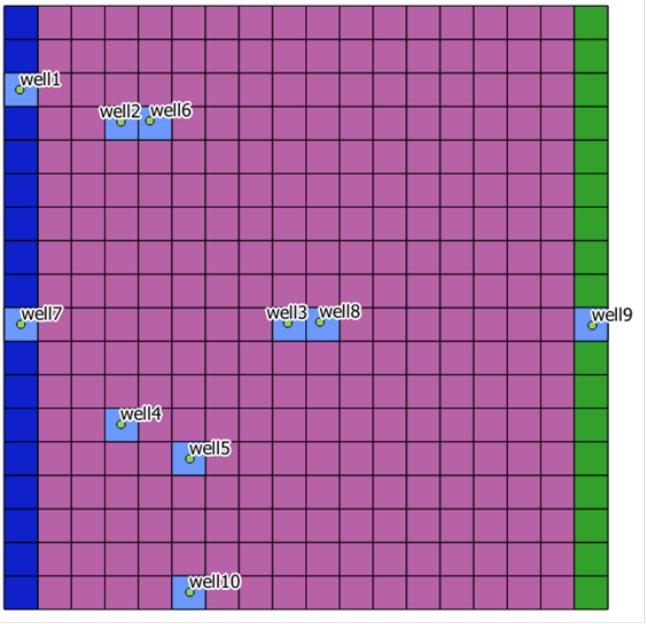


Model Name:	Name of the groundwater model
Grid Layer:	Desired grid layer

Here you can tick optionally *Use selected OAT sensor* to create the MDO directly from sensor data (refer FREEWAT Manual OAT - Volume V, Chapter 8 *Creating a HOB layer using OAT sensors*).

Point Layer:	Shapefile containing spatial information of head observations
Field of Observation Well Name:	Column of shapefile containing name of observation well (e.g. *WellName*)
Field of Top of the Screen:	Column in shapefile containing the information about top elevation of filter screen (e.g. *TopScreen*)
Field of Bottom of the Screen:	Column in shapefile containing the information about bottom elevation of filter screen (e.g. *BottomScre*)
Name of new layer:	Name of HOB layer you will create

After information is inserted, press `OK` and a new model data object (MDO) will be created in you FREEWAT project. The MDO will be called as *Name of new layer* plus the extension *_hob* with an attribute table containing the corresponding data, see figure.



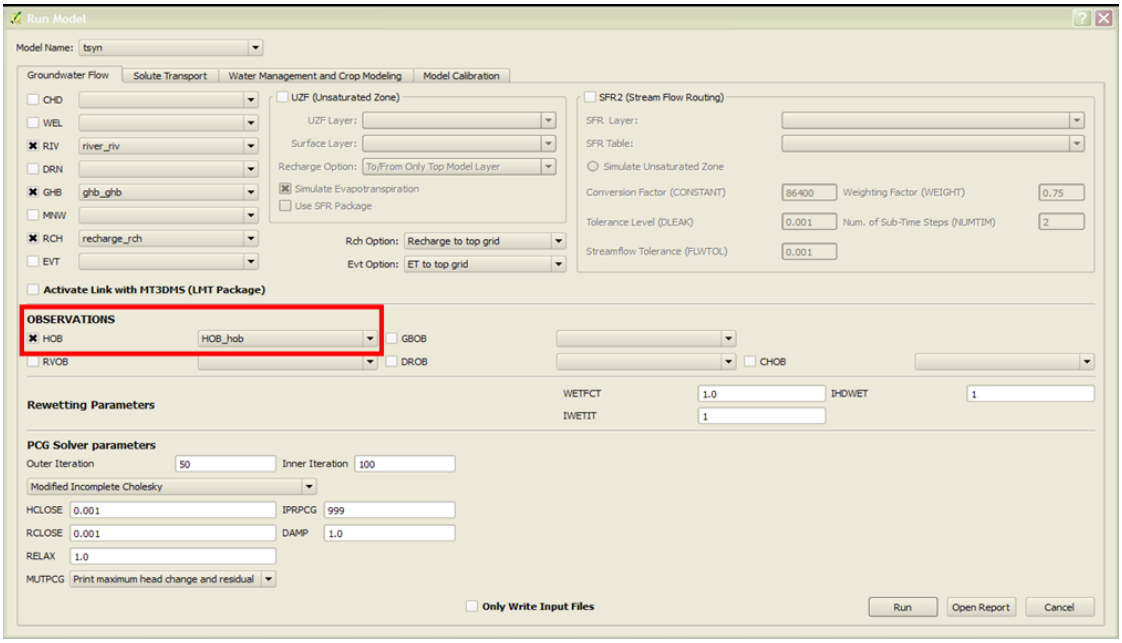
Attribute table - HOB_hob :: Features total: 10, filtered: 10, selected: 0

	ROW	COL	WELLNAME	OBSNAM	WEIGHT	STATISTICS	from_lay	to_lay	HOBS	ROFF	COFF	PR_1	PR_2	PR_3	IREFSP	TOFFSET
9	0	3	1	well1	well1_1	1.05	SD	1	1	128.0	0.006663296398...	-0.0241530470914	0.98	0	0	1	2.0
0	0	18	6	well10	well10_1	1.05	SD	3	3	142.0	-0.0115789473684	0.0184210526316	0	0	1	1	2.0
7	0	4	4	well2	well2_1	1.0025	VAR	1	1	128.0	-0.0373684210526	-0.0373684210526	0.98	0	0	1	2.0
4	0	10	9	well3	well3_1	1.05	SD	1	1	157.0	-0.0357894736842	-0.0636842105263	0.98	0	0	1	2.0
2	0	13	4	well4	well4_1	1.05	SD	1	1	125.0	-0.0184210526316	-0.0373684210526	0.98	0	0	1	2.0
1	0	14	6	well5	well5_1	1.0025	VAR	1	1	141.0	0.009473684210...	0.0184210526316	0.98	0	0	1	2.0
8	0	4	5	well6	well6_1	1.05	SD	3	3	127.0	-0.0705263157895	-0.142105263158	0	0	1	1	2.0
3	0	10	1	well7	well7_1	1.05	SD	3	3	101.0	-0.00263157894...	0.009004847645...	0	0	1	1	2.0
5	0	10	10	well8	well8_1	1.05	SD	3	3	158.0	-0.0689473684211	-0.102105263158	0	0	1	1	2.0
6	0	10	18	well9	well9_1	1.05	SD	3	3	176.0	0.0305263157895	0.0215789473684	0	0	1	1	2.0

The attribute table (*_hob*) contains information of the csv-file, name and observation name, assigned weights their statistic method, groundwater head observation (*HOBS*), as well as new information as model row (*ROW*), column (*COL*) and layer (*from_lay*, *to_lay*) of the location of the observation well, shift from cell center (*ROFF*, *COFF*), reference stress period of the observation (*IREFSP*) and the timeoffset (*TOFFSET*) and *PR(I)*, the proportion of the simulated hydraulic head in layer *MLAY(I)* that is used to calculate simulated multilayer head. The sum of all PR values for a given observation equals 1.0.

Applying the MODFLOW HOB package in FREEWAT

In order to apply the Head Observation package in a groundwater model run, open the *Run Model* window under *FREEWAT -> Run Model* and select the *Groundwater Flow* tab. Select and set everything as for a regular run, but under the section *OBSERVATIONS* tick *HOB* and select the desired HOB MDO (*_hob*) (see figure) and then press *Run* as regular.



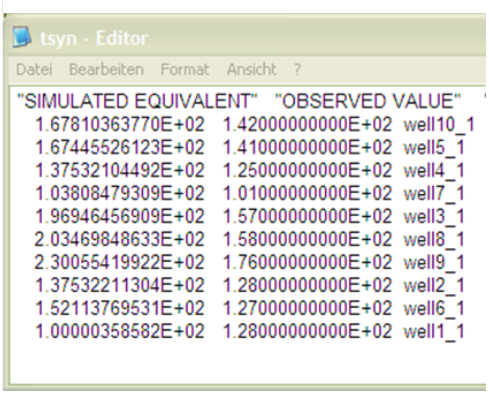
HOB package output

After a successful run, you can open the MODFLOW report (*.LST*) with the *Open Report* -button and in the bottom of this report you can now find information about the observed and simulated value of the selected head observations as well as the difference between observed and selected values and a sum of squared differences of all selected observations (see left figure).

HEAD AND DRAWDOWN OBSERVATIONS

OBSERVATION NAME	OBSERVED VALUE	SIMULATED VALUE	DIFFERENCE
well10_1	142.00000000	157.47305298	-15.473052979
well5_1	141.00000000	157.54983521	-16.549835205
well4_1	125.00000000	138.97160339	-13.971603394
well7_1	101.00000000	102.95048523	-1.9504852295
well3_1	157.00000000	174.75590515	-17.755905151
well8_1	158.00000000	178.08007812	-20.080078125
well9_1	176.00000000	191.66963196	-15.669631958
well2_1	128.00000000	138.97160339	-10.971603394
well6_1	127.00000000	147.96478271	-20.964782715
well1_1	128.00000000	100.02256012	27.977439880

HEAD/DRAWDOWN SUM OF SQUARED DIFFERENCE: 3.01898E+03



The observed and simulated equivalent value information is also contained in a file called *.obh* which has been created in your working folder (see right figure) and can be opened with a text editor.

Note: Before proceeding to any executions in the *Run Model -> Model Calibration* tab a groundwater model run has to have been executed with the desired HOB dataset in order to create the *.obh*-file.

Implementing flow observations

Flow observations are estimates of fluxes in or out of the aquifer, for river segments (RIV), drains (DRN), general head boundaries (GHB) and constant head boundaries (CHD).

Implementing river flow observations (MODFLOW RVOB package)

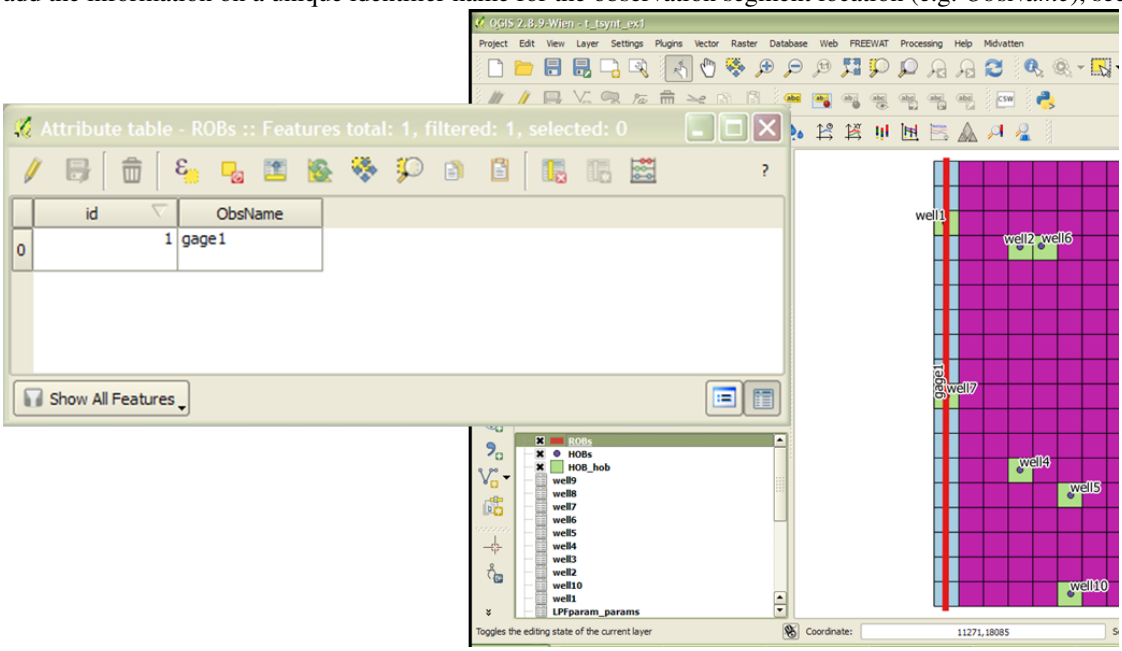
River observations (RVOB) represent fluxes between a river segment and the aquifer.

- A positive value represents seepage from the river into the aquifer, a loss of river flow.
- A negative value discharge from the aquifer to the river, which equals the gain of river flow.

A RVOB value is calculated from the difference in discharge between two discharge measurement stations, e.g. with the OAT tool (See FREEWAT manual Volume V OAT).

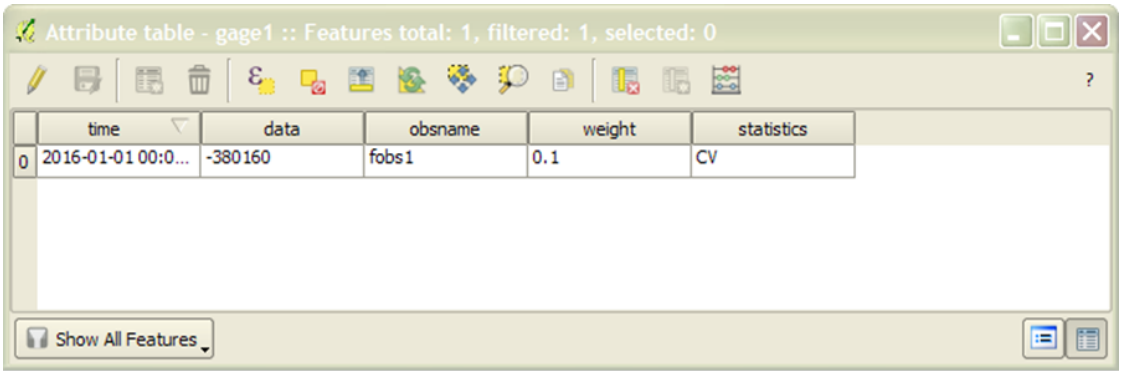
Prepare shapefile

To implement river observations into your FREEWAT groundwater model prepare a line shapefile, referenced to the geographic coordinate system of your model project. For each river observation segment add a row in the shapefile and add the information on a unique identifier name for the observation segment location (e.g. *ObsName*), see figure.



Prepare csv-files

The actual observation information is saved in comma-seperated-value files (csv-files). Such a csv-file needs to be given the same name as the observation identifier name (*ObsName*) in the shapefile and contain the following columns: *time*, *data*, *obsname*, *weight* and *statistics*. A csv-file can contain only one row, if there is only an observation at one point in time, or multiple rows representing several observations in time at this specific location (see figure).



Attribute table - SPAGu :: Features total: 9, filtered: 9, selected: 0

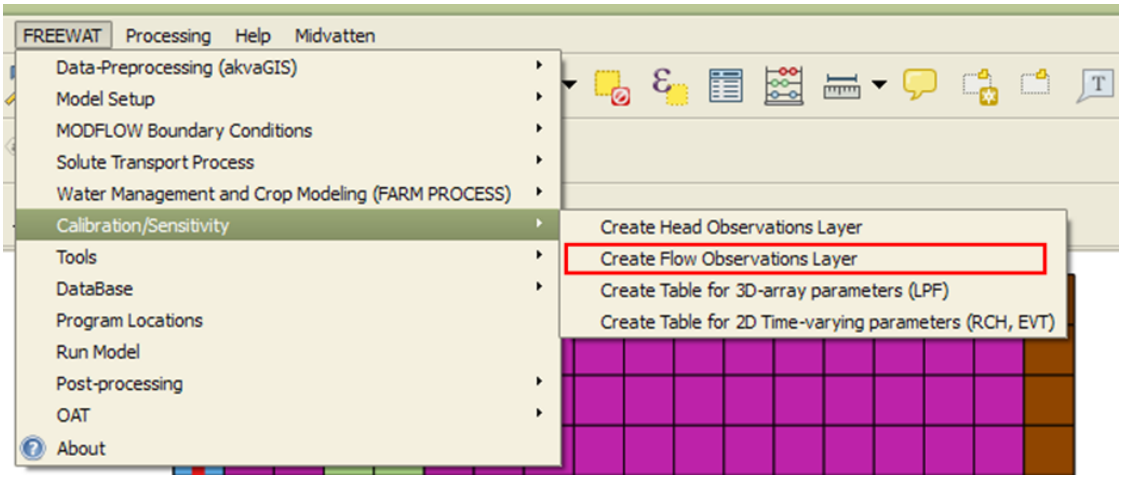
	time	data	obsname	weight	statistics
0	2010-07-06 01:00:00	-1.1	SPA_21	1.05	VAR
1	2010-07-16 01:00:00	-1.62	SPA_22	1.05	VAR
2	2010-07-26 01:00:00	-1.91	SPA_23	1.05	VAR
3	2010-08-05 01:00:00	-1.61	SPA_24	1.05	VAR
4	2010-08-15 01:00:00	-0.79	SPA_25	1.05	VAR
5	2010-08-25 01:00:00	-1.52	SPA_26	1.05	VAR
6	2010-09-04 01:00:00	-2.11	SPA_27	1.05	VAR
7	2010-09-14 01:00:00	-2.41	SPA_28	1.05	VAR
8	2010-09-24 01:00:00	-2.11	SPA_29	1.05	VAR

Show All Features

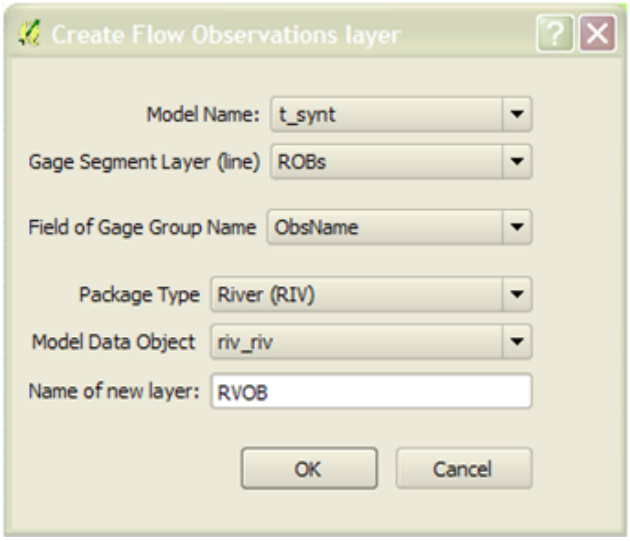
time:	date and time at which the specific observation is recorded, important the format has to be `YYYY-MM-DD hh:mm:ss` e.g. for the 3rd of January 2016 at Midnight `2016-01-03 00:00:00` (Note: It is needed for the Time Offset calculation (TOFFSET) with respect initial date and time of simulation)
data:	observed water level in length unit of model
obsname:	Identifier name of time specific flow observation, the name needs to start with a letter (e.g. flow_1)
weight:	weighting value of the specific observation
statistic:	statistical method for the calculation of the observation weighting, the available methods are either variance (VAR), standard deviation (SD) or coefficient of variation (CV)

Creating the River Flow Observations Layer

The river flow observations layer, which is read as input for the FREEWAT model is created under *FREEWAT -> Calibration/Sensitivity -> Create Flow Observations Layer*.

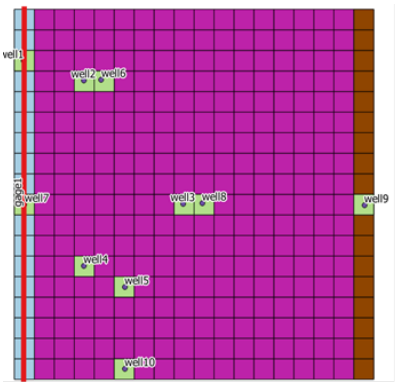


The following window opens:



Model Name:	Name of the groundwater model
Gage Segment Layer (line):	Line shapefile containing spatial information of the location of the flow obersvations segments
Field of Gage Group Name:	Column of shapefile containing name of flow observation segment (e.g. *ObsName*)
Package Type:	Select River (RIV)
Model Data Object:	Select the desired river MDO with the extension *_riv*
Name of new layer:	Name of RVOB layer you will create

After information is inserted, press *OK* and a new model data object (MDO) will be created in you FREEWAT project. The MDO will be called as *Name of new layer* plus the extention *_rvob* with a corresponding attribute table (see figure).



Attribute table - RVOB_rvob :: Features total: 18, filtered: 18, selected: 0

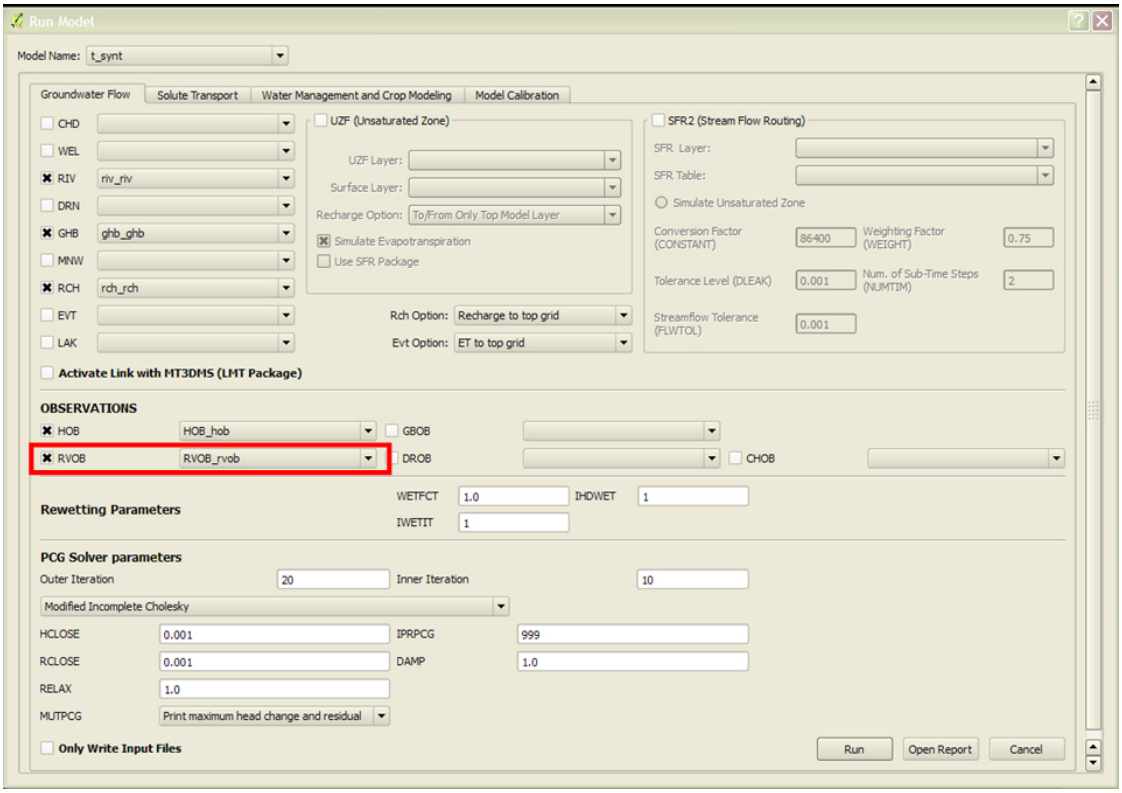
	PKUID	ID	ROW	COL	layer	GAGENAME	OBSNAM	FLOWOBS	WEIGHT	STATISTICS	TOFFSET	IREFSP
0	1	0	18	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
1	2	0	17	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
2	3	0	16	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
3	4	0	15	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
4	5	0	14	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
5	6	0	13	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
6	7	0	12	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
7	8	0	11	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
8	9	0	10	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
9	10	0	9	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
10	11	0	8	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
11	12	0	7	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
12	13	0	6	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
13	14	0	5	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
14	15	0	4	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
15	16	0	3	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
16	17	0	2	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1
17	18	0	1	1	1	gage1	fobs1	-380160.0	0.1	CV	0	1

Show All Features

The attribute table (*_rvob*) contains information of the csv-file, as observation segment name (*GAGENAME*) and observation name (*OBSNAM*), flow observation value (*FLOWOBS*), assigned weights their statistic method, as well as new information as model row (*ROW*), column (*COL*) and layer (*from_lay*, *to_lay*) of the location of the flow observation, reference stress period of the observation (*IREFSP*) and the timeoffset (*TOFFSET*).

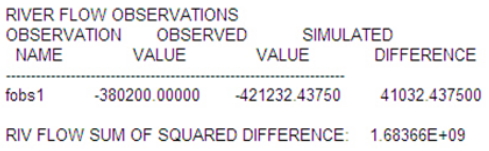
Applying the MODFLOW RVOB package in FREEWAT

In order to apply the River Flow Observation package in a groundwater model run, open the *Run Model* window under *FREEWAT -> Run Model* and select the *Groundwater Flow* tab. Select and set everything as for a regular run, but under the section *OBSERVATIONS* tick *RVOB* and select the desired RVOB MDO (*_rvob*) (see figure) and then press *Run* as regular.



RVOB package output

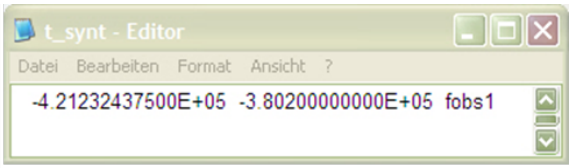
After a successful run, you can open the MODFLOW report (*.LST*) with the *Open Report* button and in the bottom of this report you can now find information about the observed and simulated value of the selected river flow observations as well as the difference between observed and selected values and a sum of squared differences of all selected observations (see figure).



RIVER FLOW OBSERVATIONS

OBSERVATION NAME	OBSERVED VALUE	SIMULATED VALUE	DIFFERENCE
fobs1	-380200.00000	-421232.43750	41032.437500

RIV FLOW SUM OF SQUARED DIFFERENCE: 1.68366E+09



The observed and simulated equivalent value information is also contained in a file called *.obr* which has been created in your working folder which can be opened with a text editor. Note: before proceeding to any executions in the *Run Model -> Model Calibration* tab a groundwater model run has to have been executed, in order to create the *.obr* file.

Implementing drain flow observations (MODFLOW DROB package)

Drain observations (DROB) represent fluxes from a drain segment to the aquifer, they are given as positive value represents seepage from the drain into the aquifer.

For the implementation refer to Chapter *Implementing river flow observations (MODFLOW RVOB package)*, the implementation process and output is the same, but select *Package Type DRN*.

Implementing general head boundary flow observations (MODFLOW GHOB package)

General head boundary observations (GHOB) represent fluxes between a GHB segment and the aquifer.

- A positive value represents a flow through the GHB boundary into the aquifer.
- A negative value a flow through the GHB boundary out of the aquifer.

For the implementation refer to Chapter *Implementing river flow observations (MODFLOW RVOB package)*, the implementation process and output is the same, but select *Package Type GHB*.

Implementing constant head flow observations (MODFLOW CHOB package)

Constant head boundary observations (CHOB) represent fluxes between a CHD segment and the aquifer.

- A positive value represents a flow through the CHD boundary into the aquifer.
- A negative value a flow through the CHD boundary out of the aquifer.

For the implementation refer to Chapter *Implementing river flow observations (MODFLOW RVOB package)*, the implementation process and output is the same, but select *Package Type CHD*.

CHAPTER 3

SENSITIVITY ANALYSIS AND PARAMETER ESTIMATION: Theory

What is UCODE_2014 and how does it work?

UCODE is one of a set of inverse modeling codes supported by the U.S. Geological Survey. UCODE was developed for models in which the number of parameters is less than the number of observations. It supports a wide range of parameterization capabilities through its template file and derived parameter capabilities, and emphasizes the utility of a range of sensitivity and uncertainty analysis methods. FREEWAT is designed to execute UCODE_2014 for further detail on the code refer to the UCODE_2005 (Poeter et al. 2005) and UCODE_2014 (Poeter et al. 2014) documentations.

Two other inverse modeling codes supported by the U.S. Geological Survey are PEST++ (Welter et al., 2012) and bgaPEST (Fienen et al., 2013). Both support methods with which the number of parameters can exceed the number of observations. It is hoped that making a range of methods readily available to users will enable the kind of experimentation needed to understand how to enhance the predictive skill and process understanding models ideally provide. There are also a number of freely available programs from outside the U.S. Geological Survey with similar capabilities. These include, for example, PEST (Doherty, 2010) and OSTRICH (Mattot, 2010). Users are encouraged to consider this rich set of alternatives as they develop their models.

The UCODE code is public domain, open-source software and can be downloaded from the Internet at URL http://igwmc.mines.edu/. The performance of the code has been tested in a variety of applications. Future applications, however, might reveal errors that were not detected in the test simulations. Users are requested to notify the IGWMC (Integrated Groundwater Modeling Center) of any errors found in the report or the computer codes. Updates might occasionally be made to both the report and to the codes. Users can check for updates on the Internet at URL http://igwmc.mines.edu/.

Process Model

Both the UCODE_2005 documentation and the UCODE_2014 report use the phrase *process model* to describe the model run by UCODE and for which UCODE estimates parameter values. Consider this within the ongoing debate in many fields of environmental science about three types of models: statistical models based on probability distribution functions (pdfs), conceptual models based largely on if/then rules, and process-based models based largely on differential equations. The authors of UCODE have used process-based models throughout their careers, and when defining a term by which to differentiate the model run by UCODE and the inverse model embodied by UCODE, it was natural to call the model run by UCODE a process model. However, UCODE is not limited in any way, and is equally capable of being used with statistical and conceptual models (for example, Foglia et al., 2013 evaluate a range of conceptual models that differ in how aspects of a system are simulated). Thus, UCODE is not limited to process models as defined in some scientific disciplines, despite the use of the term *process model*. Of concern is whether the parameters to be estimated and the observations used in the estimation are real numbers (UCODE applies) or discrete (UCODE does not apply). In some cases with discrete parameter values or for other aspects of model construction for which discrete alternatives are of interest (for example, alternative ways of calculating recharge or alternative conceptualizations of

boundary conditions or geometry of system characteristics), constructing alternative models that represent the discrete alternatives and using UCODE and another code called Multi-Model Analysis (MMA) (Poeter and Hill, 2007) can be useful. For an example, see Foglia et al. (2013).

Sensitivity Analysis

While Saltelli et al. (2008) limit sensitivity analysis to identifying sources of prediction uncertainty, a broader definition is embraced here that includes identifying parameters important to fitting the observations and observations important to estimating parameters. Once important parameters and observations are identified, further analyses such as regression, GLUE, or MCMC can be posed in a way that increases the chance of obtaining useful results.

Here we show how sensitivity analysis is used to design regressions. The sensitivity analysis implemented here is suggested by Hill and Tiedeman (2007), and includes computationally frugal local, or gradient, methods. Local sensitivity analysis methods use the sensitivities (derivatives) of simulated values with respect to parameters, and the sensitivities are evaluated at a specific set of parameter values. Sensitivities can be calculated using central or forward differences. The sensitivities themselves are not useful for sensitivity analysis (Saltelli et al., 2008, p. 15), but statistics calculated using the sensitivities are useful. The sensitivity analysis statistics implemented in UCODE_2014 and therefore in FREEWAT are described below and are divided into the categories fit-independent and fit-dependent.

Fit-Independent Statistics

Fit-independent statistics are calculated without using residuals (observed minus simulated values), so that the analysis is likely to be useful even when the model does not fit the observations well, as can occur with an uncalibrated model. Fit-independent statistics account for observation type, time, and location, but not the observed value. This paper uses three fit-independent statistics: composite scaled sensitivities (CSS), parameter correlation coefficients (PCC), and leverage. Composite scaled sensitivities (CSS) are calculated using dimensionless scaled sensitivities (DSS).

For a diagonal weight matrix, dimensionless scaled sensitivity for observation i and parameter j are calculated as

$$DSS_{ij} = (\partial y_i'/\partial b_j)|_b \, b_j \omega_{ii}^{1/2} \quad i = 1, n \; j = 1, p$$

where i is the observation index; y'_i is the simulated value being compared to the ith observation; b_j is the j^{th} estimated parameter; $(\partial y'_i / \partial b_j)$ is the sensitivity of the ith simulated value with respect to the j^{th} parameter, evaluated for b; b is a vector of parameter values; ω_{ii} is the weight for the j^{th} observation; n is the number of observations; and p is the number of parameters. The equation for DSS when the weight matrix is full is presented by Hill and Tiedeman [2007, p. 49] and can be implemented using, for example, UCODE_2005. It is suggested by Saltelli et al. [2008, p.15] that scaling by the parameter value in equation (1) should be replaced by the parameter standard deviation, and Hill and Tiedeman [2007, pp. 56-57] also suggest this scaling. While scaling using the standard deviation is useful when investigating the parameter contribution to uncertainty, scaling by the parameter value often is more useful when the goal is to determine the likely success of parameter estimation.

Composite scaled sensitivity (CSS) for any parameter j is calculated as

$$CSS_j = [\textstyle\sum_{i=1}^{n} (DSS_{ij})^2|_b / n]^{1/2} \qquad j = 1, p$$

where DSSij is from the previous equation. Larger CSS values identify parameters for which more information is provided by all observations for each parameter. CSS provides no information on whether coordinated changes in parameter values would produce the same model fit, which results in parameter value nonuniqueness.

This type of nonuniquness can be detected using parameter correlation coefficients (PCC), which are calculated as

$$PCC_{k,l} = cov(b_k, b_l)/[var(b_k)^{1/2} var(b_l)^{1/2}] \qquad k = 1, p \; l = 1, p$$

where cov(b_k, b_j) are the covariances and var(b_k) are the variances of the square, symmetric parameter variance-covariance matrix, V(b). V(b) is calculated as

$$V(b) = \sigma^2 (X^T \omega X)^{-1}$$

where σ^2 is the calculated error variance (referred to as CEV below), X is an n by p matrix of sensitivities defined after the equation above, and ω is an n by n weight matrix which was assumed to be diagonal to obtain equation (1). Absolute values of PCC close to 1.00 (greater than 0.95, with increasing assurance as values approach 1.00) identify parameters for which it may not be possible to estimate uniquely the defined parameters given the information provided by the observations. Many extremely correlated parameter pairs for which the same parameters occur in different combinations indicate correlation among a set of parameters.

$$h_{ii} = x_i^T (X^T X)^{-1} x_i \qquad i = 1, n$$

where h_{ii} is the leverage for observation i, and $x_i$is the transpose of the ith row of the sensitivity matrix as defined in the equation. Values of leverage range from 0.0 to 1.0. Larger values identify observations that are potentially more important to estimating the parameter values.

Fit-Dependent statistics

Fit-dependent statistics are calculated using residuals and include all so-called influence statistics. For fit-dependent statistics, model fit is important and generally a calibrated model is used.

Parameter Estimation

Parameter estimation refers to the process of optimizing a selected set of parameters using a nonlinear regression and objective function is the sum of squared weighted residuals, which are calculated as

$$S(b) = \sum_{i=1}^{nh} \omega_i (q_i - q_i'(b))^2 + \sum_{i=1}^{nq} \omega_i (q_i - q_i'(b))^2 + \sum_{i=1}^{npr} \omega_i (P_i - P_i'(b))^2$$

where S(b) is the objective funtion, b the selected model parameter and ω_i the observation weight; while h_i and h'_i are observed and simulated heads, q_i and q'_i are observed and simulated flows and P_i and P'_i are observed and simulated prior information.

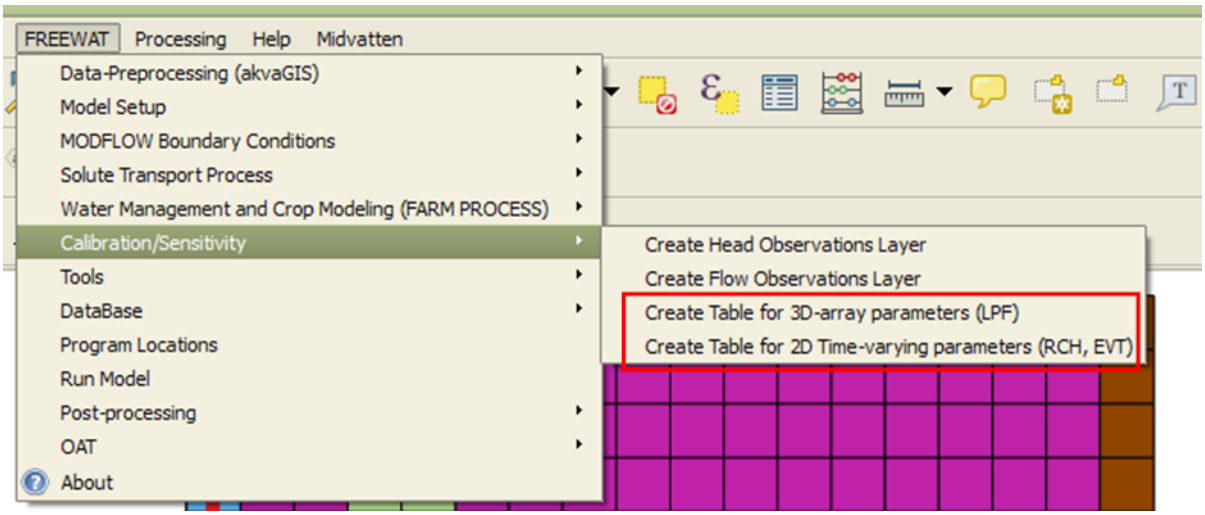
Goal of the regression is to find a set of parameters b which minimized S(b), applying the modified Gauss-Newton method. UCODE uses a forward- or central-difference perturbation technique, the method is described by Hill and Tiedeman (2007). UCODE also provides the following additional ways to improve regression performance. First, dynamic omission of insensitive parameters can be used so that insensitive parameters do not disrupt regression performance. Second, unique criteria for each parameter can be specified that govern the maximum fractional amount that the parameter value can change in one parameter-estimation iteration. Smaller values may be useful for insensitive parameters. Third, a quasi-Newton or trust region modification of the Gauss-Newton method can be used to reduce the number of parameter-estimation iterations needed and, in some cases, achieve successful regressions (see Poeter et al. 2005).

CHAPTER 4

SENSITIVITY ANALYSIS AND PARAMETER ESTIMATION: Implementation

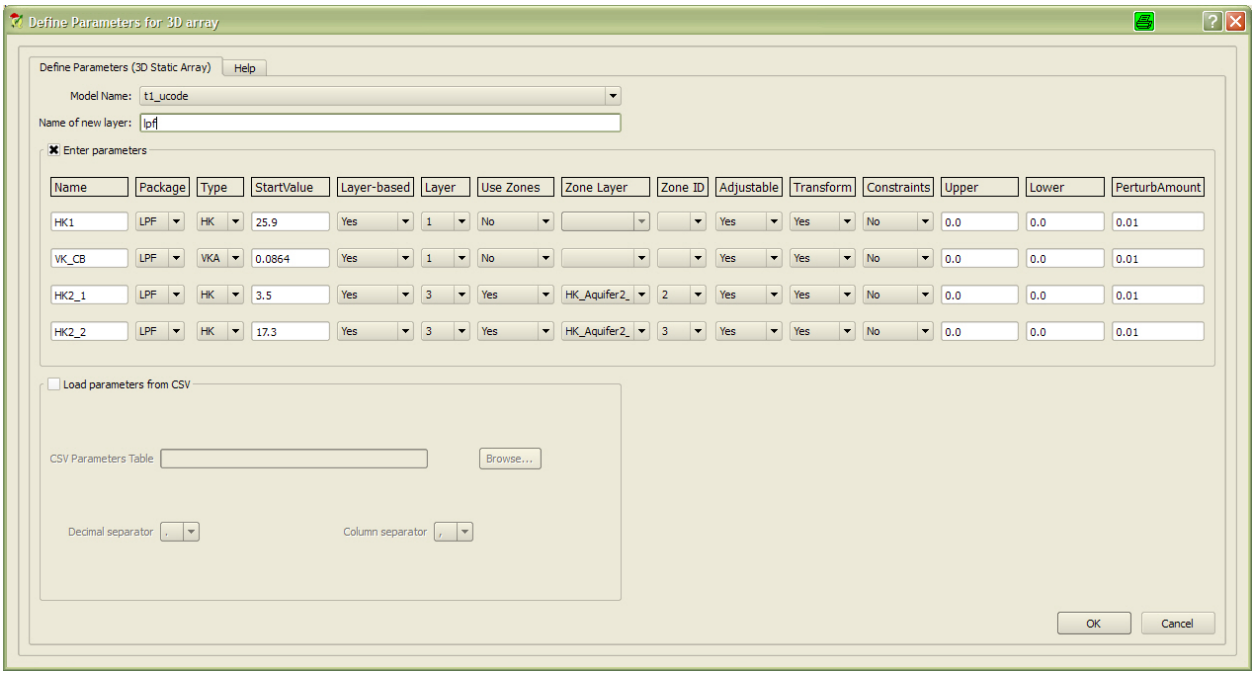
Selecting groundwater model parameters for sensitivity analysis and parameter estimation

For the calibration, meaning the execution of a sensitivity analysis or parameter estimation with UCODE, next to the implementation of observations (see Chapter 2), the desired groundwater model parameters have to be selected. There are two categories of parameter arrays which can be created 3D-arrays and 2D-arrays. 3D-arrays are containing parameters of the MODFLOW Layer Properties Flow (LPF) package while the 2D-arrays contain time-varying parameters such as recharge (RCH) and evapotranspiration (EVT). The two options are selected under *FREEWAT -> Calibration/Sensitivity -> Create Table for 3D-array parameters (LPF)* or *Create Table for 2D Time-varying parameters (RCH, EVT)* (see figure).



Create tables for 3D-array parameters (LPF)

When selecting *Create Table for 3D-array parameters (LPF)* the following window opens:



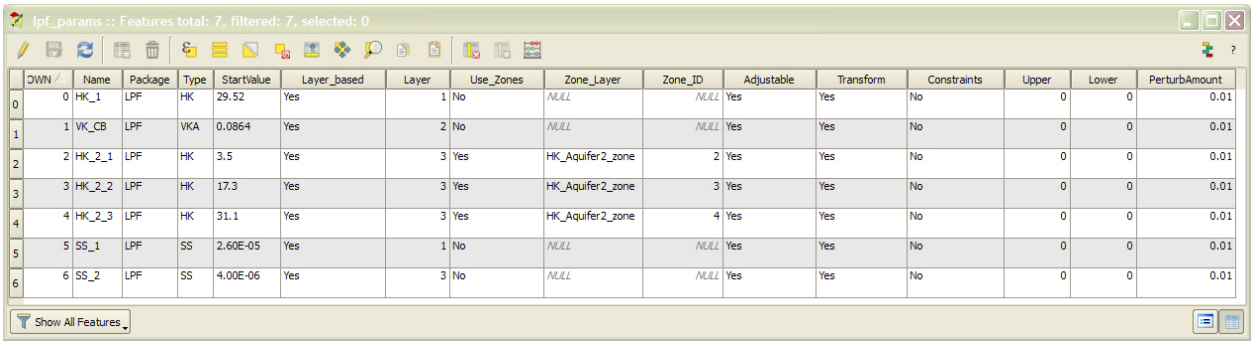
Model Name:	Name of the groundwater model
Name of new layer:	Name of parameter layer to be created

You can choose between entering up to four parameters manually selecting **Enter Parameters** or as alternative select **Load parameters from CSV** and browse to a prepared csv-file containing columns as described below and either separate columns by point or comma and use the opposite symbol as decimal separator.

Name:	User-defined name of parameter
Package:	Select LPF from dropdown menu
Type:	Select HK, VAK, SS, SY from dropdown menu
StartValue:	Enter starting parameter value (e.g. value from initial model)
Layer-based:	Select from dropdown menu **Yes**, will apply parameter for whole layer; **No**, use a zone layer
Layer:	Select layer number containing the parameter
Use Zone:	Select from dropdown menu **Yes**, will enable the selection of a zone layer; **No**, apply parameter to whole layer
Zone Layer:	If *Use Zone* is **Yes** select a zone layer with the desired *Zone IDs* set
Zone ID:	Select zone ID as described in **Zone Layer**
Adjustable:	Select **Yes** if this parameter should be used in a sensitivity analysis or parameter estimation, and **No** if not
Transform:	Select **Yes** if this parameter should be log transformed, and **No** if not
Constraints:	Select **Yes** if this parameter should be constraint, and **No** if not
Upper:	Value of upper constraint
Lower:	Value of upper constraint
PerturbAmount:	Fractional amount of parameter value to perturb to calculate sensitivity

An attribute table with the extension *_params* will be created containing all the entered information (see figure).

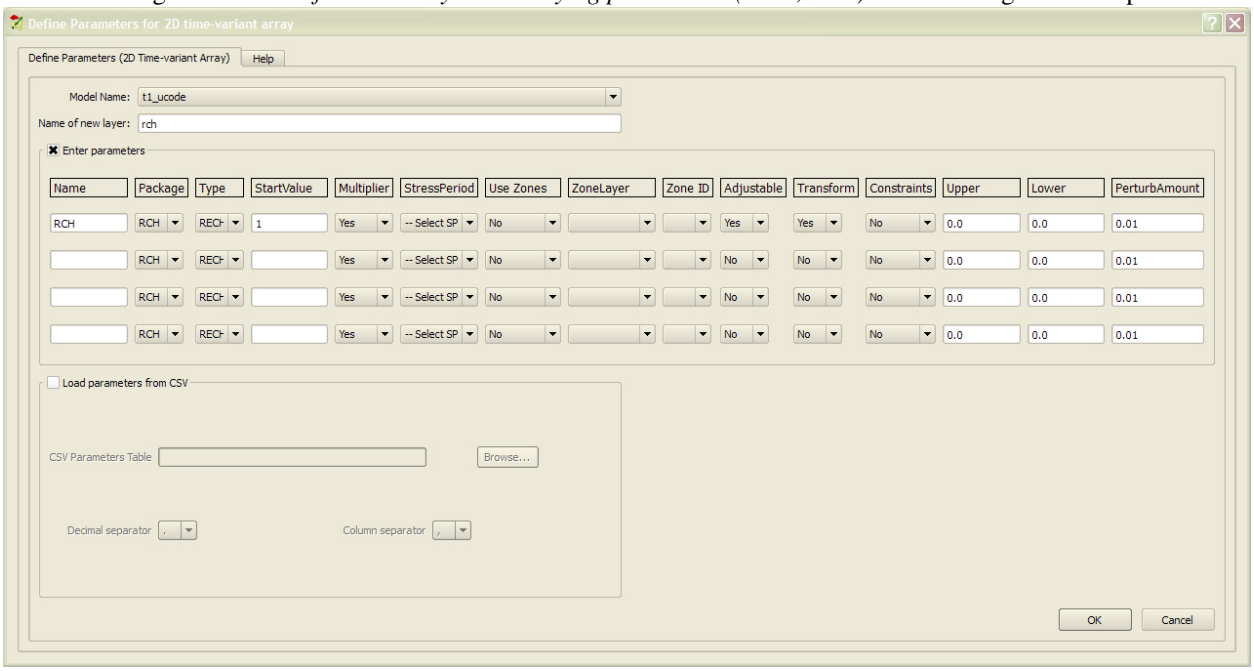
Note: This table can be used to change for example the starting values (StartValue) or if a parameter will be adjustable.



FID	Name	Package	Type	StartValue	Layer_based	Layer	Use_Zones	Zone_Layer	Zone_ID	Adjustable	Transform	Constraints	Upper	Lower	PerturbAmount
0	HK_1	LPF	HK	29.52	Yes	1	No	NULL	NULL	Yes	Yes	No	0	0	0.01
1	VK_CB	LPF	VKA	0.0864	Yes	2	No	NULL	NULL	Yes	Yes	No	0	0	0.01
2	HK_2_1	LPF	HK	3.5	Yes	3	Yes	HK_Aquifer2_zone	2	Yes	Yes	No	0	0	0.01
3	HK_2_2	LPF	HK	17.3	Yes	3	Yes	HK_Aquifer2_zone	3	Yes	Yes	No	0	0	0.01
4	HK_2_3	LPF	HK	31.1	Yes	3	Yes	HK_Aquifer2_zone	4	Yes	Yes	No	0	0	0.01
5	SS_1	LPF	SS	2.60E-05	Yes	1	No	NULL	NULL	Yes	Yes	No	0	0	0.01
6	SS_2	LPF	SS	4.00E-06	Yes	3	No	NULL	NULL	Yes	Yes	No	0	0	0.01

Create tables for 2D-array Time-varying parameters (RCH, EVT)

When selecting *Create Table for 2D-array Time-varying parameters (RCH, EVT)* the following window opens:



Model Name:	Name of the groundwater model
Name of new layer:	Name of parameter layer to be created

You can choose between entering up to four parameters manually selecting **Enter Parameters** or as alternative select **Load parameters from CSV** and browse to a prepared csv-file containing columns as described below and either separate columns by point or comma and use the opposite symbol as decimal separator.

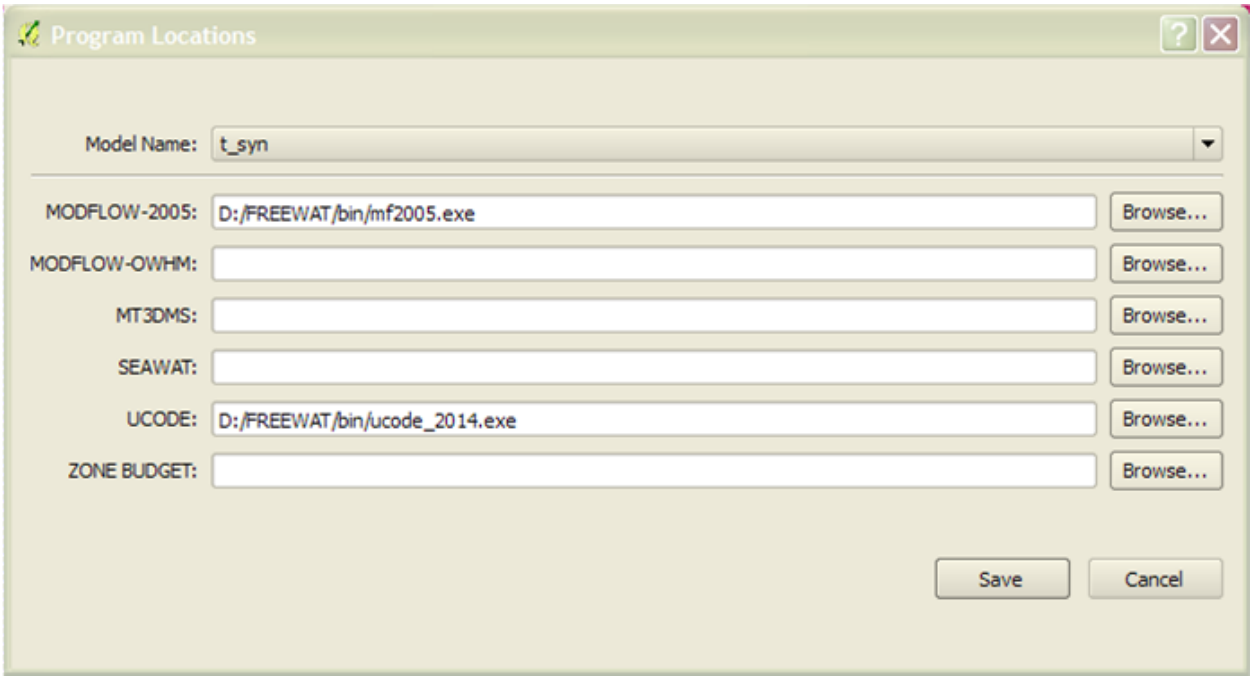
Name:	User-defined name of parameter
Package:	Select RCH or EVT from dropdown menu
Type:	Select RECH, EVTR, EXDP or SURF from dropdown menu
StartValue:	Enter starting parameter value (e.g. value from initial model)
Multiplier:	Select from dropdown menu **Yes**, will apply parameter for whole layer; **No** will not use the multiplier option (select when *Use Zone = Yes*)
StressPeriod:	Select the stress period from the dropdown menu
Use Zone:	Select from dropdown menu **Yes**, will enable the selection of a zone layer; **No**, apply parameter to whole layer (select when *Multiplier = Yes*)
Zone Layer:	If *Use Zone* is **Yes** select a zone layer with the desired *Zone IDs* set
Zone ID:	Select zone ID as described in **Zone Layer** (Note: Zone IDs can only be used if set to the uppest layer)
Adjustable:	Select **Yes** if this parameter should be used in a sensitivity analysis or parameter estimation, and **No** if not
Transform:	Select **Yes** if this parameter should be log transformed, and **No** if not
Constraints:	Select **Yes** if this parameter should be constraint, and **No** if not
Upper:	Value of upper constraint
Lower:	Value of upper constraint
PerturbAmount:	Fractional amount of parameter value to perturb to calculate sensitivity

Note: Currently the option of setting *Multiplier = No* and *Use Zone = No*, which allows a constant value for the uppest layer is not active yet.

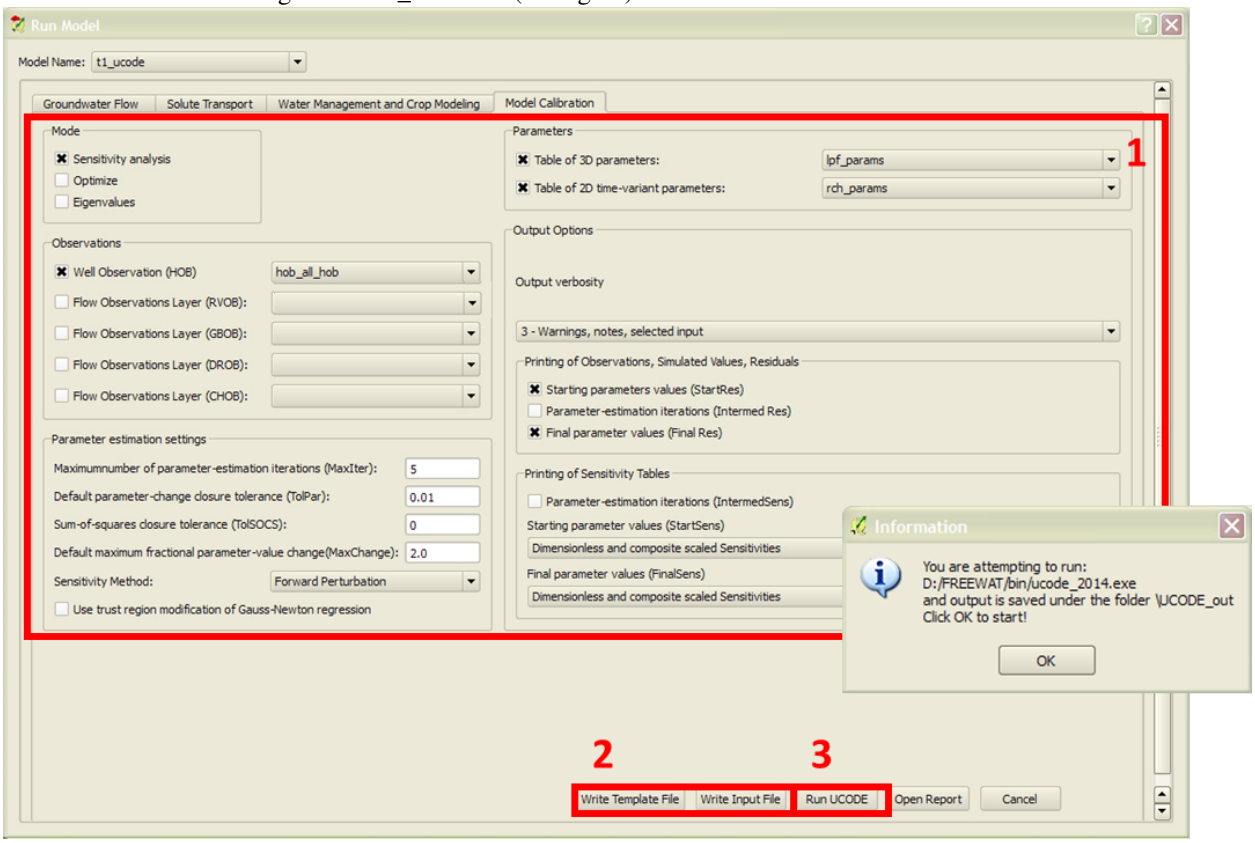
An attribute table with the extension *_params* will be created containing all the entered information (see figure). This table can be used to change for example the starting values (StartValue) or if a parameter will be adjustable.

Executing a sensitivity analysis

A sensitivity analysis is executed to gain information on the quantitative relationship between parameters and observations (see Chapter 3). In order to execute a Sensitivity Analysis you need to implement observations into your groundwater flow model and select the parameters you want to analyze (see Chapter 1 and 2). If this input is prepared open the under *FREEWAT -> Run Model* the **Model Calibration** tab. There are three major steps to follow (marked in figure) 1) define setting in the **Model Calibration** tab, 2) **Write Template File** and **Write Input File** as well as 3) **Run UCODE**. Note: Update template file if you change something concerning the parameter tables, update input file if you change something regarding the observations files and the parameter settings.



Important: Before attempting the execution make sure you have set the program location to the correct executables. Under *FREEWAT -> Program Locations* set the program location of the groundwater flow model e.g. mf2005.exe and the UCODE executable e.g. UCODE_2014.exe (see figure).



Setting options of the Model Calibration tab

The **Model Calibration** tab contains the following sections: Mode, Observations, Parameter estimation settings,

Parameters, Output Options and Printing of Sensitivity Tables.

Mode

Here you need to select the mode **Sensitivity Analysis**.

Note: You can also check no box, which will execute a forward run of your groundwater model, with the initial values you selected in the parameter table. This option can be useful if you want to check whether your groundwater model will run successfully.

Observations

In the observations section you check the observation types and observations set for each type you want to use in the sensitivity analysis.

The options are:

Well Observations (HOB)	Refers to head observations (HOB) and a MDO with the extension *_hob*
Flow Observations Layer (RVOB)	Refers to river flow observations (RIV) and a MDO with the extension *_rvob*
Flow Observations Layer (GBOB)	Refers to general head boundary (GHB) flow observations and a MDO with the extension *_gbob*
Flow Observations Layer (DROB)	Refers to drain (DRN) flow observations and a MDO with the extension *_drob*
Flow Observations Layer (CHOB)	Refers to constant head boundary (CHD) flow observations and a MDO with the extention *_chob*

Parameter estimation settings

Parameter estimation setting are not needed for the execution of a sensitivity analysis.

Parameters

In the Parameters section you check the parameter tables you want to use in the Sensitivity Analysis. There is the option of choosing one table for *3D parameters* and *2D time-variant parameters*. Be careful to select the right parameter table, because there is no distinction in the table name extension both types have the extension *_params*.

Output Options

In the Output Options section you can select an output verbosity, which defines how detailed your output report will be. You can choose between:

0-	No extraneous output
1-	Warnings
2-	Warnings, notes
3-	Warnings, notes, selected input (default option)
4-	Warnings, notes, all input
5-	All available output

Further you have the option to choose under *Printing of Observations, Simulated Values, Residuals* between:

Starting parameters values (StartRes)

Parameter-estimation interations (Intermed Res)

Final parameters values (FinalRes)

Printing of Sensitivity Tables

In the Printing of Sensitivity Tables section you can select among:

Parameter-estimation iterations (IntermedSens)

Starting parameter values (StartSens) dropdown-menu:

Dimensionless and composite scaled sensitivities (default option)

Composite scaled sensitivities

One-percent scaled sensitivities and composite scaled sensitivities

All sensitivity tables

Final parameter values (FinalSens) dropdown-menu:

Dimensionless and composite scaled sensitivities (default option)

Composite scaled sensitivities

One-percent scaled sensitivities and composite scaled sensitivities

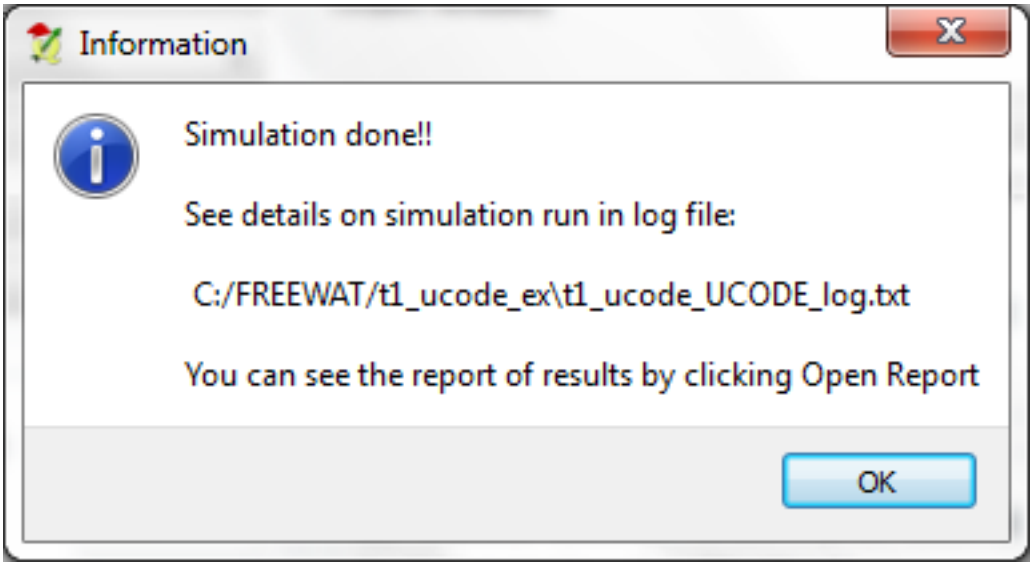
All sensitivity tables

Write UCODE input files

The **Model Calibration** tab window contains two button (see figure) called **Write Template File** and **Write Input File**. After defining your desired settings (see above), press both of these buttons. The order is not relevant and if you already created one file type and did not change the settings you do not need to recreate before a new run.

Execute UCODE

After creating the UCODE input files you can press the **Run UCODE** button, this will enable an external execution window, which is now executing the UCODE code. After a run you will see an information window (see figure).

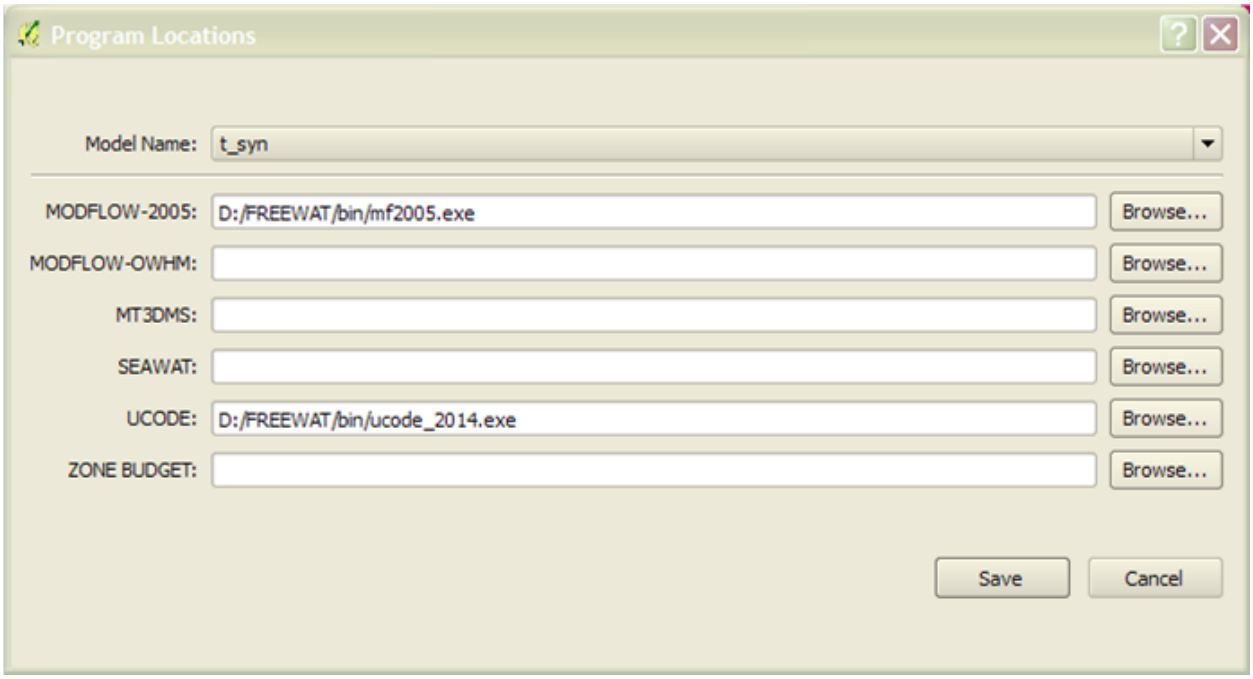


To obtain the output of the Sensitivity Analysis press the **Open Report** button on the **Run Model** window **Model Calibration** tab, this will open the UCODE output report (*.#uout*). For visualization you can proceed to *FREEWAT -> Post-processing -> Plot Calibration Results* (see Chapter 5).

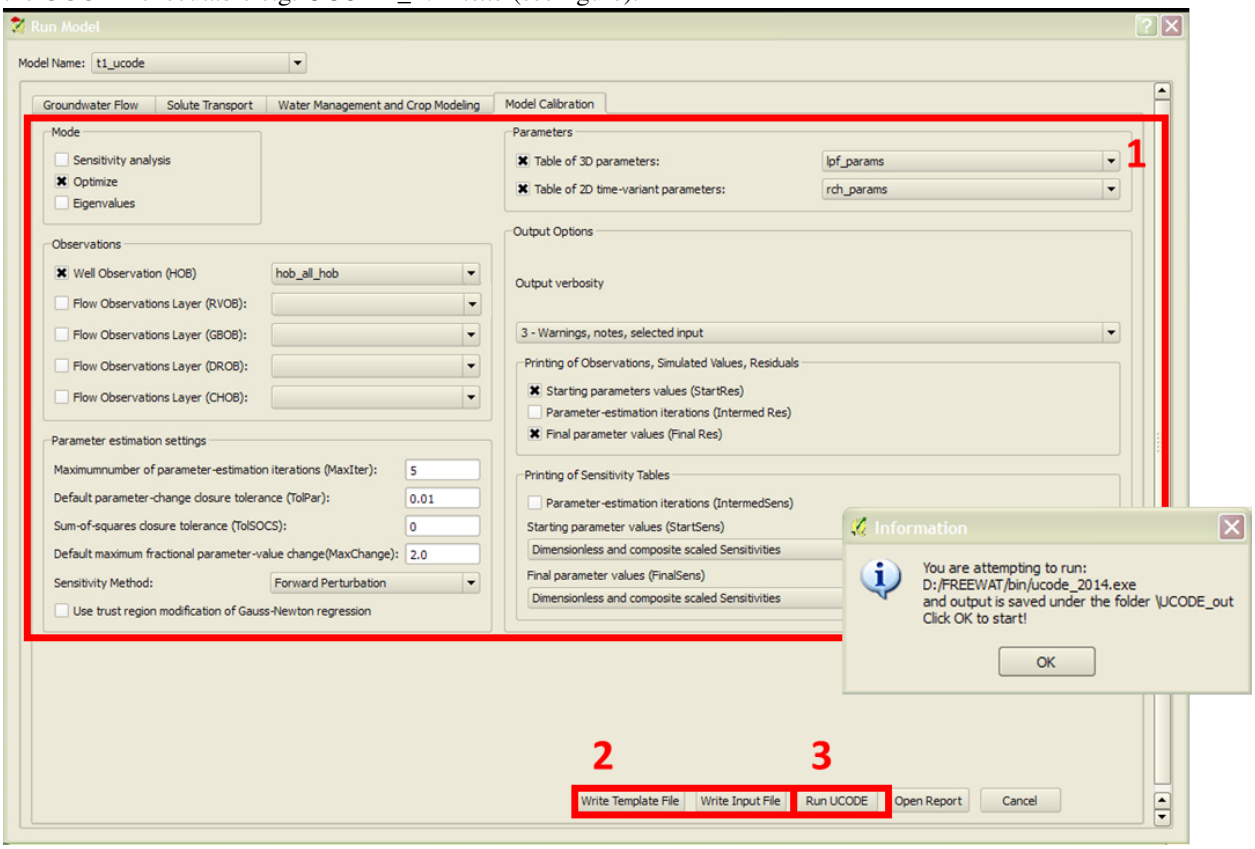
Executing a parameter estimation

Parameter estimations are executed to obtain the set of parameters which give the best fit between observed and simulated values of the square weighted residuals regression. In order to execute a parameter estimation you need to implement observations into your groundwater flow model and select the parameters you want to optimize (see Chapter 1 and 2). If this input is prepared open the under *FREEWAT -> Run Model* the **Model Calibration** tab. There are three

major steps to follow (marked in figure) 1) define setting in the **Model Calibration** tab, 2) **Write Template File** and **Write Input File** as well as 3) **Run UCODE**.



Important: Before attempting the execution make sure you have set the program location to the correct executables. Under *FREEWAT -> Program Locations* set the program location of the groundwater flow model e.g. *mf2005.exe* and the UCODE executable e.g. *UCODE_2014.exe* (see figure).



Setting options of the Model Calibration tab

The **Model Calibration** tab contains the following sections: Mode, Observations, Parameter estimation settings, Parameters, Output Options and Printing of Sensitivity Tables.

Mode

Here you need to select the mode **Optimize**.

Note: You can also check no box, which will execute a forward run of your groundwater model, with the initial values you selected in the parameter table. This option can be useful if you want to check

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whether your groundwater model will run successfully.

Observations

In the observations section you check the observation types and observations set for each type you want to use for the parameter estimation. The options are:

Well Observations (HOB)	Refers to head observations (HOB) and a MDO with the extension *_hob*
Flow Observations Layer (RVOB)	Refers to river flow observations (RIV) and a MDO with the extension *_rvob*
Flow Observations Layer (GBOB)	Refers to general head boundary (GHB) flow observations and a MDO with the extension *_gbob*
Flow Observations Layer (DROB)	Refers to drain (DRN) flow observations and a MDO with the extension *_drob*
Flow Observations Layer (CHOB)	Refers to constant head boundary (CHD) flow observations and a MDO with the extention *_chob*

Parameter estimation settings

Under Parameter estimation settings you can define settings for the following:

Maximum number of parameter-estimation iterations (MaxIter):	Maximum number of iterations (MaxIter) has to be set, default is 5. Modified Gauss-Newton optimization typically converges within a number of iterations equal to five or twice the number of parameters, whichever is greater.
Default parameter-change closure tolerance (TolPar):	Convergence is achieved when the parameter values change only a small amount from one parameter-estimation iteration to the next. This indicates that at the current regression iteration, the parameter values lie in a relatively flat area that is a minimum in the objective-function space. This condition is satisfied if, for all parameters, max-calculated-change (TolPar) is less than max-allowed-change. Preferably, this convergence is achieved in the final calibrated model with a criterion value no larger than 0.01 (default value).
Sum-of-squares closure tolerance (TolSOCS):	In the second convergence criterion, the nonlinear regression converges if the model fit changes little over the course of two parameter-estimation iterations. If three consecutive values of the least squares objective function change less than a user-defined amount (**TolSOCS**) the regression converges. As default this criterion is 0 and is only recommended to use if parameter estimation does not converge otherwise.
Default maximum fractional parameter-value change (MaxChange):	The maximum fractional change allowed in one regression iteration. If MAX-CHANGE=2 (default value) and the parameter value=1.1, the new value is allowed to be between 1.1(2x1.1), or between -1.1 and 3.3.
Sensitivity Method:	From the dropdown menu choose between **Forward Perturbation** and **Central Perturbation**, the latter does a forward and backward perturbation
Use trust region modificiation of Gauss-Newton regression:	Dogleg: use the trust-region modification with the double dogleg step-size strategy or Hookstep: use the hookstep modification

Parameters

In the Parameters section you check the parameter tables you want to optimize in the parameter estimation. There is the option of choosing one table for **3D parameters** and **2D time-variant parameters**. Be careful to select the right parameter table, because there is no distinction in the table name extension both types have the extension *_params*.

Output Options

In the Output Options section you can select an output verbosity, which defines how detailed your output report will be. You can choose between:

0-	No extraneous output
1-	Warnings
2-	Warnings, notes
3-	Warnings, notes, selected input (default option)
4-	Warnings, notes, all input
5-	All available output

Further you have the option to choose under **Printing of Observations, Simulated Values, Residuals** between:

Starting parameters values (StartRes)

Parameter-estimation interations (Intermed Res)

Final parameters values (FinalRes)

Printing of Sensitivity Tables

In the Printing of Sensitivity Tables section you can select among:

Parameter-estimation iterations (IntermedSens)

Starting parameter values (StartSens) dropdown-menu:

Dimensionless and composite scaled sensitivities (default option)

Composite scaled sensitivities

One-percent scaled sensitivities and composite scaled sensitivities

All sensitivity tables

Final parameter values (FinalSens) dropdown-menu:

Dimensionless and composite scaled sensitivities (default option)

Composite scaled sensitivities

One-percent scaled sensitivities and composite scaled sensitivities

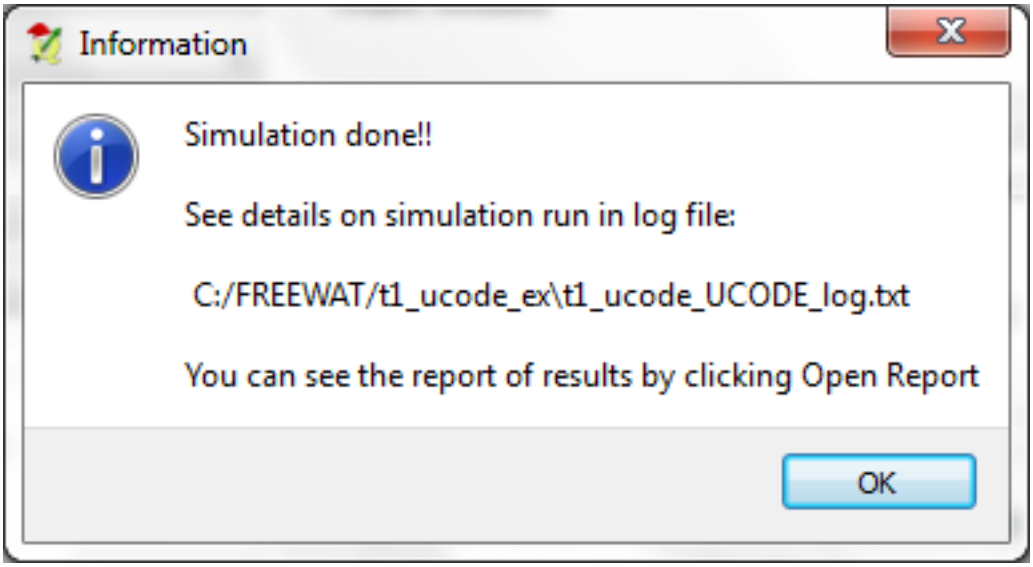
All sensitivity tables

Write UCODE input files

The **Model Calibration** tab window contains two button (see figure) called **Write Template File** and **Write Input File**. After defining your desired settings (see above), press both of these buttons. The order is not relevant and if you already created one file type and did not change the settings you do not need to recreate before a new run.

Execute UCODE

After creating the UCODE input files you can press the **Run UCODE** button, this will enable an external execution window, which is now executing the UCODE code. After a run you will see an information window (see figure).



To obtain the output of the Parameter Estimation press the **Open Report** button on the **Run Model** window **Model Calibration** tab, this will open the UCODE output report (*.#uout*). For visualization you can proceed to *FREEWAT -> Post-processing -> Plot Calibration Results*.

UCODE output files and post-processing options

After a successful UCODE run you will have produced a set of UCODE output files and you will want to visualize those output files. For visualization you have the option of **Chart Plots**, which are graphs of your results and **Map Plots**, which are GIS layers of certain outputs (residuals and leverage) which can be visualized spatially distributed for each head observation in your project.

Output files

The UCODE run produces the following output files in your working folder, all marked with an underscore _:

Graphical analysis of model fit to observations

_nm	Weighted residuals and probability plotting positions
_os	Unweighted simulated equivalents and observed or prior values[1]
_r	Unweighted residuals[2]
_w	Weighted residuals for observations and prior information[2]
_w_presd	Copy of _w based on parameters used to start SVD
_ws	Simulated equivalents and weighted residuals[1]
_ww	Weighted simulated equivalents and weighted observations or prior information[1]

Commonly used for sensitivity analysis

_pcc	Large parameter correlation coefficients (+/- 0.85) formatted for presentation[1]
_sc	Composite scaled sensitivities for each parameter[1]
_scgrp	Grouped composite scaled sensitivities for each parameter[1]
_sc_svd	Decomposition of CSS using SVD of scaled[wt^0.5][X][1]
_sc_svd_presvd	Copy of _sc_svd based on parameters used to start SVD
_sd	Dimensionless scaled sensitivities for each observation and each parameter[1]
_so	Leverage statistics with observations and, if defined, prior information[2]
_s1	One-percent scaled sensitivities[1]
_svd	Singularvalues and vectors of [$wt^{0.5}$][X]{b} matrix[1]
_svd_presvd	Copy of _svd based on parameters used to start SVD
_svd-id	SVD-ID statistics for a range of SVDnumber
_svd-id_presvd	Copy of _svd-id based on parameters used to start SVD

Information from each parameter-estimation iteration

_pa	All defined parameters: values formatted in columns[1]
_pasub	All defined parameters: formatted to substitute in Parameter_Values input block
_ss	Sum of squared weighted residuals[1]

Final results

_paopt	All defined parameters
_paopt_presvd	Copy of _paopt based on parameters used to start SVD
_pc	Adjusted parameters
_summary	Summary of regression progress
_summary_presvd	Summary of regression progress for run to start SVD

Files used for model development and testing

_dm	Information related to model structure, fit and parsimony
_dm_presvd	Copy of _dm based on parameters used to start SVD
_gm	Defines observation groups

Used by other programs; rarely by users

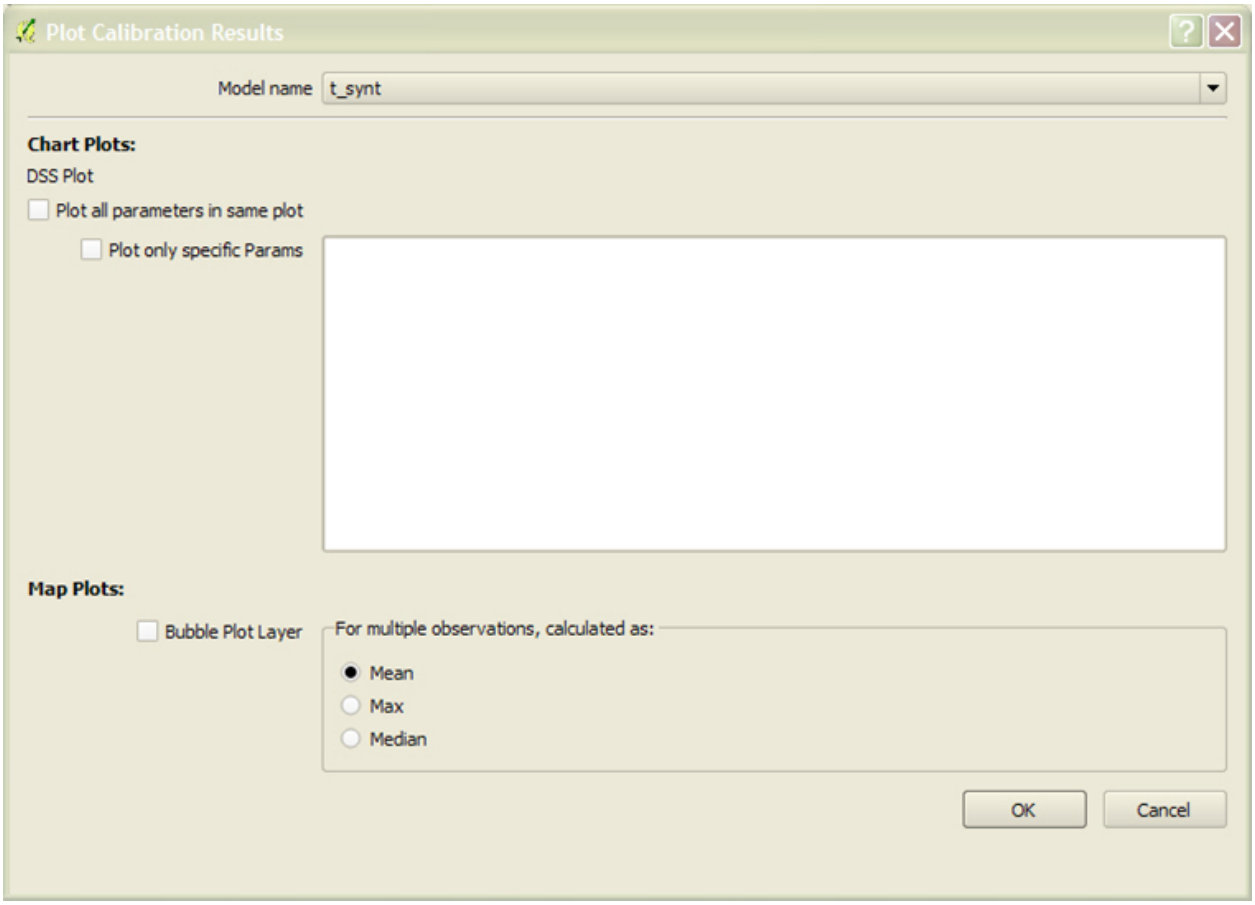
_b1	Parameter sets for calculating Beale's measure of linearity
_init	Like _paopt but for a non-optimal parameter set
_mc	Parameter correlation coefficient matrix
_mv	Parameter variance-covariance matrix
_mv_presvd	Copy of _mv based on parameters used to start SVD
_su	Unscaled sensitivities for observations
_su_presvd	Copy of _su based on parameters used to start SVD
_wt	Weighting for observations
_wt_presvd	Copy of _wt based on parameters used to start SVD

[1]this output-file is represented as chart plot

[2]this output-file is represented as chart and map plot

Post-processing options

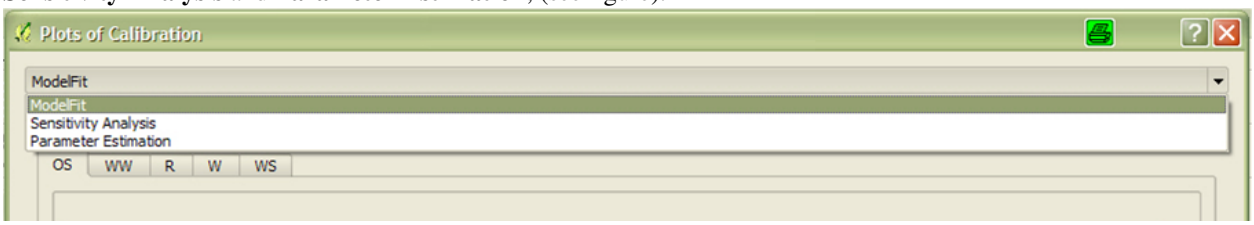
The most important of the listed output-files can be visualized using a post-processing tool. Under *FREEWAT -> Post-Processing -> Plot Calibration Results* you can open the following window:



The window contains the two options of creating either **Chart Plots** or **Map Plots** and further options to specify settings for some of the plots. There is the option of saving the plots as .png or .pdf file by right clicking and selecting *Save Plot*.

Chart plots

The chart plots are graphs of the calculated UCODE outputs, which are sorted by the three categories **Model Fit**, **Sensitivity Analysis** and **Parameter Estimation**, (see figure).



Model Fit

Model Fit contains the following flow options:

OS:	Observed values vs. simulated equivalent
WW:	Weighted observed values vs. simulated equivalent
R:	Residuals or observed and simulated equivalents
W:	Weighted residuals or observed and simulated equivalents
WS:	Weighted residuals vs. simulated equivalents

Sensitivity Analysis:

The Sensitivity Analysis Section contains the following flow options:

SD:	Observation importance, based on Dimensionless Scaled Sensitivity
SC:	Parameter importance to Observations, based on Composite Scaled Sensitivity
SC_GRP:	Grouped parameter importance to observations, based on Composite Scaled Sensitivity
SC_SVD:	Composite Scaled Sensitivity Singular Value Decomposition
SVD:	Process Model Parameter Contribution to each SVD Parameter
PCC:	Parameter dependence, based on Parameter Correlation Coefficient
SO:	Observation Dominance, based on Leverage

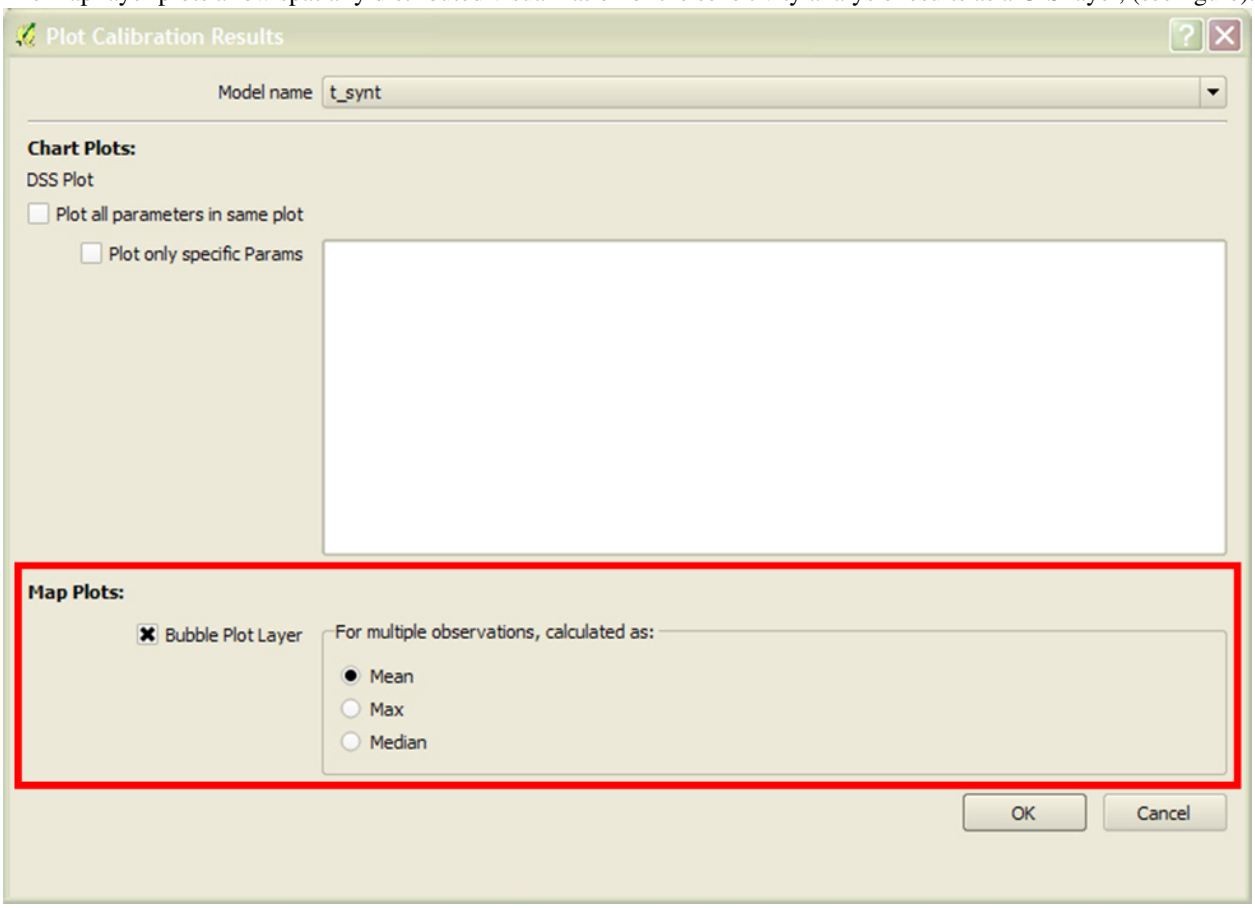
Parameter Estimation:

The Parameter Estimation Section contains the following flow options:

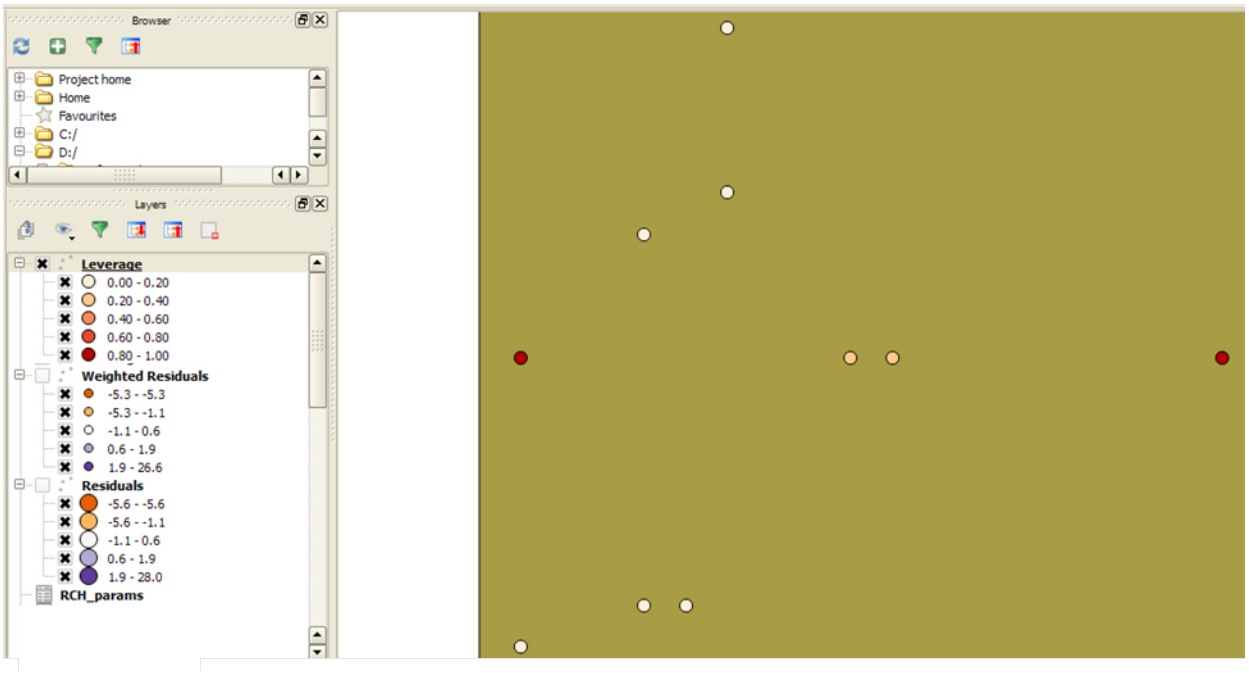
PA:	Estimated parameter for each iteration step
SS:	Squared weighted residuals for each iteration step

Map layer plots

The map layer plots allow spatially distributed visualization of the sensitivity analysis results as a GIS layer, (see figure).



For head observations you have the option to visualize Residuals, Weighted Residuals and Leverage with a color coding/as bubble charts. If there are multiple observations for one observation location, you can select the statistical method of calculation (mean, maximum or median).


Browser
Project home
Home
Favourites
C:/
D:/
Layers
Leverage
0.00 - 0.20
0.20 - 0.40
0.40 - 0.60
0.60 - 0.80
0.80 - 1.00
Weighted Residuals
-5.3 - -5.3
-5.3 - -1.1
-1.1 - 0.6
0.6 - 1.9
1.9 - 26.6
Residuals
-5.6 - -5.6
-5.6 - -1.1
-1.1 - 0.6
0.6 - 1.9
1.9 - 28.0
RCH_params

References

Doherty, J., 2010, PEST, Model-independent parameter estimation User manual (5th ed., with slight additions) and addendum: Brisbane, Australia, Watermark Numerical Computing. http://www.sspa.com/PEST/index.html

Fienen, M.N., D'Oria, Marco, Doherty, J.E., and Hunt, R.J., 2013, Approaches in highly parameterized inversion: bgaPEST, a Bayesian geostatistical approach implementation with PEST Documentation and instructions: U.S. Geological Survey Techniques and Methods, book 7, section C9, 86 p., available online at http://pubs.usgs.gov/tm/07/c09

Foglia, L., S. W. Mehl, M. C. Hill, and P. Burlando, 2013, Evaluating model structure adequacy: The case of the Maggia Valley groundwater system, southern Switzerland, Water Resour. Res., 49, doi:10.1029/2011WR011779.

Harbaugh, A.W., 2005, MODFLOW-2005, The U.S. Geological Survey modular ground-water model the Ground-Water Flow Process: U.S. Geological Survey Techniques and Methods 6-A16, variously p.

Hill, M.C., Banta, E.R., Harbaugh, A.W., and Anderman, E.R., 2000, MODFLOW-2000, the U.S. Geological Survey modular ground-water model – User guide to the Observation, Sensitivity, and Parameter-Estimation Processes and three post-processing programs: U.S. Geological Survey Open-File Report 00-184, 210 p.

Hill, M. C., and C. R. Tiedeman (2007), Effective Calibration of Groundwater Models, With Analysis of Data, Sensitivities, Predictions, and Uncertainty, John Wiley, New York.

Matott, L. S., 2010, OSTRICH: An Optimization Software Tool. Accessed 12/27/2010 at http://www.civil.uwaterloo.ca/lsmatott/Ostrich/OstrichMain.html

Poeter, E.P., Hill, M.C., Banta, E.R., Mehl, Steffen, and Christensen, Steen, 2005, UCODE_2005 and Six Other Computer Codes for Universal Sensitivity Analysis, Calibration, and Uncertainty Evaluation: U.S. Geological Survey Techniques and Methods 6-A11, 283p.

Poeter, E.P. and Hill, M.C., 2007, MMA, a computer program for multi-model analysis: U.S Geological Survey Techniques and Methods 6-E3 113p. http://typhoon.mines.edu/freeware/mma/.

Poeter, Eileen P., Mary C. Hill, Dan Lu, Claire R. Tiedeman, and Steffen Mehl, 2014, UCODE_2014, w ith new capabilities to define parameters unique to predictions, calculate weights using simulated values, estimate parameters with SVD, evaluate uncertainty with MCMC, and more: Integrated Groundwater Modeling Center Report Number GWMI 2014-02

Saltelli, A., M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisona, and S. Tarantola (2008), Global Sensitivity Analysis: The Primer, 292 pp., John Wiley, Chichester, U. K.

Welter, D.E., Doherty, J.E., Hunt, R.J., Muffels, C.T., Tonkin, M.J., and Schreder, W.A., 2012, Approaches in highly parameterized inversion: PEST++, a Parameter ESTimation code optimized for large environmental models. U.S. Geological Survey Techniques and Methods, book 7, section C5, 47 p. http://wi.water.usgs.gov/models/pestplusplus/