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Numerical modelling of evaporation from shallow aquifers: laboratory tests and field examples

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Summary

1 Introduction

Hydrogeology plays an important role in the land-atmosphere system. In order to gain a better understanding of this complex system, it is important to carefully analyze all the processes involved, namely: precipitation, evaporation, transpiration, infiltration and run-off. Most of these processes have been detailed studied in the past and still attract scientific attention from different disciplines, such as run-off processes or near surface evapotranspiration. Nevertheless, a limited number of studies have so far addressed the problem of direct evaporation processes from shallow groundwater bodies (Alkhaier et al., 2012; Kollet & Maxwell, 2008; Mengistu et al., 2018).

Evapotranspiration is the largest terrestrial water flux, typically accounting for more water than runoff and for about 60% of precipitation. It's a substantial portion of the global land-energy budget as latent heat flux (Maxwell & Condon, 2016). It represents a key process in the hydrologic cycle influencing the mass exchange between the land surface and the atmosphere and the energy balance of terrestrial surface. Hence, its impact to the micro-climate is inevitable (Mengistu et al., 2018).

Evapotranspiration can be divided in three components: surface evaporation (E_s), which includes evaporation from surface water and from water intercepted by plants; subsurface evaporation (E_{ss}), evaporation of water from below the ground surface; and transpiration of water by plants (T_{ss}). T_{ss} and E_{ss} together are defined as subsurface evapotranspiration (ET_{ss}). ET_{ss} can be further divided in groundwater evapotranspiration (ET_g) and unsaturated water evapotranspiration (ET_u). The process of separating different components of ET is called partitioning which remains a key uncertainty in the terrestrial water balance (Balugani et al. 2017).

To estimate evapotranspiration different methods exist, most estimates of crop evapotranspiration and bare soil evaporation are based on semi-empirical models such as that of Penman-Monteith (Ward & Robinson, 1990; Allen et al., 1998). It is recommended to use meteorological data as inputs to the Penman-Monteith methodology for estimating the potential evapotranspiration for a reference crop; then evapotranspiration for other crops is estimated by multiplying the reference by crop coefficients which frequently vary during the growing season and fall significantly at harvest. A non-varying crop coefficient is used to estimate bare soil potential evaporation from potential evapotranspiration; this coefficient is K_e=1.05 (Allen et al., 1998). When solar radiation data, relative humidity data and/or wind speed data are missing potential evapotranspiration can be estimated using the Hargreaves equation (Hargreaves & Samani, 1985), which requires the maximum and minimum daily temperatures and it also takes account of the latitude and the elevation of the sun. A reformulation of the Monteith's model is the widely applied Kc-NDVI methods. Within this approach the use of the Normalized Difference Vegetation Index (NDVI) replaces that of time-varying crop coefficients (Kc). It combines meteorological and NDVI data to simulate the actual evapotranspiration of various terrestrial ecosystems, utilizing the fractional vegetation cover (FVC) derived from NDVI to separate transpiring and evaporating surfaces (Maselli et al., 2014). The development of new monitoring methods has allowed independent measurement of various water fluxes. Both the Bowen ratio [*ratio used to describe the type of heat transfer, that can either occur as sensible heat or latent heat, for a surface that has moisture* (Wikipedia)] and the eddy covariance EC methods [*statistical method used in meteorology and other applications such as hydrology to determine exchange rates of trace gases over natural ecosystems and agricultural fields, and to quantify gas emissions rates from other land and water areas. It is frequently used to estimate momentum, heat, water vapour, carbon dioxide and methane fluxes* (Wikipedia)] permit reliable measurement of latent heat flux (and therefore ET) but over relatively small areas and only in specific conditions. Besides, it is possible nowadays to estimate E_s from models applying semi-continuous soil moisture and matrix potential profile measurements, while E_s can be estimated from pan evaporation and measurement of tree interception using tipping buckets and gutters placed under a tree canopy and by interception models (Balugani et al., 2017). The rate of E_s from different water table depths can be also estimated from the water balance equation in a lysimeter (Mengistu et al., 2018).

Considering a sandy bare (with no vegetation cover) soil, only the groundwater evaporation (E_g) component has been analyzed and modelled in this work. Groundwater affects soil moisture variations and surface evaporation and may have substantial effects in areas where the water table is near or within a model's soil column (Chen & Hu, 2004).

Evaporation from bare soil is an important component of the soil-water balance and a good knowledge of it is, therefore, fundamental to the groundwater management. Especially in arid and semi-arid areas where the demand for the water is increasing, quickly depleting scarce resources stored as groundwater.

However, the evapotranspiration of groundwater resources is often underestimated, both because evaporation processes are not yet included in the theory and because transpiration from roots tapping the water table is not taken into account. The underestimation of groundwater evapotranspiration often results in the overestimation of the net recharge (Balugani et al., 2017).

Of particular significance is the substantial reduction in bare soil evaporation as the water table falls and the dependency on the soil properties (Mengistu et al., 2018). An important feature claimed by many studies for sandy soils is that the evaporation becomes negligible when the water table is more than 60 cm below the ground surface. Nevertheless, considering an evaporation extinction depth of 60 cm, it is not always a conservative choice and could lead to significantly underestimate this component of the water cycle. In fact, as it was reported in (Balugani et al., 2017), considering the vapour flow through the ''almost dry'' unsaturated zone can result in even deeper evaporation extinction depths, which means greater E_g fluxes than estimated so far.

2 Materials and methods

As it was already said, this case study deals with groundwater evaporation in a sandy bare soil reproduced in a lab tank. In order to simulate the natural process, the tank has been set up in the hydrogeology laboratory in the SIMAU Department of "Università Politecnica delle Marche". Several parameters (hydrometric height, temperature, salinity, etc..) have been monitored over a time period of 145 days, by means of different sensors inside the tank.

To numerically simulate the process, a groundwater flow simulation model was required. Processing Modflow (Chiang, 2005), which was originally developed to support the first official release of MODFLOW-88, has been used. Together with MODFLOW (Harbaugh, 2005) code, another supporting code has been utilized named SEAWAT (Langevin et al., 2008). It incorporates MT3DMS (Zheng & Wang, 1999) code and includes the effect of fluid viscosity variations on groundwater flow.

The model of the tank in the laboratory has been created and, throughout its calibration with the data collected by the sensors (water head, temperature and salinity), the evaporation rates have been evaluated.

Then, a sensitivity analysis has been carried out for some of the parameters, such as effective porosity (n_e), longitudinal dispersion, mass loading rate and extinction depth, in order to determine their impact on the evaporation process.

Finally, the results obtained with the model have been carried from laboratory to basin scale. A 2007 case study has been reanalyzed in which the Tronto basin has been modelled for the low flow and high flow period and, at the time, the evapotranspiration has been neglected. Inserting highest and lowest value of maximum evaporation rates obtained with the calibration of the tank model, a substantial change in the hydrological balance of the basin resulted. The water at the outlet, due to evaporation from the groundwater, was more than 10% of the total output considering the lowest value; and almost 30% considering the highest.

This last step of the study has shown how evaporation, and evapotranspiration in general, plays a very important role in the hydro-geological balance and in estimating the water resources of a basin and, therefore, it should not be considered negligible.

All the laboratory materials and methodologies that have been used and adopted in this case study will be fully described in this chapter, together with the model characterization analyzing all the inputs.

2.1 Laboratory experiment and instruments

2.1.1 Tank design

In order to simulate and study the natural evaporation process, a large tank has been set up at the Hydrogeological laboratory of SIMAU Department of Università Politecnica delle Marche. The tank, assembled with an internal structure of armed PVC and fixed on an external one of natural wood implemented with steel scaffolding pipes, has dimensions of 1.4x4.0x1.3 m. It has been filled with coarse sand materials (9.0 m^3 of sandy sediments and 0.5 m^3 of gravel) that have been taken from a sand pit in an alluvial plain along a meander of the Aspio river in Ancona, Italy. The relatively homogeneous nature of the sedimentary succession consists of coarsening-upward sandy sediments. The sediments have been transported at the laboratory, poured into the tank starting from the inflow gravel wall toward the outflow wall reaching a height of 1.1±0.02 m. Then they have been compacted by a large shovel and the natural compaction of sediment under saturated conditions has been monitored for two months. After an initial localized collapse near the infiltration point the compaction was found to be negligible and the collapsed part refilled. In order to apply a steady-state flux a constant head has been applied to the tank by means of an external reservoir, exploiting the two gravel walls at the inflow and at the outflow to stabilize the groundwater flux.

2.1.2 Wells and piezometers

Eight piezometers with a bottom screen of 5 cm length and four fully screened wells have been installed to form a semi-regular grid as shown in Fig.2.1.

Fig.2.1: tank in the hydrogeological laboratory in SIMAU department (Università Politecnica delle Marche)

The piezometers have an internal diameter of 2.0 cm and the wells, which have been located in the centre of the tank, of 5.0 cm. They both were equipped with high resolution multi-level samplers (MLSs), each one of them consisted of 6 HDPE tubes (4 mm i.d.) placed around the wells and piezometers as it is possible to see in the following Figure.

Fig.2.2: HDPE tubes placed around a wells and a piezometer

These tubes were connected to a micro-screen of 0.5 cm length and the sampling ports have been equally spaced every 10 cm, starting from the tank bottom to 60 cm.

2.1.3 Meter probes and data loggers

The groundwater level measurements were obtained using a freatimeter (Pasi, Città di Castello, Italy) by simply dropping the probe inside the piezometers. The sensors within the probes close a circuit when they come in contact with water, activating the warning system that allowed the operator to register the groundwater depth by mean of the graduated cable.

The MLSs have been sampled for salinity measurement only once to minimize the perturbation of the ongoing experiment, while the groundwater heads, temperature and electrical conductivity every 10 minutes using a Soil & Water Diver® water level data-logger (Eijkelkamp, Giesbeek, The Netherlands).

Fig.2.3: Soil & Water Diver water level data-logger that has been employed

This water level data logger is the world's most widely used and compact instruments for automatic measurement and registration of groundwater level, electrical conductivity and temperature. Here some of its feature are illustrated: it has no mechanical parts and no wear; no air vent; it ranges vary from 5 – 100 meters; it can be read on site or in-situ with DDC cable; it can be combined with telemetry; software enables easy data in and output; it has many output formats; barometric logs of air pressure variations; it is deal for wells and it is also applicable in open water (Eijkelkamp Foundation, 2011). The values from the data logger need to be corrected for atmospheric pressure changes via Barologger® (Eijkelkamp, Giesbeek, The Netherlands) placed at the soil surface.

In order to monitor volumetric water content (VWC), Temperature (T) and Soil Bulk Electrical Conductivity (ECb) in the vadose zone, three 5TE® Meter probes (Meter Environment, Pullman, WA, USA) have been installed inside the tank respectively at 5, 20 and 40 cm; each probes were connected to a Meter data logger (ECH_2O) recording every 10 min.

Fig.2.4: meter group ECH20 5TE soil moisture sensor

Previously known as Decagon 5TE Soil Moisture Sensor, the 5TE lets us monitor bulk electrical conductivity (EC), in addition to volumetric water content (VWC) and soil temperature. Monitoring salt levels can be as important as monitoring soil moisture in water-limited areas. The 5TE allows us to measure salt levels through bulk electrical conductivity. In the following table the sensor features are described (Pessl instruments, 1984).

Volumetric water content (VWC)	**Range**	Mineral soil calibration: 0.0-0.1 m3/m3
		Soilless media calibration: 0.0-1.0 m3/m3
		Apparent dielectric permittivity: 1 (air) to 80 (water)
	Resolution	0.0008 m3/m3 from 0%-50% VWC
	Accuracy	Generic calibration: ± 0.03 m3/m3
		Medium-specific calibration: ± 0.02 m3/m3
		Apparent dielectric permittivity: 1-40 (soil range), ±1 εa (unitless) 40–80, 15% measurement
Temperature	**Range**	–40 to +60 °C
	Resolution	0.1 °C
	Accuracy	±1 °C
Bulk electrical conductivity (EC)	**Range**	0–23 dS/m (bulk)
	Resolution	0.01 dS/m from 0–7 dS/m, 0.05 dS/m from 7–23 dS/m
	Accuracy	±10% from 0–7 dS/m, user calibration required from 7–23 dS/m
Dimensions		10.9 cm (4.3 in) lenght; 3.4 cm (1.3 in) width; 1.0 cm (0.4 in) height
Prong length		5.0 cm (1.9 in)
Operating temperature range		-40 °C to 60 °C
Cable length		5 m (standard)
Supply voltage		3.6 VDC to 15.0 VDC
Current drain (asleep)		Typical: 0.03 mA
Current drain (measurement)		0.5 mA to 10.0 mA (typical: 3.0 mA)
Measurement duration		Typical: 150 ms; Maximum: 200 ms

Tab.2.1: meter group ECH20 5TE soil moisture sensor features

According to the model of Hilhorst (2000), soil's ECb have been converted in EC and then into salinity using a standard conversion factor (APHA, 2017).

2.1.4 Physical parameters and hydraulic properties

Physical parameters (grain size, bulk density, porosity, etc...) have been retrieved via dry sieving and gravimetric measurements on 5 randomly collected samples.

A soil sample was randomly taken from the tank and, after oven drying at 105 °C for 24 hours and quartering, it was placed -into the top sieve of a column, which has the largest screen mesh size. Each lower sieve in the column has smaller mesh size than the one above. In order to obtain the complete screening of the material, this column is placed in a mechanical shaker (Fig 2.5).

Fig.2.5: column of sieves placed in a mechanical shaker

After the shaking is complete the material on each sieve is weighed. The mass of the sample of each sieve is then divided by the total mass to give a percentage retained on each sieve. The size of the average particle on each sieve is then analysed and the results of this test are used to describe the properties of the aggregate.

As it is possible to see in the following Table, a small variability in the grain size distribution has been registered with a low coefficient of uniformity (C_U).

Parameter	Tank sediments
Sand (0.63-2 mm)	98.5±8.6
Silt (2-63 μm)	1.4±1.7
Clay (<2 μm)	0.1±0.1
Dry bulk density (kg/dm3)	1.68±0.1
Residual water content (%)	0.05±0.01
Saturated water content (%)	29.1±1.7
CU (-)	3.1±1.6
D10 (mm)	0.45±0.24
D60 (mm)	1.09±0.17

Tab.2.2: sediment parameters and their standard deviation from quintuplicate samples

These sediments, following the Wentworth classification, can be defined as coarse to medium sands.

Thereafter, the saturated hydraulic conductivity (K) distribution have been estimated in different ways: by slug tests, by rate pumping test and by means of Kozeny-Carman formula (Freeze & Cherry, 1979; Rosas et al., 2014), exploiting all the sediments parameters retrieved. This last methodology will be explained below.

A number of empirical formulas, some dating back over a century, have been proposed which attempt to relate the hydraulic conductivity K of an unconsolidated geologic material (granular sediment or soil) to its grain size distribution obtained from sieve analysis.

Equations for estimating K from grain size commonly use two metrics from a grain size distribution plot: D_{10}, the grain diameter for which 10% of the sample is finer (90% is coarser), and D_{60}, the grain diameter for which 60% of the sample is finer (40% is coarser). D_{10} is frequently taken as the effective diameter of the sample while the ratio $CU=D_{60}/D_{10}$ is known as the coefficient of uniformity.

The equation attributed to Kozeny and Carmen that has been used in this study to estimate the hydraulic conductivity of sediments and soils is:

$$K_{KC} = C_{KC}\frac{g}{\nu}\frac{n^3}{(1-n)^2}D_{10}^2$$

where

$-$ K_{KC} is hydraulic conductivity (m/s);

- C_{KC} is an empirical coefficient equal to 1/180 [dimensionless];
- g is gravitational acceleration (m/s²);
- ν is kinematic viscosity of water (m²/s);
- n is total porosity (-).

This formula is assumed to be valid for sediments and soils composed of silt, sand and gravelly sand.

Finally, relative humidity data collected from the online Marche Region Meteorological-Hydrological Information System (SIRMIP, 2020) every 30 minutes, averaging the values of the two nearby meteorological stations.

2.2 Numerical codes

As modelling tool PMWIN 8.0 (Processing Modflow for Windows, Simcore Software) has been used to numerically simulate the natural process of evaporation occurring inside the tank in the laboratory. The software was developed by Chiang and Kinzelbach in 1998 and it consists in a graphical user-interface interacting with several supported program such as MODFLOW (for groundwater flow modelling), MT3DMS (for groundwater solute transport models), SEAWAT (for density dependent flow and transport models), PEST (for models calibration) and others. PMWIN is one of the most complete groundwater simulation systems with a series of independent subroutines named modules grouped into packages to deal with features of the hydrologic system that need to be modelled. All the supporting program and codes that have been used in the simulation of this case study will be characterized in the following paragraphs, including theoretical fundamentals.

2.2.1 MODFLOW

MODFLOW is a modular three-dimensional finite-difference groundwater model published by the U.S. Geological Survey. The first public version of MODFLOW was released in 1988 as MODFLOW-88. MODFLOW-88, but nowadays it is available the most recent version MODFLOW-2005 (Simcore Software, 2012). This version has a modular structure, in which each package (wells, areal recharge, evapotranspiration, drains, etc...) deals with a different element of the hydrogeological system. The program is able to simulate steady and transient flow in a system in which aquifer layers can be confined, unconfined, or a combination of the two. Hydraulic conductivities or transmissivities for any layer may differ spatially and be anisotropic (restricted to

having the principal directions aligned with the grid axes), and the storage coefficient may be heterogeneous.
The partial differential equation of groundwater flow on which MODFLOW is based on is (McDonald & Harbaugh, 1988):

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t}$$

Where:
- K_{xx}, K_{yy} , K_{zz} are the values of hydraulic conductivity along x-, y- and z-coordinate axes $\left(\frac{L}{T}\right)$;
- h is the hydraulic head (L);
- S_s is the specific storage (L^{-1});
- t is time (T);
- W is the volumetric flux per unit volume, representing sources and/or sinks of water (T^{-1}).

This combined with boundary and initial conditions, describes transient three-dimensional ground-water flow in a heterogeneous and anisotropic medium, provided that the principal axes of hydraulic conductivity are aligned with the coordinate directions (Harbaugh et al., 2000). MODFLOW solves it by means of the finite-difference method: the hydraulic head is calculated for each node of the model domain. In order to do this, it requires as inputs the values of hydraulic conductivity, both for vertical and horizontal direction, and the value of specific storage. It needs the boundary conditions characterization (i.e. the interaction between the domain area and its external environment), together with the initial conditions (i.e. values of the variable at initial time) to obtain a unique solution.
Three general types of boundary condition are considered in MODFLOW:
- *Specified head (Dirichlet Condition)*, in which heads are specified along the boundary for the entire duration of the stress period. It acts as a source or sink of water entering or leaving the model domain;
- *Specified flow boundary (Neumann Condition)*, which is implemented when the flow exchanged in the model domain is known;

- *Head-dependent flow or General Head Boundary (Cauchy Condition)*, which is a kind of combination of the previous ones, in which both heads and flow along the boundary are known.

In solving flow equations, it is needed to take into consideration that MODFLOW is based on various assumptions, such as:

- laminar flow, so Darcy's law is valid;
- the standard expression for specific storage in a confined aquifer is applicable;
- the porous medium is assumed to be fully saturated with water and isothermal conditions prevail;
- a single, fully miscible liquid phase of very small compressibility is also assumed.

2.2.2 MT3DMS/SEAWAT

MT3DMS is a further development of MT3D. MT3D stands for Modular 3-Dimensional Transport model and the abbreviation MS denotes the Multi-Species structure for accommodating add-on reaction packages. MT3DMS includes three major classes of transport solution techniques, three-dimensional numerical model for simulating changes in concentrations of miscible contaminants in complex hydrogeological settings and it is capable of modelling advection, anisotropic dispersion and linear and nonlinear sorption in complex steady-state and transient flow fields.

The basic assumptions on which this program is based on are the same of MODFLOW, with the additional assumption that the diffusive approach to dispersive transport based on Fick's law can be applied.

The partial differential equation which governs the transport of contaminants of species *k* in 3-dimensions transient groundwater flow systems can be written as:

$$\frac{\partial(\theta C^k)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C^k}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(\theta v_i C^k) + W C_s^k + \sum R_n$$

Where:

- θ is the porosity of the subsurface medium;

- C_k is the dissolved concentration of species k $\left(\frac{M}{L^3}\right)$;

- t is time (T);

- $x_{i,j}$ is the distance along the respective Cartesian coordinate axis (L);

- D_{ij} is hydrodynamic dispersion coefficient tensor $\left(\frac{L^2}{T}\right)$;

- v_i is the linear pore water velocity $\left(\frac{L}{T}\right)$;

- W is volumetric flow rate per unit volume of aquifer, and it represents fluid sources (if positive) or sinks (if negative) (T^{-1});

- C_s^k is the concentration of the source or sink flux for species k $\left(\frac{M}{L^3}\right)$;

- $\sum R_n$ is chemical reaction term $(ML^{-3}T^{-1})$, which can be used to include the effect of biochemical and geochemical reactions on contaminant fate and transport.

Like MODFLOW, MT3DMS consists of a main program and independent subroutines, which are grouped into a series of "packages". Each of these packages deals with a single property of the transport simulation, so that it is possible to simulate advection, dispersion/diffusion, source/sink mixing, and chemical reactions separately.

SEAWAT, also included in PMWIN, is a combined version of MODFLOW and MT3DMS designed to simulate three-dimensional, variable-density, saturated groundwater flow and transport. Similar to previously described programs, also SEAWAT is organized in a modular scheme. Thanks to the coupling, the numerical methods used by MT3DMS to simulate solute transport in a constant density flow field are directly used in SEAWAT to simulate solute transport in a variable-density flow field.

The governing equation for flow and transport is:

$$\nabla * \left[\rho \frac{\mu_0}{\mu} K_0 \left(\nabla h_0 + \frac{\rho - \rho_0}{\rho_0} \nabla z\right)\right] = \rho S_{s,0} \frac{\partial h_0}{\partial t} + \theta \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} - \rho_s q_s'$$

Where:

- ρ_0 is the fluid density (ML^{-3}) at the reference concentration and reference temperature;
- μ is dynamic viscosity ($ML^{-1}T^{-1}$);
- K_0 is the hydraulic conductivity tensor of material saturated with the reference fluid (LT^{-1});
- h_0 is the hydraulic head (L) measured in term of the reference fluid of a specific concentration and temperature;
- t is time (T);
- $S_{s,0}$ is the specific storage (L^{-1});
- θ is the porosity;
- C is salt concentration (ML^{-3});
- $q_s^{'}$ is a source or sink (T^{-1}) of fluid with density ρ_s.

This equation of state, which relates fluid density to solute concentration, temperature, and pressure, is typically written as a function of the volumetric expansion coefficient for solute concentration (*βC*), temperature (*βT*), and pressure (*βP*), which are:

$$\beta_C = \frac{1}{\rho}(\frac{\partial\rho}{\partial C})_{T,P};$$

$$\beta_T = \frac{1}{\rho}(\frac{\partial\rho}{\partial T})_{C,P};$$

$$\beta_P = \frac{1}{\rho}(\frac{\partial\rho}{\partial P})_{C,T}.$$

where *T* is temperature (ºK) and *P* is pressure ($ML^{-1}T^{-2}$) (Langevin et al., 2008). SEAWAT includes both explicit and implicit methods for coupling the flow and solute-transport equations. With the implicit coupling method, solutions to the flow and transport equations are repeated, and concentrations and densities are updated within each time step until the maximum difference in fluid density at a single cell for consecutive iterations is less than a user-specified value.

With the explicit one, fluid densities are calculated with solute concentrations from the previous time step. Advective fluxes from the flow solution for the current time step are then used in the current solution to the transport equation. This cycling mechanism results in an explicit coupling of the flow and transport equations.

Although MT3DMS and SEAWAT are not explicitly designed to simulate heat transport, temperature can be simulated as one of the species by entering appropriate transport coefficients. For example, the process of heat conduction is mathematically analogous to Fickian diffusion. Heat conduction can be represented in SEAWAT by assigning a thermal diffusivity for the temperature species.

2.3 Model setup and inputs

In this section of the thesis it will be explained how the tank was modelled in order to simulate the natural evaporation process which was occurring in the laboratory. The first steps in the groundwater modelling process are to define the goals of the model (evaporation process), select a computer code (PMWIN) and, after the collection of the necessary data, create a conceptual model of the system. Following the grid, the parameters and the models menu, it is possible to implement the various input needed in the simulation. All the menus will be fully described below.

2.3.1 The grid menu

2.3.1.1 Mesh Size

After creating a new model and saving it in a folder of the project with the file extension *.PM5, it is needed to spatially discretize and design the grid of the model. Anderson and Woessner discuss the steps in going from aquifer systems to a numerical model grid, Zheng and Bennett (2002) describe the design of model grids, which are intended for use both in flow and transport simulations. In the block centered finite difference method, an aquifer system is replaced by a discretized domain consisting of an array of nodes and associated finite difference blocks (cells).

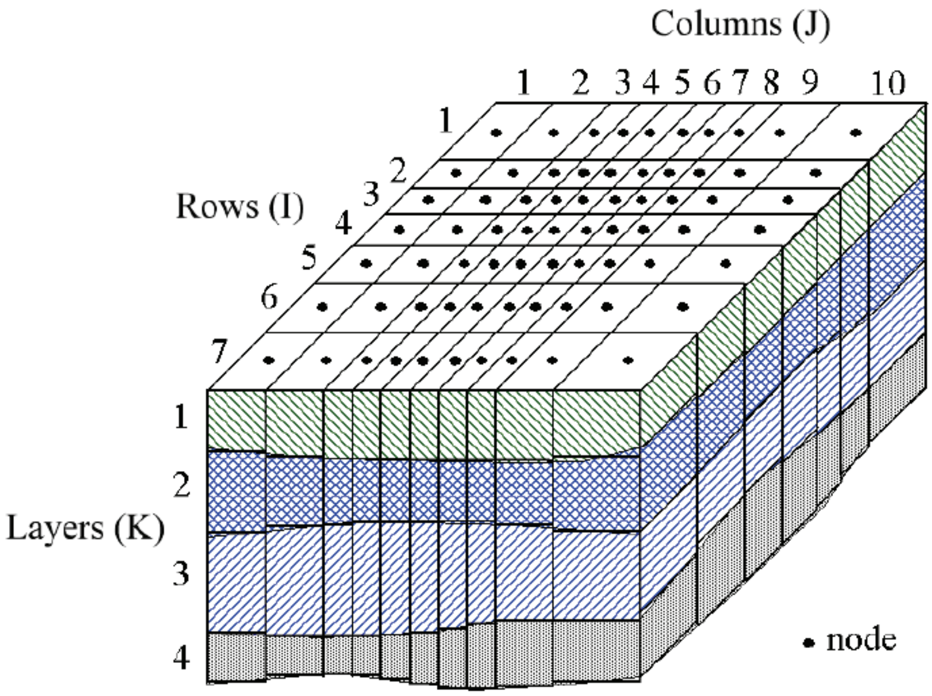


Fig.2.6: spatial discretization of fan aquifer system and the cell indices

Fig. 2.6 shows the spatial discretization scheme of an aquifer system with a mesh of cells and nodes at which hydraulic heads are calculated. The nodal grid forms the framework of the numerical model. Hydrostratigraphic units can be represented by one or more model layers. The thickness of each model cell and the width of each column and row can be specified. The locations of cells are described in terms of layers, rows, and columns. PM uses an index notation [Layer, Row, Column] for locating the cells. For example, the cell located in the first layer, 6th row, and 2nd column is denoted by [1, 6, 2]. To generate or modify a model grid, select Grid/Mesh Size. If a grid does not exist, a Model Dimension dialog box (Fig. 2.7) appears for specifying the extent and number of layers, rows, and columns of the model grid. After specifying the data and clicking the OK button, the Grid Editor shows the model grid.

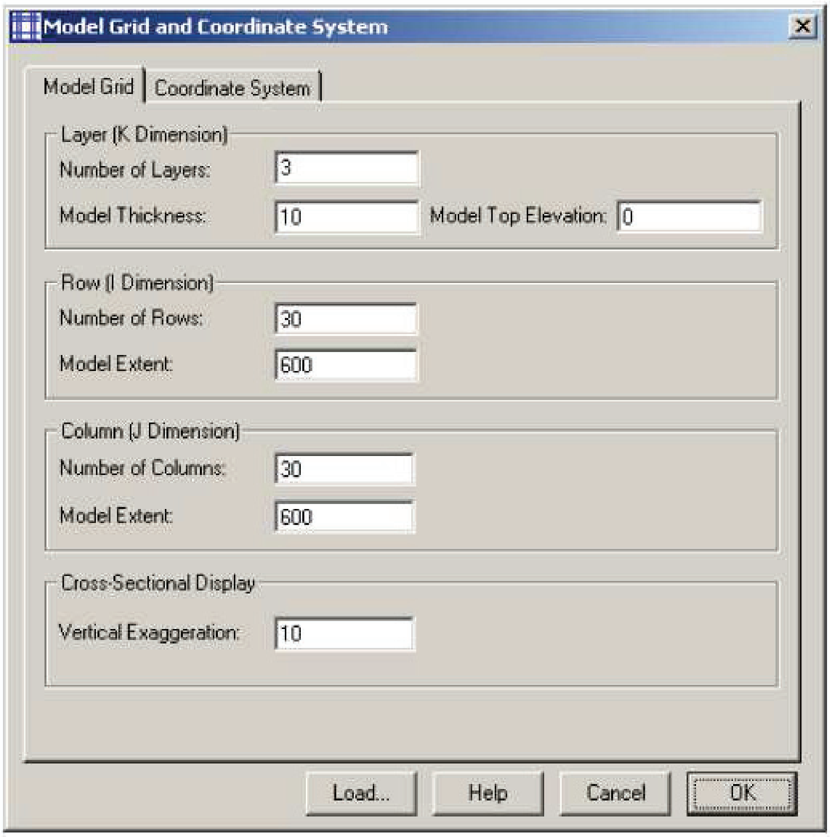


Fig.2.7: model dimension dialog box

In this case study, in order to reproduce the tank, the very simple grid is defined by 28 columns, 80 rows and 22 layers of equal thickness. Each cell measures 0.05x0.05x0.05 m, reaching the volume of 1.4x4.0x1.1 m of the porous media inside the tank.

2.3.1.2 Layer Property

The layer properties are defined in the Layer Property dialog box (Fig. 2.8). Many settings of this dialog box depend on the selection between the Block Centered-Flow (BCF) and Layer Property Flow (LPF) packages. When the LPF Package is used, the columns Transmissivity, Leakance and Storage Coefficient are dimmed to indicate that their settings are ignored, because the LPF package only uses HK, VK, Ss and Sy. When the BCF package is used, the column Vertical Anisotropy is dimmed since it is not supported by the BCF package.

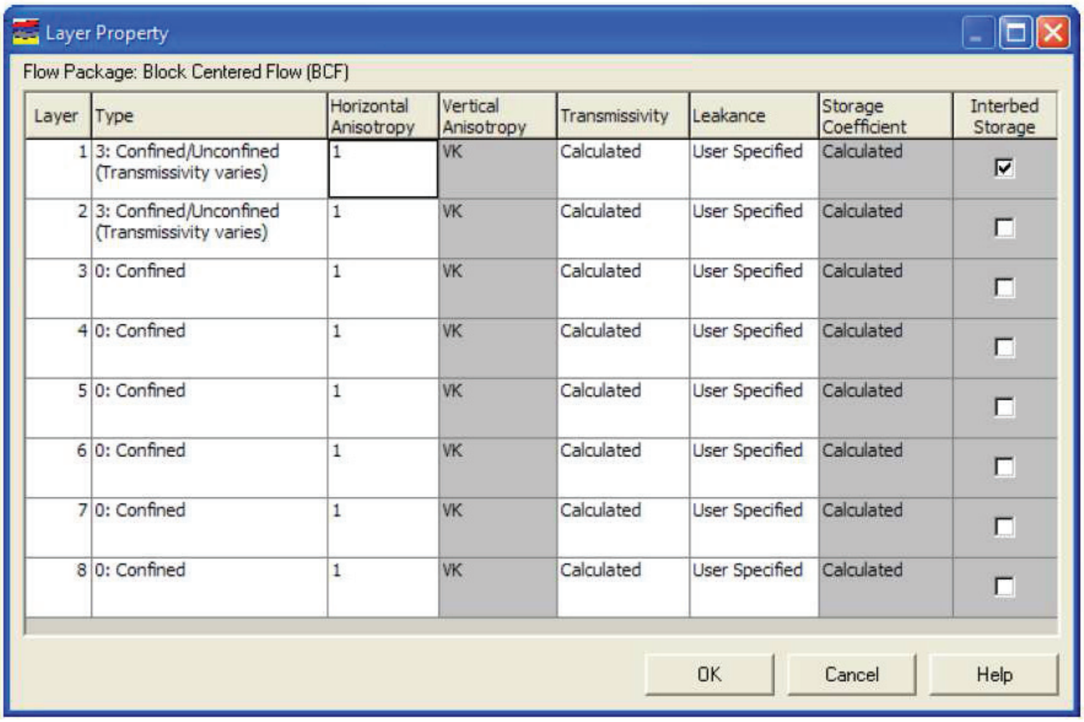


Fig.2.8: Layer Property dialog box

The available layer types are:

- Type 0: The layer is strictly confined. For transient simulations, the confined storage coefficient is used to calculate the rate of change in storage. Transmissivity of each cell is constant throughout the simulation.
- Type 1: The layer is strictly unconfined. The option is valid for the first layer only. Specific yield is used to calculate the rate of change in storage for this layer type. During a flow simulation, transmissivity of each cell varies with the saturated thickness of the aquifer.
- Type 2: A layer of this type is partially convertible between confined and unconfined. Confined storage coefficient is used to calculate the rate of change in storage, if the layer is fully saturated, otherwise specific yield will be used. Transmissivity of each cell is constant throughout the simulation. Vertical leakage from above is limited if the layer desaturates.
- Type 3: A layer of this type is fully convertible between confined and unconfined. Confined storage coefficient is used to calculate the rate of change in storage, if the layer is fully saturated, otherwise specific yield will be used. During a flow simulation, transmissivity of each cell varies

with the saturated thickness of the aquifer. Vertical leakage from above is limited if the layer desaturates.

The layers in the dialog box of the model domain of this case study have been all set to Type 3.

2.3.1.3 Cell Status

The flow model MODFLOW requires an IBOUND array, which contains a code for each model cell. A positive value in the IBOUND array defines an active cell (the hydraulic head is computed), a negative value defines a constant head or fixed head cell (the hydraulic head is kept constant at a given value throughout the flow simulation) and the value 0 defines an inactive cell (no flow takes place within the cell). It is suggested to use 1 for active cells, 0 for inactive cells and -1 for constant head cells. Any outer boundary cell, which is not a constant head cell, is automatically a zero-flux boundary cell.

All the cells of the study area representing the tank are active cells (value 1).

The transport model MT3DMS requires an ICBUND array, which contains a code for each model cell. A positive value in the ICBUND array defines an active concentration cell (the concentration varies with time and is calculated), a negative value defines a constant-concentration cell (the concentration is constant) and the value 0 defines an inactive concentration cell (no transport simulation takes place at such cells). It is suggested to use the value 1 for an active concentration cell, -1 for a constant-concentration cell, and 0 for an inactive concentration cell.

All cells in the model were assigned value 1, to allow the transport.

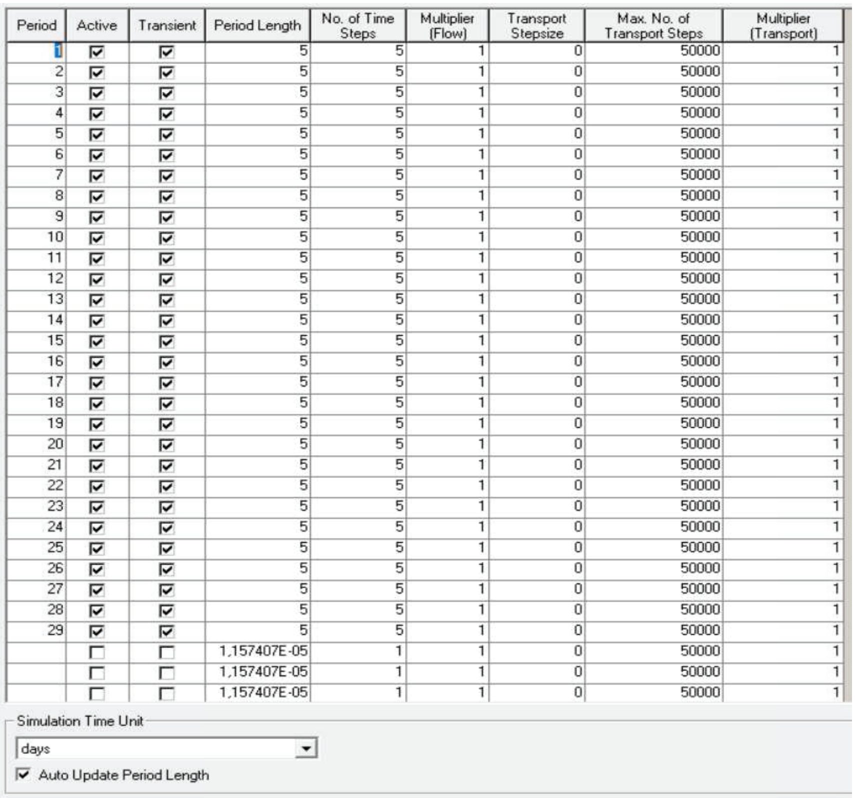
2.3.2 The parameters menu

This menu is used to input time, initial hydraulic head values, and aquifer parameters. Depending on the settings of the layer properties, it is possible that an aquifer parameter is required only for certain model layers or is not required for any of the model layers. All the parameters that have been inserted will be fully illustrated below.

2.3.2.1 Time

The appearance of the time dialog box is affected by the setting of the Modflow. When the Modflow Version is set to ”MODFLOW-2000/MODFLOW-2005”, the Transient column appears in the table and the Simulation Flow Type group of this dialog box is dimmed and deactivated since MODFLOW-2000 allows individual stress periods in a single simulation to be either transient or steady state instead of requiring the entire simulation to be either steady state or transient. Steady state and transient stress periods can occur in any order. Commonly the first stress period is steady state and produces a solution that is used as the initial condition for subsequent transient stress periods.

MODFLOW divides the simulation time into stress periods, which are, in turn, divided into time steps. The length of stress periods and time steps is not relevant to steady state flow simulations. However, if transport simulations need to be done at a later time, the actual period length should be entered.



Period	Active	Transient	Period Length	No. of Time Steps	Multiplier (Flow)	Transport Stepsize	Max. No. of Transport Steps	Multiplier (Transport)
1	☑	☑	5	5	1	0	50000	1
2	☑	☑	5	5	1	0	50000	1
3	☑	☑	5	5	1	0	50000	1
4	☑	☑	5	5	1	0	50000	1
5	☑	☑	5	5	1	0	50000	1
6	☑	☑	5	5	1	0	50000	1
7	☑	☑	5	5	1	0	50000	1
8	☑	☑	5	5	1	0	50000	1
9	☑	☑	5	5	1	0	50000	1
10	☑	☑	5	5	1	0	50000	1
11	☑	☑	5	5	1	0	50000	1
12	☑	☑	5	5	1	0	50000	1
13	☑	☑	5	5	1	0	50000	1
14	☑	☑	5	5	1	0	50000	1
15	☑	☑	5	5	1	0	50000	1
16	☑	☑	5	5	1	0	50000	1
17	☑	☑	5	5	1	0	50000	1
18	☑	☑	5	5	1	0	50000	1
19	☑	☑	5	5	1	0	50000	1
20	☑	☑	5	5	1	0	50000	1
21	☑	☑	5	5	1	0	50000	1
22	☑	☑	5	5	1	0	50000	1
23	☑	☑	5	5	1	0	50000	1
24	☑	☑	5	5	1	0	50000	1
25	☑	☑	5	5	1	0	50000	1
26	☑	☑	5	5	1	0	50000	1
27	☑	☑	5	5	1	0	50000	1
28	☑	☑	5	5	1	0	50000	1
29	☑	☑	5	5	1	0	50000	1
	☐	☐	1.157407E-05	1	1	0	50000	1
	☐	☐	1.157407E-05	1	1	0	50000	1
	☐	☐	1.157407E-05	1	1	0	50000	1

Simulation Time Unit

days

☑ Auto Update Period Length

Fig.2.9: Time Parameters dialog box

In the previous Figure it is represented the time dialog box of the model. In the case study, 29 stress periods of 5 days each have been activated reaching the simulation time of 145 days.

2.3.2.2 Initial & Prescribed Hydraulic Heads

MODFLOW requires initial hydraulic heads at the beginning of a flow simulation. Initial hydraulic heads at constant head cells are used as specified head values of those cells and remain constant throughout the flow simulation. For transient flow simulations, the initial heads must be the actual values, since they are used to account for the storage terms. For steady-state flow simulations, the initial heads are used as starting values for the iterative equation solvers. The initial heads at the constant head cells must be the actual values while all other values can be set at an arbitrary level. For an unconfined or convertible layer (layer type 1 or 3), the initial hydraulic head of a constant head cell should be higher than the elevation of the cell bottom, because MODFLOW does not convert a dry fixed-head cell to an inactive cell. If any constant-head cell becomes dry, MODFLOW will stop the flow simulation (Simcore Software, 2012).

In this case study, in order to apply a steady-state flux, a constant head has been applied to the tank by means of an external reservoir, exploiting the two gravel walls at the inflow and at the outflow to stabilize the groundwater flux. The initial hydraulic heads of the water in the tank have been set to be around 0.5 m and measured as it is represented in Fig.2.10.

2.3.2.3 Horizontal Hydraulic Conductivity

Horizontal hydraulic conductivity, which is required for layers of types 1 or 3, is the hydraulic conductivity along model rows. It is multiplied by an anisotropy factor specified in the Layer Property dialog box to obtain the hydraulic conductivity along model columns.

Talking about our case study, the horizontal hydraulic conductivity (K) distribution have been estimated in different ways: by slug tests, by rate pumping test exploiting the inflow and outflow gravel wall to balance the fluxes and by means of Kozeny-Carman formula, exploiting all the sediments parameters retrieved. Finally, a mean value of around 60 m/d for the sand and a value around 660 m/d for the gravel (Fig.2.11).

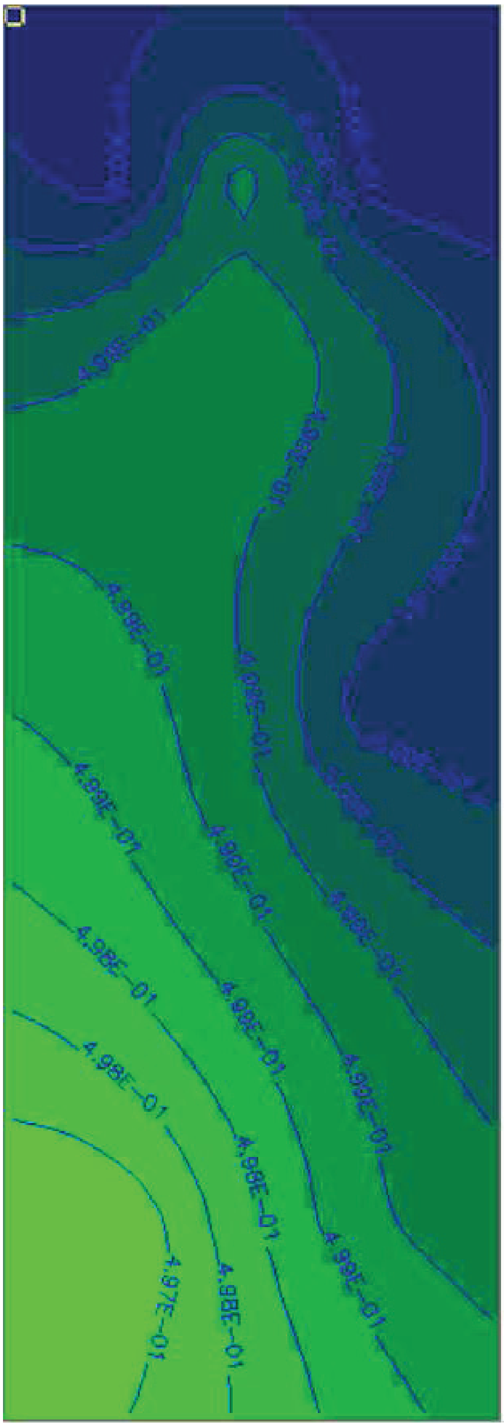


Fig.2.10: Initial Hydraulic Heads

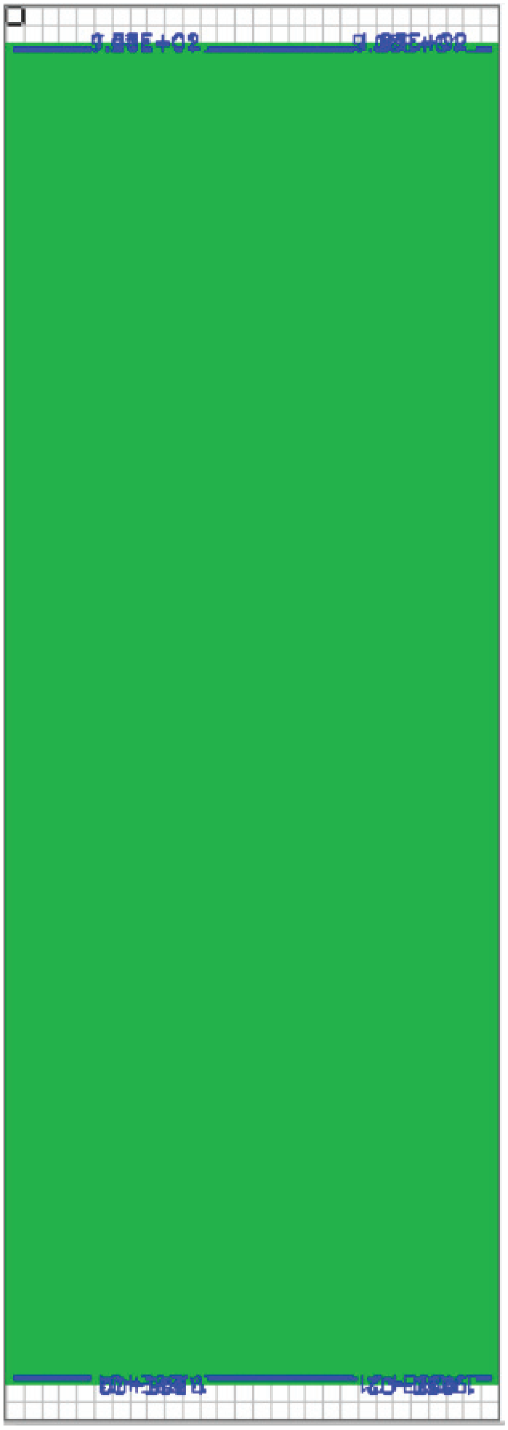


Fig.2.11: Horizontal Hydraulic Conductivity

2.3.2.4 Vertical Hydraulic Conductivity

The Layer-Property Flow (LPF) package supports the use of the cell-by-cell vertical hydraulic conductivity or vertical anisotropy, which is the ratio of horizontal hydraulic conductivity along rows to vertical hydraulic conductivity for the model layer. When Vertical Anisotropy of a layer in the Layer Property dialog box (Fig. 2.8) is VK, the cell-by-cell vertical hydraulic conductivity of that layer is used in the simulation. When Vertical Anisotropy is VANI, the cell-by-cell vertical anisotropy of the layer is used (Simcore Software, 2012).

In this case study, the vertical hydraulic conductivity distribution has been estimated to be around 30 m/d for the sand and around 330 m/d for the gravel.

2.3.2.5 Specific Storage

For transient flow simulations, MODFLOW requires dimensionless storage terms specified for each layer of the model. For a steady state simulation, these menu items are not used and are therefore dimmed. In a confined layer, the storage term is given by storativity or confined storage coefficient. The storativity is a function of the compressibility of the water and the elastic property of the soil matrix. The specific storage or specific storativity is defined as the volume fraction of water that a unit column of aquifer releases from storage under a unit decline in hydraulic head. The specific storage ranges in value from 3.3×10^{-6} 1/m of rock to 2.0×10^{-2} 1/m of plastic clay. Layers of types 0, 2 and 3 require the confined storage coefficient. PM uses specific storage and the layer thickness to calculate the confined storage coefficient, if the corresponding Storage Coefficient setting in the Layer Property dialog is Calculated.

In the model a value of 1.0×10^{-4} 1/m has been set up.

2.3.2.6 Effective Porosity

If the total unit volume V V of a soil matrix is divided into the volume of the solid portion V_S and the volume of voids V_V, the porosity n is defined as $n = \frac{V_V}{V}$.

Effective porosity (with the respect to flow through the medium) is normally smaller than porosity, because part of the fluid in the pore space is immobile or partially immobile. This may occur when the flow takes place in a fine-textured medium where adhesion (i.e., the attraction to the solid surface of the porous matrix by the fluid molecules adjacent to it) is important. On a more macroscopic scale the effective porosity also has to accommodate the fact that unresolved conductivity variations lead to a reduction of effective porosity.

Transport models use effective porosity to calculate the average velocity of the flow through the porous medium.

In this case study a value of 0.2 has been chosen as effective porosity.

2.3.2.7 Specific Yield

Specific yield is defined as the volume of water that an unconfined aquifer releases from storage per unit surface area of aquifer per unit decline in the water table. Specific yield is a function of porosity (and is not necessarily equal to porosity), because a certain amount of water is held in the soil matrix and cannot be removed by gravity drainage.

In the model a value of 0.226 has been set up.

2.3.2.8 Bulk Density

The bulk density is can be divided in layer-by-layer bulk density and cell-by-cell one. The layer-by-layer bulk-density data are used by the Chemical Reaction package of MT3D or RT3D (version 1) for calculating the retardation factor or for calculating the first-order irreversible (radioactive decay or biodegradation) rate of the adsorbed phase. The cell-by-cell bulk-density data, which was specified (1700 kg/m^3) in our model, are used by the Chemical Reaction package of MT3DMS, MT3D99, PHT3D, SEAWAT, and RT3D (version 2 and later) for simulating sorption effects.

2.3.3 The models menu | MODFLOW

The only flow package input that have been set up for this case study is the evapotranspiration one.

2.3.3.1 Flow Packages | Evapotranspiration

The Evapotranspiration package simulates the effects of plant transpiration and direct evaporation in removing water from the saturated groundwater regime. Considering that inside the tank there is a sandy bare soil with no vegetation at all, the transpiration contribution has been considered to be null and the study have been focused only on the evaporation contribution. Anyway, the term "Evapotranspiration" will be used again in this paragraph.

Evapotranspiration is defined by assigning the following parameters to each vertical column of cells. The input parameters are assumed to be constant during a given stress period. For transient flow simulations involving several stress periods, the input parameters can be different from period to period, as in our case study. Note that the user may move to other layers within the Data Editor and examine the grid configuration in each layer, although the values are specified for each vertical column of cells.

This package removes water from the saturated groundwater regime based on the following assumptions:

1. when groundwater table is at or above the elevation of the ET surface h_S, evapotranspiration loss from the groundwater table is at the maximum ET Rate (R_{ETM});
2. no evapotranspiration occurs when the depth of the groundwater table below the elevation of the ET surface exceeds the ET extinction depth (d);
3. in between these two extremes evapotranspiration varies linearly with the groundwater table elevation.

The input values that are needed to be specified are:

- Maximum ET Rate (R_{ETM}) [LT^{-1}];
- Elevation of the ET Surface (h_S) [L];
- ET Extinction Depth (d) [L];
- Layer Indicator (IET) [-];
- Parameter Number [-].

These values, which represent the result of the case study, have been found after being set and corrected many times following a calibration procedure. This calibration process, together with the retrieved evaporation parameters will be explained and presented in the next chapter.

2.3.3.2 Solvers

To calculate heads in each cell in the finite-difference grid, MODFLOW prepares one finite difference equation for each cell, expressing the relationship between the head at a node and the heads at each of the six adjacent nodes at the end of a time step. Because each equation may involve up to seven unknown values of head, and because the set of unknown head values changes from one equation to the next through the grid, the equations for the entire grid must be solved simultaneously at each time step. The system of simultaneous finite difference linear equations can be expressed in matrix notation as:

$$\underline{A} \cdot \underline{x} = \underline{b}$$

where A is a coefficient matrix assembled by MODFLOW using user-specified model data; b is a vector of defined flows, terms associated with head-dependent boundary conditions and storage terms at each cell; x is a vector of hydraulic heads at each cell.

In this case study the Geometric Multigrid Solver (GMG) package has been used, which is only implemented in MODFLOW-2000 and MODFLOW-2005.

2.3.3.3 Head Observations

In order to specify the locations of the head observation boreholes and their associated observed data (measurements), the Head Observations dialog box has to be opened from the MODFLOW menu (Fig.2.12). The options of this dialog box are described below:

- *Observation Borehole*: The name and the coordinates (expressed in the world coordinates according to the user-defined coordinate system) of each borehole are given in this table.

- The *Observation Data* group contains two tables - Layer Proportion and Head Observation(s). By means of the *Layer Proportions* table, PM supports multi-layer observations. For a single-layer borehole, simply specify a non-zero proportion value to the layer, where the borehole is screened and assign a proportion value of zero to all other layers. If the proportion values of all layers are zero, the observation borehole is considered as "inactive" and thus no graphical display can be generated for this borehole. The *Head Observation*(s) table is the section where the data collected in the field at the time of simulation could be entered. Time, HOBS and weight have to be inserted. The observation *Time*, to which the measurement pertains, is measured from the beginning of the model simulation. *HOBS* is the hydraulic head observed at the observation time. The *Weight* of an observation gives a relative confidence level of the observed value.

After a simulation, the user may select View | Head Scatter Diagram from Modflow menus to compare the calculated and observed values.

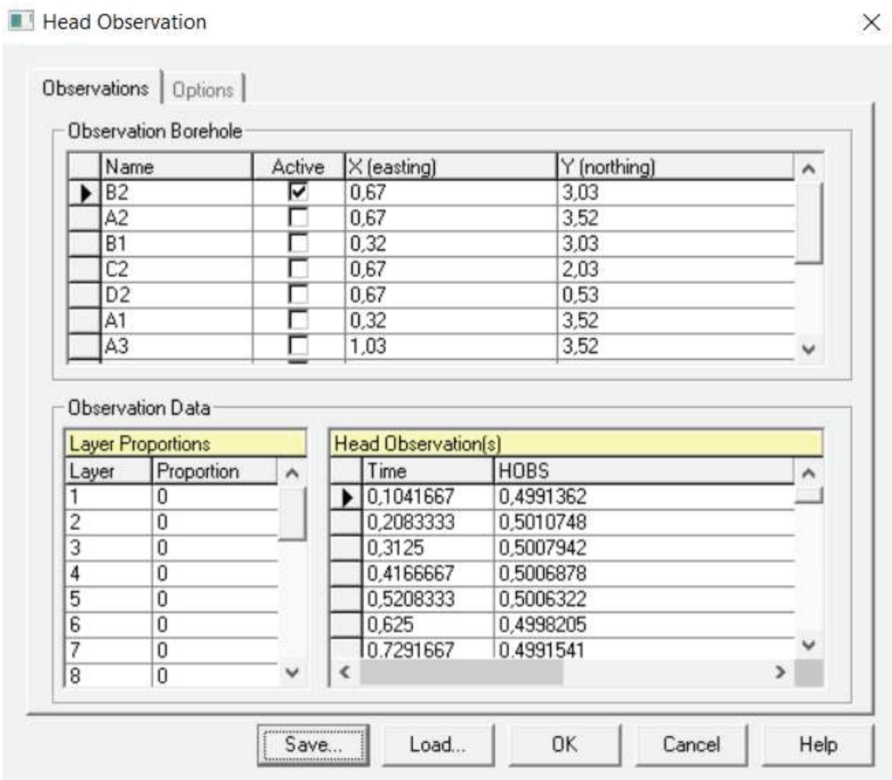


Fig.2.12: Head Observation dialog box

2.3.3.4 Output Control

The primary output file of MODFLOW is the run listing file OUTPUT.DAT. MODFLOW calculates a volumetric water budget for the entire model at the end of each time step, and saves it in the run listing file. The volumetric water budget provides an indication of the overall acceptability of the numerical solution. In numerical solution techniques, the system of equations solved by a model actually consists of a flow continuity statement for each model cell. Continuity should therefore also exist for the total flows into and out of the entire model or a sub-region. This means that the difference between total inflow and total outflow should equal the total change in storage (Simcore Software, 2012).

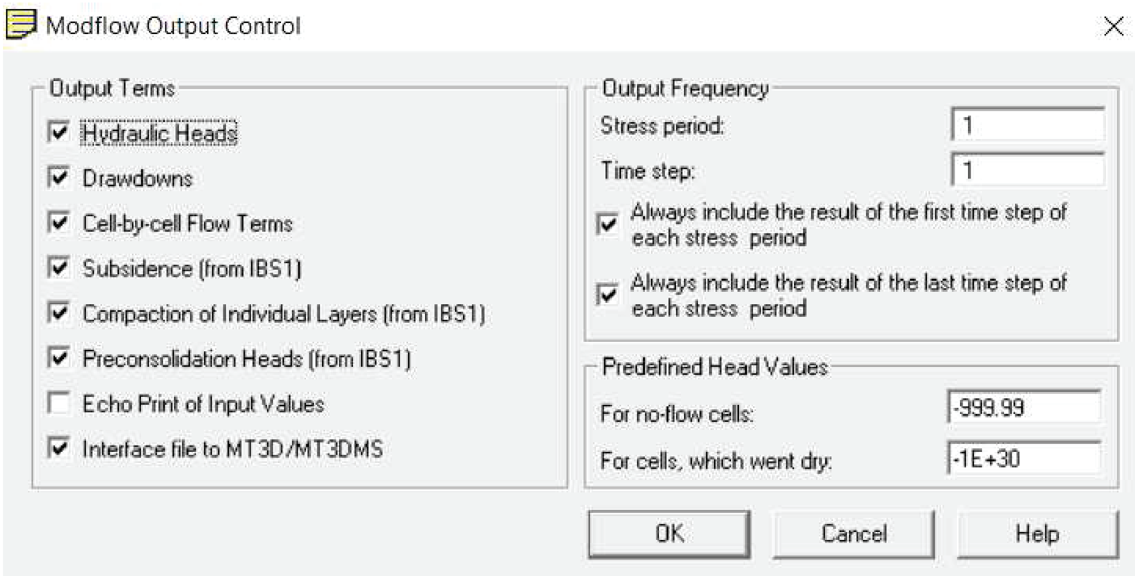


Fig.2.13: Modflow Output Control dialog box

2.3.3.5 Run

Selecting this menu item to open the Run Modflow dialog box, it will be possible to run the flow simulation with MODFLOW or to check the model data. The available settings of the dialog box are described below. The File Table has three columns:

- Generate: Prior to running a flow simulation, PM uses the user-specified data to generate input files for MODFLOW and MODPATH. An input file will be generated if it does not exist or if the corresponding Generate box is checked. Normally, we do not need to worry about these boxes since PM will take care of the settings

- Description gives the names of the packages used in the flow model.
- Destination File shows the paths and names of the input files of the flow model.

The Options are:

- Regenerate all input files: Check this option to force PM to generate all input files regardless the setting of the Generate boxes.
- Generate input files only, don't start MODFLOW: Check this option, if the user does not want to run MODFLOW.
- Check the model data: If this option is checked, PM will check the geometry of the model and the consistency of the model data
- OK: Click OK to generate MODFLOW input files. 2.3.4 The models menu | MT3DMS/SEAWAT

2.3.4 The models menu | MT3DMS/SEAWAT

2.3.4.1 Simulation Settings

The Simulation Settings dialog box (Fig. 2.14) controls the type of reaction and the species involved in the simulation. It also controls whether variable density flow and/or transport should be simulated. The available settings are described as follows.

Simulation Mode:

- *Constant Density Transport with MT3DMS*: If this option is selected, the constant density flow solution of MODFLOW will be used by MT3DMS to simulate solute transport processes. It is assumed that the solution concentration does not affect the fluid density and the flow field.
- *Variable Density Flow and Transport with SEAWAT*: If this option is selected, SEAWAT will be used to simulate coupled variable-density flow and solute transport. With this option, fluid density is calculated by using an equation of state and the simulated solute concentration values of involved species.

Type of reaction:

- *No kinetic reaction is simulated*: To turn off the simulation of kinetic reactions.
- *First-order irreversible reaction*: Simulates radioactive decay or biodegradation.

Then there are three tabs: the Species tab, the Stoichiometry tab and the SEAWAT tab.

The columns of the Species table are described below:

- *Number*: displays the (read-only) species number.
- *Active*: to add a species to the simulation.
- *Description*: to type the name or description of the species.
- *Density On*: item used by SEAWAT only. Check the box to include the concentration of the simulated species in the fluid density calculation.
- *DRHODC*: used by SEAWAT only. DRHODC is the slope that relates fluid density to solute concentration.
- *CRHOREF*: used by SEAWAT only. CRHOREF is the reference concentration for the species. For most simulations, CRHOREF should be specified as zero.

Fig. 2.14 shows the simulation settings of our case study in which Salinity and Temperature are the two species involved in the simulation.

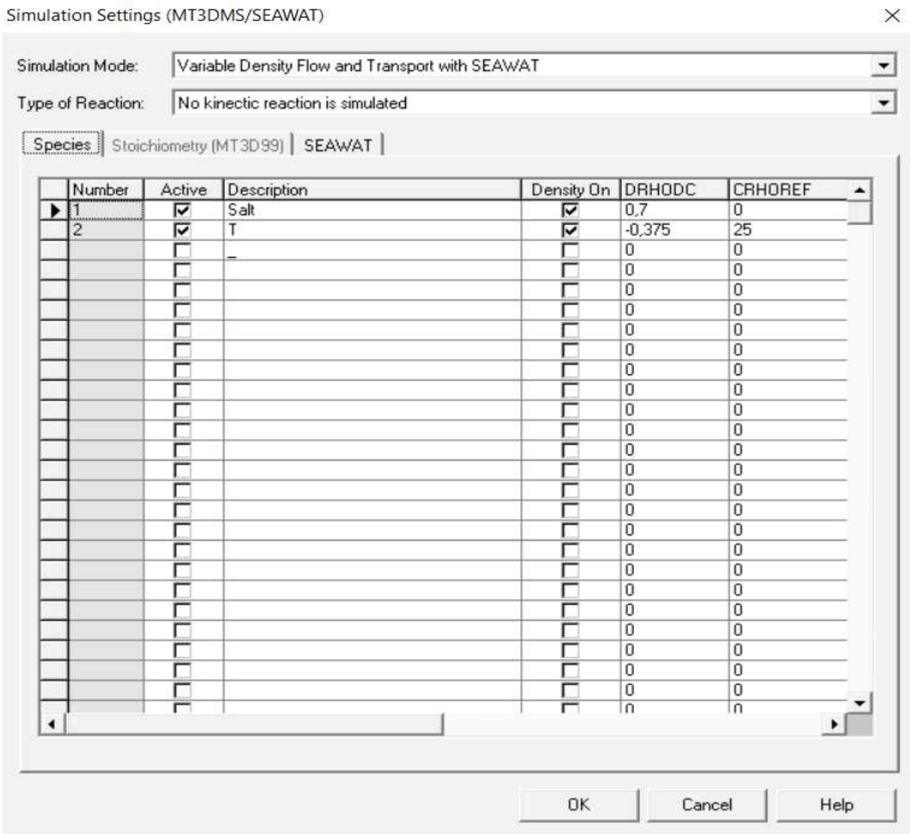


Fig.2.14: Simulation Settings Species tab

2.3.4.2 Initial Concentration

At the beginning of a transport simulation, MT3DMS and SEAWAT require the initial concentration of each active species at each active concentration cell.

In our case study Salt and Temperature Initial Concentration have been monitored and represented in the figures below.

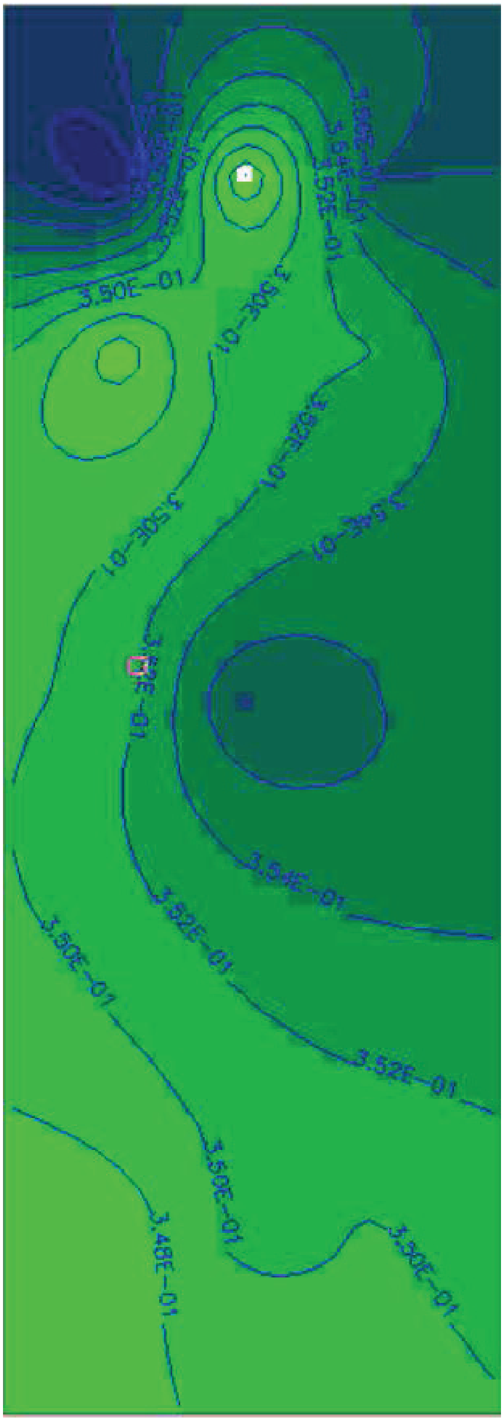


Fig.2.15: Initial TDS distribution

Fig.2.16: Initial Temperature distribution

2.3.4.3 Advection

The available settings of the Advection Package dialog box (Fig. 2.17) are described below.

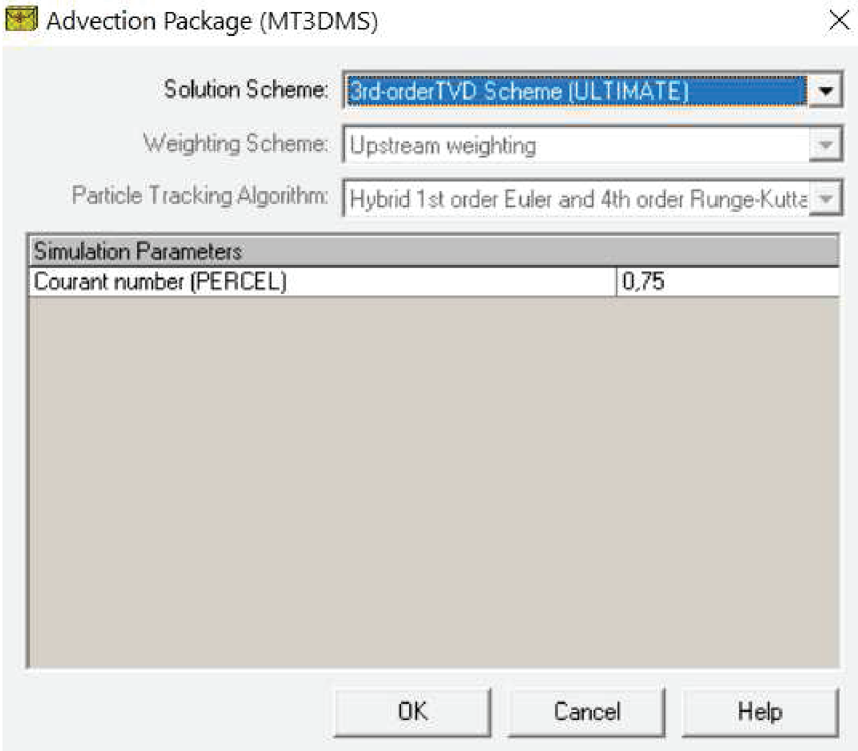


Fig.2.17: Advection Package dialog box

MT3DMS provides five *Solution Schemes* for the advection term. *The third-order TVD method*, based on the ULTIMATE algorithm, is the one that has been chosen for this case study. With the ULTIMATE scheme, the solution is mass conservative, without excessive numerical dispersion and artificial oscillation.

The *Weighting Scheme* is needed only when the implicit finite-difference method is used.

Particle Tracking Algorithm is used in combination with the method of characteristics.

Finally, depending on the selected Solution Scheme, one or more *Simulation Parameters* may be required. Courant number (PERCEL) is the number of cells (or a fraction of a cell) any particle will be allowed to move in any direction in one transport step. Generally, $0.5 \leq PERCEL \leq 1$. As it is possible to see in the Figure above, a value of 0.75 has been chosen.

2.3.4.4 Dispersion

The following values must be specified for each layer in the Dispersion Package dialog box (Fig.2.18).

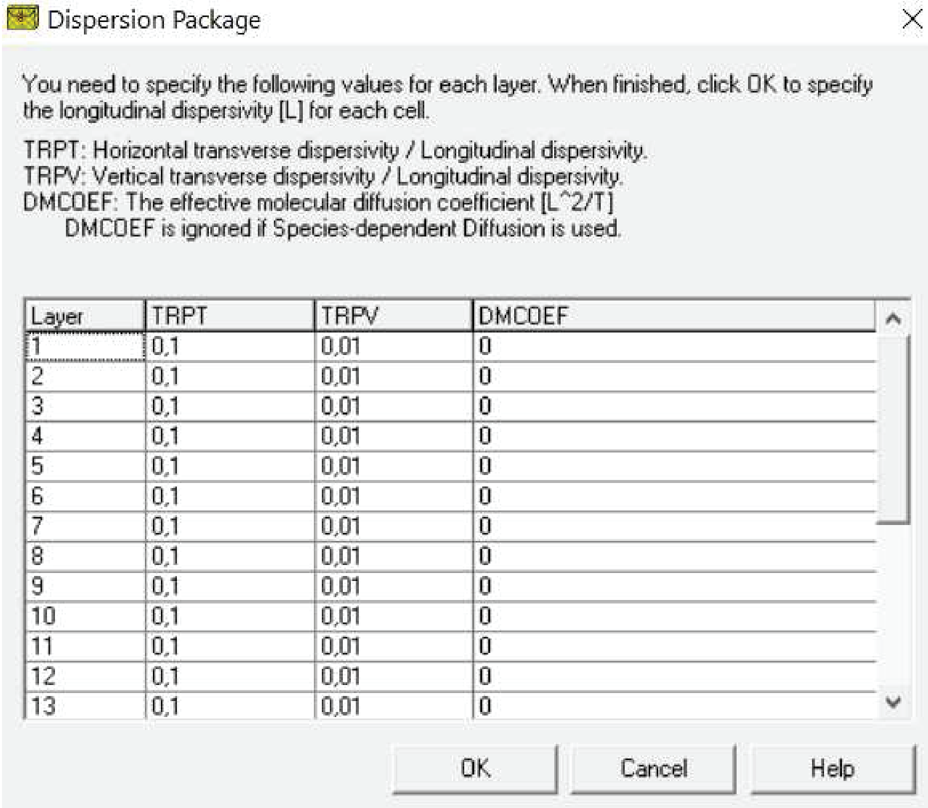


Fig.2.18: Dispersion Package dialog box

TRPT is the ratio of the horizontal transverse dispersivity to the longitudinal dispersivity. Longitudinal dispersivity is used to approximate the spreading of the solute concentration in groundwater caused by the irregular shape of the interconnected pore space and the velocity variations at the microscopic level as well as the unresolved macroscopic level.

TRPV is the ratio of the vertical transverse dispersivity to the longitudinal dispersivity.

DMCOEF is the effective molecular diffusion coefficient D [L^2T^{-1}]. It describes the diffusive flux of a solute in water from an area of greater concentration toward an area where it is less concentrated.

2.3.4.5 Species Dependent Diffusion

Selecting this item, a diffusion coefficient can be entered for individual species. The specified data will be used by MT3DMS or SEAWAT to replace the effective molecular diffusion coefficient in the Dispersion package only if it is activated. The specified data are $2.0\text{x}10^{-4}$ m^2/d for the salt and 0.15031 m^2/d for the temperature.

2.3.4.6 Chemical Reaction

The Chemical Reaction package can be used to simulate sorption and chemical reactions. The type of reaction is selected in the Simulation Settings dialog box (Fig. 2.14). As it is possible to see in the figure, *no kinetic reaction is simulated*. The type of sorption and the parameters for sorption are defined in the Chemical Reaction dialog box (Fig.2.19).

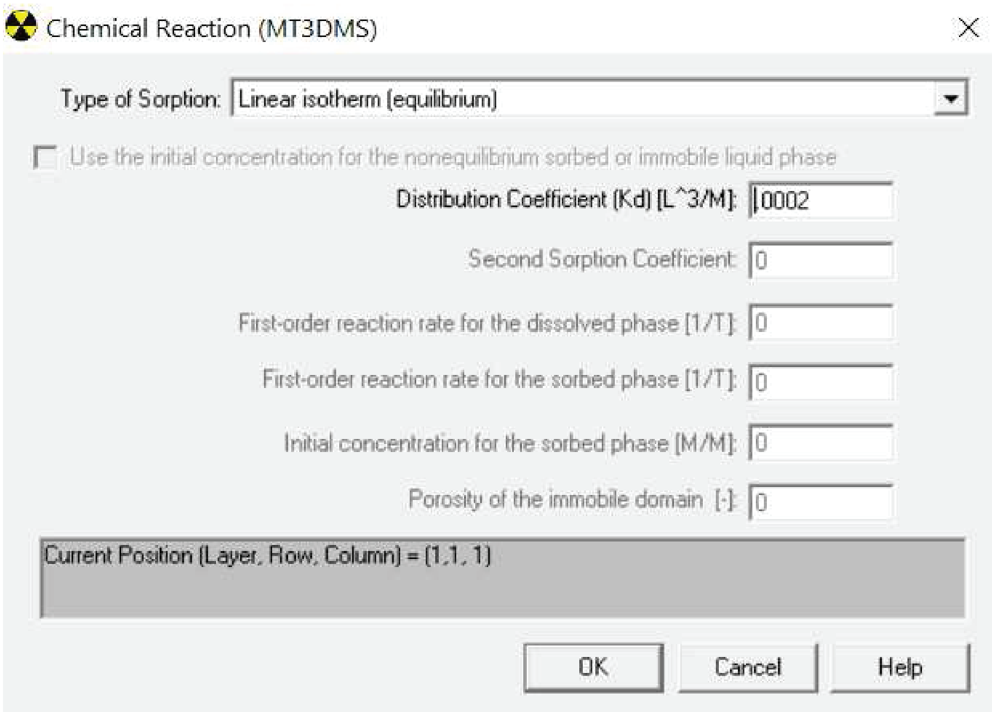


Fig.2.19: Chemical Reaction dialog box

In this case study a Linear isotherm (equilibrium) type of sorption has been selected, together with a value of 0 and $2.0\text{x}10^{-4}$ m^3/g of the Distribution Coefficient respectively for salt and temperature. The Distribution Coefficient depends on the solute species, nature of the porous medium, and other conditions of the system.

2.3.4.7 Sink/Source Concentration

This menu is used for specifying the concentration associated with the fluid of point or spatially distributed sources or sinks. The concentration value of a particular source or sink is specified in the Data Editor. Point sources include wells, general head boundary cells, fixed-head cells, rivers and streams. Recharge is the only spatially distributed source whereas evapotranspiration is the only sink whose concentration can be specified. The concentration of a sink cannot be greater than that of the groundwater at the sink cell. If the sink concentration is specified greater than that of the groundwater, it is automatically set equal to the concentration of the groundwater.

For the *Evapotranspiration* a value of 0.3 kg/m^3 has been set for the salt and, considering that the model allows to simulate the temperature as one of the species, a value $20°C$ for temperature. The value of 0.3 g/l of the Specified Concentration of Evaporation Flux represent how much of the salt evaporate together with the water. If a value of 0 g/l is set, only the water will be allowed to evaporate and, consequently, the salt concentration in the tank will increase a lot.

Finally using the menu item *Time Variant Specified Concentration*, it is possible to define constant concentration cells anywhere in the model grid and different concentration values may be specified for different stress periods. A time varying specified concentration cell is defined by setting the following data in the Data Editor:

- Flag: a nonzero value indicates that a cell is specified as a constant concentration cell. In a multiple stress period simulation, a constant-concentration cell, once defined, remains a constant-concentration cell during the simulation, but its concentration value can be specified to vary in different stress period. To change the concentration value in a particular stress period, simply set a non-zero value to Flag and assign the desired concentration value to Specified Concentration.

- Specified Concentration: this value is the concentration in the cell from the beginning of a stress period.

In this case study, the temperature [°C] has been set as specified concentration [ML^{-3}] in those layer where a non zero value of the flag has been indicated (groundwater table) considering an averaged value for each stress period. The depletion of the groundwater due to evaporation has been also taken into account setting a nonzero value of the flag for the underlying layers which correspond to the water table.

2.3.4.8 Mass-Loading Rate

Instead of specifying a source concentration associated with a fluid source, the mass loading rate [MT^{-1}] into the groundwater system can directly be specified by using this menu item.

In this case study, a value of 1.667×10^{-9} kg/d has been set for the first three layers and a value of 5.0×10^{-9} kg/d for all the others.

2.3.4.9 Solver

MT3DMS includes a general-purpose iterative solver based on the generalized conjugate gradient method for solving the system of the transport equations. The solver is implemented in the Generalized Conjugate Gradient package. This solver must always be activated. Using this solver, dispersion, sink/source, and reaction terms are solved implicitly without any stability constraints on the transport step size.

2.3.4.10 Concentration Observations

Selecting this menu item from the MT3DMS menu, it will be possible to specify the locations of the concentration observation boreholes and their associated observed (measurement) data in a Concentration Observations dialog box. Its use is identical to the Head Observation dialog box (see Section 2.3.3.3). The only difference is that the head observations are replaced by concentration observations.

2.3.4.11 Output Controls

In order to set the output options of MT3D it is possible to use the Output Control dialog box (Fig. 2.20). The options in this dialog box are grouped under three tabs described below.

- Output Terms: the MT3DMS transport model always generates a listing file OUTPUT. MTM, which documents the details of each simulation step. All output terms denoted by (ASCII) are also saved in the listing file.
- Output Times: the value of the output frequency, NPRS, indicates whether the output is produced in terms of total elapsed simulation time or the transport step number. If NPRS=0, simulation results will only be saved at the end of simulation.
- Misc.: it includes CINACT, which is the predefined concentration value for an inactive concentration cell (ICBUND = 0); THKMIN, which is the minimum saturated thickness in a cell, expressed as the decimal fraction of the model layer thickness, below which the cell is considered inactive; and NPRMAS, which indicates how frequently the mass budget information should be saved in the mass balance summary file MT3Dnnn.MAS, where n is the species number.

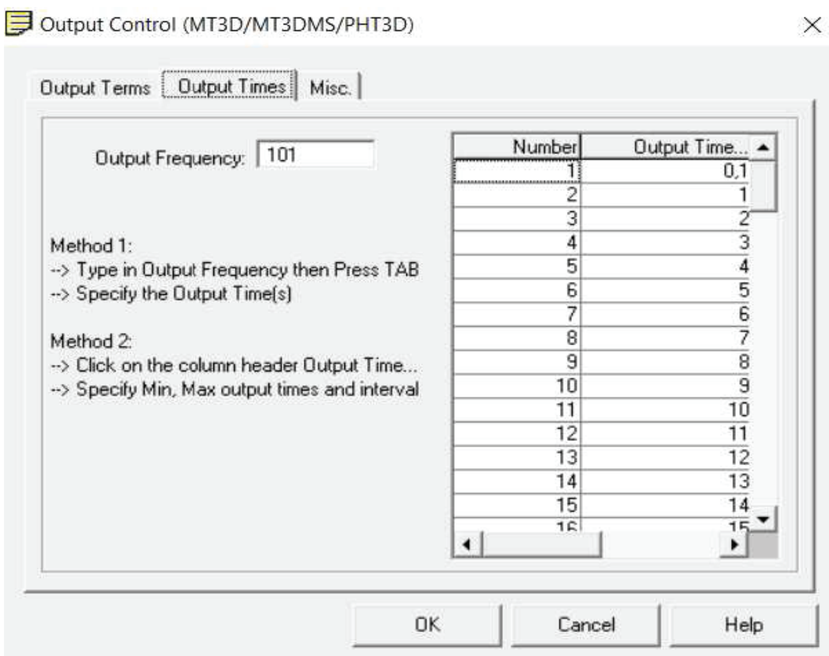


Fig.2.20: Output Control (MT3D/MT3DMS) dialog box

2.3.4.12 Run

If the Simulation Mode is set as Constant Density Transport with MT3DMS, the Run MT3DMS dialog box will be displayed. If the Simulation Mode is set as Variable Density and Transport with SEAWAT as in this case study, the Run SEAWAT dialog box (Fig.2.21) will be displayed in place of the Run MT3DMS dialog box.

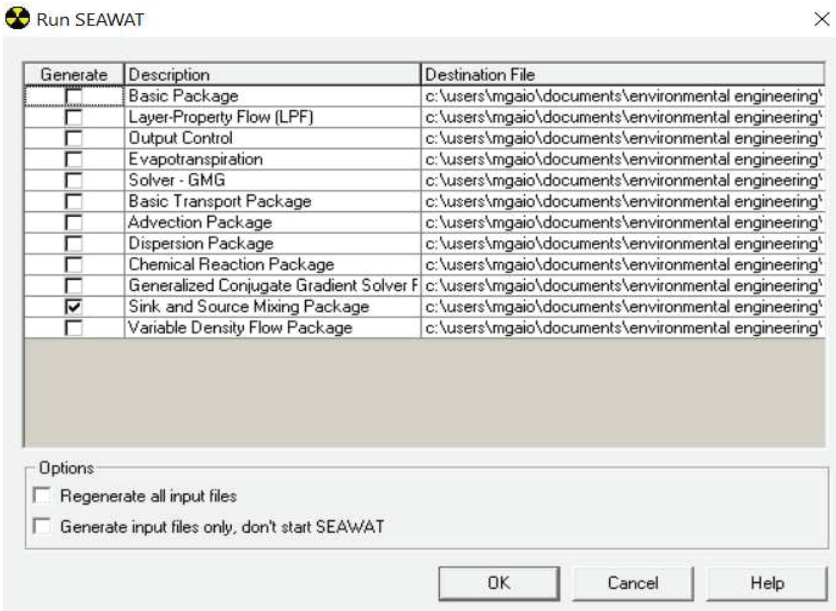


Fig.2.21: Run SEAWAT dialog box

The available settings of the Run SEAWAT dialog box are described below.

The *File Table* has three columns:

- *Generate*: prior to running a transport simulation, PM uses the user-specified data to generate input files for SEAWAT. An input file will be generated if it does not exist or if the corresponding Generate box is checked. Normally, there is no need to worry about these boxes since PM will take care of the settings.
- *Description* gives the names of the packages used in the model.
- *Destination File* shows the paths and names of the input files of the model.

Options:

- *Regenerate all input files*: checking this option it will be possible to force PM to generate all input files regardless the setting of the Generate boxes. This is useful if the input files have been deleted or overwritten by other programs.
- *Generate input files only, don't start SEAWAT*: checking this option, the user does not want to run SEAWAT. The simulation can be started at a later time or can be started at the Command Prompt (DOS box) by executing the batch file SEAWAT.BAT.

OK: clicking OK it is possible to generate SEAWAT input files. In addition to the input files, PM creates a batch file SEAWAT.BAT in the model folder. When all input files are generated, PM automatically runs SEAWAT.BAT in a Command Prompt-window (DOS box).

3 Results

In this chapter all the results will be presented and discussed, together with the calibration process through which the evaporation values have been retrieves. Finally, a sensitivity analysis has been performed in order to estimate the impact that some of the input parameters have on the evaporation process.

3.1 Calibration of the model

The calibration is the process to adjust the input parameters in order to obtain a good fit between the model results and the observed field data.
The measured data from the tank to be compared with the results of the model are:

- Hydraulic Head
- TDS concentration
- Temperature

Since only the evaporation stress has been taken into account as model input, the calibration process resulted to be simple and fast. It was carried out manually taking evaporation parameters from literature, increasing or decreasing them till the model results fit the observed field data. In order to check if the measured results match the observed ones and so the evaporation input parameters are correct, the Scatter Diagram dialog box and the Time Series Curves dialog box has been opened for each one of the measured data (Hydraulic Head, TDS concentration and Temperature).

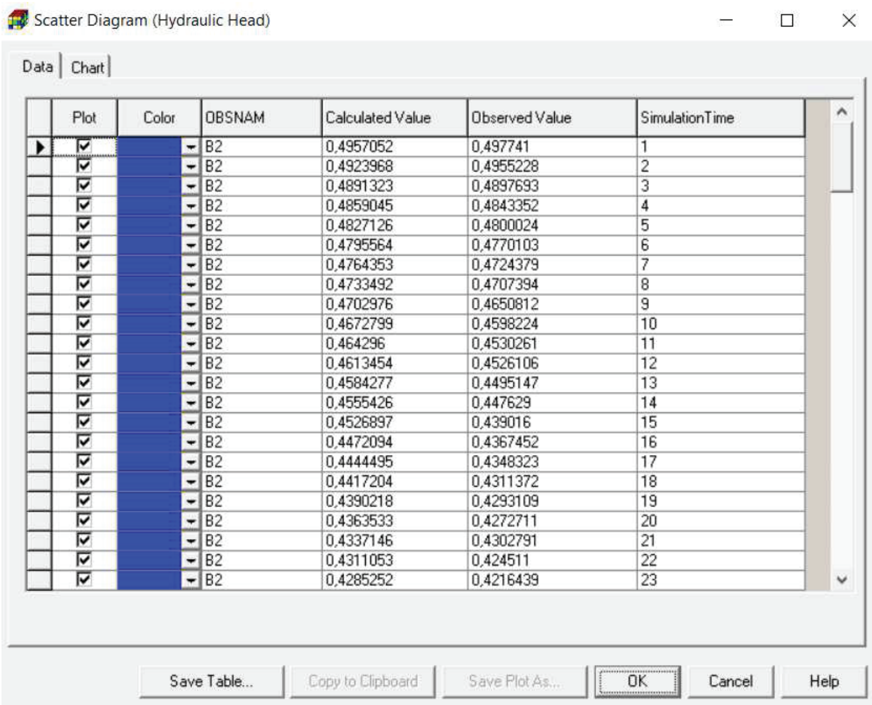
3.1.1 Hydraulic Head calibration

After running the MODFLOW model simulation, the menu item **MODFLOW | View | Head Scatter Diadram** has been selected to open the Scatter Diagram (Hydraulic Head) diagram box. This menu item is available only if Head

Observations have been defined. The options are grouped under two tabs – Data and Chart – as described below.

The Data Tab (Fig. 3.1) contains a table showing the observed and calculated values at active observation boreholes. The columns of this table are listed:

- Plot: A borehole will be displayed on the scatter diagram only when its Plot box is checked.
- Colour: Defines the plot colour for each borehole.
- OBSNAM: Displays the name of each observation borehole specified in the Head Observation dialog box (Fig. 2.12).
- Calculated value: Displays simulated head values at observation boreholes.
- Observed Value: The user-specified observed values in the Head Observations dialog box are linearly interpolated to the simulation times and displayed in this column.
- Simulation Time: Displays the times at the end of each stress period or time step, to which the calculated values and observed values pertain.



Plot	Color	OBSNAM	Calculated Value	Observed Value	SimulationTime
☑		B2	0,4957052	0,497741	1
☑		B2	0,4923968	0,4955228	2
☑		B2	0,4891323	0,4897693	3
☑		B2	0,4859045	0,4843352	4
☑		B2	0,4827126	0,4800024	5
☑		B2	0,4795564	0,4770103	6
☑		B2	0,4764353	0,4724379	7
☑		B2	0,4733492	0,4707394	8
☑		B2	0,4702976	0,4650812	9
☑		B2	0,4672799	0,4598224	10
☑		B2	0,464296	0,4530261	11
☑		B2	0,4613454	0,4526106	12
☑		B2	0,4584277	0,4495147	13
☑		B2	0,4555426	0,447629	14
☑		B2	0,4526897	0,439016	15
☑		B2	0,4472094	0,4367452	16
☑		B2	0,4444495	0,4348323	17
☑		B2	0,4417204	0,4311372	18
☑		B2	0,4390218	0,4293109	19
☑		B2	0,4363533	0,4272711	20
☑		B2	0,4337146	0,4302791	21
☑		B2	0,4311053	0,424511	22
☑		B2	0,4285252	0,4216439	23

Fig.3.1: Data tab of the Scatter Diagram (Hydraulic Head) dialog box

The Chart Tab (Fig. 3.2) displays the scatter diagram using the calculated and observed data. Scatter diagrams are often used to present the quality of calibration results. The observed values are plotted on one axis against the corresponding calculated values on the other. If there is an exact agreement between measurement and simulation, all points lie on a 45° line. The narrower the area of scatter around this line, the better is the match. Variance is the mean squared error between observed and calculated value of Plot-marked observations, which are displayed on the scatter diagram.

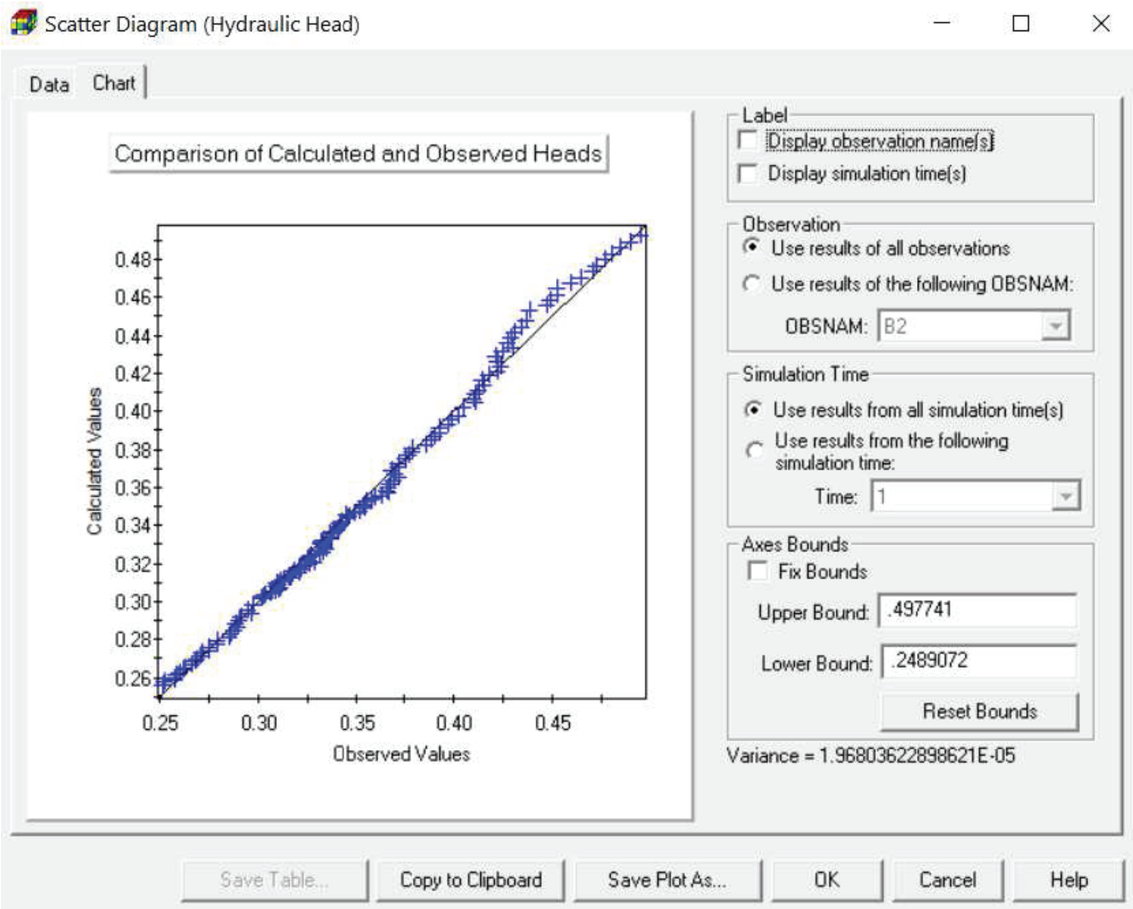
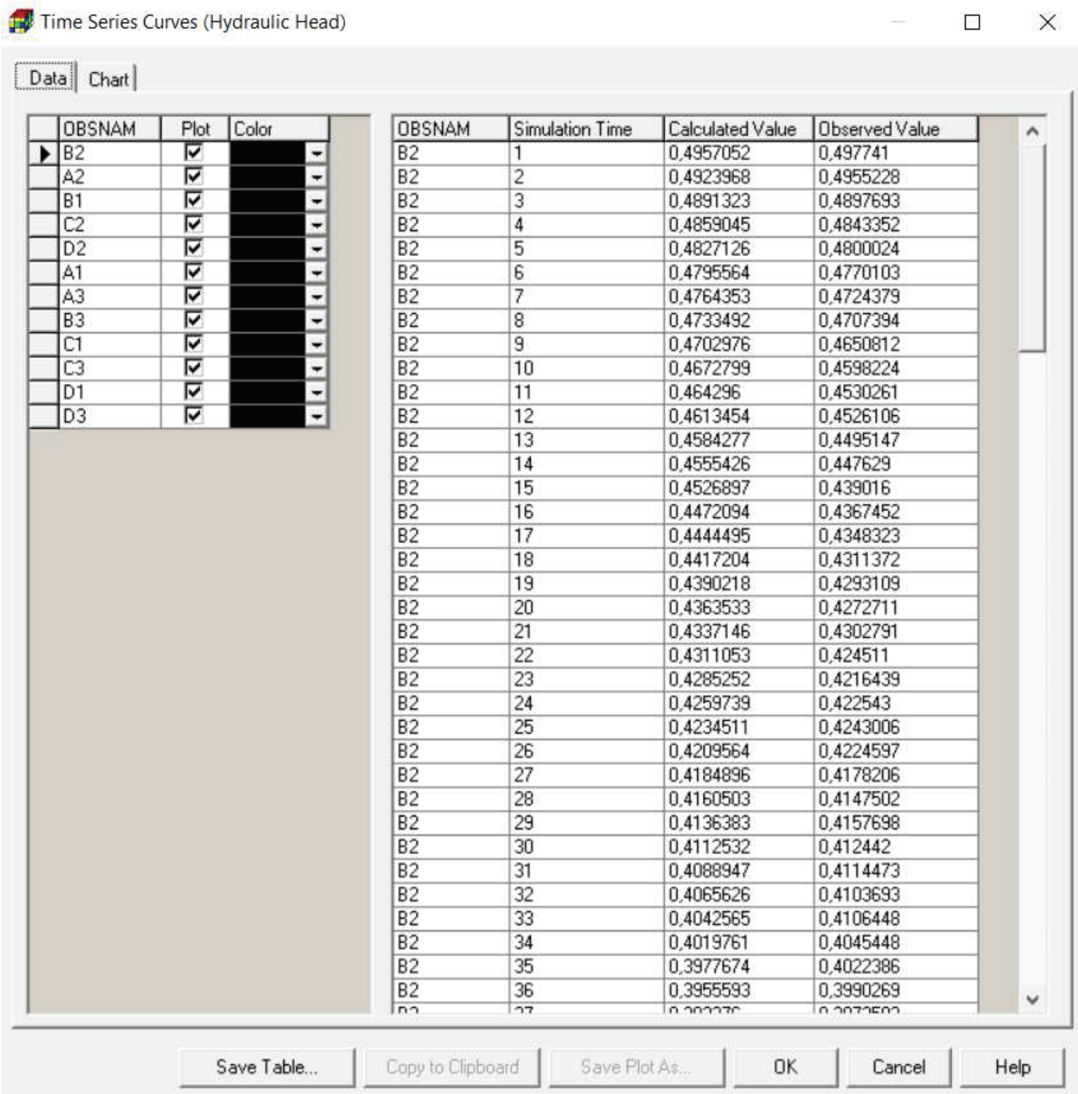


Fig.3.2: Chart tab of the Scatter Diagram (Hydraulic Head) dialog box

In order to check if the calculated Hydraulic Head values fit the observed ones over the observation time, the menu item **MODFLOW | View | Head-Time Curves** has been selected to open the Time Series Curves (Hydraulic Head) dialog box. Also this menu item is available only if Head Observations have been defined. The options are grouped under two tabs: Data and Chart as described below.

The Data tab (Fig. 3.3) contains two tables. The table to the left shows the names (OBSNAM) of the observation boreholes and their Plot and Colour settings. The table to the right shows the Observation Time, Calculated Values and Observed Values.



OBSNAM	Plot	Color
B2	☑	
A2	☑	
B1	☑	
C2	☑	
D2	☑	
A1	☑	
A3	☑	
B3	☑	
C1	☑	
C3	☑	
D1	☑	
D3	☑	

OBSNAM	Simulation Time	Calculated Value	Observed Value
B2	1	0,4957052	0,497741
B2	2	0,4923968	0,4955228
B2	3	0,4891323	0,4897693
B2	4	0,4859045	0,4843352
B2	5	0,4827126	0,4800024
B2	6	0,4795564	0,4770103
B2	7	0,4764353	0,4724379
B2	8	0,4733492	0,4707394
B2	9	0,4702976	0,4650812
B2	10	0,4672799	0,4598224
B2	11	0,464296	0,4530261
B2	12	0,4613454	0,4526106
B2	13	0,4584277	0,4495147
B2	14	0,4555426	0,447629
B2	15	0,4526897	0,439016
B2	16	0,4472094	0,4367452
B2	17	0,4444495	0,4348323
B2	18	0,4417204	0,4311372
B2	19	0,4390218	0,4293109
B2	20	0,4363533	0,4272711
B2	21	0,4337146	0,4302791
B2	22	0,4311053	0,424511
B2	23	0,4285252	0,4216439
B2	24	0,4259739	0,422543
B2	25	0,4234511	0,4243006
B2	26	0,4209564	0,4224597
B2	27	0,4184896	0,4178206
B2	28	0,4160503	0,4147502
B2	29	0,4136383	0,4157698
B2	30	0,4112532	0,412442
B2	31	0,4088947	0,4114473
B2	32	0,4065626	0,4103693
B2	33	0,4042565	0,4106448
B2	34	0,4019761	0,4045448
B2	35	0,3977674	0,4022386
B2	36	0,3955593	0,3990269

Fig.3.3: Data tab of the Head-Time Series Curves (Hydraulic Head) dialog box

The Chart tab (Fig. 3.4) displays time-series curves using the calculated and observed values.

The reduction of the Hydraulic Head in time fitting the monitored reduction in the tank due to evaporation is well represented by the model simulation.

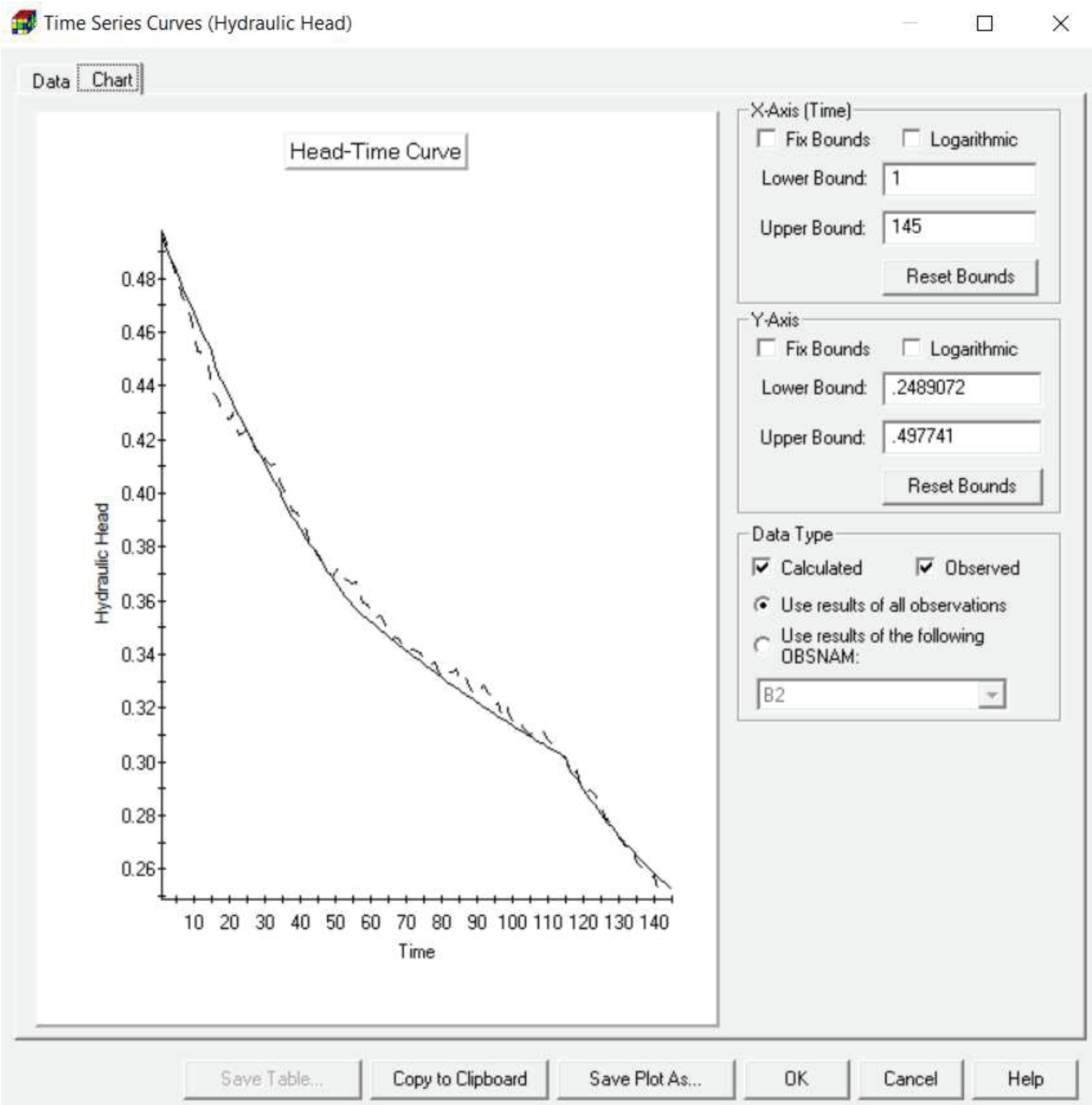


Fig.3.4: Chart tab of the Head-Time Series Curves Diagram dialog box

3.1.2 TDS concentration and Temperature calibration

After running the MT3DMS/SEAWAT model simulation, in order to check if the calculated concentration (TDS and Temperature) values fit the observed ones over the observation time, the menu item **MT3DMS/SEAWAT | View | Concentration-Time Curves** has been selected to open the Time Series Curves (Concentration) dialog box, both for TDS concentration (Fig. 3.5) and Temperature (Fig. 3.6). Also these menu items are available only if Concentration Observations have been defined and they are identical to the Time Series Curves (Hydraulic Head) dialog box (Fig. 3.4), except the concentration values replace the head values.

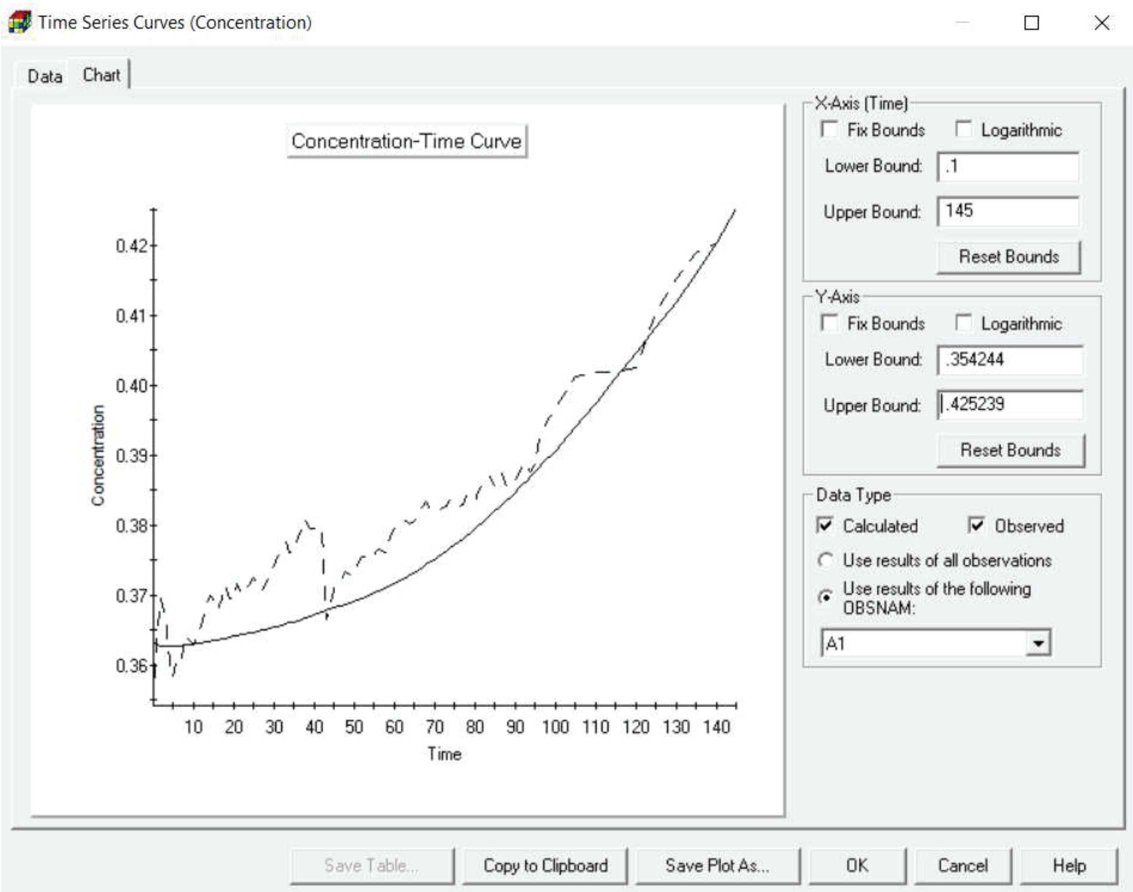


Fig.3.5: TDS Concentration-Time Series Curves Diagram dialog box

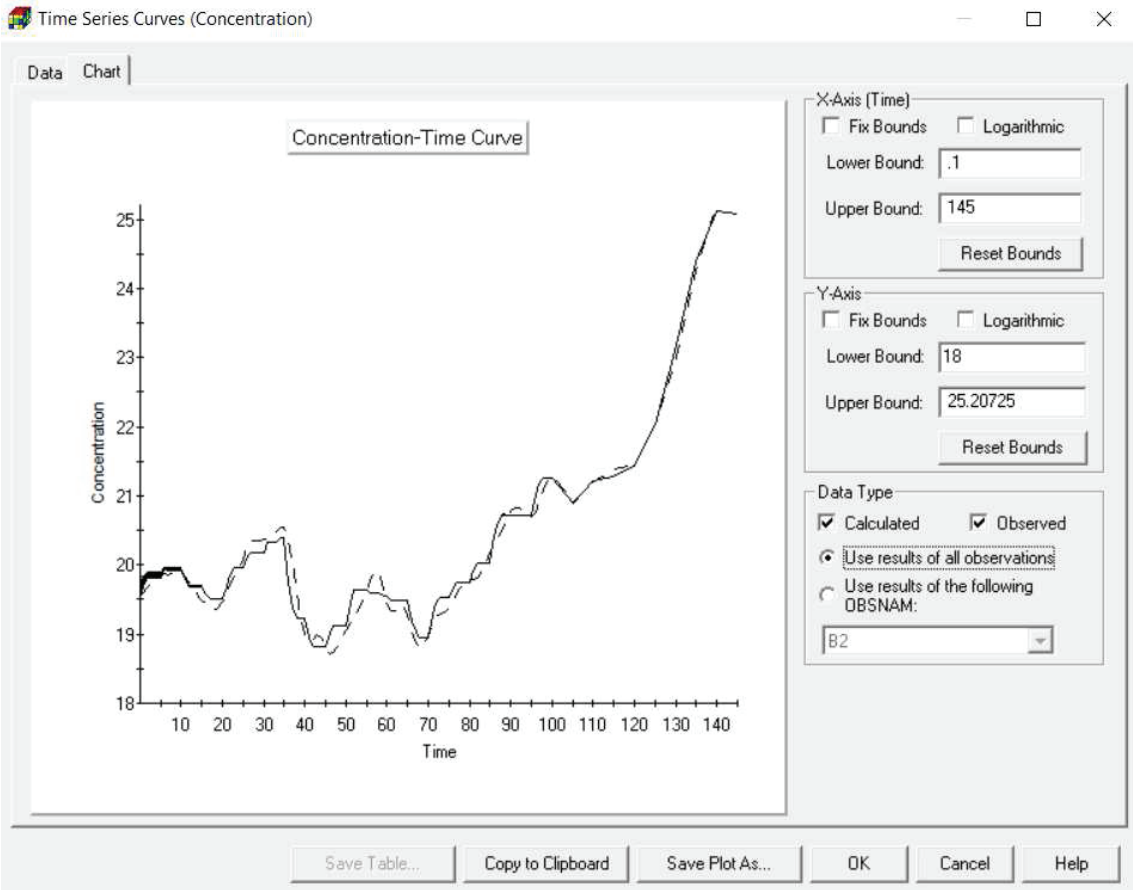


Fig.3.6: Temperature-Time Series Curves Diagram dialog box

3.2 Discussion

As it is possible to see in the Time Series Curves dialog boxes shown in the previous paragraph, a good model calibration has been reached. The lowering of the water head in the tank due to evaporation has been almost perfectly reproduced by the model simulation; the same for the temperature variation and for the rising of the TDS concentration considering a value of 0.3 g/l of the Specified Concentration of Evaporation Flux.

Allowing this model calibration that has been fully described above, the following evapotranspiration input values have been retrieved.

Three different Maximum ET Rate (R_{ETM}) and Parameter Number have been set for three different stress period activated: respectively 2.3×10^{-3} m/d and 1 for the stress period 1, $1.15x10^{-3}$ m/d and 2 for the stress period 12, $4.4x10^{-3}$ m/d and 3 for the stress period 24.

The Elevation of the ET Surface (h_S) is 1.1 m, the ET Extinction Depth (d) 0.9 m and the Layer Indicator (IET) 0 for all the stress periods activated.

The first thing that it is possible to notice after the calibration process is that the highest R_{ETM} was the one associated with the stress period 24. This is due to the increasing of temperature during the last part of the observation time because of the beginning of the summer (Fig. 3.6).

The other input parameter, which it is important to focus on, is the ET Extinction Depth (d). This parameter changes depending on soils type and land covers. As it is shown in the Figure (Shah et al. 2007) below, fine-textured soils have greater extinction depth than coarse textured soils for a similar land cover.

Extinction Depths for Different Soil Land Covers [cm]			
Soil Type	**Bare soil**	**Grass**	**Forest**
Sand	50	145	250
Loamy sand	70	170	270
Sandy loam	130	230	330
Sandy clay loam	200	300	400
Sandy clay	210	310	410
Loam	265	370	470
Silty clay	335	430	530
Clay loam	405	505	610
Silt loam	420	515	615
Silt	430	530	630
Silty clay loam	450	550	655
Clay	620	715	820

Tab. 3.1: Extinction Depths for Different Soil Land Covers (Shah et al. 2007)

After that the terrain inside the lab tank has been investigated, it was defined, following the Wentworth classification, as coarse to medium sands. Therefore, the ET Extinction Depth (d) should be around 50 cm. In fact, an important feature claimed by many studies for sandy soil is that the evaporation becomes negligible when the water table is more than a value around 60 cm below the ground surface.

However, in this case study a value of d=90 cm has been retrieved for the Extinction Depth after the calibration process. So, even if a bare and coarse-sandy soil has been tested, the evaporation from groundwater can't be considered negligible when the water table fall down the value of 60 cm below the ground surface. Considering it negligible leads to significantly underestimate its magnitude and its role in the hydro-geological balance.

It is also important to highlight that, by working in lab condition, the experiment was carried out in conservative condition. In fact, conducting the experiment inside the SIMAU department, the tank was not subjected to solar radiation and wind, both factors that promote and increase the evaporation from groundwater. The only parameters that were varying inside the lab during the observation time were temperature, pressure and relative humidity that have been monitored as described in the Chapter 2.

3.3 Sensitivity analysis

A sensitivity analysis has been carried out for some of the input model parameters [ET Extinction Depth (d), Mass Loading Rate, Longitudinal Dispersivity and Effective Porosity (n_e)] in order to determine their impact on the evaporation process and to check if the model would be equally calibrated.

Sensitivity analysis is defined as "the study of how the uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input" (Saltelli et al. 2004).

The first input parameter that has been analysed was the Extinction Depth. Values of 0.8 m and 1 m have been inserted as input in the Evapotranspiration Flow Package of MODFLOW and the model simulations were run. For each model simulation, the menu item MODFLOW | View | Head-Time Curves has been selected to open the Time Series Curves (Hydraulic Head) dialog box. Then, the three calculated curves with different values of d have been plotted in the same graph by means of excel (Fig. 3.7).

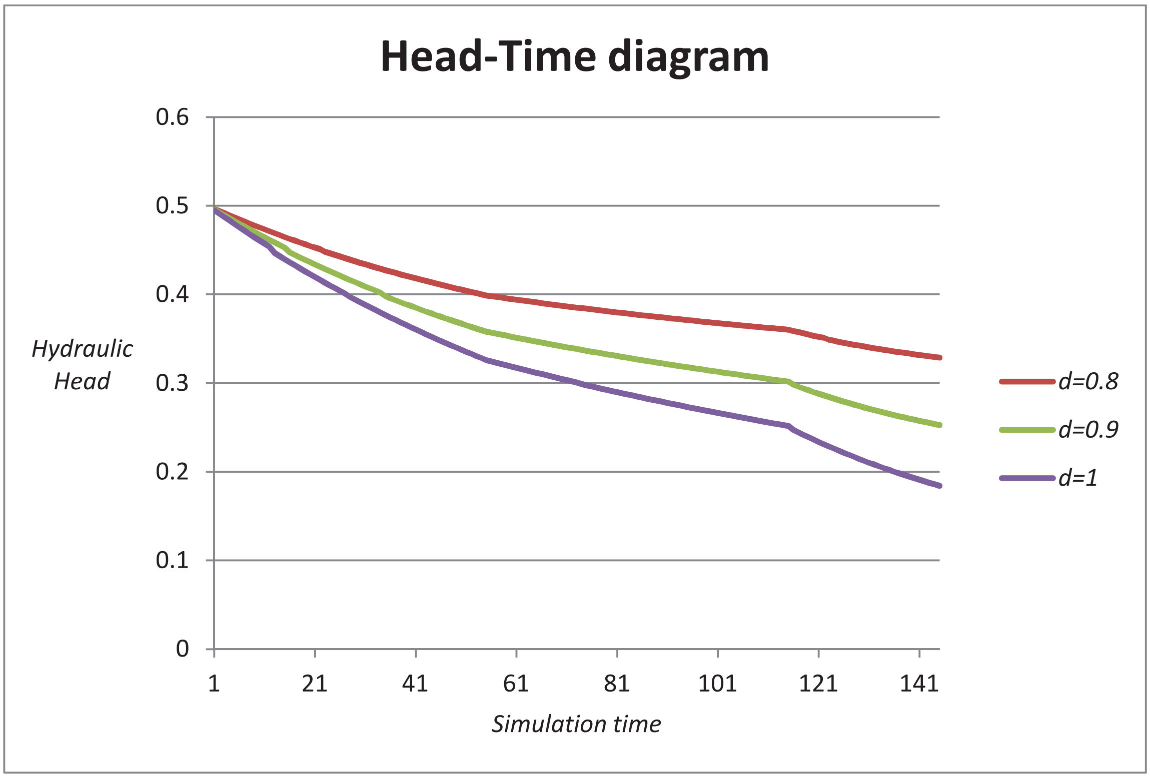


Fig.3.7: Head-Time Curves with different extinction depth values (0.8, 0.9 and 1 m)

As it is possible to see in the Figure, when the extinction depth is reduced the groundwater head drawdown will be less pronounced and the relative Head-Time Curve will be above the calibrated one with a final distance of the order of 0.1 m; vice versa if d is increased. This result underline the importance of d impact on the evaporation process.

In order to check the sensitivity of the transport parameters the Mass Loading Rate and the Longitudinal Dispersivity have been analysed.

Considering the Mass Loading Rate of salt, the values of 1.66×10^{-9} kg/d for the first three layers and 5.0×10^{-9} kg/d for all the others have been doubled and halved and the model simulations were run. For each model simulation, the menu item MT3DMS/SEAWAT | View | Concentration-Time Curves has been selected to open the Time Series Curves (TDS concentration) dialog box and to estimate the changes in salinity over time. Then, the three calculated curves with different values of Mass Loading Rate have been plotted in the same graph by means of excel (Fig. 3.8).

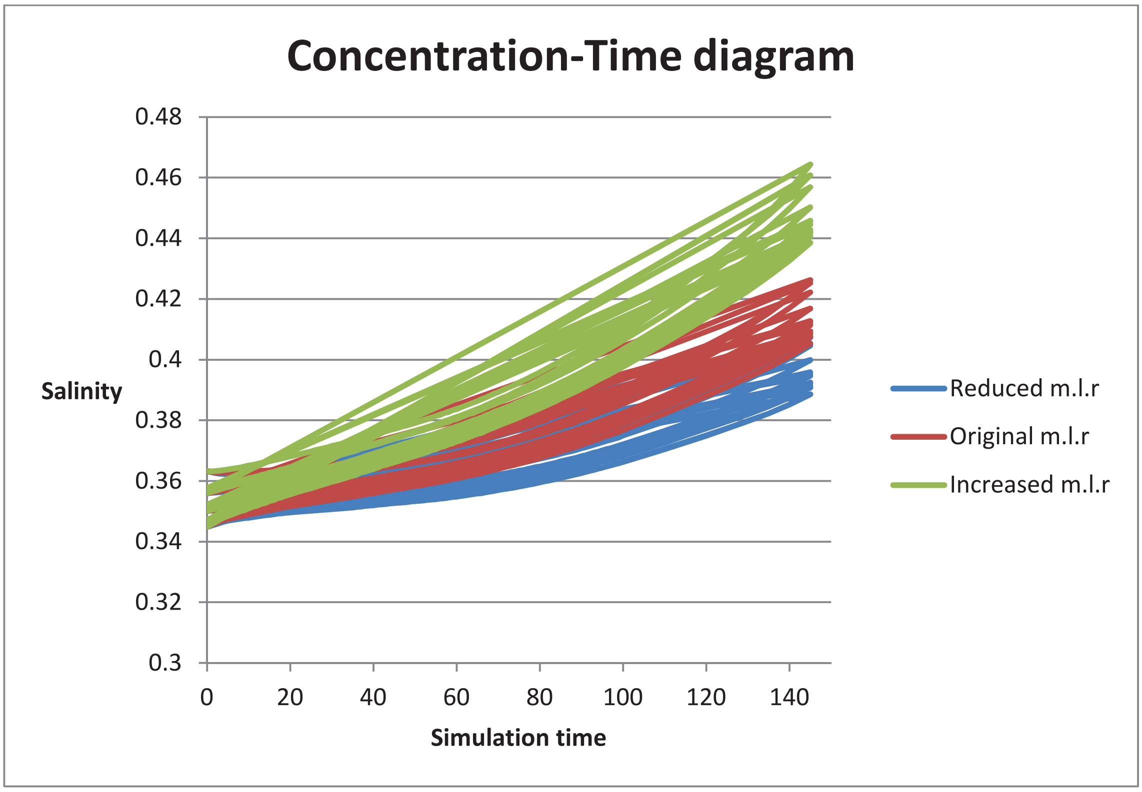


Fig.3.8: TDS concentration-Time Curves with different mass loading rate values (halved, calibrated and doubled values)

As shown in the Figure, the Mass Loading Rate affects the salinity concentration and, therefore, the evaporation process. In fact, the larger are the Mass Loading Rate values the larger will be the TDS evapoconcentration; vice versa if smaller values are taken.

Considering the Longitudinal Dispersivity, the same procedure has been followed, the values of 0.1 have been doubled and halved and the model simulations were run. For each model simulation, the Time Series Curves (TDS concentration) dialog box has been opened and the three calculated curves have been plotted in the same graph by means of excel (Fig. 3.9).

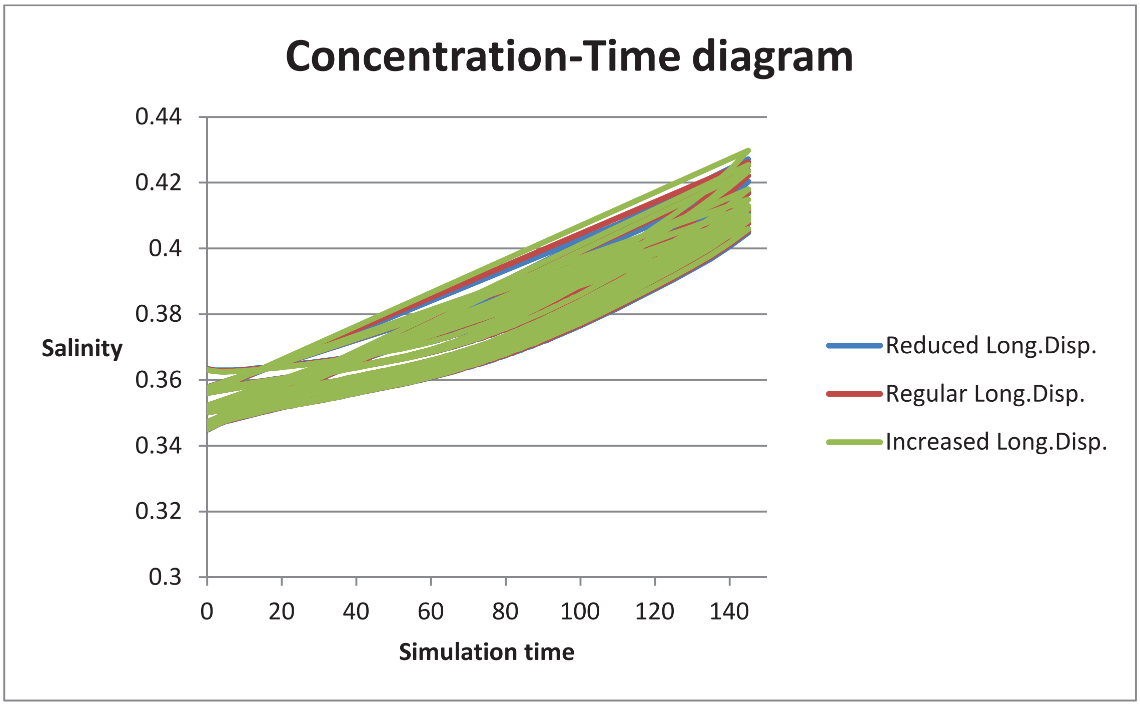


Fig.3.9: TDS concentration-Time Curves with different longitudinal dispersivity values (halved, calibrated and doubled values)

As it is possible to see in the Figure, the Longitudinal Dispersivity seems to not affect the TDS evapoconcentration and, therefore, it does not impact the calibration of the model.

The last input parameter that has been analysed was the Effective Porosity. Values of 0.18 and 0.22 have been inserted as input in the Parameters Menu and the model simulations were run. For each model simulation, the menu item MT3DMS/SEAWAT | View | Concentration-Time Curves has been selected to open the Time Series Curves (TDS concentration) dialog box and to estimate the changes in salinity over time. Then, the three calculated curves with different values of n_e have been plotted in the same graph by means of excel (Fig. 3.10).

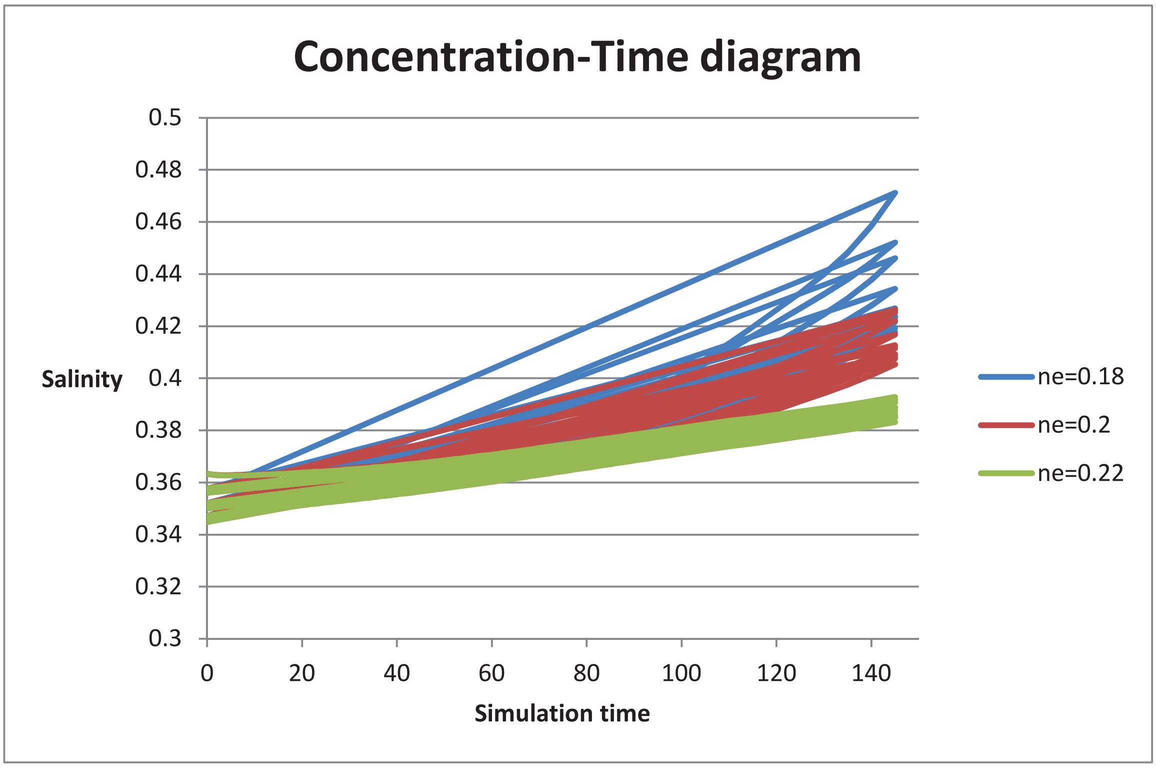


Fig.3.10: TDS concentration-Time Curves with different effective porosity values (0.18, 0.2 and 0.22)

As shown in the Figure, the effective porosity affects the salinity concentration and, therefore the evaporation process. In fact, the smaller is n_e the larger is the TDS evapoconcentration; vice versa if a larger value is taken.

4 Testing the evaporation rates on a large scale model

The results obtained with the tank model simulation have been carried from laboratory to basin scale. A 2007 case study has been reanalyzed in which the Tronto basin has been modelled for the low flow (June, 2007) and high flow (January, 2007) period and, at the time, the evapotranspiration has been neglected.
The characterization of the Tronto river basin, together with the model input, procedures and results will be fully described in this chapter.

4.1 Tronto river basin

The drainage basin of Tronto river extends for 1192 km^2 between Abruzzi and Marche regions and is elongated WSW–ENE. The maximum elevation is reached at Mount Vettore (2476 m), which is the highest summit of the Sibillini Mountains, while the mean elevation is about 784 m. The basin is characterised by 39.9% of terrain with a prevalent arenaceous composition. The rest of the area is covered by 30.2% pelitic sediments, 7.3% marls and 5.4% limestones, from the Sibillini Mountains (Coltorti & Farabollini, 2008).

Similarly to many Adriatic valleys, it has the north side characterised by a sequence of terraces at progressive elevations above the valley floor and the south side characteristically very steep and covered by a number of landslides of large dimensions (Coltorti et al., 1991a, b).
The area has been subdivided into three sectors: piedmont, mid-valley and coastal (Fig. 4.1).

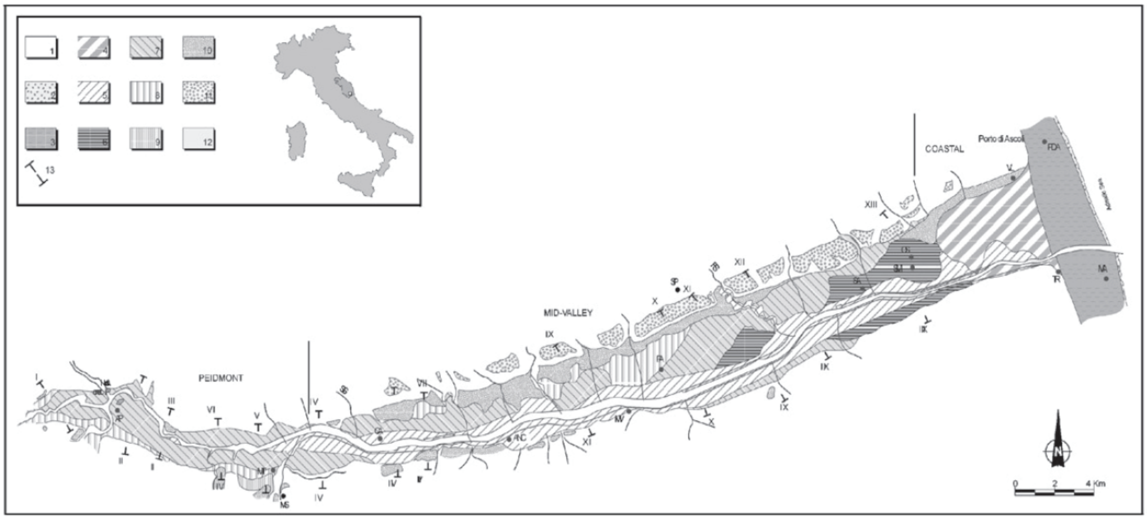


Fig.4.1: Geo-morphological map of the lower Tronto River Valley characterised by 12 Holocene alluvial deposits (all these deposits will be translated in the model into two different zone with different horizontal hydraulic conductivity): (1) thalweg; (2) present-day beach deposits; (3) barrier beach and deltaic deposits; (4) lagoon, swamp and overbank deposits; (5) present-day alluvial plain (IV-e terrace in the middle and pedemontan sector); (6) IV-d terrace; (7) IV-c terrace; (8) IV-b; (9) IV-a terrace; (10) III order (Late Pleistocene alluvial terrace); (11) II and I order (Late Middle and Middle Pleistocene alluvial deposits); (12) bedrock. (Modified by Coltorti & Farabollini, 2008).

The piedmont sector, about 6 km long, is characterised by a relatively steep longitudinal profile (H/d=0.006) and a narrow thalweg delimited by a high and vertical scarp that creates a small gorge. In the mid-valley sector, 21 km long, the thalweg enlarges progressively and is bordered by a large alluvial plain; it has a gentler longitudinal profile (H/d=0.005-0.004) and confined terraces. The coastal sector, about 4 km long, is characterised by a very reduced gradient (H/d up to 0.025), a greater width of the valley and an elongated sandy coastline (Coltorti & Farabollini, 2008).

The rivers along the Adriatic side are characterised by at least four terraces located up to over 100 m above the valley floor and numbered from the older to the younger according to their progressive elevation on the valley floor.

Flowing northwards and then turning to the East, cutting transversely the major Apennine structures, the Tronto river is one of the major rivers of the Adriatic side of Central Italy south of the Po plain. It has its source in the sector located between the ‘‘Laga Mountains’’, a chain belonging to the Southern Apennines composed of Miocene sandstones and marls, and the Sibillini Mountains, composed of limestone rocks, that represent the southern tip of the northern Apennine.

The river is 115 km long and flows into the Adriatic Sea at Porto D'Ascoli. It has a mean gradient of 2.1 % and a 32 km alluvial plain, oriented E–W with a mean gradient of 0.4 %, downstream from the mountain tract.

The climate of the Tronto is of the ''central-southern Adriatic'' type in the lower valley and ''Apennine'' in the mountainous part (Mori, 1957). As most Mediterranean regions, it has mild winters and hot dry summers (Bisci et al., 1999). At the Folignano di Marino town, 28 km from the mouth, the maximum peak discharge is 1320 m^3/s, the mean is 17.8 m^3/s and the mean low is 2.5 m^3/s (Coltorti & Farabollini, 2008).

A quarry (Fig. 4.2) has recently been opened in the alluvial plain 500 m from the channel, near Ponte di Ancarano. The stratigraphy exhibited by the sediments exposed in the quarry is characterised by medium to fine planar and trough cross-bedded gravels (Miall, 1985, 1995). Local layers of horizontally bedded gravels are also present.

Fig.4.2: Opened quarry at "Ponte di Ancarano" (Modified by Coltorti & Farabollini, 2008).

4.2 Model input

In this section of the thesis it will be explained how the Tronto basin was modelled throughout PMWIN, describing all the input parameters both for low (June 2007) and high flow periods (January 2007). Following the grid, the parameters and the model menu, it was possible to implement the various input needed in the simulation.

4.2.1 The grid menu

All the input values of this menu are the same both for low and high flow period.

4.2.1.1 Mesh Size

The grid is defined by 300 columns 100 rows and 1 layer with a specified top and bottom for each cell (see Paragraph 4.2.1.4). In the Figure below is shown the geo-referenced grid together with Environment Options dialog box.

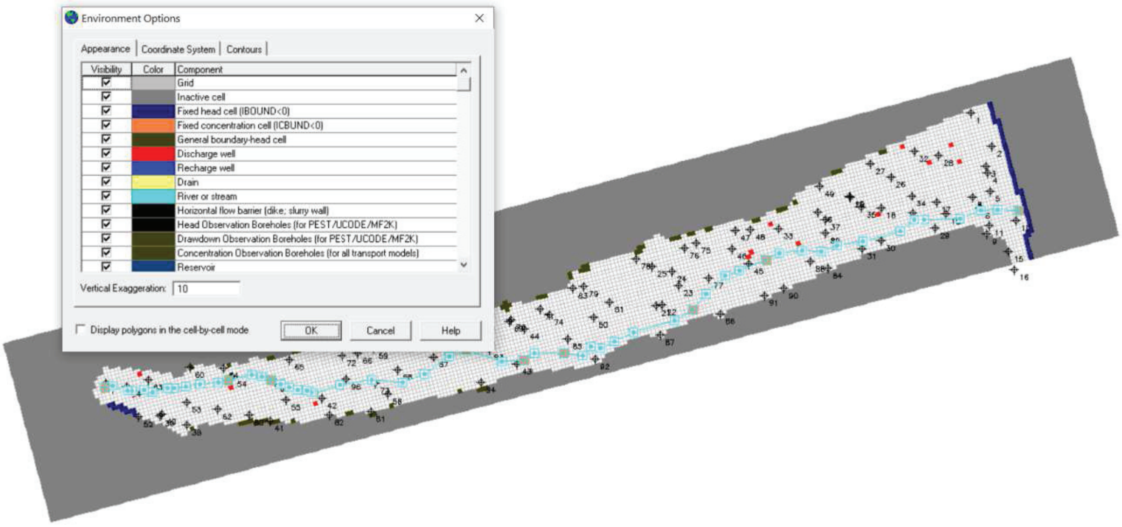


Fig.4.3: Geo-referenced study area and Environment Options dialog box

4.2.1.2 Layer Property

The layer properties are defined in the Layer Property dialog box (Fig. 4.4). A type 3 layer was set which is fully convertible between confined and unconfined.

Confined storage coefficient is used to calculate the rate of change in storage, if the layer is fully saturated, otherwise specific yield will be used.

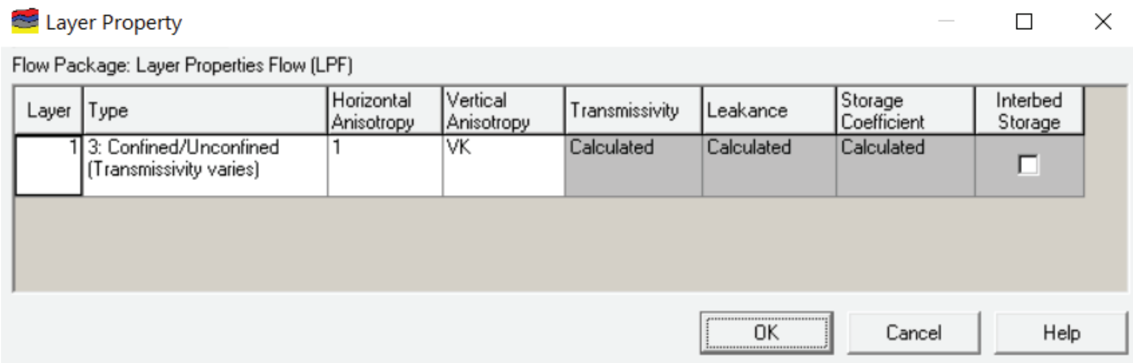


Fig.4.4: Layer property dialog box

4.2.1.3 Cell Status

As it was already said in the second chapter, the flow model MODFLOW requires an IBOUND array, which contains a code for each model cell. A positive value in the IBOUND array defines an active cell (the hydraulic head is computed), a negative value defines a constant head or fixed head cell (the hydraulic head is kept constant at a given value throughout the flow simulation) and the value 0 defines an inactive cell (no flow takes place within the cell). It is suggested to use 1 for active cells, 0 for inactive cells and -1 for constant head cells. Any outer boundary cell, which is not a constant head cell, is automatically a zero-flux boundary cell.

As it is possible to see in Fig. 4.3, the cells in grey are the inactive cells (0), the cells in blue are the fixed head cells (-1) and all the other cells are active cells (1) and the hydraulic head was computed.

4.2.1.4 Top (TOP) and Bottom of Layers (BOT)

In order to define the vertical model domain the Digital Terrain Model (DTM) has been entered into the software. In the two Figures below, both the Top and Bottom of the layer are graphically represented.

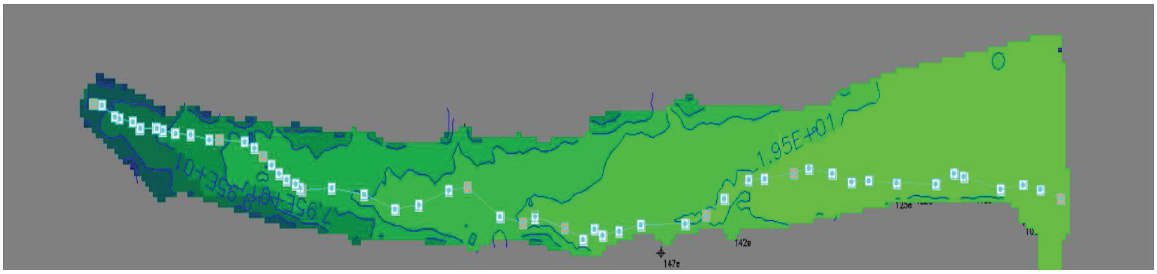


Fig.4.5: Top of Layer (TOP)

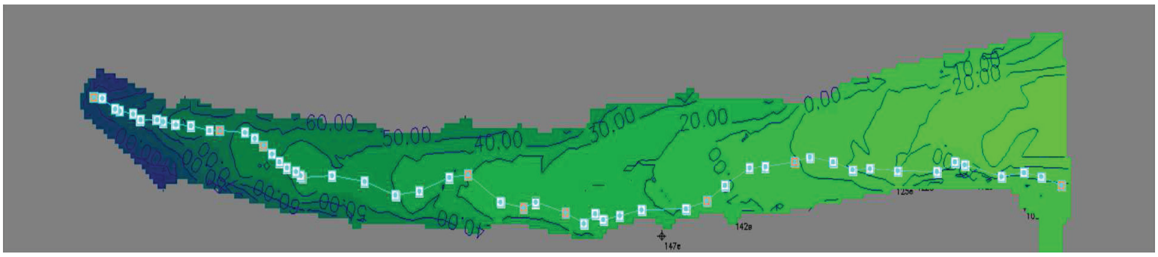


Fig.4.6: Bottom of Layer (BOT)

4.2.2 The parameters menu

This menu is used to input time, initial hydraulic head values, and aquifer parameters. The input values of this menu are the same both for low and high flow period.

4.2.2.1 Time

MODFLOW-2000 allows individual stress periods in a single simulation to be either transient or steady state instead of requiring the entire simulation to be either steady state or transient. Steady state and transient stress periods can occur in any order. Commonly the first stress period, as in this case study, is steady state and produces a solution that is used as the initial condition for subsequent transient stress periods. The length of stress periods and time steps is not relevant to steady state flow simulations.

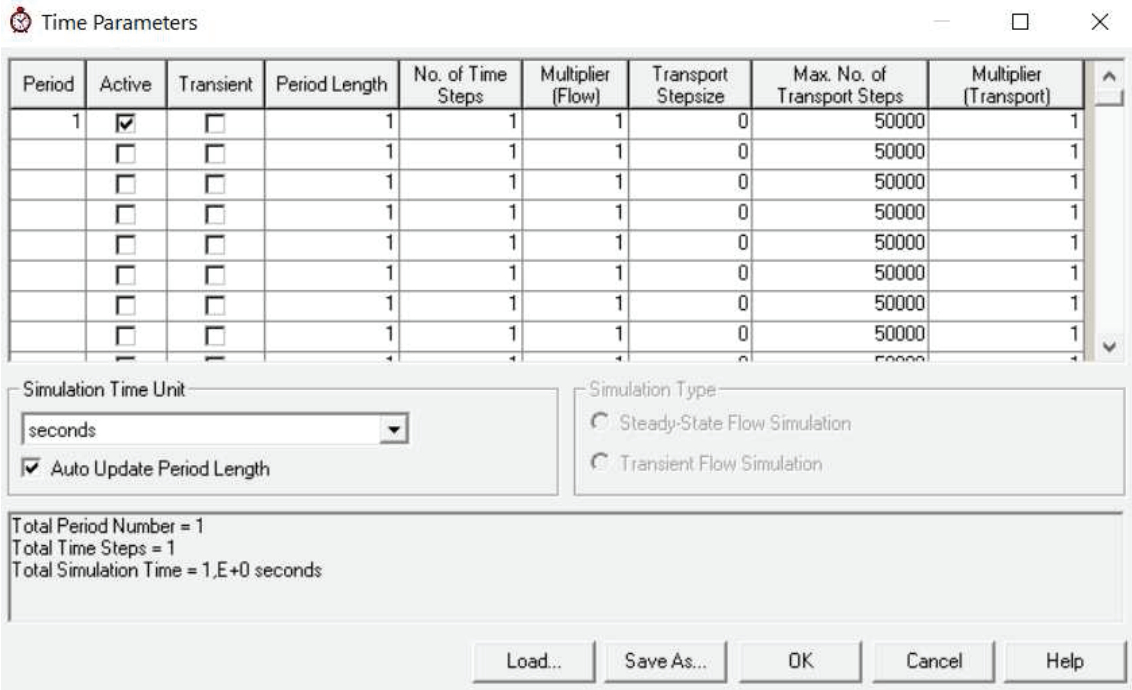


Fig.4.7: Time Parameters dialog box

4.2.2.2 Initial & Prescribed Hydraulic Heads

As already said, MODFLOW requires initial hydraulic heads at the beginning of a flow simulation. Initial hydraulic heads at constant head cells are used as specified head values of those cells and remain constant throughout the flow simulation. In this case study, in order to apply a steady-state flux, a constant head has been applied in order to ensure that all the cells begin the simulation not being dry.

4.2.2.3 Horizontal Hydraulic Conductivity

It is important to underline that all the Holocene deposits of the Tronto river valley (Fig.4.1) have been translate into two zone with different Horizontal Hydraulic Conductivity. As it is possible to see in the Figure below, the active cells of the grid were divided into two different areas: the green zone, which represent the less permeable one, has a value of Horizontal Hydraulic

Conductivity of 3.3×10^{-4} m/s and the blue zone that, with a value of 2.7×10^{-3} m/s, represents the more permeable one.

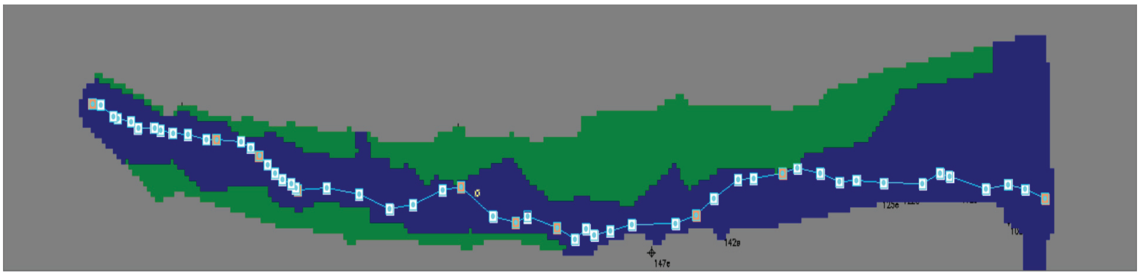


Fig.4.8: Horizontal Hydraulic Conductivity distribution

4.2.2.4 Effective Porosity

The value of n_e was set at 25% for all cells both for low and high flow period.

4.2.3 The models menu

4.2.3.1 MODFLOW | Flow Packages | Evapotranspiration

In 2007 the evapotranspiration has been considered negligible and the relative flow package has not been edited. Nevertheless, by means of the evapotranspiration input parameters retrieved throughout the calibration process of the tank model, it was possible to integrate the Tronto case study considering also the evapotranspiration process.

Evapotranspiration is defined by assigning the parameters that have already been described in the second Chapter (see paragraph 2.3.3.1), to each vertical column of cells. The input parameters are assumed to be constant during a given stress period.

Considering that three different Maximum ET Rate (R_{ETM}) values have been found corresponding to three different stress period activated (see paragraph 3.1), two scenarios have been analyzed for both the flow periods. In the first scenario the highest R_{ETM} value (4.40×10^{-3} m/d=5.1×10^{-8} m/s) has been entered in the Evapotranspiration Package (Fig 4.9). In the second scenario the lowest value (1.50×10^{-3} m/d=1.74×10^{-8} m/s) has been entered (Fig 4.10).

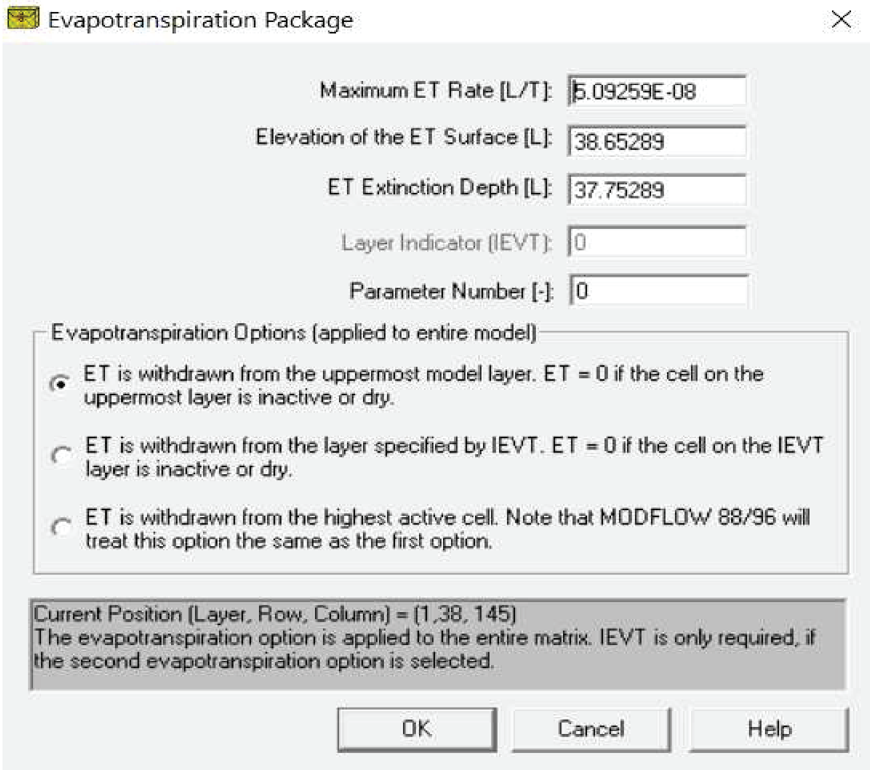


Fig.4.9: Evapotranspiration Package dialox box with highest R_{ETM} value

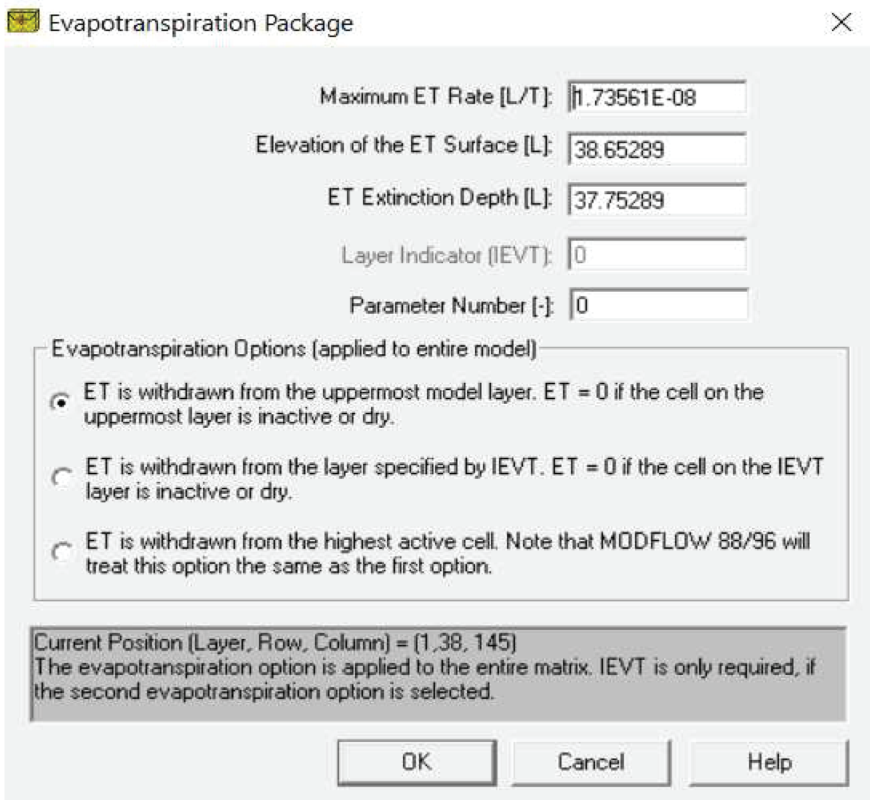


Fig.4.10: Evapotranspiration Package dialox box with lowest R_{ETM} value

In order to consider and enter in the Evapotranspiration Package the retrieved value of the ET Extinction Depth (d) 0.9 m, the topography of the layer (TOP) has been loaded as Elevation of ET Surface (Fig. 4.11) and as ET Extinction Depth and then, throughout the Search and Modify dialog box (Fig. 4.12), the value of 0.9 m has been subtracted.

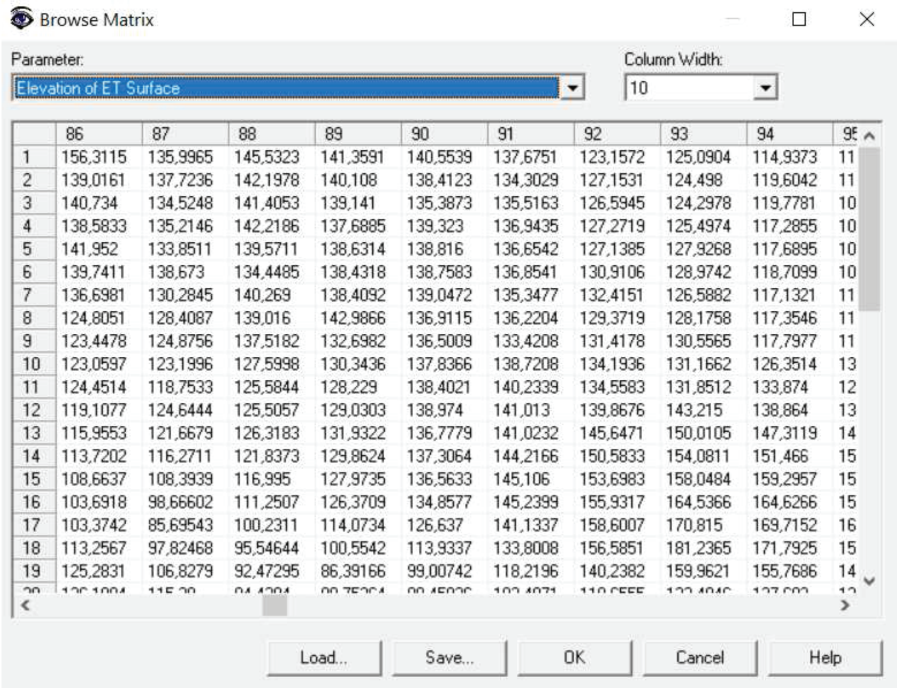


Fig.4.11: Elevation of ET Surface Matrix dialog box

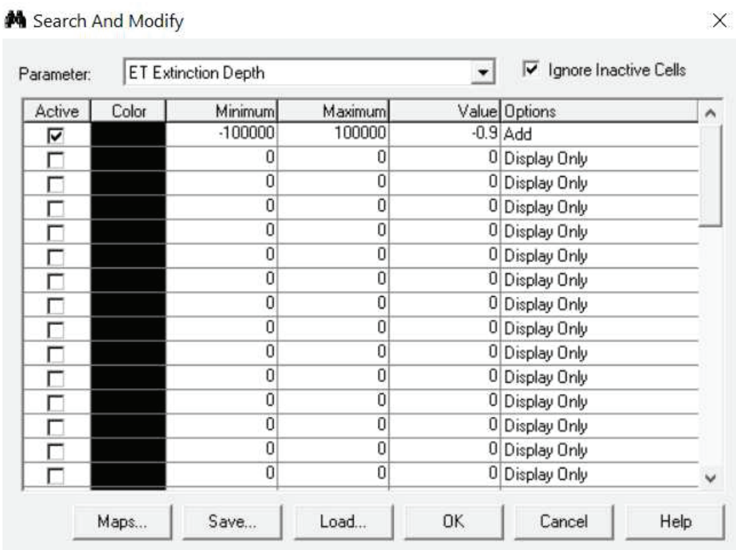


Fig.4.12: Search and Modify dialog box

4.2.3.2 MODFLOW | Flow Packages | General-Head Boundary

The General-Head Boundary (GHB) package is used to simulate head-dependent flow boundaries (Cauchy boundary conditions), where flow into or out of a GHB-cell from an external source is provided in proportion to the difference between the head in the cell and the head assigned to the external source. The input parameters are assumed to be constant during a given stress period and the input methods require different parameters.

The General Head Boundary conceptually is a fixed head far from the model where it is assumed as a fixed head with time. The purpose of using this boundary condition is to avoid unnecessarily extending the model domain outward to meet the element influencing the head in the model.

When using the Cell-by-cell or Polygon input methods, the parameters in Fig. 4.13 and 4.14 are to be assigned to model cells of a general-head boundary (see the dark green cells in Fig. 4.3).

General head conditions are specified by assigning a head and a conductance to a selected set of cells. If the water table elevation rises above the specified head, water flows out of the aquifer. If the water table elevation falls below the specified head, water flows into the aquifer. In both cases, the flow rate is proportional to the head difference and the constant of proportionality is the conductance.

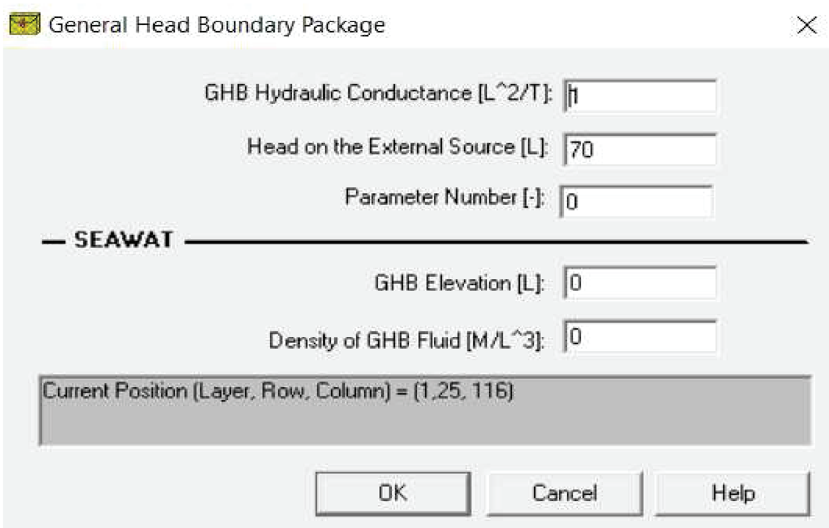


Fig.4.13: General-Head Boundary Parameters dialog box set for the high flow period (0107)

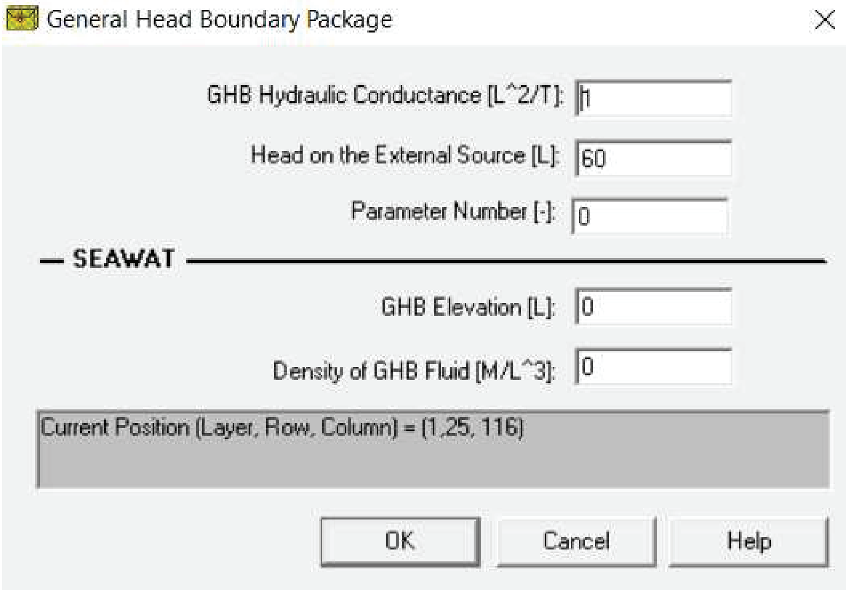


Fig.4.14: General-Head Boundary Parameters dialog box set for the low flow period (0607)

In this case study, as shown in the two Figures above, the Head on the External Source values set for the high flow period (January 2007) are higher than the values set for the low flow period (June 2007) considering the same cell (1,25,116).

It is also important to highlight that not considering these heads leads to a worse model calibration.

4.2.3.3 MODFLOW | Flow Package | Recharge

The Recharge package is designed to simulate distributed recharge to the groundwater system. Recharge is defined by assigning the following data to each vertical column of cells. The input parameters (Fig. 4.15) are assumed to be constant during a given stress period.

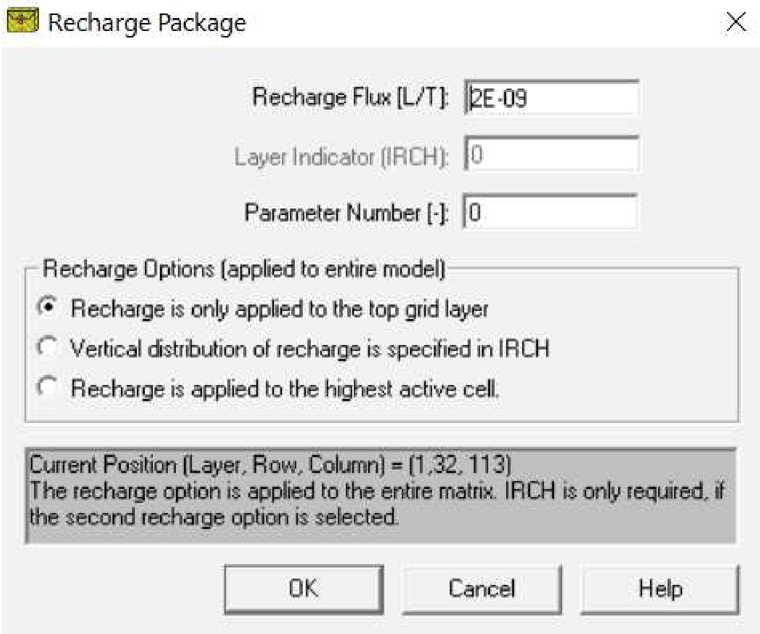


Fig.4.15: Recharge Package dialog box

In the simplest situation, the water table is located in the top layer of the model, the top layer is designated as unconfined and an array of Recharge Flux I_R is specified for that layer.

There are no differences between the high and low flow periods.

4.2.3.4 MODFLOW | Flow Package | River

The purpose of the River package is to simulate the effect of flow between groundwater and surface-water systems, such as rivers, lakes or reservoirs. Using the Data Editor, a river is defined by using the Cell-by-Cell or Polygon input methods to assign parameters to model cells or, as in this case study, by using the Polyline input method and assigning parameters to vertices of the polylines along the trace of the river. The input parameters are assumed to be constant during a given stress period.

When using the Polyline input method, it is needed to specify its properties in the River Parameters dialog box (Fig. 4.16 and 4.17). If the properties are assigned to one vertex only, the properties of all vertices of the polyline are assumed to be the same.

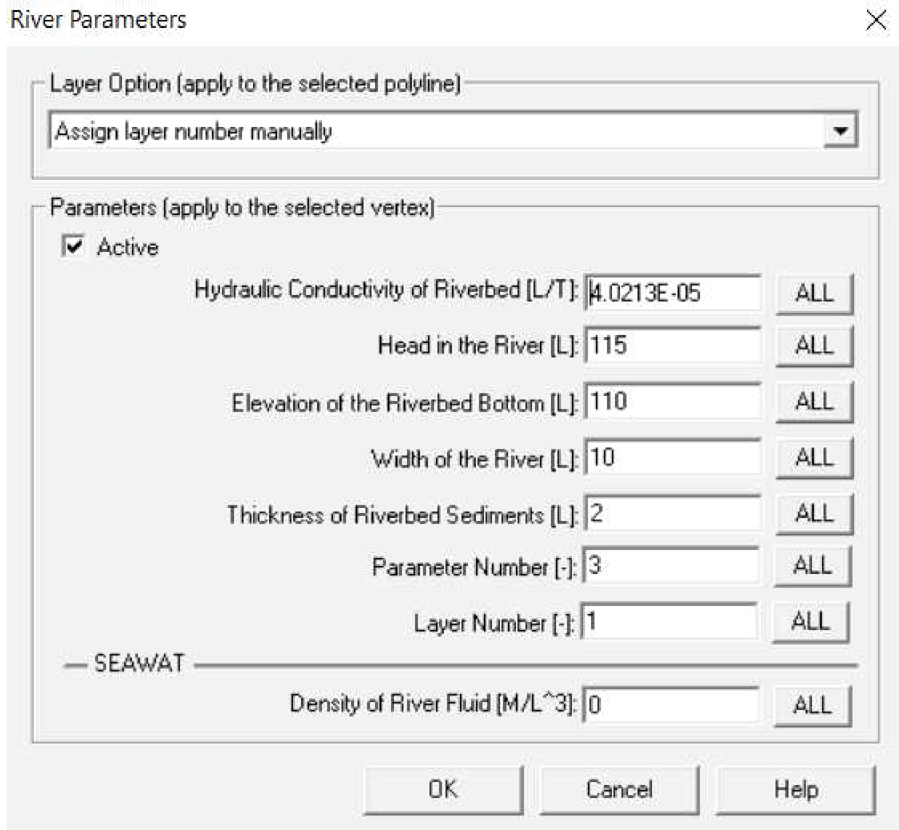


Fig.4.16: River Parameters dialog box (0107)

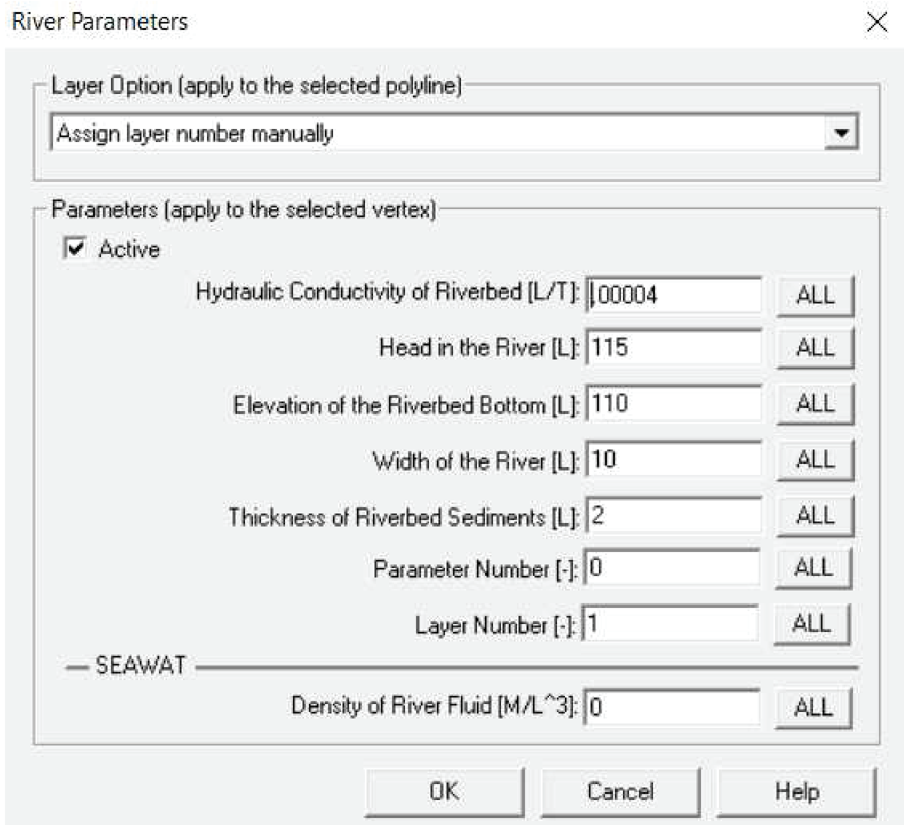


Fig.4.17: River Parameters dialog box (0607)

The settings of the dialog box are described below.

- Layer Option and Layer Number: Layer Option controls how the layer number of a river is determined. If Layer Option is "Assign layer number manually", the value of Layer Number defines the model layer number for all model cells downstream from a vertex until the next vertex redefines the layer number.
- Active: by checking this box is possible to activate a vertex. The properties of an active vertex will be used in the simulation. The properties of an inactive vertex are ignored.
- Hydraulic Conductivity of Riverbed (K_{riv}) [LT^{-1}], Head in the river (H_{riv}) [L], Elevation of the Riverbed bottom (B_{riv}) [L], Width of the river (W_{riv}) [L], and Thickness of the riverbed (M_{riv}) [L]: the value K_{riv} describes all of the head loss between the river and the aquifer. It depends on the material and characteristics of the riverbed itself and the immediate environment. Since the river package requires the input of H_{riv}, B_{riv}, and river hydraulic conductance (C_{riv}) to each cell of a river, the input values K_{riv}, H_{riv} and B_{riv} at active vertices are linearly interpolated or extrapolated to each cell along the trace of the polyline and the value C_{riv} is obtained by

$$C_{riv} = \frac{K_{riv} \cdot L \cdot W_{riv}}{M_{riv}}$$

  where L is the length of the river within a cell.

- Parameter Number [-]: Since C_{riv} is usually unknown, it must be estimated. Parameter Number is used to group cells, where the C_{riv} values are to be estimated. The value of Parameter Number is assigned to all model cells downstream from a vertex until the next vertex redefines the parameter number.
- Density of River Fluid [M/L^3]: This value represents the prescribed density of fluid entering the groundwater system from the river. This value is used by SEAWAT only if it is running in a uncoupled mode.

- The ALL button: clicking the ALL button of a property it is possible to copy the property value to all other active vertices.

As shown in the two Figures above, considering the same vertex of the polyline, the only difference between high and low flow period is the parameter number.

4.2.3.5 MODFLOW | Flow Package | Well

An injection or a pumping well is defined by using the Cell-by-Cell or Polygon input methods of the Data Editor to assign the following parameters to model cells (see red cells in Fig. 4.3). The input parameters are assumed to be constant during a given stress period.

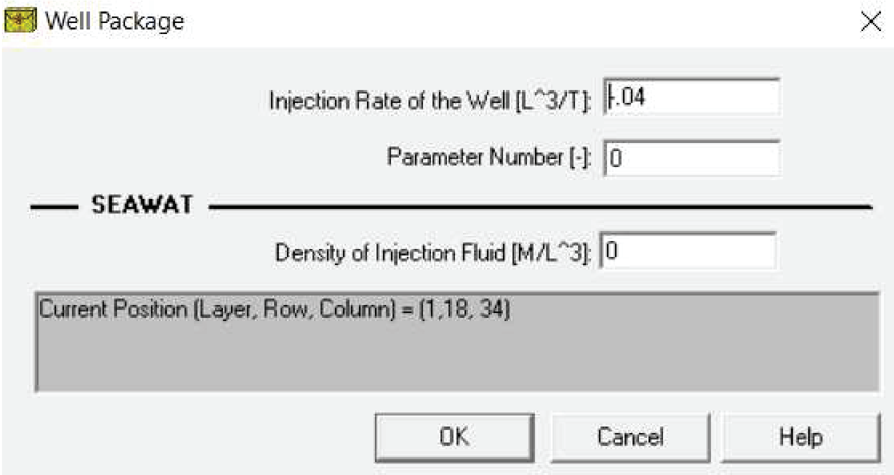


Fig.4.18: Well Parameters dialog box

- Injection rate of the well (Q_w) [L^3T^{-1}]: negative values are used to indicate pumping wells, while positive cell values indicate injection wells. The injection or pumping rate of a well is independent of both the cell area and the hydraulic head in the cell. MODFLOW assumes that a well penetrates the full thickness of the cell.
- Parameter Number [-]: Parameter Number is used to group cells, where the Q_w values are to be estimated by the parameter estimation programs.

- Density of Injection Fluid [M/L^3]: This value is used by SEAWAT only if it is running in a uncoupled mode.

Concerning this parameter, different wells are characterized by different injection rate, but there are no differences between high and low flow period.

4.2.3.6 MODFLOW | Head Observation

Selecting Head Observations from the MODFLOW menu, it was possible to specify the locations of the head observation boreholes and their associated observed (measurement) data in the Head Observations dialog box (see paragraph 2.3.3.3).

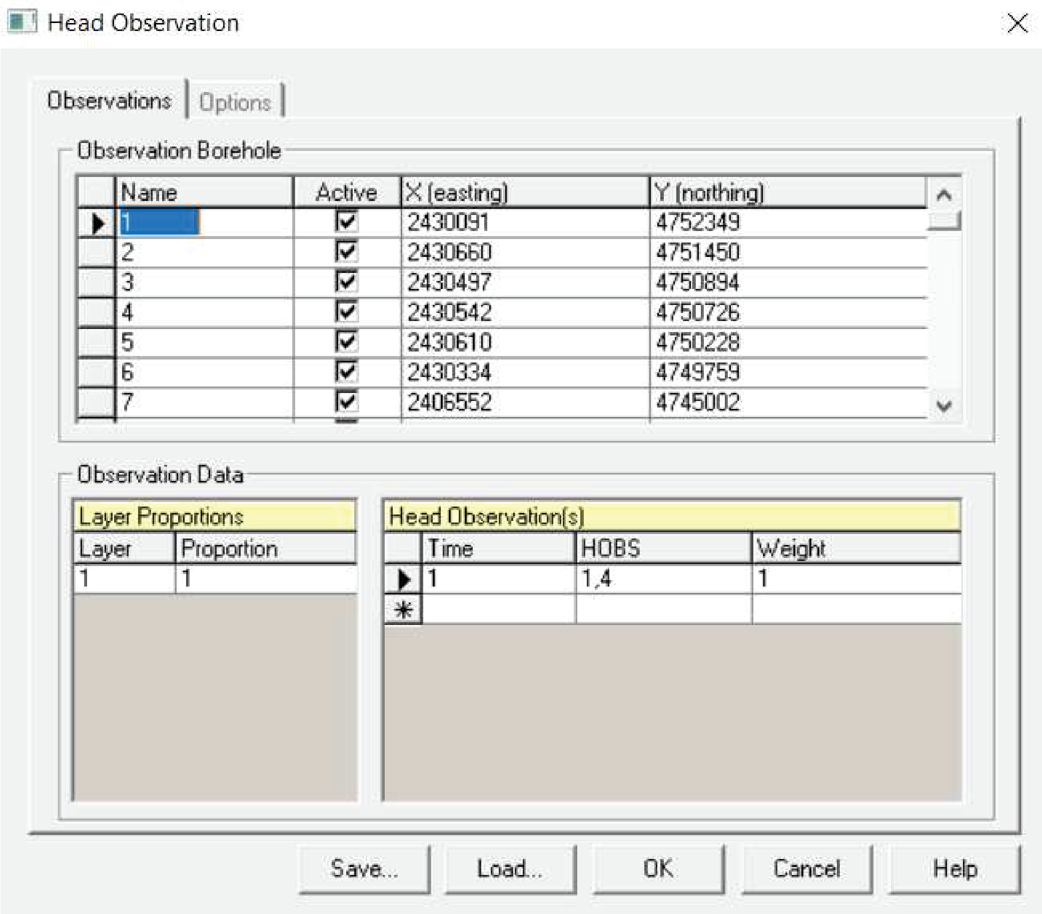


Fig.4.19: Head Observation dialog box (0107)

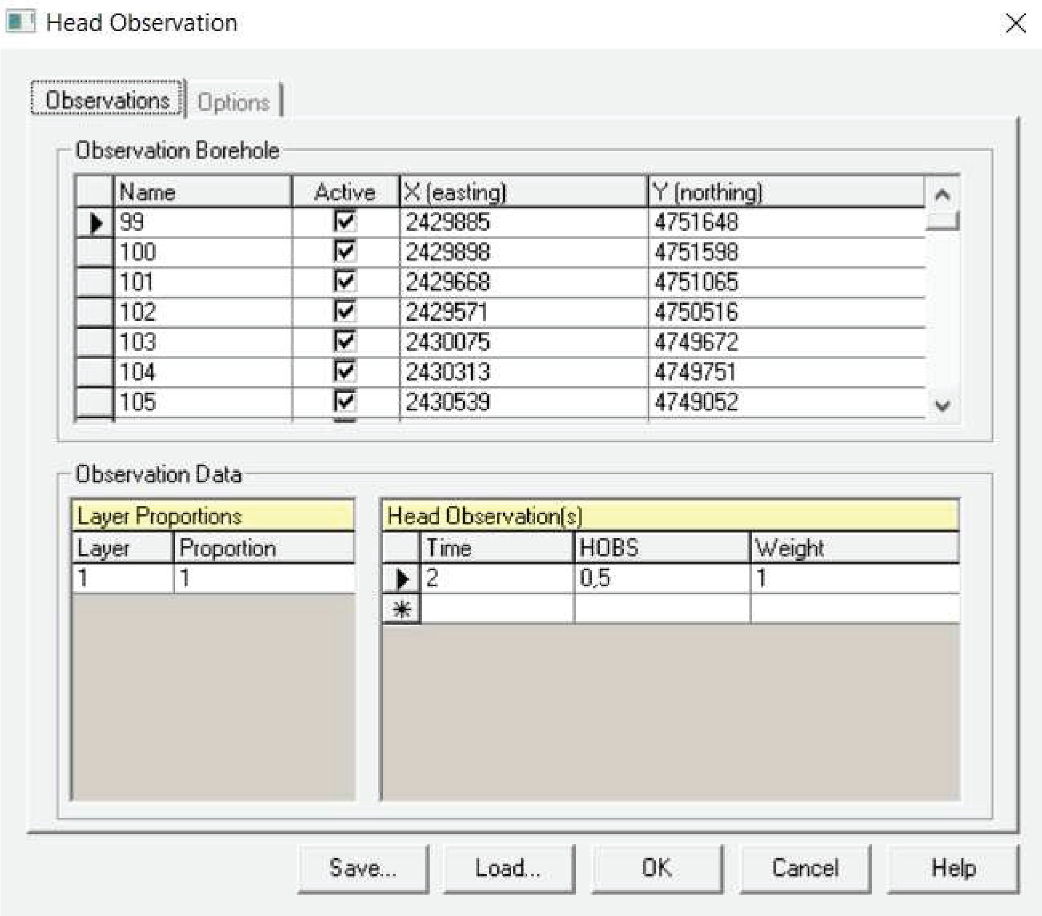


Fig.4.20: Head Observation dialog box (0607)

Since two measurement campaigns have been carried out in different season, different values for high (Fig. 4.19) and low flow period (Fig. 4.20) have been found.

4.3 Results and discussion

After entering the evapotranspiration parameters in the Evapotranspiration Package, the model was run for each scenario and the results have been compared.

First, the calibration of the models has been checked by means of the Head Scatter Diagrams. As it is possible to see in the following Figures, the editing of the Evapotranspiration Package both for high and low flow period does not affect the calibration of the model and the variance is almost the same.

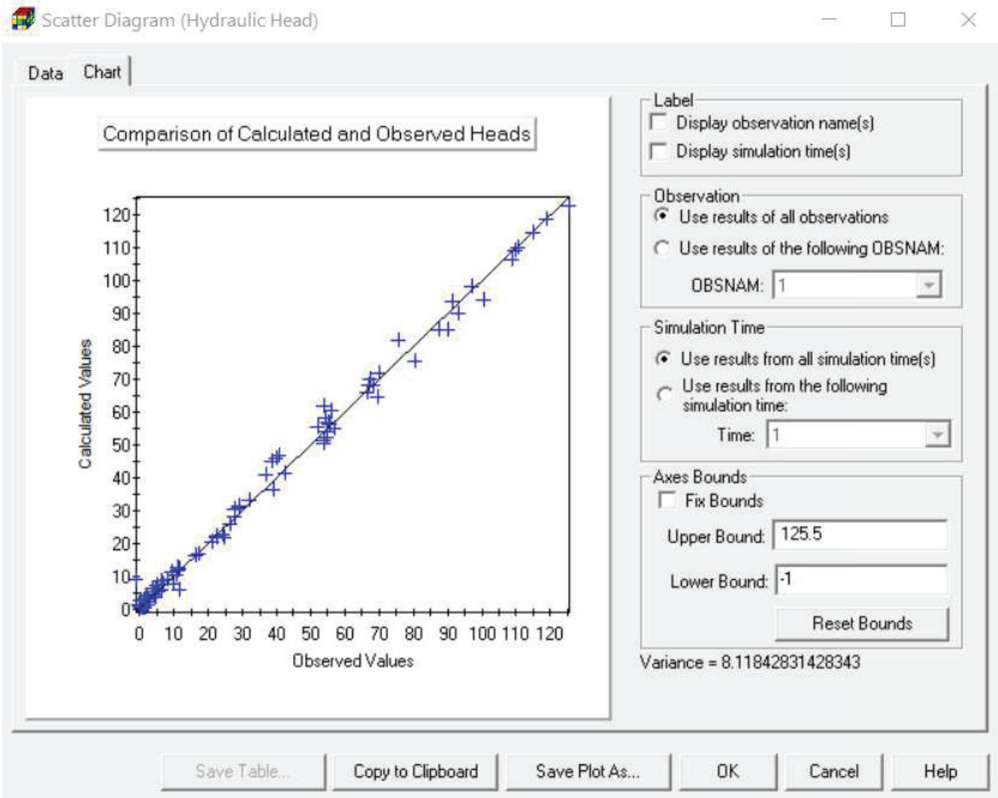


Fig.4.21: Head Scatter Diagram dialog box for high flow period (0107) without ET

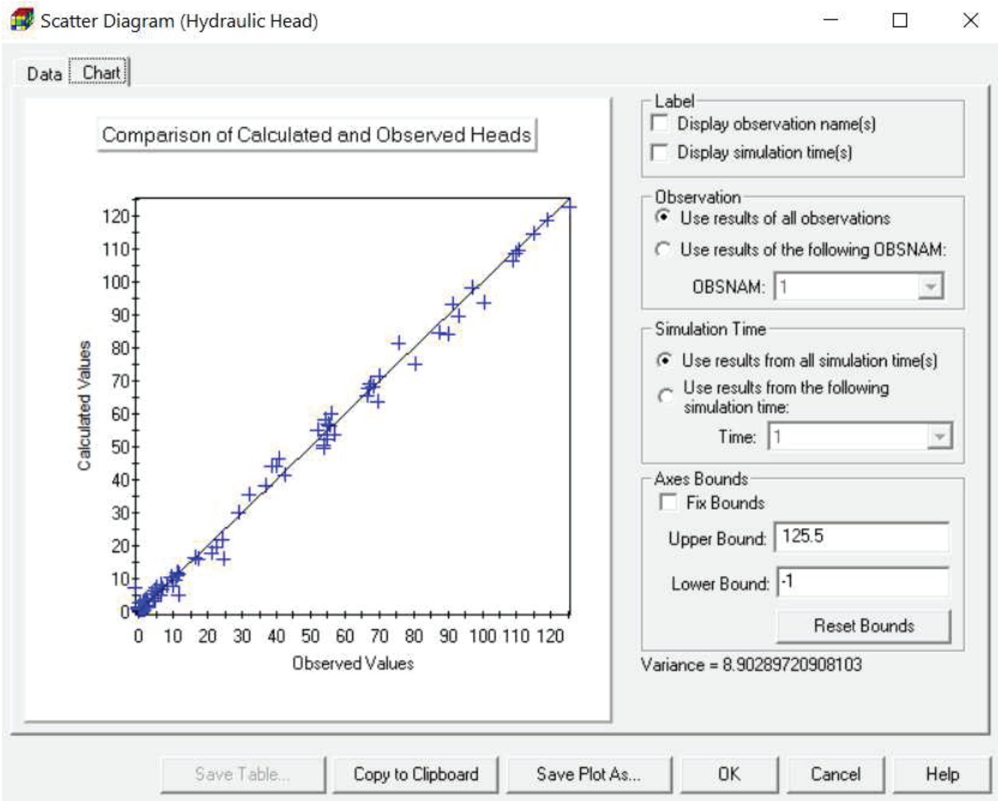


Fig.4.22: Head Scatter Diagram dialog box for high flow period (0107) with highest R_{ETM} value

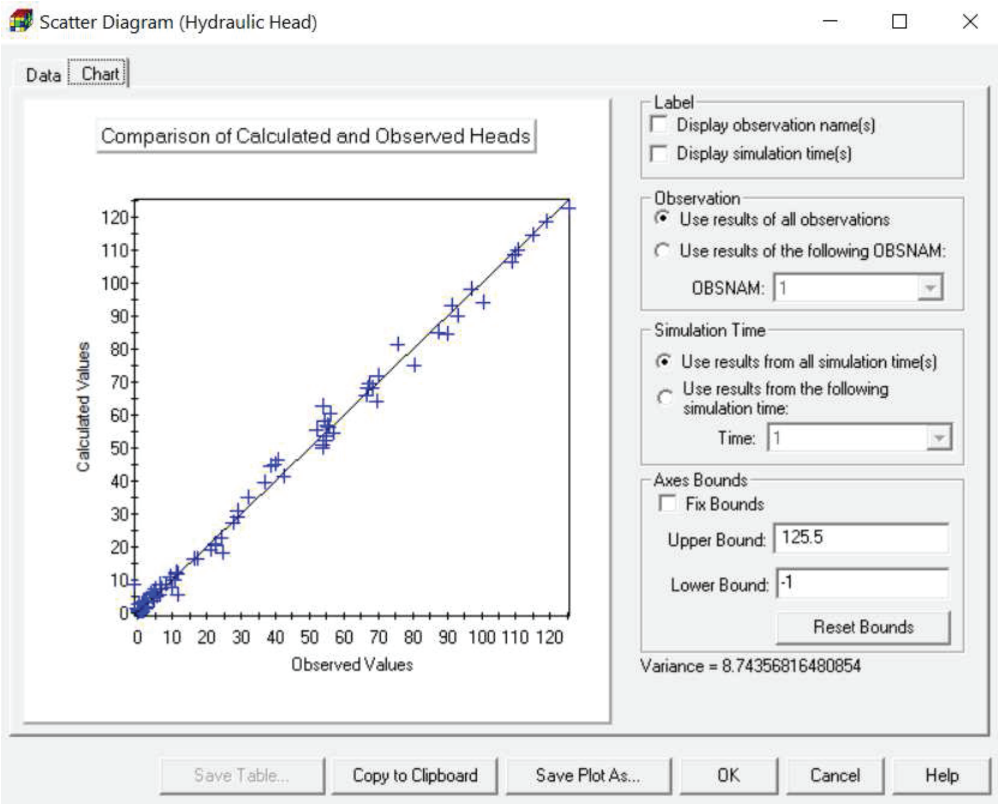


Fig.4.23: Head Scatter Diagram dialog box for high flow period (0107) with lowest R_{ETM} value

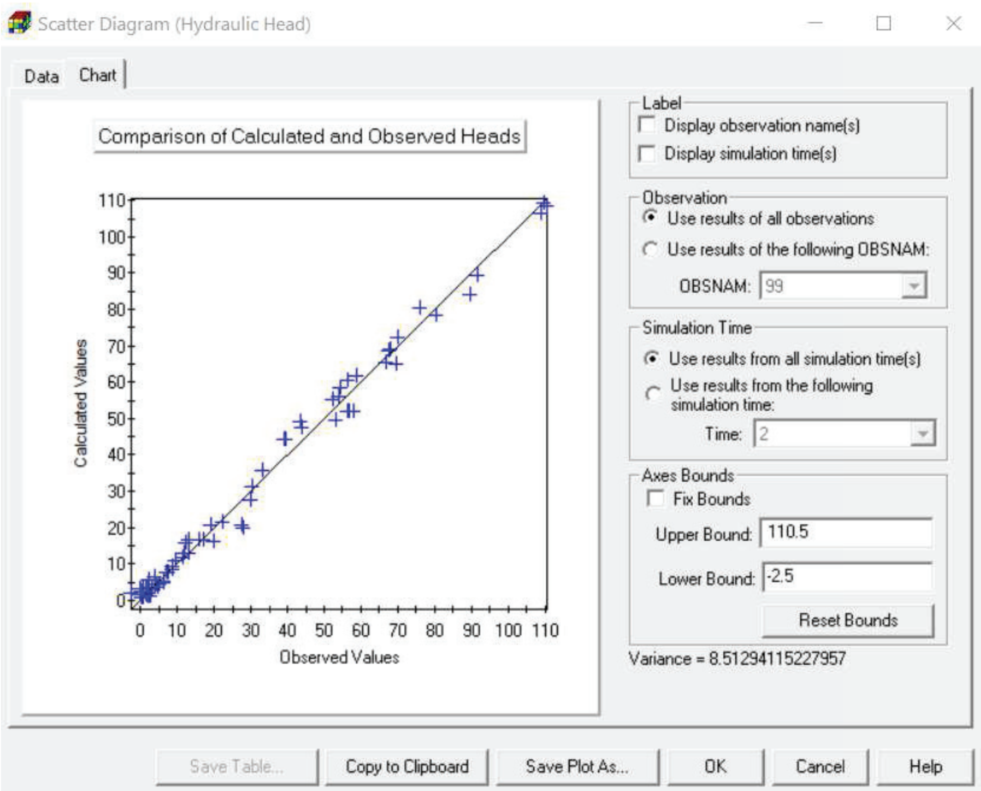


Fig.4.24: Head Scatter Diagram dialog box for low flow period (0607) without ET

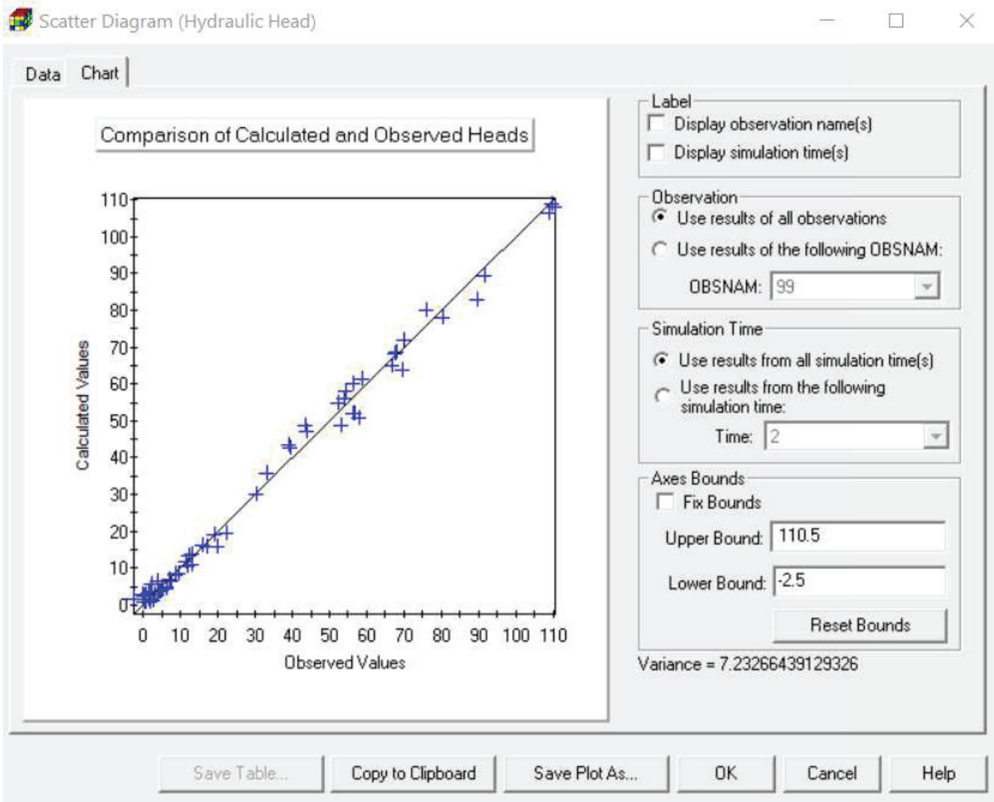


Fig.4.25: Head Scatter Diagram dialog box for low flow period (0607) with highest R_{ETM} value

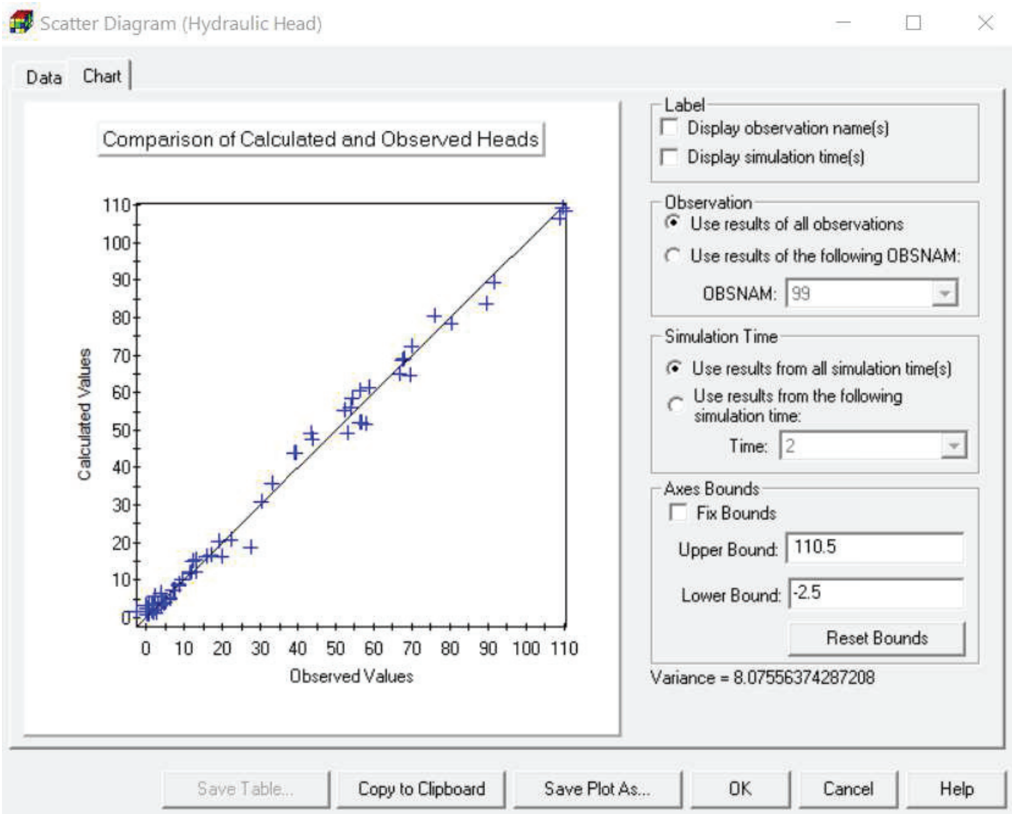


Fig.4.26: Head Scatter Diagram dialog box for low flow period (0607) with lowest R_{ETM} value

From the Hydraulic Heads point of view almost nothing has changed and the models, with or without considering the evapotranspiration, result to be well calibrated.

It was also possible to visualize the plotted Hydraulic Head by selecting the menu item Tools | 2D Visualization. This tool will load the selected model result and automatically displays the contour levels ranging from the minimum to maximum values. In Figures 4.27 and 4.28, all the scenarios are shown for both the campaigns.

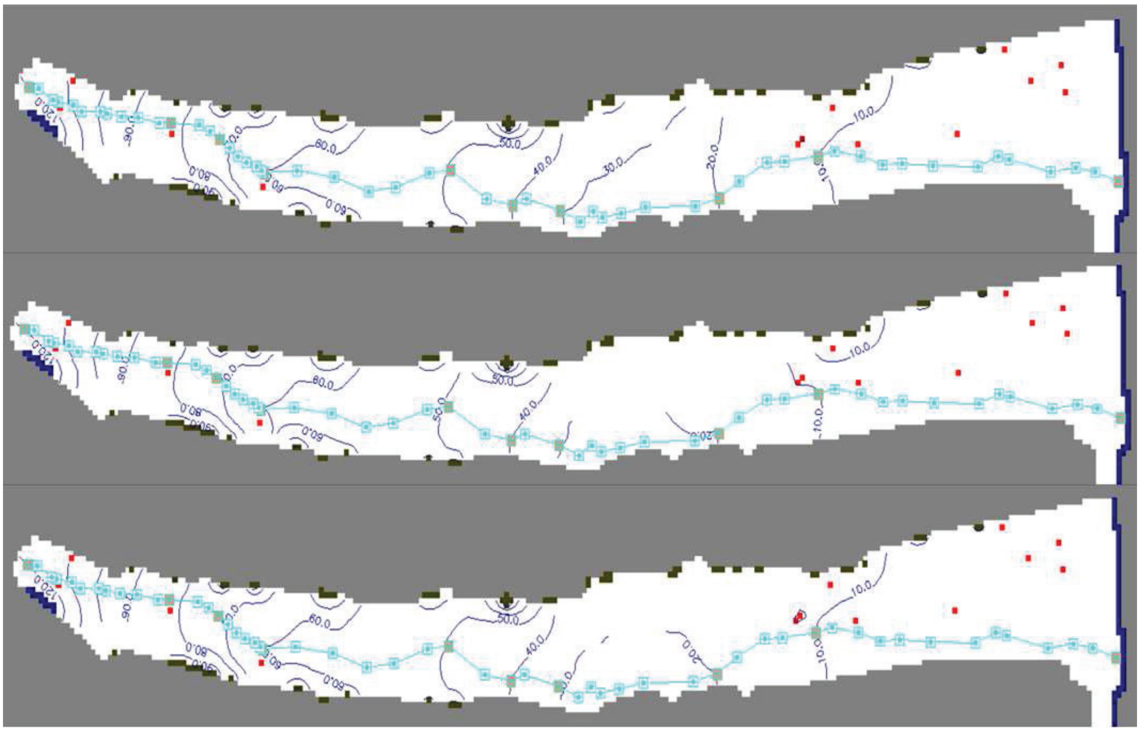


Fig. 4.27: Hydraulic Heads for the high flow period (0107) with no ET, with highest R_{ETM} and lowest R_{ETM} (from up to down)

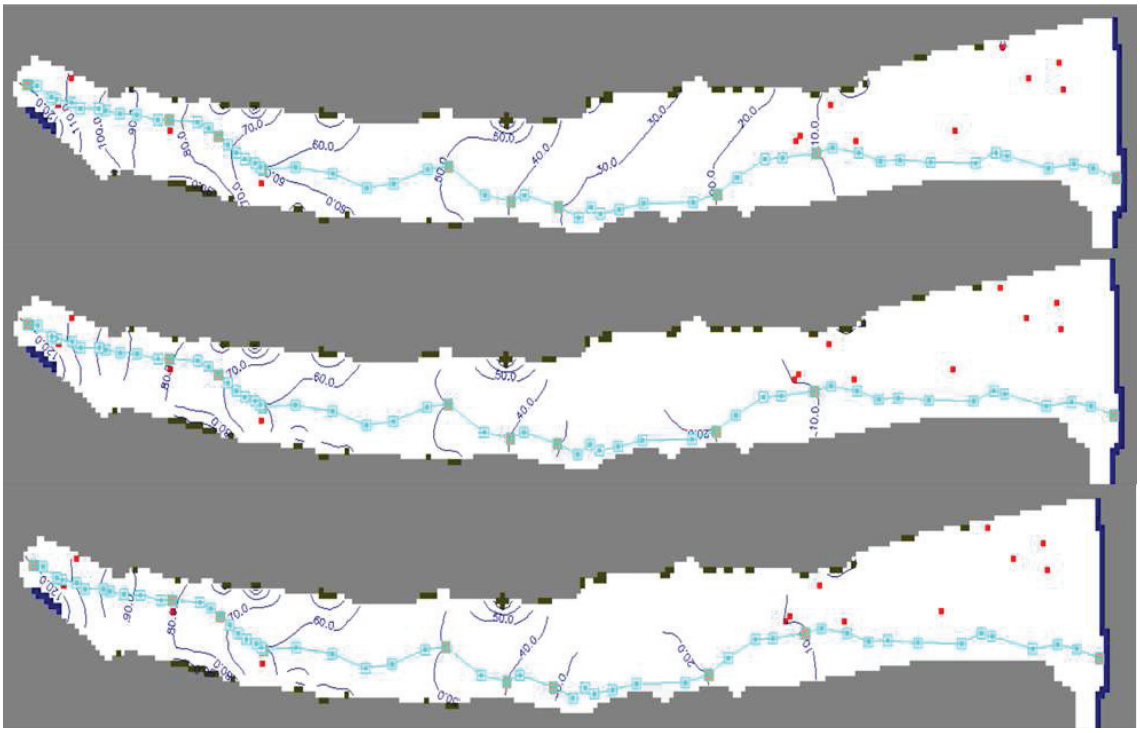


Fig. 4.28: Hydraulic Heads for the low flow period (0607) with no ET, with highest R_{ETM} and with lowest R_{ETM} (from up to down)

So, looking at the piezometry, as it is already highlighted, the models don't seem to be strongly affected by the evaporation from groundwater.

However, the analysis of the Water Budget has shown that the evaporation process strongly affects the hydrological cycle.
Water availability is an important concern nowadays and, in order to ensure sustainable water supplies, an understanding of the hydrologic cycle is required. A water budget is an accounting of the rates of water movement and the change in water storage in all or parts of the atmosphere, land surface and subsurface and represents a tool that water users and managers use to quantify the hydrologic cycle.
As shown in Figures 4.29, 4.30, 4.31, 4.32, 4.33 and 4.34, the Water Budget of each scenario for each one of the two measurement campaigns has been calculated by the model.

To facilitate such calculations, MODFLOW saved the computed flow terms for individual cells in the file BUDGET.DAT. These individual cell flows are referred to as cell-by-cell flow terms.

FLOW TERM	IN	OUT	IN-OUT
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	2.3472123E+00	2.0905931E-01	2.1381531E+00
WELLS	0.0000000E+00	6.3999999E-01	-6.3999999E-01
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	1.4718000E-01	0.0000000E+00	1.4717999E-01
ET	0.0000000E+00	0.0000000E+00	0.0000000E+00
RIVER LEAKAGE	7.3257275E-01	5.4598322E+00	-4.7272596E+00
HEAD DEP BOUNDS	3.1337912E+00	5.3121809E-02	3.0806694E+00
STREAM LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
INTERBED STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
RESERV. LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
SUM	6.3607564E+00	6.3620133E+00	-1.2569427E-03
DISCREPANCY [%]	-0.02		

Fig.4.29: Water Budget for high flow period (0107) without ET

FLOW TERM	IN	OUT	IN-OUT
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	2.1125005E+00	1.7791642E-01	1.9345841E+00
WELLS	0.0000000E+00	5.3499999E-01	-5.3499997E-01
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	1.3126000E-01	0.0000000E+00	1.3125999E-01
ET	0.0000000E+00	1.6329864E+00	-1.6329864E+00
RIVER LEAKAGE	1.2247465E+00	3.5258532E+00	-2.3011067E+00
HEAD DEP BOUNDS	2.4037446E+00	5.5453909E-04	2.4031901E+00
STREAM LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
INTERBED STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
RESERV. LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
SUM	5.8722515E+00	5.8723106E+00	-5.9127808E-05
DISCREPANCY [%]	0.00		

Fig.4.30: Water Budget for high flow period (0107) with highest R_{ETM} value

FLOW TERM	IN	OUT	IN-OUT
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	2.0921521E+00	1.8973393E-01	1.9024181E+00
WELLS	0.0000000E+00	5.3499999E-01	-5.3499997E-01
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	1.3516000E-01	0.0000000E+00	1.3516000E-01
ET	0.0000000E+00	5.9410850E-01	-5.9410852E-01
RIVER LEAKAGE	8.3454560E-01	4.0615604E+00	-3.2270148E+00
HEAD DEP BOUNDS	2.3199478E+00	1.5151652E-03	2.3184326E+00
STREAM LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
INTERBED STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
RESERV. LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
SUM	5.3818054E+00	5.3819180E+00	-1.1253357E-04
DISCREPANCY [%]	0.00		

Fig.4.31: Water Budget for high flow period (0107) with lowest R_{ETM} value

FLOW TERM	IN	OUT	IN-OUT
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	2.1048902E+00	1.9455150E-01	1.9103386E+00
WELLS	0.0000000E+00	5.7499999E-01	-5.7499999E-01
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	1.3688000E-01	0.0000000E+00	1.3688000E-01
ET	0.0000000E+00	0.0000000E+00	0.0000000E+00
RIVER LEAKAGE	7.7838618E-01	4.0093962E+00	-3.2310100E+00
HEAD DEP BOUNDS	1.7730004E+00	1.4259785E-02	1.7587407E+00
STREAM LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
INTERBED STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
RESERV. LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
SUM	4.7931566E+00	4.7932076E+00	-5.1021576E-05
DISCREPANCY [%]	0.00		

Fig.4.32: Water Budget for low flow period (0607) without ET

FLOW TERM	IN	OUT	IN-OUT
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	2.1289668E+00	1.7668062E-01	1.9522861E+00
WELLS	0.0000000E+00	5.3499999E-01	-5.3499997E-01
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	1.2868000E-01	0.0000000E+00	1.2867999E-01
ET	0.0000000E+00	1.5550156E+00	-1.5550156E+00
RIVER LEAKAGE	1.3759242E+00	3.2197798E+00	-1.8438556E+00
HEAD DEP BOUNDS	1.8606087E+00	7.7602216E-03	1.8528485E+00
STREAM LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
INTERBED STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
RESERV. LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
SUM	5.4941797E+00	5.4942365E+00	-5.6743622E-05
DISCREPANCY [%]	0.00		

Fig.4.33: Water Budget for low flow period (0607) with highest R_{ETM} value

FLOW TERM	IN	OUT	IN-OUT
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	2.1153893E+00	1.8736725E-01	1.9280220E+00
WELLS	0.0000000E+00	5.7499999E-01	-5.7499999E-01
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	1.3214000E-01	0.0000000E+00	1.3214000E-01
ET	0.0000000E+00	5.6379020E-01	-5.6379020E-01
RIVER LEAKAGE	9.7847552E-01	3.6939575E+00	-2.7154820E+00
HEAD DEP BOUNDS	1.8056071E+00	1.1612420E-02	1.7939947E+00
STREAM LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
INTERBED STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
RESERV. LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
SUM	5.0316119E+00	5.0317273E+00	-1.1539459E-04
DISCREPANCY [%]	0.00		

Fig.4.34: Water Budget for low flow period (0607) with lowest R_{ETM} value

The unit of the flows is $m^3s^{-1}[L^3T^{-1}]$. Flows are considered IN, if they are entering the model and OUT, if they are escaping it.
The percent discrepancy is simply calculated by

$$\frac{100 \cdot (IN - OUT)}{\frac{(IN + OUT)}{2}}.$$

In order to underline the evapotranspiration contribution to the budget, the percentage of OUT flows due to ET with respect to the total OUT flows has been calculated (Tab. 4.1).

	ET out (m^3/s)	TOT out (m^3/s)	Percentage %
WB 0107 max ET	1.6329864	5.8723106	27.81
WB 0107 min ET	0.5941085	5.3819180	11.04
WB 0607 max ET	1.5550156	5.4942365	28.30
WB 0607 min ET	0.5637902	5.0317273	11.20

Tab. 4.1: percentage of incidence of ET

So, as it is possible to see in the Table, evaporation contribution represents a large part of the total OUT flow escaping from the model reaching percentages of incidence of almost 30% for the scenarios with the highest R_{ETM}.

It is also interesting to show, thanks to the menu item Tools | 2D Visualization, the Evapotranspiration cell by cell in order to check the zones of the model grid characterized by the larger evapotranspiration outflow (light green cells in Fig.4.35 and 4.36).

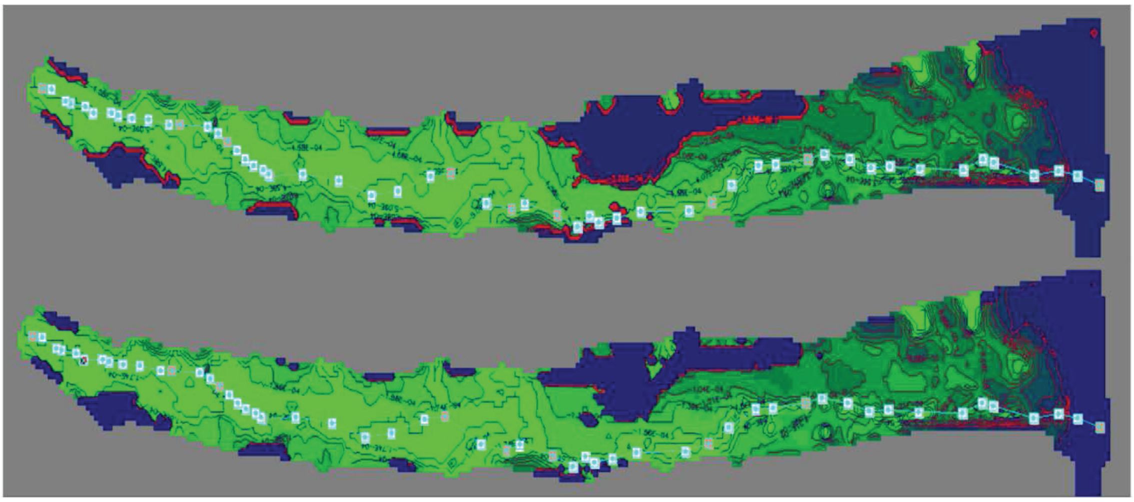


Fig.4.35: Evapotranspiration outflow cell by cell for the high flow period (0107) with highest R_{ETM} and lowest R_{ETM} (from up to down)

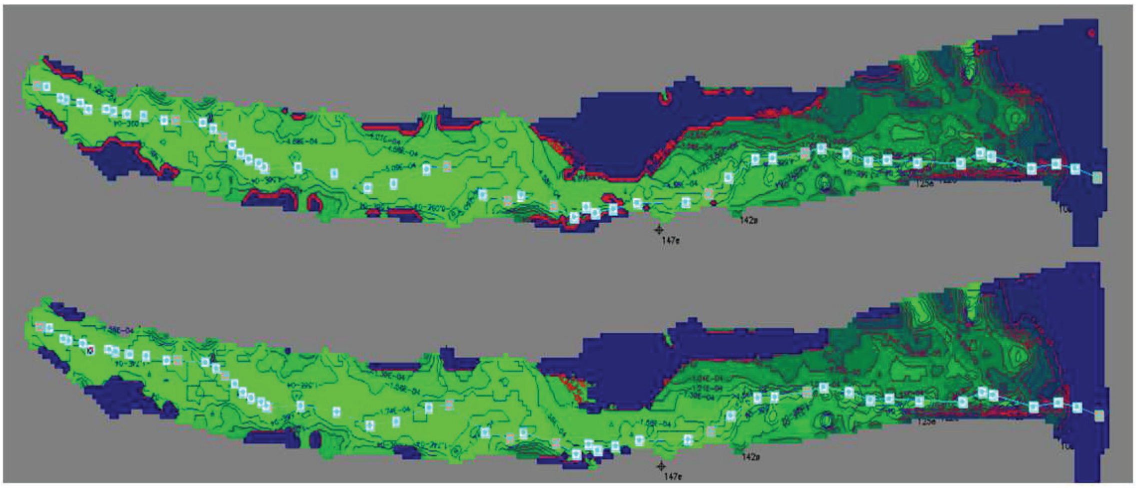


Fig.4.36: Evapotranspiration outflow cell by cell for the low flow period (0607) with highest R_{ETM} and lowest R_{ETM} (from up to down)

According to this study, the evaporation parameters estimated by calibrating the model of the tank in lab, once carried to basin scale, can have a significant impact and should not be overlooked, even if the basin investigated is characterized by granular and coarse soils with low capillary rise such as Tronto basin. The underestimation of groundwater evapotranspiration, in fact, often results in the overestimation of the net recharge and water availability.

Finally, since some differences concerning the river leakage emerged looking at the water budget with and without evapotranspiration, this parameter has been visualized cell by cell by means of the menu item Tools | 2D Visualization for every scenarios and for both the campaigns (Fig.4.38 and 4.39).

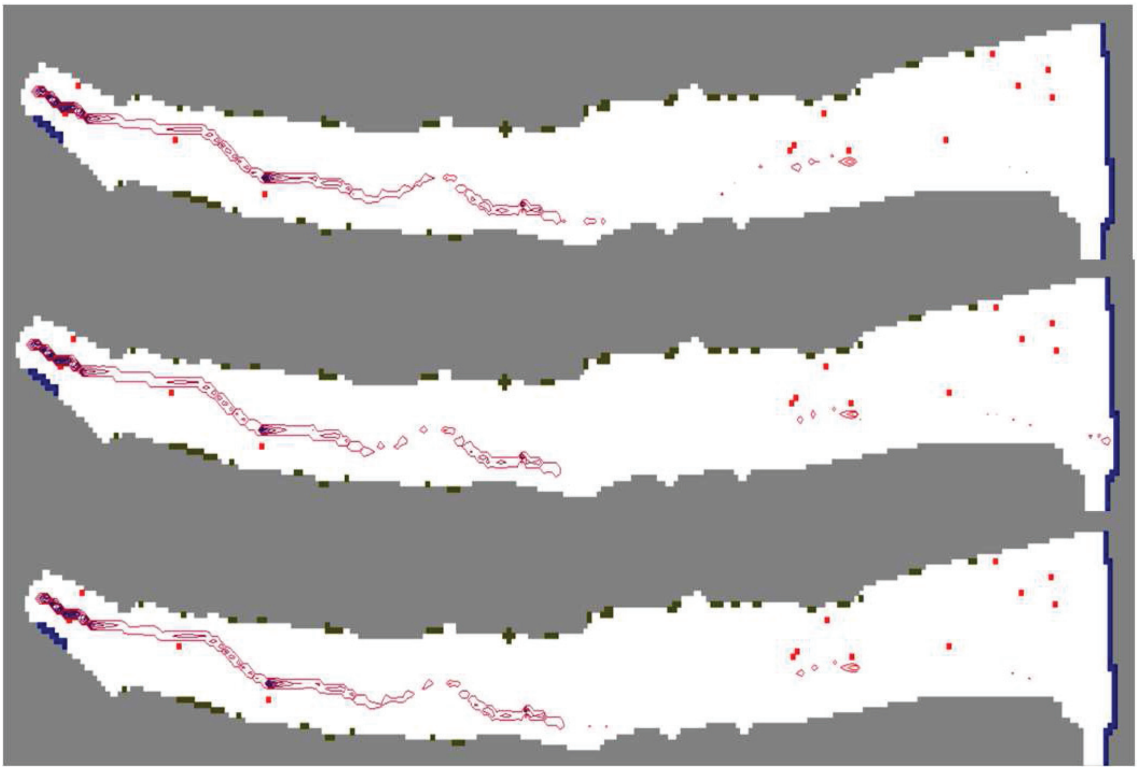


Fig.4.38: River leakage cell by cell for the high flow period (0107) with no ET, with highest R_{ETM} and lowest R_{ETM} (from up to down)

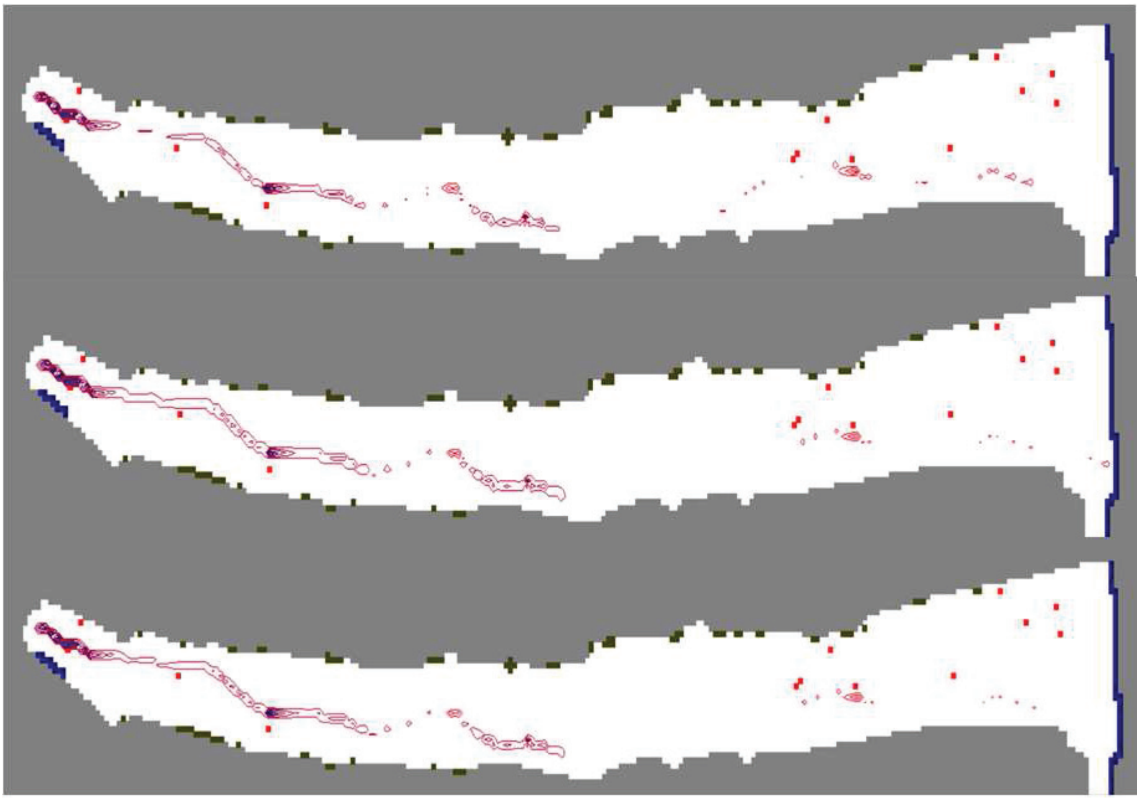


Fig.4.39: River leakage cell by cell for the low flow period (0607) with no ET, with highest R_{ETM} and lowest R_{ETM} (from up to down)

This parameter describes the exchange relation between river and groundwater. This relation and the associated river discharges can be measured and then compared with the calculated ones, in order to further validate the conceptual model.

5 Conclusions

The results of this thesis contribute to a better understanding of the subsurface flow dynamics, focusing on the evapotranspiration process that plays a key role in the land-atmosphere system. In particular the evaporation from shallow groundwater (E_g), which knowledge to groundwater management is fundamental, has been deeply analyzed. In order to do that and to simulate the natural processes, a tank has been set up in the hydrogeology laboratory in the SIMAU Department of "Università Politecnica delle Marche". The sediments that have been poured into the tank resulted to be coarse sandy sediments from grain size distribution measurements. A constant head has been applied to the tank by means of an external reservoir. Then, throughout the use of different sensors placed inside the tank, hydrometric height, temperature and TDS concentration have been monitored over the 145 days time period during which the evaporation occurred.

Thanks to the graphical user interface Processing Modflow, which incorporates MODFLOW and MT3DMS/SEAWAT codes, the tank has been modelled. By calibrating the numerical model via a trial and error procedure, the calculated values were fitted the measured ones. In this way, the evaporation parameters have been evaluated and estimated with high precision degree. Together with the Maximum ET Rates (R_{ETM}), the parameter that has been found to be critical is the Extinction Depth (d). In fact, many studies claimed that for coarse sandy soils, the latter should be around 60 cm (between 50 and 70 cm), while a value of 90 cm has been retrieved in this case study. This result means that the evaporation from shallow groundwater can't be considered negligible under 60 cm from ground surface, while neglecting such effect leads to underestimate the magnitude of the evaporation process, which in turn is a major component at the watershed scale. The sensitivity analysis has shown the dependency of the processes (both evaporation and evapoconcentration) on different values of extinction depth, mass loading rate, longitudinal dispersion and effective porosity. Which in turn affect the model calibration performance too.

Finally, the results obtained with the model have been carried from laboratory to basin scale, integrating the 2007 case study relative to the Tronto basin. The highest and lowest value of Maximum ET Rate (R_{ETM}), together with the value of the Extinction Depth (d) have been entered in the model for both the measurement campaigns. From the Hydraulic Heads point of view, the Tronto model result to be slightly affected by the evaporation process and the variance retrieved from the Head Scatter Diagrams was almost the same. However, from a groundwater budget point of view, the model resulted to be strongly affected. Considering the evaporation, in fact, a substantial change in the hydrological balance of the basin occurred. The water at the outlet due to evaporation from the groundwater was more than 10% of the total output considering the lowest value of R_{ETM} and almost 30% considering the highest value.

Therefore, according to this case study, evaporation plays a very important role in estimating the water resources of a basin and should not be considered negligible even if the basin under investigation is characterized by granular and coarse soils with low capillary rise such as the Tronto basin. This highlights also that to correctly incorporate evapotranspiration processes in subsurface groundwater flow models, independent observations datasets other than piezometric heads must be employed to further validate the conceptual model at the base of the numerical model employed. Examples of independent observations datasets could be: (i) exchange fluxes between surface water bodies (in this case the Tronto river) and aquifer, or (ii) environmental tracers ($\delta^{18}O$, $\delta^{2}H$ and Chloride) that could provide indication of evaporative processes in shallow groundwater. Although these aspects are beyond the aims and scopes of the present thesis, they could be explored in future studies.

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