Document public

Guidelines for MARTHE v7.8 computer code for hydro-systems modelling

(English version)

BRGM/RP-69660-FR
September 2020

Dominique Thiéry, Géraldine Picot-Colbeaux

Géosciences pour une Terre durable
brgm

Document public

Guidelines for MARTHE v7.8 computer code for hydro-systems modelling
(English version)

BRGM/RP-69660-FR
September 2020

Dominique Thiéry, Géraldine Picot-Colbeaux
With the collaboration of :
Quentin Guillemoto

(English translation by H.M. Kluijver and A. Sbai)

Vérificateur :	**Approbateur :**
Nom : A. Sbai	Nom : P. Audigane
Fonction : Expert en modélisation hydrogéologique	Fonction Responsable d'Unité DEPA/GDR :
Date : 07/09/2020	Date : 21/09/2020
Signature : 	Signature : 

Le système de management de la qualité et de l'environnement est certifié par AFNOR selon les normes ISO 9001 et ISO 14001.
Contact : qualite@brgm.fr

Géosciences pour une Terre durable
brgm

Keywords: MARTHE computer program, Hydrosystems modelling, Groundwater modelling, Tutorials, Pre-processor software, User's guide, WinMarthe, Managed Aquifer Recharge (MAR), Salt intrusion, Unsaturated flow, Unsaturated zone, Vadose zone, Mass transport

En bibliographie, ce rapport sera cité de la façon suivante :
(In bibliographic references, the report should be cited as follows)

Thiéry D. and Picot-Colbeaux, G. (2020) – Guidelines for MARTHE v7.8 computer code for hydro-systems modelling (English version). Report BRGM/RP-69660-FR, 246 p., 177 fig.

(English translation by H.M. Kluijver and A. Sbai)

Thanks are due to the JPI-EVIBAN and JPI-SMART-CONTROL projects.

Abstract

The finite-difference based MARTHE software (French acronym for: ***M**odélisation d'**A**quifères par maillage **R**ectangulaire en régime **T**ransitoire pour la simulation **H**ydrodynamique des **E**coulements*) developed by BRGM enables to perform three-dimensional simulations of groundwater flow, mass and energy transport in porous media.

It can model hydrosystems by integrating groundwater flow, hydro-climatic budgets and surface-water flow. The underlying schemes can be simple or complex (unsaturated flow, multiphase flow, density-dependent fluid flow, consideration of vegetation, aquifer-river interactions, etc.). The implementation of the different functionalities is described by Thiéry in related reports and publications.

The software uses a finite-difference numerical scheme using irregular parallelepipedal or rectangular stencils. This can represent complex multi-layer aquifer systems, with pinchouts and the occurrence of free surfaces in any layer. MARTHE addresses modelling of regional multi-layer systems covering several thousand square kilometres, as well as local scale modelling of porous media systems down to few cubic centimetres, with millimetre-size cells.

The object of this tutorial report is to present, explore and highlight most of the features relevant to MARTHE version 7.8. These are applied to several examples of increasing difficulty, but for relatively simple geometries. The aim is to provide the user with a first grasp on how to use the software package. This is a pre-requisite prior to being introduced to more advanced features through specific training courses. Detailed explanations of the functionalities, and the numerical implementation, of the MARTHE computer code are not the purpose of the present manual; this is documented in specific reports in the related list of references.

This tutorial is partly based on that of MARTHE version 7.8: Report BRGM/RP-69542-FR (Thiéry, 2020b, *in french*).

Additionally, the report "Tutorial for the WinMarthe v4.0" pre-processor, BRGM/RP-54652-EN (Thiéry 2007) (or the report BRGM/RP-54652-FR, Thiéry, 2006 *in French*) describes the WinMarthe preprocessor in more detail.

Recent information on BRGM's MARTHE software is available on the dedicated website: http://marthe.brgm.fr/

Sommaire

List of figures

List of tables

List of appendices (“Annexes”)

1 Introduction

The MARTHE software (***M**odélisation d'**A**quifères par maillage **R**ectangulaire en régime **T**ransitoire pour la simulation **H**ydrodynamique des **E**coulements*) simulates three-dimensional groundwater flow, mass and heat transport in porous media by a finite-difference approach. The schemes can be simple or complex (unsaturated flow, multiphase flow, density-dependent fluid flow, consideration of vegetation, aquifer-river interactions, heat transfer, etc.).

The implementation of the different functionalities is described by Thiéry (1990, 1993, 2006, 2007, 2009, 2010a, b and c, 2015a, 2015b, 2015c, 2015d, 2016, 2020a, 2020b, 2020c). This schematization in finite difference involves cells organized in stacked layers, each layer being formed of cells organized in rows and columns (as in a spreadsheet). The layer management allows modelling of complex geological systems Figure 1): layers can disappear locally creating short-circuits, deep layers can be exposed, etc.

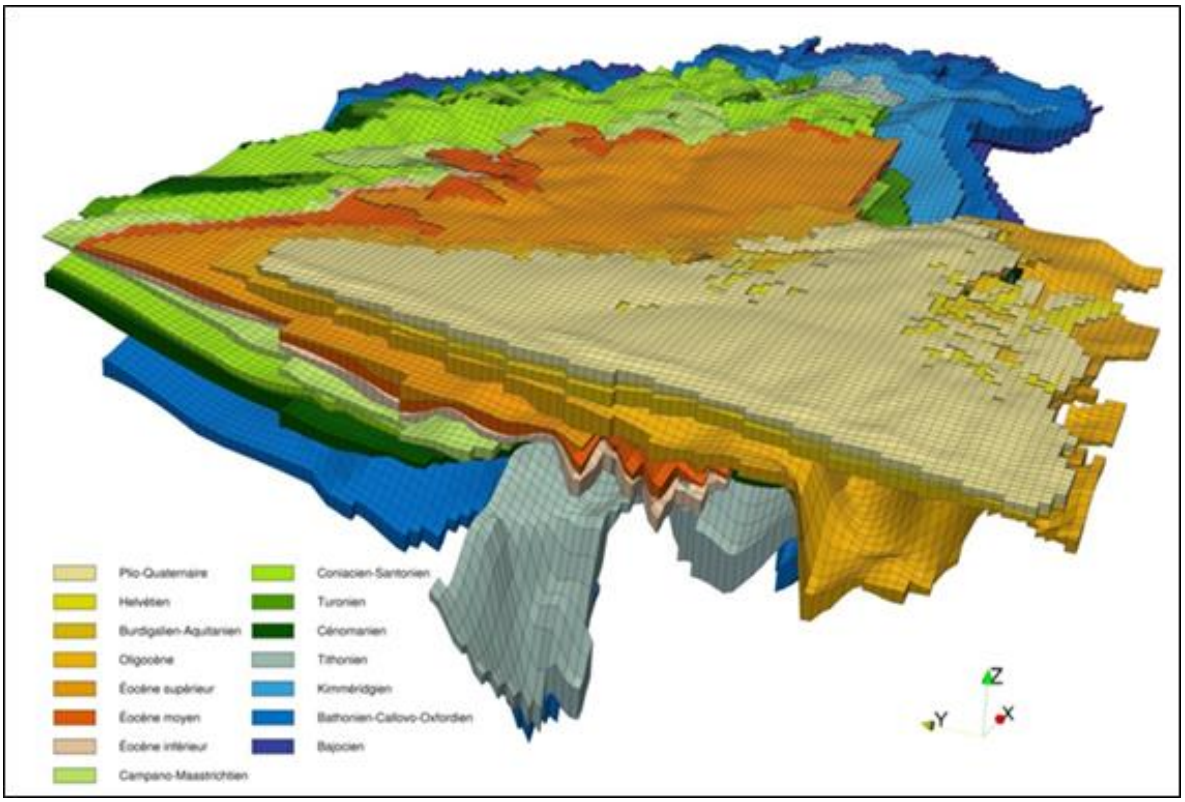


Figure 1 – 3D view of the north-Aquitaine model showing the succession of the 15 modelled aquifer layers (Saltel and Pedron, 2012).

The aim of this report is to present, explore and showcase most of the functionalities of MARTHE v7.8, as a tutorial applied to several examples of increasing difficulty. A deliberate choice was to present examples with simple geometries, but MARTHE can also model large aquifer systems (Figs. 1 and 2) of more than one million cells.

We aim at providing the user with a preliminary autonomous familiarization of the computer code, possibly before organizing specific training courses dedicated to MARTHE's advanced features. Detailed explanations of all the MARTHE computer code features is not the purpose of this report, but can be retrieved from other reports in the list of related references, in particular the MARTHE v7.8 User Guide: report BRGM/RP-69541-FR (Thiéry, 2020a, *in French)* (see References hereafter) and available on the web site: http://marthe.brgm.fr/

The report "Tutorial for the WinMarthe v4.0 pre-processor", BRGM/RP-54652-EN (Thiéry 2007) (or the report BRGM/RP-54652-FR, Thiéry, 2006, *in French*) presents the WinMarthe preprocessor in detail.

Thanks are due to Quentin Guillemoto for his contribution to this report. H.M. Kluijver and A. Sbai translated the French 'Didacticiel' into the present English version.

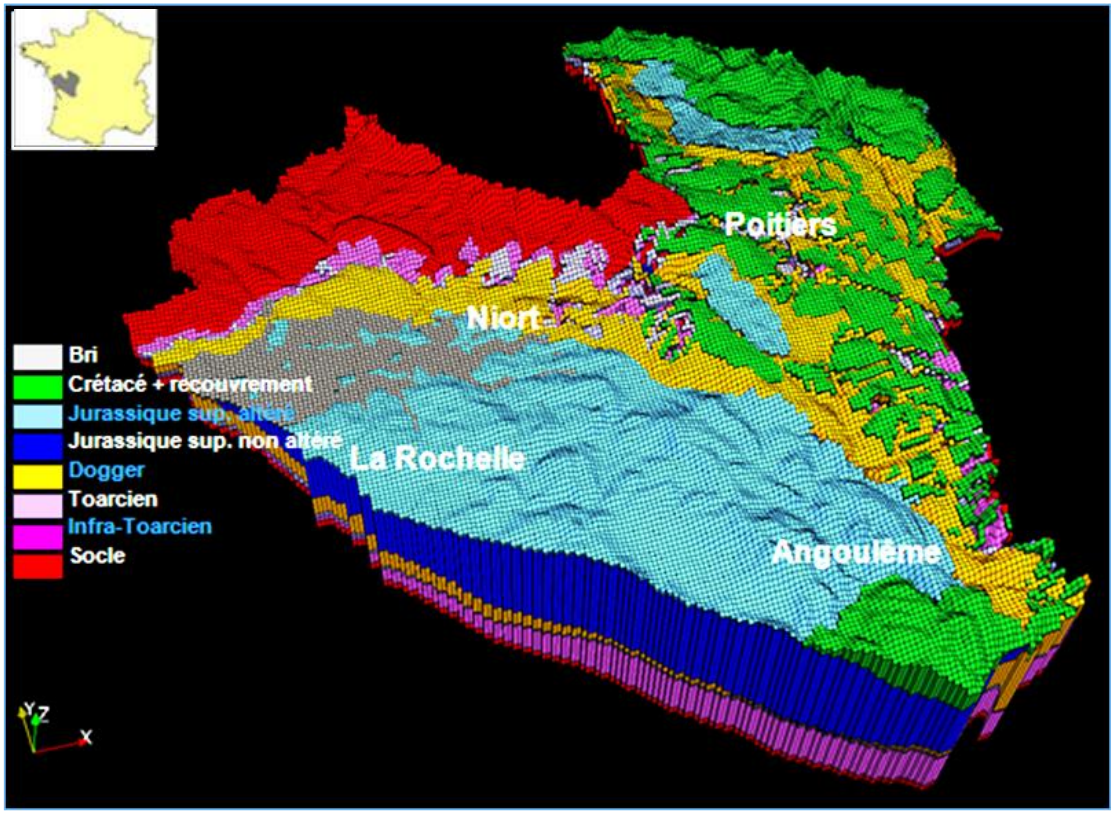


Figure 2 – 3D view of the model of the Poitou-Charentes Jurassic, 8 layers, 4 aquifers (Douez et al. 2011).

2 General description of the MARTHE computer code

2.1 FIELD OF APPLICATION OF THE MARTHE COMPUTER CODE

In version 7.8, the MARTHE computer code allows the modelling of hydrosystems, integrating both groundwater flow and river flow.

Density-dependent effects could be included in the simulations of groundwater flow, mass and heat transport (Thiéry, 2015c) in the saturated and unsaturated zones (Thiéry, 2015b), and in single-phase and two-phase flow systems (Thiéry, 2015c). It is also possible to make a reactive transport calculation (Thiéry, 2015e). Specifically, MARTHE has the following features:

- ***Standard hydraulic features**:*
  - 2D (plan, vertical cross-section, axisymmetric) or 3D grids.
  - Single- or multi-layer aquifer systems (stacked aquifers that may be separated by semi-permeable layers).
  - Unconfined, semi-confined or confined aquifers under steady-state or transient conditions.
  - Consideration of discontinuities such as surface water (lakes, gravel pits, etc.), local drying-up (and wetting) of (multi-layer) aquifer(s), aquifer overflow into rivers, springs, and water-tight walls (sheet piling, etc.).
  - Automatic progressive shut-down of pumping wells depending on the calculated hydraulic head (dewatering of the pumping screens).
  - Detailed integration of rivers and lakes networks and of drains networks.
  - Direct integration of hydro-climatic budgets.
  - Horizontal and vertical anisotropy of the aquifer hydraulic conductivity.
  - Calculation of forward and/or backward flow lines under steady-state or transient hydraulic conditions.
- ***Hydrodispersive mass transport**:*
  - Hydrodispersive migration of a solute in the aquifer and the unsaturated zone (UZ) by convection, diffusion or hydrodynamic dispersion.
  - Degradation of a solute through exponential decay over time (water-content and temperature functions).
  - Chain degradation of several solutes.
  - Invariant retarding factor or function of a linear Kd partition coefficient (adsorption-desorption phenomena).
  - Consideration of double porosity, with kinetics or in equilibrium.
  - Freundlich or Langmuir isotherms.
- ***Unsaturated zone, Density, Temperature**:*
  - Continuous modelling of both saturated and unsaturated zones.
  - Density effects induced by salinity and/or temperature gradients.
  - Temperature-dependent fluid Viscosity.
- ***Heat transport**:*
  - Heat storage and recovery, migration of a thermal plume.
  - Simulation of heat transport between geothermal doublet wells.
  - Approximating thermal walls with the Vinsome (1980) analytical solution.
- ***Automatic model calibration, Optimization**:*
  - Automatic calibration of model parameters along homogeneous zones or cell-by-cell calibration.
  - Sensitivity analysis of the calibrated parameters.

- Analysis of the simulation variance. The "Analysis of simulation variance (*Analyse des écarts de simulation*") is described in report BRGM/RP-69210-FR (Thiéry, 2020c).

- ***Geochemical reactions:***
  MARTHE is coupled with two external geochemical sets of modules:
  - The hydrogeochemical REACT modules from the LBNL's TOUGHREACT code (Xu et al. 2004).
  - The hydrogeochemical modules of the USGS's PHREEQC code (Parkhurst and Appelo, 2013; Parkhurst and Wissmeier, 2015). The physico-chemical interactions between the liquid phase and the porous matrix can be simulated at will with one of these coupled versions. The coupling with PHREEQC is described by Thiéry, (2015e).

- ***Advanced features****:*
  - Drain or tunnel networks.
  - Transport with physico-chemical interactions between water, effluents and porous matrix.
  - Two-phase flow: fresh water and saltwater, water and air, water and "oil".
  - Single-phase gas flow.
  - Development of vegetation in the root zone.
  - Simulation of vertical fractures by their equivalent transmissivity.

2.2 CHARACTERISTICS OF THE MARTHE COMPUTER CODE

2.2.1 General characteristics

Among the characteristics of the MARTHE code, the following stand out:

- 1D, 2D or 3D fluid flow.
- Irregular rectangular gridding, whereby the size of each layer can be different from that of the other ones. Vertically, all cells have the same horizontal dimensions, but this can be short-circuited when a formation disappears (lacuna, wedge).
- Nested cells can be integrated in the main grid leading to a locally refined grid (LGR) stencil.
- Simulations in steady-state and transient modes. Optionally, a steady-state simulation can precede a transient run.
- Possibility of considering a free surface (or water table) in any layer.
- Efficient simulation of local dewatering and re-saturation phenomena of the aquifer.
- Possibility of considering semi-permeable boundaries between any aquifer layers.
- Overflowing cells (springs, gravel pits, ponds, etc.).
- Equipotential zones with an unknown or variable hydraulic head (gravel pits).
- Water-tight walls (sheet piles, foundations, faults, etc.).
- Hydraulic conductivity anisotropy in the two horizontal grid directions ("north/south" and "east/west").
- Vertical anisotropy of the hydraulic conductivity.
- Possibility of introducing hydraulic conductivity anisotropy coefficients on a cell-by-cell basis.
- Coupled simulation of aquifer and river network.
- Coupling with an underground-drain network that may be under pressure.
- Integration of hydro-climatic-budget to estimate distributed aquifer recharge and surface runoff.
- WinMarthe pre-processor for data preparation and post-processing of the simulations results.
- Definition or modification of any field at any simulation time step. Such modifications can be performed on a cell-by-cell basis, by zones, by layers, or on the entire grid.
- Detailed budgets of groundwater flow, mass- and energy transport by zone.
- Calculation of groundwater flow and transport with consideration of the unsaturated zone "UZ" dynamics.

- Consideration of the vegetation land cover evolution and its effects on (evapo)-transpiration.
- Simulation of nitrate transfer.
- Coupling with external geochemical modules to simulate reactive transport.

2.2.2 User Friendliness

- Creation and modification of the finite-difference grid with the WinMarthe graphical pre-processor.
- Import of geometry produced by third-party 3D geometrical modellers or geo-modellers, such as GDM®, Multilayer®, EarthVision®, or Eclipse/Petrel®.
- Pre-processor to define the simulation parameters.
- Pre-processor to define the time stepping progression:
  - Use of absolute dates allowing consecutive simulations that can be juxtaposed,
  - Model time steps whose duration can be individually defined by the user.
- Very detailed water budgets and inflowing and outflowing flow rates that are stored and released by each cell in the model.
- Detailed water budgets in rivers and lakes.
- Possibility to modify any data file before a simulation start-up and at each time step.
- All data can be modified:
  - By reading a new file (for all layers),
  - By assigning a uniform value to all cells,
  - By assigning a uniform value to each layer,
  - By assigning a uniform value to a "geometrical zone",
    A "geometrical zone" is a set of cells, not necessarily adjacent, with the same "geometrical zone number".
  - By assigning a value per cell or "block of cells":
    A "block of cells" is a unit of adjacent cells, in a "parallelepiped" it is defined by a range of consecutive rows, a range of consecutive columns and a range of consecutive layers. For instance: columns 7:9, rows 12:15, layers 3:7 or: columns 7:9, rows *, layer 2.

The above features can be used to modify:

- The pressure head values, the river or lakes levels, the sea level;
- The index of local overflow (modification of spring flow, or the position of a drain);
- The pumped or injected flow rates to simulate evolving needs;
- The aquifer recharge flux according to hydro-climatic variations;
- The spatial extension of the simulated domain by changing the position of cells with null hydraulic conductivity;
- The spatial extension of potential fractures or gravel pits by modifying the spatial extension of associated equipotential zones;
- The prescribed boundary conditions by locally fixing or freeing a hydraulic head, a concentration, or a temperature, *via* a flow rate value coded at 9999.

No data are redundant (for instance, the bottom of a layer serves as the top of the underlying layer.

It is allowed to selectively save any data fields and results at pre-defined time steps.

Moreover, saving of the evolution at each time step of calculated fields in selected cells.

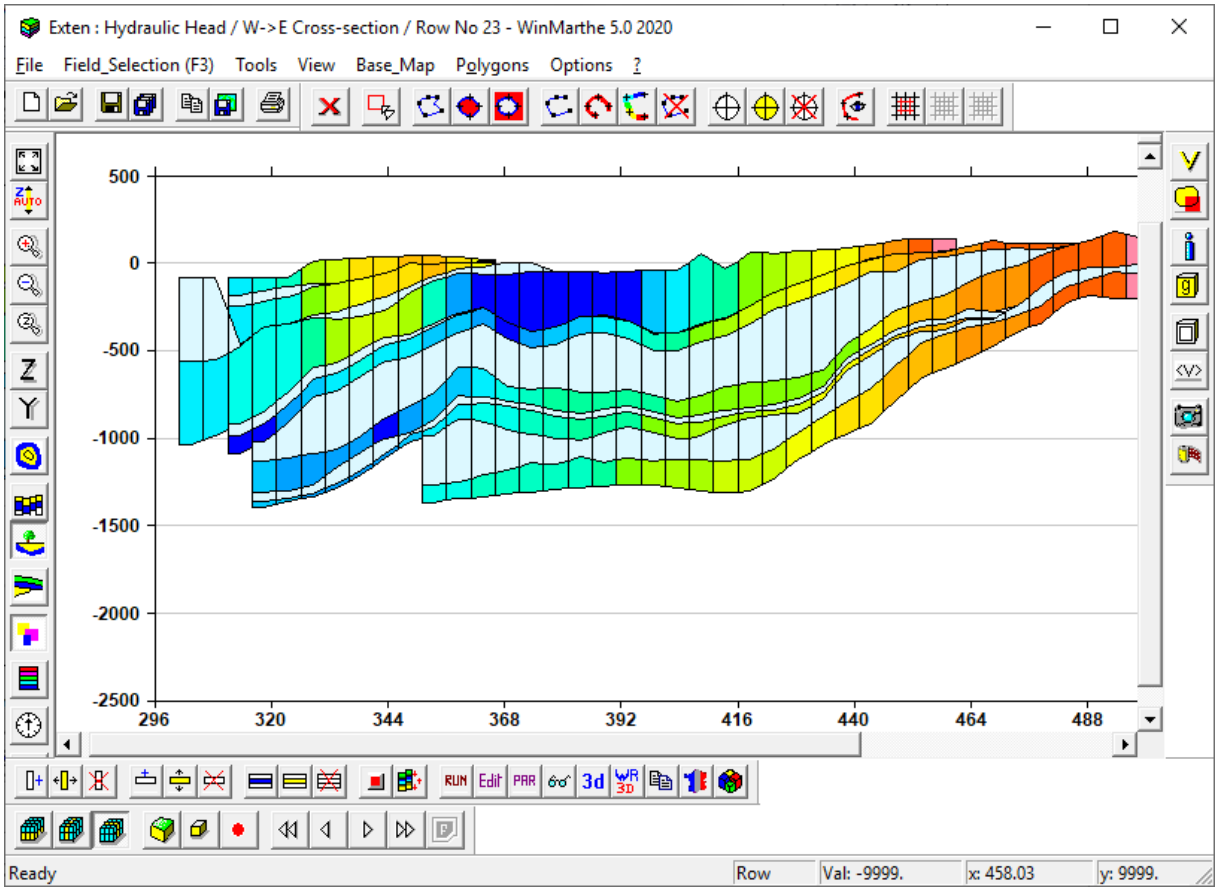


Figure 3 –WinMarthe pre-processor enabling the creation and modification of any data field.

2.2.3 Maximal dimensions

Except for the following maximal dimensions, MARTHE v7.8 was designed to be dimension independent. The underlying limitations are not exceeded in typical modelling applications.

- 999 model layers.
- 3000 rows in a grid.
- 3000 columns in a grid.
- 99 nested sub-grids in the parent grid when using the LGR approach.
- 999 spatial zones.
- 500 soil zones for the hydro-climatic budget assessment.
- 500 irrigation zones.
- 99 cultivated zones.
- 999 crop types.
- 99 equipotential zones.
- 15,000 calculated time series in cells.
- 1000 river tributaries.
- 999,999 river reaches (but different from 9999).
- 999,999 tributaries or reaches of drains (but different from 9999).
- 999,999 lakes and ponds.
- 150 chemical elements, 150 species, and 150 minerals.

The number of time steps is unlimited.
The number of meteo zones is unlimited but zone number 9999 cannot be used

2.3 GRIDS

The MARTHE software uses structured cells in the shape of grids stacked in layers. The organization of these layers allows depicting complex geometries.

Some layers of the domain may be chamfered within the modelled domain before disappearing, allowing short-circuits between two non-consecutive layers, or the outcropping of deep layers. Such layer disappearances are real and not just mimicked by a decrease in thickness, allowing more accurate simulations (Figure 4).

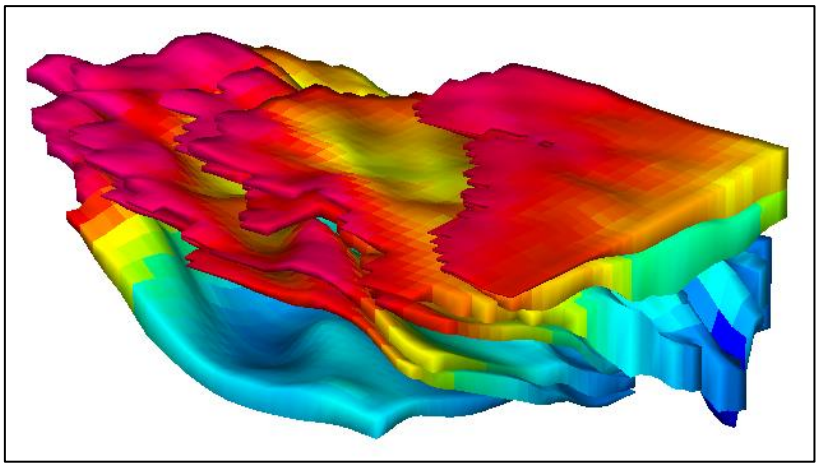


Figure 4 – Example of a complex gridding with some incomplete layers allowing short-circuits between layers.

Supported grid types are:

- "Cartesian" grids composed from irregular parallelepipeds (indexed by column, row, and layer), this is the most common case.
- Radial planar grids, 2D or 3D (indexed by radius, angle, and [layer]).
- Vertical cross-section grids (indexed by column, and layer).
- Pseudo-vertical cross-section grids (indexed by column, and row), with gravity on the oy axis.
- "Axisymmetric" vertical cross-section grids (indexed by radius, and layer or alternatively by radius, and row), with gravity on the oy axis when using an unsaturated zone (UZ) modelling scheme.

2.3.1.1 "Cartesian" grid: indexed by column, row, and layer

In a Cartesian grid, the domain to be modelled consists of irregular parallelepipeds. Seen from above, the cells are irregular rectangles (Figure 5 to Figure 7).

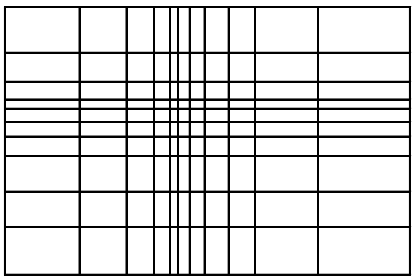


Figure 5 – Top view of an irregular rectangular grid.

The aquifer is defined as a set of layers, layer 1 being the uppermost. The cells are parallelepipeds whose dimensions are defined by:

- The width of the different columns,
- The height of the different rows,
- The thickness of the layers, variable in each cell.

This way, the height of each row and width of each column can be adapted to constraints such as (i) the local heterogeneities, (ii) the density of available data and to (ii) the required accuracy of the results.

The grids are geo-referenced and self-documented, allowing to more easily import any spatial scattered data as “x, y, value” files from geological models, interpolators, or scatter data files, etc., as well as exporting the simulation results as geo-referenced files for use by any external third-party post-processors.

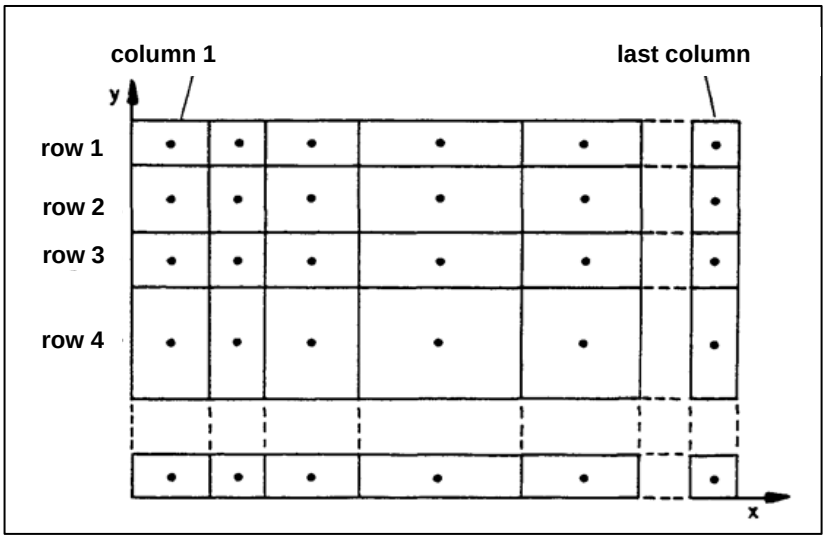


Figure 6 – Numbering of columns and rows in a 2D grid.

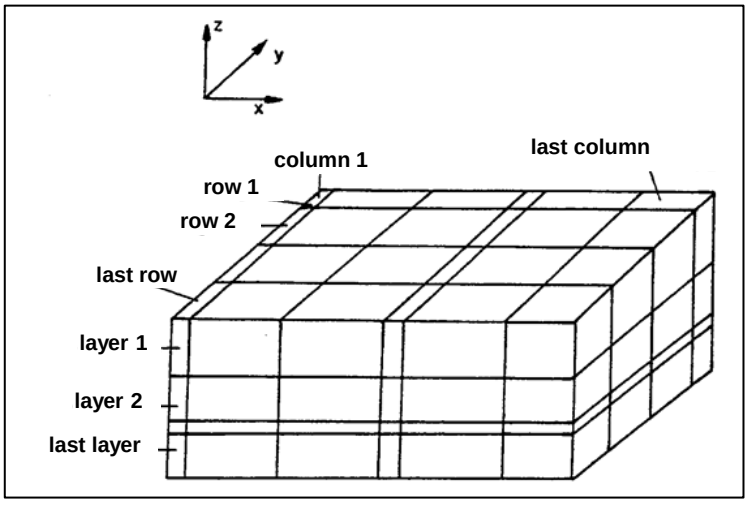


Figure 7 – Numbering of columns and rows in a 3D grid.

The grid size is limited only by the available memory and by the maximum dimensions indicated above. Within a common hardware (such as a laptop computer), it is possible to use a grid with more than one million of grid cells.

2.3.1.2 Radial Planar grid

In plan view, the grid consists of crown sectors.

In 2D, the coordinates are defined by a radius and an angle, θ.

In 3D, when there are several layers, the coordinates are the radius, the angle and the layer.

Figure 8 shows a radial grid covering a total angle sector ranging between -20° and +40°. The grid is formed from 10 radially-oriented columns growing regularly from 50 m to 500 m. Likewise, the grid is divided into 7 rows (“crowns”) of 4° to 10° angle along the θ-oriented direction.

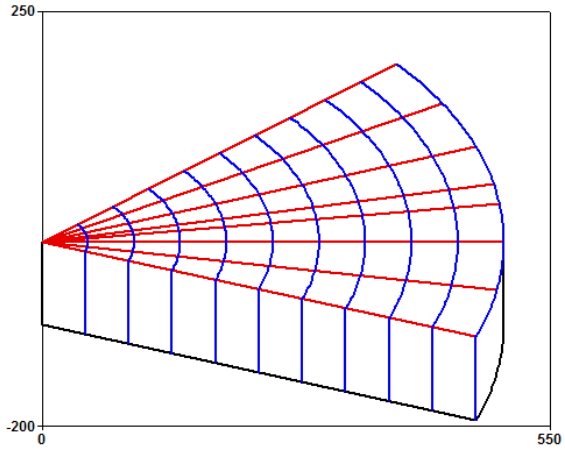


Figure 8 – Example of a radial (axisymmetric) grid in perspective view.

The calculation takes place in the radial grid.

However, for the definition of this grid types and their post-processing by WinMarthe:
- The abscissae are replaced by the distance to the origin (or to the vertical axis);
- The ordinates are replaced by the angle, in degrees, from the horizontal axis. The maximum angle value is 360°.

Figure 9 shows the representation in WinMarthe of the radial grid:
- The 10 radially-oriented columns (“crowns”) with radiuses between 0 and 500 m are represented by 10 abscissa columns from 0 to 500 m;
- The 7 θ-oriented sectors of widths between 4° to 10° are represented by 7 rows (widths of 4 to 10" units").

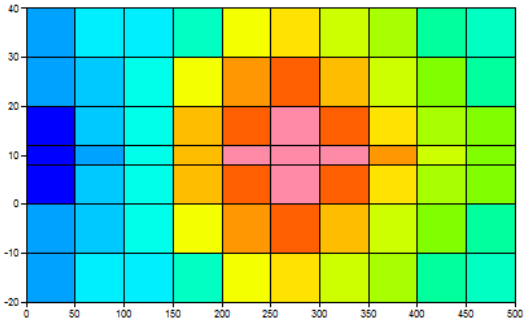


Figure 9 – Example of a planar radial grid as shown in WinMarthe Pre-processor.

When using a sector with a maximum angle of 360°, it should be noted that the North of the first row (corresponding to angle 360°) is an impervious boundary. It is not in direct contact with the South of the last row (corresponding to angle 0°), which is also an impervious boundary.

There is thus implicitly an impervious boundary between 360° and 0°. Flow therefore must be symmetrical with respect to this axis.

2.3.1.3 Vertical cross-section grid

Each cell of the grid is identified by its column and layer numbers as illustrated in Figure 10.

The results visualization follow a simple "monolayer" scheme (column and layer indices), whereas the calculation is done using the same 3D engine (using one row in the xy-plane), with several layers.

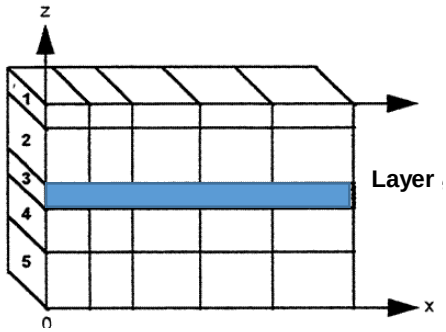


Figure 10 – Vertical cross-section gridding.

When using the unsaturated zone (UZ) modelling scheme, the hydraulic head in each cell is compared to its elevation and ***not*** to its “top elevation” or “bottom elevation”.

For vertical cross-section modelling using the UZ scheme, we use in fact a pseudo vertical cross-section modelling scheme. This is based on a plane Cartesian grid (column, row), specifying that the gravity is parallel to the downward directed oy axis (Figure 11).

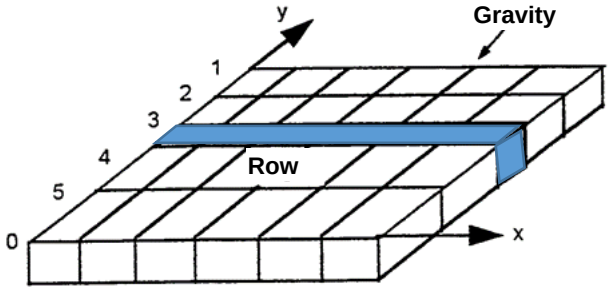


Figure 11 –Example of a pseudo-vertical cross-section grid (which is not a true vertical cross-section).

The thickness of the horizontal cut slice is normally defined by the difference between the "Topographic Elevation" and the "Elevation of the Substratum" fields. In this case, the parameters relating to the topographic surface, such as the "Soil Zones" and the "Meteo Zones", are defined in the first row (i.e. row 1). Similarly, a groundwater recharge flux can be defined by "Meteo Zones" or on a cell-by-cell basis, but only the values defined in the "outcropping" cells will be considered

The simulation is carried out in a single layer (i.e. "monolayer" scheme).

2.3.1.4 Axisymmetric Vertical cross-section grid

Each cell of the grid is defined by:

- Its radius and layer;
- Or, when using the UZ modelling scheme, by its radius and row, with the gravity direction pointing downwards on the oy axis (Figure 12).
  The calculation is then performed with a single layer. The benefit is to allow a very large number of rows, and to permit the use of nested grids.

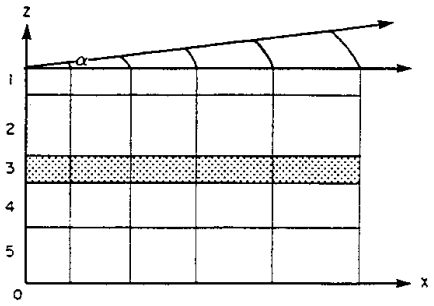


Figure 12 – Example of an axisymmetric vertical cross-section grid.

2.4 NUMERICAL CALCULATION SCHEMES

The numerical scheme is based on the standard fully implicit finite-difference method using a 7-point stencil as shown in Figure 13. The latter expresses, for a constant density fluid, the equations resulting from the conservation of fluid flows exchanged between each cell and its immediate six neighbours. The scheme is however more complex at the contact of a nested grid or in an “equipotential zone”.

In the general case, a central cell, indexed by "C", has six neighbouring cells "V": North, East, South, West, Top and Bottom (Figure 13). However, in contact with nested cells, the number of neighbouring cells may be greater than six. For example, in a partial nested grid where some cells are subdivided into 5 levels (25 sub-cells), a coarse cell will have 5 adjacent cells to the north, 5 to the east, 5 to the south and 5 to the west, for a total of 22 adjacent cells.

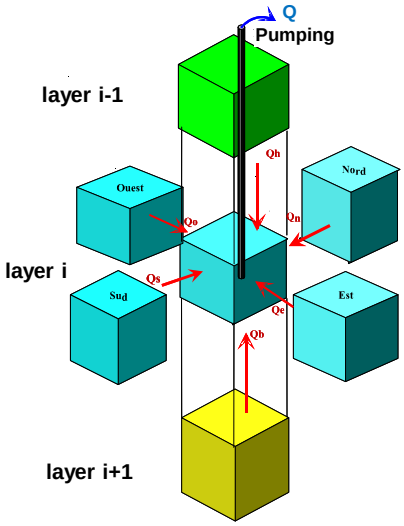


Figure 13 –Example of 7-point finite-difference scheme for flow balance between a cell and its 6 neighbours.

The mass conservation law, associated to Darcy’s law, leads to the following equations:

$$div\left(\mathrm{K}\cdot grad\ H\right)+q=S_S\cdot\frac{\partial H}{\partial t}$$ in a confined area of the aquifer,

$$div\left(\mathrm{K}\cdot grad\ H\right)+q=\frac{1}{\Delta z}\cdot S_L\cdot\frac{\partial H}{\partial t}$$ in an unconfined area of the aquifer,

With:

- K = The hydraulic conductivity,
- H = The hydraulic head,
- q = Injected or pumped flow rate (per volume unit),
- t = Time,
- S_s = The specific (confined) storage coefficient,
- S_L = The specific yield coefficient,
- Δz = The cell vertical thickness

By expressing the exchanged flows between the central cell and its neighbours, we obtain the algebraic equation:

$$Q + \sum_{V=1}^{6} T_{VC} \cdot (H_V - H_C) = Surf \cdot S \cdot \left(\frac{H_C - H_P}{dt}\right)$$

Depending on whether the aquifer is locally confined or unconfined in the cell:

$$Surf \cdot S = a_x \cdot a_y \cdot a_z \cdot S_S \quad \textit{or} \quad Surf \cdot S = a_x \cdot a_y \cdot a_z \cdot S_L$$

With:

- Q = Flow in the central cell (positive when flow is injected),
- T_{VC} = Transmissivity of exchange between cell V and cell C,
- H_P = Hydraulic head at the cell-centre and at the beginning of a time step,
- H_C = Hydraulic head at the cell-centre and at the end of a time step,
- H_V = Hydraulic head in neighbouring cell V at the end of the time step,
- dt = Duration of the time step.

The exchange transmissivities (or exchange coefficients) are described in Appendix 1.

A system of linear equations is thus obtained when the T_{VC} exchange coefficients are known. The matrix corresponding to this equation system is sparse. Generally, except in the case of nesting, it contains only 0, except in seven diagonals: the central one and the six nearby diagonals: Top, North, East, West, South and Bottom.

As the exchange coefficients are symmetrical ($T_{VC} = T_{CV}$), the matrix is symmetric as well. The solution method follows an iterative scheme, using the preconditioned conjugate gradients method. The solver can be selected from one of the proposed algorithms: The incomplete Cholesky factorization, the Eisenstat method, etc.

2.5 PRINCIPLES OF SIMULATING MASS TRANSPORT: NUMERICAL CALCULATION SCHEMES

Modelling solute transport in saturated or unsaturated media is fundamental for pollution assessments and depollution studies. The MARTHE calculation code allows modelling solute transport in 2 or 3 dimensions (2D or 3D), and in porous saturated or unsaturated media.

In the one-dimensional case, the transport equation is:

$$\frac{\partial(\theta_m \cdot C)}{\partial t} = \frac{\partial^2(D \cdot \theta_m \cdot C)}{\partial x^2} - \frac{\partial(q.C)}{\partial x} - \frac{C \cdot \theta_m}{T_d} + q_m - (\theta_f + RhoKD) \cdot \frac{\partial S_V}{\partial t}$$

$$\frac{\partial^2(D \cdot \theta_m \cdot C)}{\partial x^2} = Dispersion$$

$$-\frac{\partial(q.C)}{\partial x} = Convection$$

$$-\frac{C \cdot \theta_m}{T_d} \qquad = \text{Degradation}$$

$$-(\theta_f + \text{RhoKD}) \cdot \frac{\partial S_V}{\partial t} \; = \text{Exchange}$$

With:

- C = Concentration in mobile water (kg of solute / m^3 of mobile water);
- S_v =The volumetric concentration in the immobile phase, identical in immobile water and in the solid, (kg of solute / m^3 of immobile water) and (kg of solute / m^3 of soil);
- θ_m = Mobile water content [-];
- θ_f = Immobile water content [-];
- RhoKD = The volumetric partition coefficient = the equivalent water content of the solid [-];
- q = Darcy velocity [LT^{-1}];
- D = Dispersion coefficient [L^2T^{-1}];
- T_d = Degradation time constant [T];
- q_m = Injected mass flow per unit volume [$M.L^{-3}.T^{-1}$].

When exchanges are instantaneous, we have S_v= C; this results in the following equation:

$$\frac{\partial[(\theta_m + \theta_f + \text{RhoKD}) \cdot C]}{\partial t} = \frac{\partial^2 (D \cdot \theta_m \cdot C)}{\partial x^2} - \frac{\partial (q.C)}{\partial x} - \frac{C \cdot \theta_m}{T_d} + q_m$$

The first member can be written as:

$$\frac{\partial (R \cdot \theta_m \cdot C)}{\partial t}$$

or:

$$\frac{\partial (\theta_m \cdot C)}{\partial (t / R)}$$

with:

$$R = 1 + \frac{(\theta_f + \text{RhoKD})}{\theta_m}$$

R is the so-called retardation coefficient that is not constant if θ_m varies over time.

2.5.1 Density-dependent effects

The MARTHE 7.8 code allows considering the variations in the fluid density when the concentration has a significant impact on flow. This is called "density-dependent flow". The code works in steady-state or transient conditions and the fluid density can be taken as fixed or internally calculated as a function of concentration and/or temperature. Density effects can be considered in confined or unconfined groundwater, in the unsaturated zone, in isothermal flow, or with temperature effects. The features of mass/energy transport, and reactive transport are not described in detail here and need to be consulted in other reports (e.g. Thiéry, 2015d).

In the code, the concentrations are designated by the variable "CONCENTR", file extension [.conce]. When considering density effects, another concentration—here called "salinity"—is necessary. This is the volumetric concentration of a solute (salt) responsible for the density variation of the fluid. In MARTHE, the salinity corresponds to the variable "SALINITY", file extension [.salini].

This case of transport is analogous to the standard mass transport of the MARTHE code. However, an iterative coupling between the hydraulic head simulation and the salinity computation is necessary since the salinity depends on transport, which depends in turn on the

velocity field (therefore indirectly on the hydraulic head), which depends on the density that depends on salinity.

2.5.2 Solute transport calculation schemes available in MARTHE

In the MARTHE code, four methods are implemented for solute transport calculation:

- The standard upwind **F**inite **D**ifferences (FD) method;
- The **T**otal **V**ariation **D**iminishing method (TVD) with a flux limiter scheme;
- The **M**ethod **O**f **C**haracteristics (MOC) method;
- The **R**andom **W**alk (RW) method also known as the "random particle displacements" method. This method is only kept for archival purposes as it generally gives unsatisfactory results.

2.5.2.1 Finite-differences (FD) method

The finite-differences method, FD, discretizes the transport equation like the hydraulic equation. The obtained system of equations (one per cell) is resolved iteratively by the preconditioned Orthomin acceleration method operation with non-symmetric matrices.

The scheme used for discretizing in time is fully implicit. The spatial weighting is upwind: the incoming flow in a cell arrives with the concentration of the upwind cell; flow then exits with the concentration of the current cell. Such an upwind scheme, also called "donor cell", is unconditionally stable regardless of the dimensions of time- and space steps. It is a “monotonic scheme”: it always respects the second law of thermodynamics, i.e. in the absence of a source term the final concentration of a simulation cell is always between its concentration at the beginning of the time-step and the final concentrations of its six neighbour cells. The calculation scheme for convection and dispersion leads to a non-symmetric sparse matrix, with 9 diagonals in 2D, and 19 diagonals in 3D. Resolution of the equation system is done by the Orthomin method for non-symmetric matrices. The resolution routine by the Orthomin method from MARTHE was adapted from the Orthofem routine (operational for finite elements), transmitted by Carl A. Mendoza of the Waterloo Centre for Groundwater Research at the University of Waterloo (Ontario, Canada), (personal communication).

2.5.2.2 Total Variation Diminishing (TVD) method

The TVD method is close to the FD method, with the following differences: convection is calculated according to an explicit in time discretization scheme, while dispersion, degradation and exchanges involve an implicit scheme. Calculations are stabilized by the introduction of a flux limiter scheme that guarantees monotonicity of concentrations in the absence of source terms. This method is described by Leonard, 1988 and Zheng et al. 1999

The TVD method that has a constraint on the Courant number, is only available for transient transport simulations.

2.5.2.3 Method of Characteristics (MOC)

The Method of Characteristics consists in modelling convection and dispersion by two different methods. The calculation takes place in two successive stages: first convection by displacement of particles that are the mass in solution, and then dispersion. In the first step, particles are generated corresponding to the initial concentration in the cells and to the mass inputs, and then all particles are displaced according to the actual flow velocity, without considering dispersion. The concentrations in the cells are then calculated by counting the particles. In the second step, a pure dispersion step is calculated by a finite-difference scheme, ignoring convection. The number of particles in the cells of the modelled domain is readjusted according to calculated concentrations.

2.5.2.4 Random Walk method (for legacy)

The Random Walk (RW) method involves moving many particles according to the actual flow velocity at each point. The dispersion is modelled by adding a random term to the duration (or speed) of displacement. Each particle carries an identical elementary mass. The concentration of a cell is obtained by counting the number of particles, i.e. the solute mass in the grid, and dividing it by the volume of water in the grid (variable if the groundwater is unconfined).

The Random Walk transport method in the unsaturated zone, in 1D, with exchanges, is described by Thiéry and Iung (1990, 1991) and by Thiéry (1991).

2.5.3 Generalized Péclet and Courant numbers

When discretizing the 1D transport equation into finite differences, two dimensionless numbers appear: the “Courant number”, C_r, and the "Dispersion number", N_d:

○ The Courant number, C_r, is equal to the distance travelled by a concentration particle during a time step, divided by the dimension of a cell:
in 1D: $C_r = u \cdot dt / dx$.

The Péclet number, P_e, is equal to the ratio between solute mass flow by convection and mass flow bydispersion:
in 1D: $P_e = (q.dC) / (D. \omega \cdot dC/dx)$;

or, dividing by the numerator and denominator by the concentration variation term:
in 1D: $P_e = u \cdot dx / D$;

or even, admitting that $D \approx \alpha.u$:
in 1D: $P_e = dx / \alpha$, α being the dispersivity, of dimension [L].

These Péclet and Courant numbers can be generalized in 3D using the three following expressions:

Capacitance	= Equivalent water volume in a cell;
Conductance	= Mass discharge flowing by dispersion (conduction);
Advectance	= Mass discharge flowing by advection.

This leads to the following mathematical expressions:

$$\text{Capacitance} = R \cdot \omega \cdot dx \cdot dy \cdot dz$$

$$\text{Conductance} = \sum_{v} \frac{\omega \cdot D \cdot A}{dx}$$

$$\text{Advectance} = \sum_{a} q \cdot A$$

With:
- R = Retardation coefficient,
- ω = Kinematic porosity,
- D = Dispersion coefficient,
- q = Darcy velocity,
- u = Pore velocity = q / ω
- A = Cell area in the direction perpendicular to flow,
- a = Index of upstream cells,
- v = Index of neighbouring cells.

We now can define the Péclet (P_e) and Courant (C_r) numbers as equivalent to:

$$P_e = 2 \cdot \frac{\text{Advectance}}{\text{Conductance}}$$

$$C_r = \frac{\text{Advectance} \cdot dt}{N_a \cdot \text{Capacitance}}$$

With:

dt = Duration of a simulation time step

N_a = Number of upstream cells.

In 1D these expressions are equal to the standard expressions:

$$P_e = 2 \cdot \frac{q \cdot A}{2 \cdot \frac{\omega \cdot D \cdot A}{dx}} = \frac{\mathbf{u \cdot dx}}{\mathbf{D}}$$

$$C_r = \frac{q \cdot A \cdot dt}{1 \cdot R \cdot \omega \cdot A \cdot dx} = \frac{\mathbf{u \cdot dt}}{\mathbf{R \cdot dx}}$$

In 3D, with an isotropic coefficient D and square cells, we also obtain:

$$P_e = 2 \cdot \frac{3 \cdot q \cdot A}{6 \cdot \frac{\omega \cdot D \cdot A}{dx}} = \frac{\mathbf{u \cdot dx}}{\mathbf{D}}$$

$$C_r = \frac{3 \cdot q \cdot A \cdot dt}{3 \cdot R \cdot \omega \cdot A \cdot dx} = \frac{\mathbf{u \cdot dt}}{\mathbf{R \cdot dx}}$$

In 3D, for mono-dimensional flow with a velocity u, we obtain:

$$C_r = \frac{q \cdot A \cdot dt}{1 \cdot R \cdot \omega \cdot A \cdot dx} = \frac{\mathbf{u \cdot dt}}{\mathbf{R \cdot dx}}$$

$$P_e = 2 \cdot \frac{q \cdot A}{2 \cdot \frac{\omega \cdot A}{dx} \cdot \left[D_0 + \frac{q}{\omega} \cdot (\alpha_L + 2\alpha_T)\right]}$$

When neglecting molecular diffusion D_0:

$$P_e = 2 \cdot \frac{q \cdot A}{2 \cdot \frac{\omega \cdot A}{dx} \cdot \frac{q}{\omega} \cdot (\alpha_L + 2\alpha_T)} = \frac{\mathbf{dx}}{\boldsymbol{\alpha_L + 2\alpha_T}}$$

- The "Dispersion number", N_d, is the ratio: $N_d = C_r / P_e$.

In 1D we have:

$$N_d = \frac{C_r}{P_e} = \frac{D \cdot dt}{dx^2}$$

The ratio between time-step duration *dt* divided by the dispersion “characteristic time” in the cell is:

dx^2 / D.

2.5.4 Numerical dispersion

Numerical dispersion is an additional dispersion term generated by some numerical schemes. It is due to an unappropriated choice of the spatial discretization (dimension *dx* of the cells) and the temporal discretization (duration of the *dt* time steps). Numerical dispersion always tends to increase the mechanical dispersion. Indeed, if we introduces a dispersivity "α" as modelling

parameter, the resulting calculations will be (approximately) identical to a simulation made with tiny cells and very small time-steps, but with an “apparent” dispersion:

α_apparent = α + Numerical dispersion.

This shows that it would not be appropriate to increase α in order to reduce the effects of numerical dispersion. In practice, if possible, one should try to select such a spatial and temporal discretization that the numerical dispersion is much lower than the real one. For example, a numerical dispersion not exceeding 25% of the actual dispersion α.

For instance: If the real dispersion is $2\ 10^{-3}$ m^2/s and if the simulation generates a numerical dispersion equal to $0.2\ 10^{-3}$ m^2/s, the simulation will be nearly perfect, without numerical dispersion, with a dispersion of $2.2\ 10^{-3}$ m^2/s, i.e. 10% too big.

Numerical Dispersion depends upon:

- The numerical scheme selected to solve the transport equation,
- The discretization in time and space (cell dimension).

The FD method, while remaining simple and efficient, can generates a relatively large amount of numerical dispersion. The TVD and MOC methods, however, are much more accurate, but have some limitations.

A reasonable numerical dispersion generally is not an alarming issue, as the actual dispersivity values are usually hard to determine accurately, and as such values depend upon the dimension of interest.

2.5.5 Simulation time steps

Mass transport simulations can be run in steady or transient states, independently of the hydrodynamic (hydraulic head) simulation that can also be performed in the steady or transient states.

When the flow and transport simulation are carried in transient mode, the computational time steps (defined in the time-step file) are identical. Otherwise, when the flow simulation is in steady-state and one wishes to run a transient mass transport simulation, the transport time steps will be defined in the time-step file, extension [.pastp]. This definition of time steps is done with the "Non-meshed parameters" module ("Paramart” module), by clicking the button 

located in the lower WinMarthe’s toolbar.

2.6 EXTENSION OF THE AQUIFER DOMAIN

The aquifer boundaries are naturally defined by positive hydraulic conductivity values in the aquifer domain and by null values outside.

All cells with a hydraulic conductivity equal to the code value 9999 lie outside the domain. In the 3D grid, a cell with a hydraulic conductivity equal to 9999 allows isolating groundwater flow between two adjacent layers.

Lateral boundaries can be different from one layer to the next, without superposition (Figure 14).

In summary:

- A cell with a hydraulic conductivity greater than 0 is part of the aquifer domain;
- A cell with a hydraulic conductivity = 0 (or 9999) lies outside the aquifer domain;
- In a 3D, or multilayer, grid one should distinguish between:
  - Hydraulic conductivity = 0 => Inexistent cell (transparent to flow),
  - Hydraulic conductivity = 9999 => Impermeable cell (can separate 2 layers).

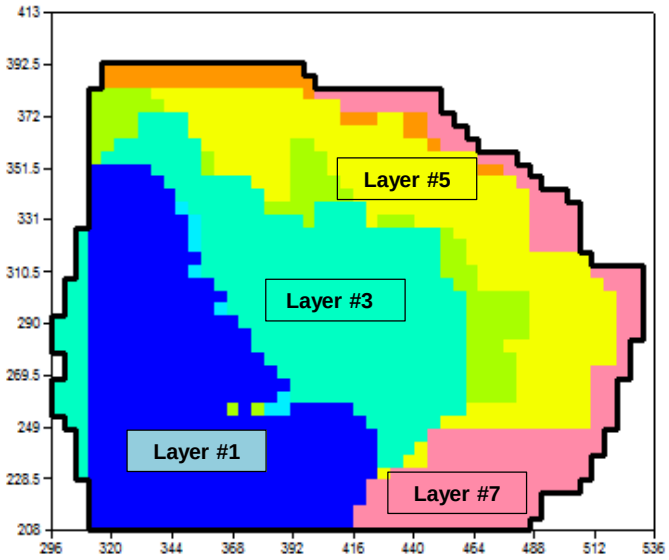


Figure 14 – North-Aquitaine aquifer system with 7 layers of different extension.

2.7 BOUNDARY CONDITIONS

2.7.1 Boundary conditions for groundwater flow

A "lateral boundary cell" lies next to at least one impermeable cell (hydraulic conductivity = 0 or 9999). In a lateral boundary cell:

- If we impose nothing specific, the boundary is by default "watertight" (with regards to the neighbouring cell lying outside the domain).
- If we want to impose a hydraulic head (corresponding to a "fixed potential") in such a lateral boundary cell, we must do it in two consecutive steps:
  - Assign a dummy “flow rate” equal to the value code 9999,
  - Assign the desired hydraulic head.

In any other cell that is not adjacent to a lateral boundary cell, we can impose the hydraulic head in the same way:

- Assign a dummy “flow rate” equal to the value code 9999,
- Assign the desired hydraulic head.

In all cases, when a hydraulic head is imposed in a cell, even though this cell may be located inside the domain, it is by definition a "boundary cell". This because for imposing its hydraulic head there must be an adjacent inflowing or discharging flow rate (which is calculated by the simulation code).

It is not possible to specify a flow rate in a "fixed hydraulic head cell" as the simulation code automatically determines this flow value. Therefore, these cells are defined by an initially unknown flow rate with a value code equal to 9999. In any other cell where the hydraulic head is not prescribed, it is possible to specify an injection (positive) or a pumping (negative) flow rate.

In MARTHE, "fixed flow rate" cells are regular cells that receive an additional "source term". For example in a 2D domain, all cells can receive an aquifer recharge flux from precipitation. In the same way, we do not speak of cells "with no flow rate", since such cells do not require any particular action.

2.7.2 Boundary conditions for mass transport

Boundary conditions for mass transport are independent from boundary conditions for a groundwater flow simulation. There are two types of boundary conditions and in addition, source terms can be introduced in any given cell of the computational domain.

2.7.2.1 Fixed concentration

A concentration value can be fixed in any cell of the domain. This results in introducing an associated mass flux that is internally calculated by the computer code. This is necessary to maintain this fixed concentration considering the neighbouring concentrations. To impose a concentration in a cell, it suffices, after having assigned this concentration, to define an "external concentration" with a code value equal to 9999.

N.B.: This approach is similar to that used by MARTHE to assign a fixed hydraulic head by setting an "external flow" equal to the value code 9999.

2.7.2.2 Watertight boundary for mass transport

This boundary blocks all mass exchanges, e.g. at the edge of an aquifer bounded by an impermeable medium, or on the sidewalls of an infiltration gauge. Such a boundary is automatic (i.e. by default) in MARTHE.

2.7.2.3 "Source" terms

Mass flux

A mass flux can be fixed in each cell of the domain through the field QMASS_CONC, file extension [.qmasc]. A mass flux is a mass per unit time ($M.T^{-1}$), expressed in as the ratio of mass and time in user-specified units.

Using a parameter from the "General Parameters" file, it is, however, possible to express a mass flux per square metre of a cell surface. Such mass flux, like most MARTHE fields, can be introduced:

- by grid;
- by layer;
- by geometric area;
- by infiltration zone;
- by irrigation area;
- on a cell-by-cell basis.

Remark 1: It is not possible to fix a mass flux on a cell with a fixed concentration: this would be a contradictory.

Remark 2: With the TVD and FD transport schemes, a negative mass flux can be applied. This would be, for instance, corresponding to solute decay at a constant rate or pumping. This is not possible within the MOC and RW particle schemes.

Instantaneous mass injection (Dirac)

In any cell of the domain, an instantaneous mass input can be fixed as a "Dirac": field MASS_CONCEN file extension [.mconc]. This mass injection is expressed in mass user-input unit. It is however possible, using a parameter from the "General Parameters" file, to express the mass injection per square metre of the cell area, in which case it can be more easily defined by a grid, zone or layer, independently from the cell area.

As for a mass flux, it is not possible to fix an instantaneous mass injection in a cell with a fixed concentration; in the TVD and FD transport methods the mass injection value may be negative, whereas it must remain always positive with the MOC and RW particle schemes.

With particle (MOC or RW) transport schemes, an instantaneous mass injection is an instantaneous addition, at the start of specified time steps, of the number of particles corresponding to the injected mass, independent of the duration of the time step. In the TVD and FD methods, an instantaneous injection is a mass flux distributed over the duration of the simulation step.

N.B.: In MARTHE, all fields defined at a given time remain unchanged until their subsequent modification. An instantaneous mass injection (Dirac) is an exception to this rule, since it is a discontinuous field. If we inject a mass at the start of a simulation, or at a given date, this injection will be considered only for the current time step.

External concentration

In any cell of the domain, the concentration of an external inflowing fluid, called "External concentration" can be defined. This is the concentration at which water enters the domain. It has a default value of zero. This water flow can get into the cell:

- By an injection flow rate (from a borehole, for instance);
- By inflow into a cell with a fixed hydraulic head.

If, at a given time step, a cell receives no external fluid flow, or if it is subjected to outflow (i.e. a pumping well, or through a boundary), the value of the “external concentration” is not used.

It should be noted that an external mass flow resulting from an external concentration does not correspond to a fixed concentration in that cell, except in steady-state conditions and without hydrodynamic dispersion effects.

The advantage of using this source term type is that it is physically sound. Thus, avoiding to fix a concentration or a mass flux if it is not known a priori whether the exchanged fluxes are inflowing or outflowing. The direction of exchanged rates is not always obvious, for instance in the unsaturated zone, near the sea, or in a transient hydraulic regime.

The external concentration corresponds to the field CONCEN_EXT, and has a file extension [.conex].

Like the other MARTHE fields, it can be defined by a grid, a layer, a zone or on a cell-by-cell basis. An external concentration of 9999, is a code that allows fixing the concentration of that cell at the input value at the start of a given time step. If one would wish to set an external concentration of 9999 (kg/m^3 for instance), it suffices to set it at a very slightly different value such as 9999.1.

Recharge concentration

This is the concentration of the infiltrating water (or groundwater recharge) where it is positive. A recharge concentration only applies to infiltration and not to excess irrigation. However, in case of need, it could then be possible to define the excess irrigation as an equivalent to recharge.

The concentration of the recharge (field CONCEN_RECH) can be defined only by Soil Zone or Meteo Zone and not on a cell-by-cell-basis. There is no corresponding recharge concentration grid file.

Remark 1: We can define simultaneously in the same cell:

- A fixed mass flux;
- An instantaneous mass injection;
- A concentration of an external fluid (or “External concentration”);
- A recharge concentration.

Remark 2: We note as "*Surf*" the horizontal cell area or surface, as "*dt*" the duration of the time step, as "Q_I" the flow injected in a cell, and as "*Infiltr"* the infiltration, which gives the following equivalents (not considering the units):

CONC_MASS_FL = Q_I . EXT_CONCEN

Q_I . EXT_CONCEN = Infiltr . Surf . RECH_CONCEN

CONC_MASS_FL . dt = CONCEN_MASS

Initialization

At the start of a solute transport simulation, an initial concentration is defined. This is a field named "CONCENTR", with file extension [.conce], which can be changed during the calculations. If the transport numerical scheme is the TVD or FD methods, the concentration can be negative. Such a negative concentration can be used during geochemical calculations for representing the concentration difference with respect to a reference state, or for representing the electric charge. If transport is by particle methods (MOC or RW), the concentration must be positive or zero as the number of particles in a cell, obtained by dividing the mass in solution by the mass of a particle, must be positive.

2.8 LAYERS CONFIGURATION

MARTHE can handle up to 999 layers in a system, the uppermost one being layer 1. The lateral boundaries of each layer can be different for each layer, without being superimposed. Some layers can locally disappear forming pinchouts. For instance, layers 3 and 4 can wedge out, making layers 2 and 5 in direct contact.

Some layers can be separated by semi-permeable formations denoted by “aquitards” or “semi-pervious layers”, which are ***not*** computational layers forming the grid, but this functionality is only used in specific systems. The following text thus concerns the grid cells of the general case, without “semi-pervious layers”.

To avoid any redundancy, the top of one layer is the bottom of the overlying one, we proceed as follows:

- The description of the system to be modelled is from top to bottom (in the direction of the precipitation or recharge) i.e. from the (highest) first layer to the lowest (last) in the hydrogeological pile.
- Each cell of a layer has a bottom elevation.
- The top of a cell is thus formed by the bottom of the immediately overlying layer.
- When a cell is exposed, there is no overlying layer and no bottom that can be used for confining its top. The software then uses the "topography". This "topography" is the upper boundary of the aquifer system. It concerns the total extension of the domain, formed by the combination, or projection, of all layers. This total extension is called the fictitious layer number 0.
- In fact, the "topography" does not actually coincide with the elevation of the surface topography but, in each cell, the elevation of the "upper boundary of the top aquifer layer".
- If the top aquifer layer is covered by an impermeable layer: the "topographic elevation" will be the base of this impermeable layer.
- Each time that an aquifer formation is exposed, it is this topography that serves as its top.

On Figure 15, layer 6 (light blue) wedges out to the east bringing layer 7 (dark blue) in direct contact with layer 5 (dark green). In addition, layer 5 is outcropping farther east.

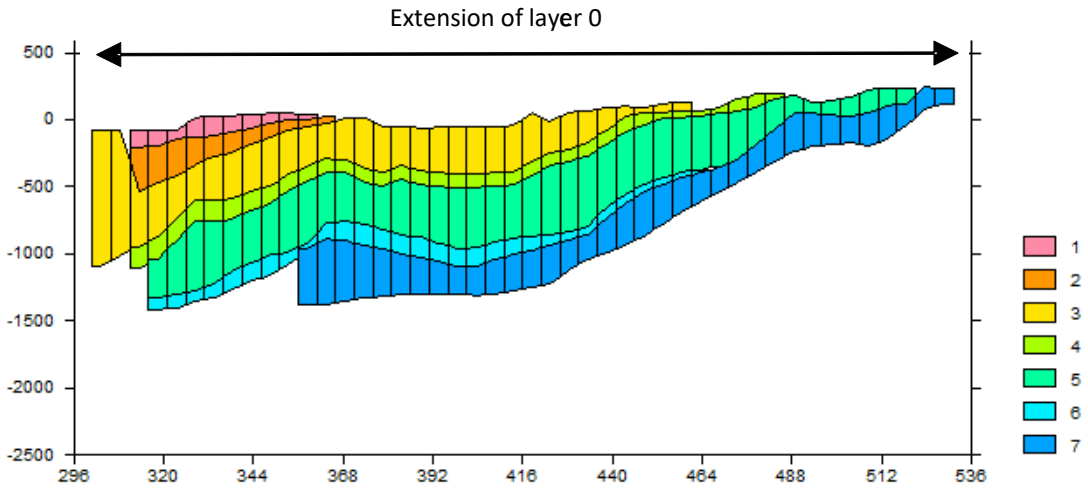


Figure 15 – A vertical cross-section through the 7-layer North-Aquitaine aquifer system. Layer 0 covers all other layers.

Figure 16 shows an example of a complex geometry, the aquifer layers being in white.

In the hydraulic conductivity data files, a positive value is assigned to hydraulically active cells. Conversely, we do not assign a value to cells outside the extension of a layer, the hydraulic conductivity of the missing cells being by default "0". MARTHE considers that two active superimposed cells are in hydraulic connection, whether or not they belong to consecutive layers. To simulate the wedging out of a formation and the induced 'short circuit' between surrounding formations, it suffices not to assign a hydraulic conductivity value to the cells corresponding to the formation gap: the over- and underlying active cells are then automatically put in hydraulic connection.

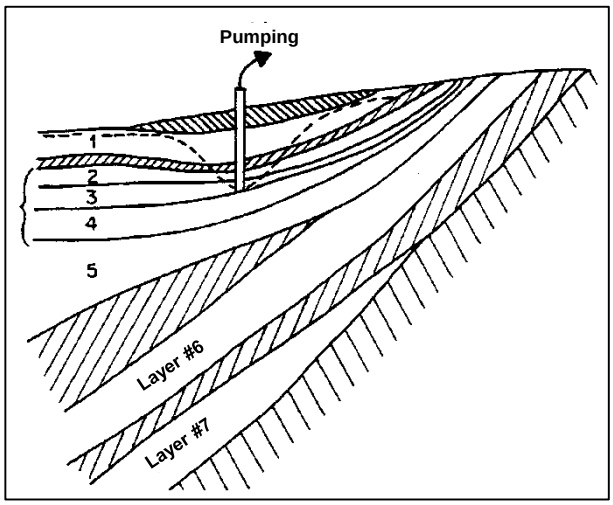


Figure 16 – Example of a complex aquifer system that can be modelled with MARTHE.

However, it is possible to indicate that, apart from the aquifer extension of a layer, the layer exists but is impermeable and isolates any layers above and below. The value code "9999" is then assigned to the hydraulic conductivity of such a zone. (Figure 17).

- A hydraulic conductivity equal to code value "9999" indicates a cell whose hydraulic conductivity is "infinitely small"; no hydraulic head calculation will take place in such a cell. For instance, in the eastern part of Figure 17, layer 3 first separates layers 2 and 4, and then layers 1 and 4.

- A hydraulic conductivity of 0 indicates a cell that doesn't exist and thus is taken as inactive in the model. For instance, in the western part of Figure 17, layer 2 has a hydraulic conductivity of 0, bringing layer 1 in direct contact with layer 3. The top of layer 3 then is automatically the bottom of layer 1

  In summary:

  - A hydraulic conductivity of 0 indicates a cell that does not exist. This is the generally preferred case.
  - A hydraulic conductivity of 9999 in a multilayer or 3D system isolates cells vertically (like "fresh granite" or completely impermeable clay), *which is relatively rare*.
  - In a single layer aquifer, an impermeable cell (hydraulic conductivity = 9999) is equivalent to a non-existent cell (hydraulic conductivity = 0).

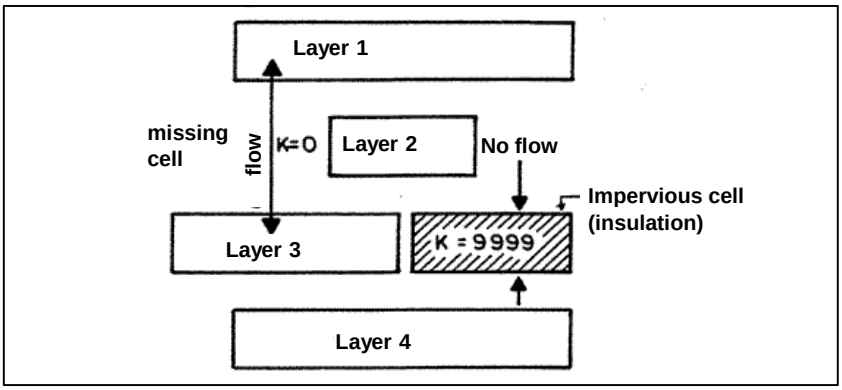


Figure 17 – Vertical cross-section, illustrating the difference between a hydraulic conductivity equal to 0 and a hydraulic conductivity equal to 9999.

Remark 1: For maximum clarity in this document, we always use the following non-geological terms:

- "top" for indicating the upper limit of a layer, and
- "bottom" for indicating the lower limit of a layer.

Remark 2: Layer 0 is a fictional layer on the surface of the modelled domain, whose extension covers the total area of all layers. This "number zero" layer is used for defining the outcrop conditions: topographic elevation, possibility of confinement or overflow, meteo zone numbers, soil zone numbers, irrigation zone numbers. In practice, in the files the layer 0 data are stored in layer 1, but they are relative to the total extension of the domain.

Remark 3: In a "vertical cross-section" or "pseudo vertical cross-section" grids, row 1 corresponds to this layer number 0 (Figure 18).

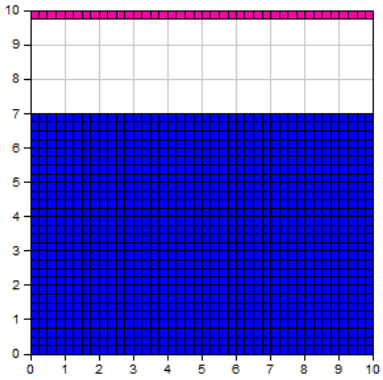


Figure 18 – "Vertical cross-section" or "pseudo vertical cross-section" grids:
Row 1, pink, corresponds to layer 0.
Soil Zones, Meteo Zone, Overflow-Index, etc. numbers must be defined in this row.

2.9 DATA IMPORT AND EXPORT

The cells of the modelled domain are automatically associated to geographic coordinates, which allows to easily import and export data sets.

2.9.1 Data import

It is possible to import the geometry resulting from third-party 3D geometric modellers or from geo-modelling software such as GDM ®, Multilayer ®, EarthVision ®, or Eclipse/Petrel ®. (Figure 19)

WinMarthe: "Tools" ➔ "Others" ➔

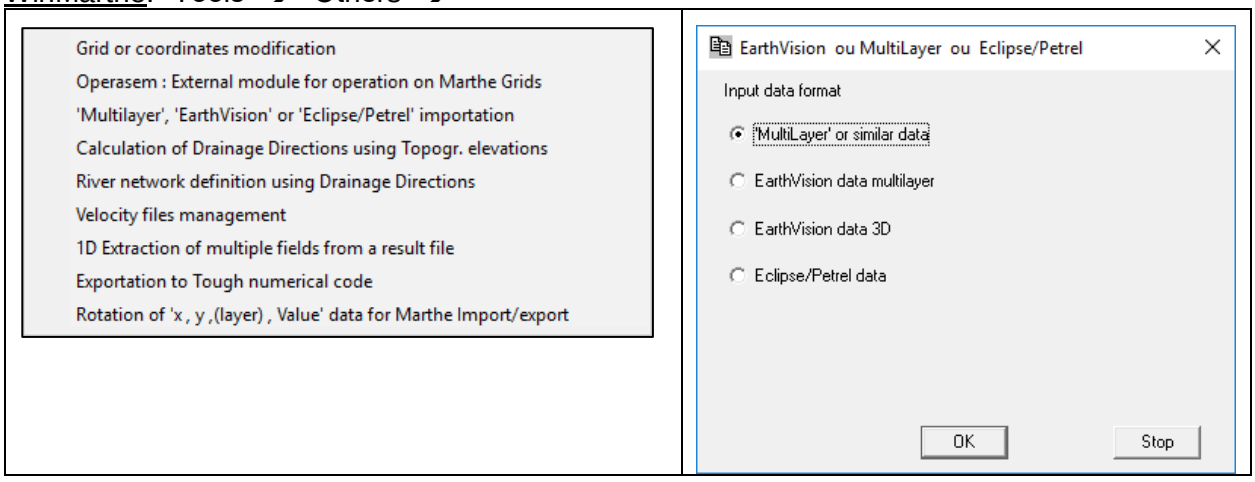


Figure 19 – Importing data from a geo-modeller (Multilayer, EarthVision, Eclipse/Petrel).

It is also possible to import polygons or background geometrical features in the "mif" format of QGIS ® or Mapinfo ®, or of the "bln" format of Surfer® in the "Polygons management" module activated by the WinMarthe's button  .

If a regular single layer grid is used, it is possible to directly import fields resulting from ArcGIS® (in text format [.asc]), or the grids generated by Surfer ®, file extension [.grd]. Only the files in text format (Ascii) can be imported (Figure 20).

The following restrictions apply:

- ArcGIS [.asc] files: the grids are composed of regular square cells.
- Surfer [.grd] files in Ascii format: the grids consist of regular rectangular cells, all rectangles being the same.

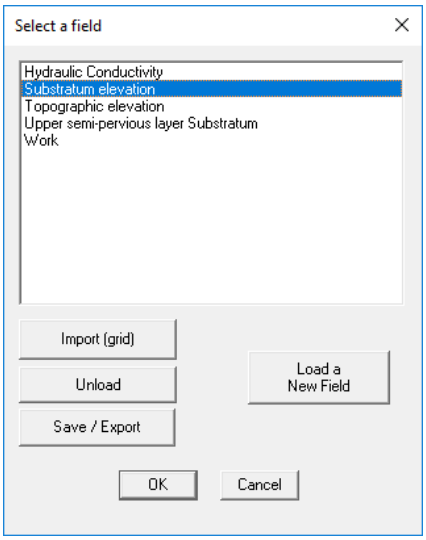


Figure 20 – Importing [.asc] or Surfer® files in the Marthe grid.

From within the WinMarthe pre-processor, we can import the data in the **(X Y value)** or (**X Y Layer value** formats: WinMarthe: "File" ➔ "Import values in the current field" ➔ "(x, y, value) or (x, y, layer, value)".

2.9.2 Data export

As the cells of the modelled domain are associated with geographic coordinates, we can superimpose the initial data and the simulation results onto cartographic reference backgrounds. The results of the simulation are saved in "text files". These can be graphically shown with the WinMarthe post-processor, or exported for visualization with an external graphical presentation software.

The procedure is shown in Figure 21:

WinMarthe: "File" ➔"Export the values of the current field" ➔

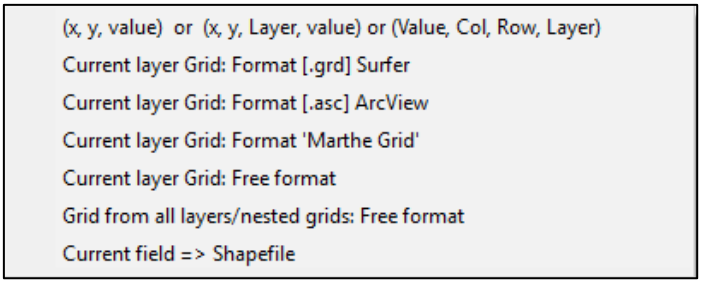


Figure 21 – Exporting the current field in WinMarthe

The current field can be exported as a:

- Single "shapefile" file (all layers and nested grids) for direct visualization with QGIS ® or ArcGIS ® software (any grid type);
- [.grd] file for visualization with Surfer ® software (current layer; a grid composed of only regular rectangular cells);
- [.asc] file for visualization with QGIS ® or ArcGIS ® software (current layer; grid composed from only regular square cells).
- "x, y, value" or "x, y, layer, value" or "value, column, row, layer" files.

The simulated fields can also be exported with the dedicated exporting facilities:

- WinMarthe:  : as a single "shapefile" file for direct visualization with QGIS ® or ArcGIS ® (or with mif/mid files for visualization with Mapinfo ®);
- WinMarthe:  : in 2.5D representation with a VRML viewer;
- WinMarthe:  : in 3D representation with 3Dview ®, VTK, Paraview ®, Tecplot ®.

The "shapefile" file export functionality is described in a dedicated report BRGM/RP-69210-FR (Thiéry, 2020c).

Time series of the simulated fields in specific cells can also be saved. The files containing these series, name extension [.prn], can be imported directly into Excel ® or equivalent. The values of these [.prn] files are always separated by "tabulations", never by "commas". In addition, decimal numbers are represented by "decimal points", never by “commas”.

2.10 RUNNING AND STOPPING SIMULATIONS

After preparing the data with the WinMarthe pre-processor, the simulation is run by clicking on the 

button, located on the first row of the toolbar located at the bottom of the main window. It is also possible to run the simulation, from outside WinMarthe, directly from the "Start menu", by invoking the "RunMarthe" command. If you have created a "Marthe_R8" button on the desktop, you can run the simulation by double-clicking directly on this button.

Directly running the computational engine outside WinMarthe frees computer memory to carry out the simulation, which is useful and recommended for large grids associated with simulations taking extended CPU times.

2.10.1 Running in "batch" mode (advanced users)

For special use, to link successive simulations for instance, MARTHE can be run in batch mode. For that, one must create a small file script ([.bat] file), for instance a file called "Run_my_Simul.bat" containing the following line:

If you are in the folder containing the project files:

"%bin_Marthe%\marth_R8.exe" My_Project.rma

Don’t forget the quotation marks on either side of: “%bin_Marthe%\marth_R8.exe”.

"**bin_Marthe**" is the environmental variable corresponding to the installation file containing the executables of MARTHE. This "environmental variable" is automatically created during the installation of MARTHE

Or, if you run the simulation from another folder:

"%bin_Marthe%\marth_R8.exe" My_File\My_Project.rma

(or)

"%bin_Marthe%\marth_R8.exe" My_Project.rma * My_File

Don't forget the quotation marks on either side of: "%bin_Marthe%\marth_R8.exe".

Don't forget the asterisk "*****" between the project name and the file name).

N.B.: A file name must be defined between quotation marks when it contains spaces. In any case, names with spaces are *not* recommended.

If one wishes to launch several successive runs in batch mode in the same file, for instance:

"%bin_Marthe%\marth_R8.exe" Project_1.rma

"%bin_Marthe%\marth_R8.exe" Project_2.rma

it will be necessary to rename the result files with a generic name between two runs, such as:

```
"%bin_Marthe%\marth_R8.exe"   Project_1.rma
Ren flowbalance.txt           flowbalance_1.txt
Ren gridsimul.out             gridsimul_1.out
Ren historiq.prn              historiq_1.prn
REM
"%bin_Marthe%\marth_R8.exe"   Project_2.rma
Ren flowbalance.txt           flowbalance_2.txt
Ren gridsimul.out             gridsimul_2.out
Ren historiq.prn              historiq_2.prn
```

2.10.2 Running in automatic "batch" mode (advanced users)

For a special use in automatic "*batch*" mode, it is possible to add to the project folder a file called: **nom_proj_marthe.defrma**" (or **nom_proj_marthe**").

Remark: The name "*nom_proj_marthe.defrma*" (or "*nom_proj_marthe*") is a fixed name that is identical in the French or the English version of the MARTHE code.

This file "nom_proj_marthe.defrma" must contain only one or two lines:

- Line 1: The name of the project file to be used, such as "my_project.rma".
- Line 2 *optional*: The name of the resulting project file at the end of simulation, for instance "Final_State_For_Restart.rma".
- When Marthe is launched, it runs automatically without any keyboard interaction.

This option is only possible with the "batch" version of Marthe (non-interactive version).

Example of file "nom_proj_marthe.defrma":

```
Automatic_Run_Albian.rma
Final_State_For_Restart.rma
```

2.10.3 Halting a running simulation

When the simulation is complete, the computational engine stops and the user is returned to the WinMarthe pre-processor, if the simulation was run from WinMarthe.

Exceptionally, one can halt a running simulation, in case of problems. To that end, keep pressing the "F9" key. After few seconds a dialog box appears asking to confirm that we want to stop the simulation and cancelling out from the computational engine.

3 Data organization

Hereafter, we will make a semantic distinction between:

- A "spatialized field", or "gridded field", for instance hydraulic head or hydraulic conductivity, with a value in the centre of each cell of the domain.
- A "parameter", such as the number of time steps or the flow rate unit, which is not spatialized.

3.1 THE DIFFERENT DATA TYPES OF THE MARTHE CODE

MARTHE handles several types of data:

- Constant options or parameters;
- Data from gridded fields;
- Other data that are neither constant, nor from gridded fields.

3.1.1 Constant options or parameters

Such constant options or parameters are for instance:

- The code id (or name) of the solver selected for simulating groundwater flow;
- The maximum possible number of iterations used by the solver;
- The tolerance to achieve convergence;
- A logical value (0/1) to choose whether pathlines are calculated or not;
- etc.

Because there are many parameters (several hundreds), they are grouped in several sections headed with paragraphs in a text file called "General Parameters" with the extension [.mart].

There are also constant options or parameters in the file "Parameters for automatic optimization or calibration".

3.1.2 Data from gridded fields

These are the data from all cells of the domain for a given field. For instance, the initial hydraulic head data, the bottom elevation data, the initial concentration data, etc.

In the MARTHE 7.8 version, more than 200 fields of different data are supported.

- Only the fields needed for the selected model type must be defined. For Instance, it is neither necessary to define a concentration if one does not calculate mass transport, nor to define salinity if one does not consider density effects.
- The data for each field are stored in a separate file. For instance, the hydraulic head field is stored in an extension file [.charg], the hydraulic conductivity field in an extension file [.permh], etc. Such "extensions" of the file names are recommended as they facilitate the identification of these datasets. Though they are the ones used by default, they are not mandatory.
- By default, all fields are initialized at zero. It is therefore not necessary to create a file for a field whose values are all equal to zero.
- The names of all data files are grouped in MARTHE's "Project file", which is simply a "directory" containing the list of file names for each data field.
- It is not necessary to create a file for a field whose domain cells have the same value. Just give it a fictitious name in the file project, like "= value". For instance, if all cells have a specific yield coefficient of 5 (in user-input units), we can give a dummy file name "=5", (without the quotation marks).

- For each non-uniform spatialized field, the "Grids file" contains the data, layer by layer, from the top layer # 1 to the last layer at the bottom, (like the pages of a closed book). The data of each layer appear as a "grid" consisting of NR rows of NC columns each.
- The data of each field can be modified, in part or in whole, at any time step. For instance, one can modify pumping rates or rainfall, but also hydraulic conductivity, river lengths, river bed hydraulic conductivity, porosity, boundary conditions, etc.

3.1.3 Data that are neither from gridded fields nor constant

These are non-gridded data files. In particular, these files contain:

- The description of the end dates of all time steps, and any modifications of the associated fields: file "Time Steps".
- The description file of aquifer layers: file "Aquifer layers and nested grids".
- The list of "Cells with time series", i.e. cells for which the simulated values of some fields are recorded at each time step during a transient simulation: file "Cells with time series", extension [.histo].
- The list of starting points of flow pathlines: file "Pathline departures".
- River or drain connections: file: "River and Lakes tributaries connection tree" or "Drain tributaries connection tree".
- The user profile: file "User profile".
- The file of impervious connections.
- etc.

3.2 THE MARTHE FILE PROJECT

The MARTHE "file project", extension [.rma], assembles the names of all files used for simulation:

- The file of "General Parameters".
- The file of "Time Steps".
- The files of gridded fields.
- The files of specific non-gridded data.

3.3 MODIFYING THE DATA OF A GRIDDED FIELD

The data of a gridded field can be modified, in part or in whole, at any time step. These changes may also appear in time step zero, that is, before the start of simulation.

Data can be changed:

- By grid,
- By layer: we assign a uniform value to a given layer,
- By zone: we assign a uniform value to a given zone,
- By cell: we assign a uniform value to a given cell or a group of cells ("block of cells"),
  - A "block of cells" is a unit of adjacent cells, in a "parallelepiped" defined by a range in rows, a range in columns and a range in model layers. For instance: columns 7:9, rows 12:15, layers 3:7, or: columns 7:9, rows *, layer 2.
  - The number of rows "12:15" means "from row # 12 to row # 15".
  - The row number "*****" signifies "all rows".
- By list of cells we assign different values to a list of cells, defined with no particular format, by their column-, row-, layer- or nested grid number, or defined by their X,Y coordinates.

Such data modifications can be introduced into the "time step" file, extension [.pastp].

They can also be introduced at the end of the "General Parameters" file, extension [.mart], in the paragraph "Initialization before simulation".

3.4 DIRECT DATA DEFINITION IN A GRIDDED FIELD, WITHOUT CREATING A FILE

To define a simple gridded field, it is not necessary to create a grid file. Simple fields can be directly defined as modifications, placed:

- At the end of the "General Parameters" file [.mart] in paragraph "Initialization before simulation",
- Or at the start of the "Time steps" [.pastp] file, at time step zero.

Even though the effect is the same, it is advised to define:

- Physical data (hydraulic conductivity, porosity, storage coefficient, boundary conditions, concentration and initial temperature):
  - At the end of the "General Parameters" file,
  - Or, if necessary, in a file "Initial modifications before simulation".
- Forcing data (rainfall, evapotranspiration, pumping discharge, etc.):
  - At the beginning of the "time step" file, at time step number zero.

N.B.: **Only gridded data in grid files are graphically viewable by the WinMarthe pre-processor**.

Any gridded-data changes introduced in the "General Parameters" and "time step" files, are formatted by the "Non-meshed parameters" pre-processor and used by the MARTHE computational engine, but they cannot be viewed graphically.

N.B.: The hydraulic conductivity field, even if it is simple or uniform, must be defined in a grid file. This grid file defines the number of rows and columns of the grids, as well as the heights of the rows and the widths of the columns.

If we define in several places gridded data relating to the same cells, only the last definition will be taken into account.

When running the simulation, the order of definitions considered is as follows:

- MARTHE starts by reading the data fields in the files whose names are given in the [.rma] project file. (These are the fields that can be viewed with WinMarthe).
- MARTHE then reads (in this project file) the name of the "General Parameters" [.mart] file. It then reads the paragraph "initialization before simulation" at the end of this [.mart] file. It then considers any field changes assigned to certain cells. These values then replace the values that could be defined in the data files for each field.
- MARTHE then reads (in the project file) the name of the "time Steps" file [.pastp], and reads any field changes assigned to certain cells. These values then replace the values that could be defined in the data files for each field, in the "initialization before simulation" paragraph at the end of the [.mart] file.

In summary, the order of assignment is:

- Reading the data files for all fields and for all cells.
- Reading any data modifications in the "initialization before simulation" paragraph of the [.mart] file.
- Reading any data modifications of the time step 0.
- Calculations with modifications of specific data during the following time steps.

Assignments are done sequentially. If we define several times the value of a cell, the last definition will prevail.

For instance:
/PERMEABILITY/LAYER C= 3:7 V = 0.1; (we assign *value 0.1 in layers 3 to 7)*

Then:
/PERMEABILITY/CELL C= 25L= 63P= 5V= 0.5;
(Permeability *in the cell: column 25, row 63, layer 5: => value = 0.5*)
("C=" = Column, "L=" = Row, "P=" = Plan, or "layer")
⇨ Value 0.1 of cell *column 25, row 63, layer 5* was replaced by value 0.5.

However:
/PERMEABILITY/CELL C= 25L= 63P= 5V= 0.5;
(Permeability *in the cell: column 25, row 63, layer 5: => value = 0.5*)

Then:
/PERMEABILITY/LAYER C= 3:7 V= 0.1; (we assign value *0.1 to all cells of layers 3 to 7)*
⇨ Value 0.5 of cell *column 25, row 63, layer 5* is **overridden** by the more general value 0.1.

3.5 EXAMPLES OF MODIFICATION OR CREATION OF A GRIDDED FIELD, WITHOUT FILE GENERATION

Example 1: To define a discharge field with only one pumping well of value 50 in a given cell, and with fixed hydraulic heads (discharge = 9999) in row 1.

/DISCHARGE/GRID: = 0
(*Discharge in the entire domain (all "grids"]: value = 0*)
(*"N" means name of the grid file: here dummy file: uniform grid = 0*)

/DISCHARGE/CELL C= 25L= 63P= 1V= -50;
(*Discharge in the cell: column 25, row 63, layer 1: value = -50*)
("C=" = Column, "L=" = Row, "P=" = Plan, or "Layer")

/DISCHARGE/CELL C= *****L= 1P= 1V= 9999;
(*Discharge: in the cells: all Columns, Row 1,*
Layer 1, value = 9999)
(***"*" means "all", here all columns.***)

These "modifications" are introduced automatically with the "Non-meshed parameters" pre-processor that automatically manages formats. It is ***strongly discouraged*** to introduce such modifications with a text editor. This is because, such data are formatted.

Example 2: To define a uniform hydraulic conductivity value in different formations:

/PERMEABILITY/GRID N = 1 (*we start by assigning value 1 to the entire grid*)

/PERMEABILITY/ZONE Z = 43:63 V= 6; (*we assign value 6 in zones 43 to 63)*

/PERMEABILITY/LAYER C = 3:7 V= 0.1; (*then we assign value 0.1 in layers 3 to 7)*

Example 3: To define discharge values per "list of cells".

The list of cells is in a free format, such as:
- value, Column, Row [Layer, Nest]
- x, y, value
- x, y, Layer, value
- x, y, z, value

The shape of the data in a "list of cells" file must be uniform. This shape is defined in MARTHE by a parameter managed by the pre-processor.

Each line of the "list" file corresponds to a cell. For instance, for the format "Value, Column, Row, Layer" the file has the following shape:

10 10 7 1 (*value 10 in the cell: column 10, row 7, layer 1*).
10 5 14 1 (*value 10 in the cell: column 5, row 14, layer 1*).
9999. * 21 1 (*value 9999 in the cells of **all** columns, of row 21, layer 1*)

3.6 THE FILES THAT ARE ALWAYS NEEDED FOR A SIMULATION

To run a simulation, some files are mandatory. Their number depends on the features which are used for the simulation. For instance, a river network with mass transport and thermal transfer coupled with a hydro-climatic evaluation will require far more files than a simulation of just the hydraulic heads in a single layer aquifer.

The names of all files that will be used for the simulation (with a few exceptions) are listed in MARTHE's "project file". This project file is automatically created by the WinMarthe pre-processor. It has the automatic extension [.rma] (**r**epertory for **ma**rthe). It is a text file that could potentially be modified by an external text editor, if necessary.

The project file may contain data-file names that will not be used. The presence of a file name in the file project is usually not enough for activating a simulation feature. It is necessary to activate this feature by a parameter from the "General Parameters" file.

For instance, adding a concentration file name into the project file does not directly imply a subsequent mass transport simulation.

The simplest simulation that can be performed is a “hydraulic calculation” (also called “hydrodynamic calculation”) to obtain the hydraulic head and discharge fields in an aquifer system. To perform such a simple simulation, the necessary files are at least the following:

- Some files of spatialized fields defining the geometry, including at least:
  - A gridded "Hydraulic conductivity" that defines in particular the extension of the grid, the cell dimensions, and the aquifer extension within the grid. This "Permeability" file also enables automatic detection of active and inactive cells.
  - A gridded “Bottom elevation” file of the modelled layers.
  - A gridded “Topographic elevation” file of the elevation of the outcropping layers at the top of the domain.
- A "(Nested) aquifer layers" file for describing the number of layers and the type of grid. This file is automatically created when creating a new project in WinMarthe. Afterwards, it can be modified with the "Non-meshed parameters" module.
- A “User profile" file is an optional ‘comfort’ file for facilitating the simulation of simple problems. This file is created and modified with the "Non-meshed parameters" module.
- A “General Parameters” file for selecting the program features, and defining the options and constant non-spatialized parameters. This file is created and modified with the "Non-meshed parameters" module.
- A file describing the “Time Steps” of the model. This file can be created and modified with the "Non-meshed parameters" module. It allows defining the dates of the time steps, and their duration. It also describes the actions to be triggered during these time steps:
  - Occasional data modifications at the start of a time step, such as modification of pumping discharge, modification of precipitation flux, etc.
  - Saving some simulated fields at the end of a time step, such as saving the amplitude of the flow velocity, saving the simulated hydraulic heads, etc.

- A file for defining “Cells with Time Series” is optional and useful for saving the evolution histories of certain simulated fields in cells of particular interest, to follow their temporal evolution, on a time step basis.

  This file can be created and modified with the "Non-meshed parameters" module.

4 Getting started

4.1 DESCRIPTION OF THE MODEL DOMAIN AND OF THE REQUIRED DATA

We consider an unconfined aquifer system of infinite extension in which we want to simulate the influence of a pumping well for a time span of 120 hours.

The aquifer characteristics are as follows:
- Permeability = 10^{-4} m/s over the major part (0.1 10^{-4} m/s in a restricted zone at the north-eastern side),
- Specific yield = 5%,
- Hydrogeologists storage coefficient = 5 10^{-4} (dimensionless),
- Elevation of the topographic surface = 10 m,
- Elevation of the bottom = 50 m (60 metres of thickness),
- Initial hydraulic head +0 m (so at 50 metres above the bottom).

The pumping characteristics are as follows:
- Pumping well flow rate = 100 m^3/h,
- Duration of pumping = 120 hours.

Selecting the domain to be modelled and the boundary conditions:

The aquifer has an infinite extension, but we opt for modelling a square domain in which the boundaries are placed far away, such they are not significantly affected by the drawdown.

The theoretical range of pumping in an infinite medium is greater than the following “Radius of action” **R_a** value:

$$R_a \geq 1.5 \sqrt{t \cdot \frac{T}{S}}$$

With:

t = 120 h = 4.32 10^5 s,
T = 50 m x 1 10^{-4} m/s,
S = 0.05,

we get: $R_a \geq 312.8$ m.

As this is a minimum theoretical value, we increase it and choose a radius of action equal to 510 m, hence the square to be modelled is 1020-m long at each side. The pumping well is placed in the middle of the domain.

A grid of 51 columns x 51 rows of 20 m square cells is adopted.

The domain boundaries are not reached by the pumping effect after 120 hours, so any type of boundary conditions can be chosen. As a demonstration, fixed hydraulic head boundaries are established on the left and bottom sides (west and south), and sealed boundaries are assumed on the right and top sides (east and north).

4.2 CREATION OF THE PROJECT

Double-click on button  to start WinMarthe, and then on the following button  , or on "File ➔ New", to create a new model.

In the new window "Definition of the MARTHE file project", clicking the button allows selecting the file where the model will be saved.

The button then allows creating a specific file. We select, for instance, the "Didactic" folder where all model files will be stored.

Give a file name for the model to be created (automatic extension .rma), for example the name **Didact_Monocar** (in the **Didactic** folder), and a dialog box then opens for defining the grid to be created (Figure 22):

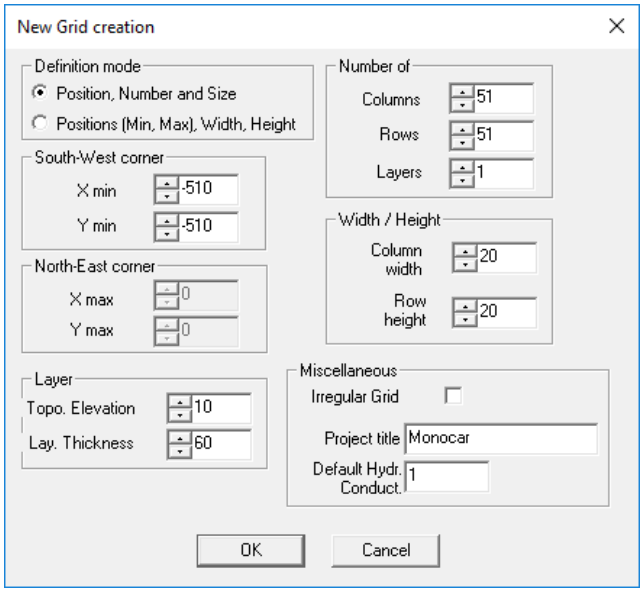


Figure 22 – Creation of the grid.

Define the coordinates of the lower left corner (-510 m, -510 m), the numbers of columns and rows (51 and 51), with a single layer and the cell dimensions (20 m, 20 m). We define the topographic elevation at +10 m, and the thickness at 60 m (or a bottom elevation at -50 m)

Call the project ***Monocar*** (in the "Various" box, lower right).

Keep the default Hydraulic conductivity = **1** (i.e. the uniform **hydraulic conductivity** = 1) as we will select a hydraulic conductivity unit equal to 10^{-4} (1e-4) in the "General Parameters" file.

Click on **OK**: the regular grid has been generated and is shown on screen (Figure 23, left part). The field on the right of Figure 23 is the hydraulic conductivity field.

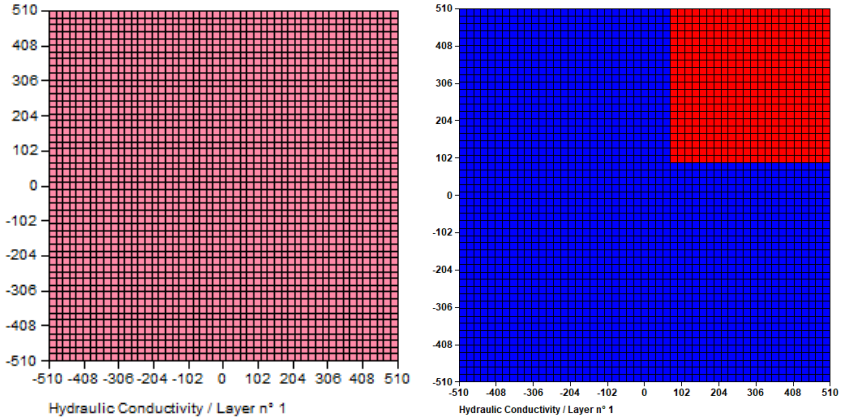


Figure 23 – Left: grid. Right: Selected zone in the hydraulic conductivity file.

In the hydraulic conductivity field, select columns 30 to 51 of rows 1 to 22. For this, we use the "select by rectangle" button; if necessary, this selection can be done in several steps with corrections. The selected cells appear in red: Figure 23, right side.

Then use button "Assign value to selected cells" for attributing the value **0.1** (10^{-4} m/s) to the selected cells: Figure 24.

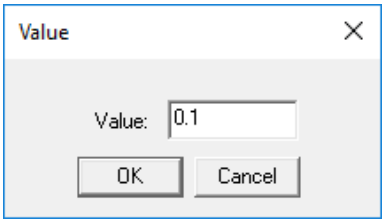


Figure 24 – Assigning a value to selected cells.

4.3 DEFINITION OF DOMAIN BOUNDARIES

To set an impervious boundary on the edge of the domain, there is nothing to do because it is the default option.

To set a limit for the prescribed hydraulic head (also called "fixed potential boundary"), the cells of this boundary must be assigned a dummy flow rate value code 9999; the prescribed head is then equal to the head declared in the "Hydraulic head" field, unless it is changed afterwards.

To define boundaries with a fixed hydraulic head, proceed as follows: select the field "Flow Rate" ("F3" on toolbar at the top), and then click on the "Load New Field" button: it is called "Aquifer Flow" and accepts the creation of this new field.

To assign 9999 values, we use button "Selection by column" (bottom toolbar). Double-click on column 1 (left) that is selected (all layers) and changes to red. With button , the 9999 value is assigned. This column now become grey as value 9999 is a "code" value.

To assign value 9999 in the last row (row 51), double-click with button on the last (lower) row, and use button for assigning the value 9999.

The obtained flow rate field is shown on Figure 25.

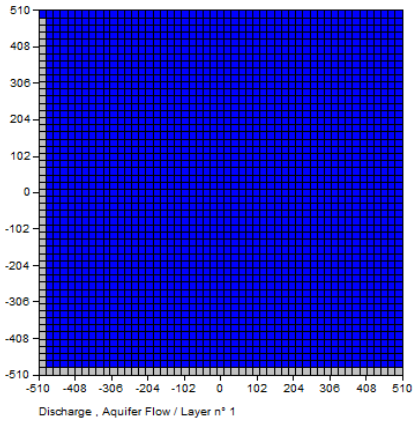


Figure 25 – Flow rate field. Prescribed hydraulic heads are shown on the left and lower boundaries.

4.4 DEFINITION OF GRIDDED FIELDS

The values must be defined of:

- The specific yield coefficient (5% in the entire domain): Select a user unit in "%" in the "General Parameters" file.
- The confined storage coefficient ($5x10^{-4}$ in the entire domain): Select a user unit in "10^{-4}" in the "General Parameters" file.
- The initial hydraulic head value, which is 0 m. As this is the default value for all fields, there is nothing to do in this case.

Specific yield coefficient:

Select the "Specific yield coefficient" field ("F3" on top toolbar), then click on the button "Load a new field" and select "Specific yield coefficient".

This selects all cells of the domain, for which we can use:

- Button  : selects entire domain,
- Or button  : selects current layer,
- Or the keyboard shortcut "Control-A" (for: control-All)

All cells are now selected and appear in red: Figure 26.

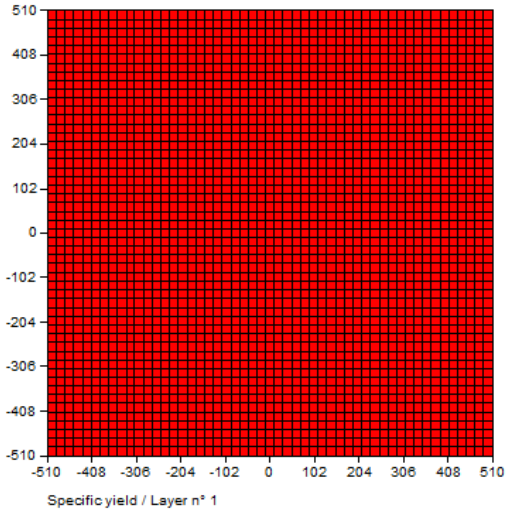


Figure 26 – Selection of all cells to assign them a uniform "Specific yield coefficient" value.

Using the preceding method, we now assign the value 5 ("%").

Confined storage coefficient.

Proceed in the same manner as above for the confined storage coefficient: Assign the value 5 ("10^{-4}") to all cells of the domain.

At this stage, it is recommended to save all data entered in the model by clicking on button  of the top toolbar.

4.5 DEFINITION OF "NON-MESHED PARAMETERS"

Access to the modelling "Non-meshed parameters" module is via button  on the bottom toolbar. This shows the general menu in Figure 27.

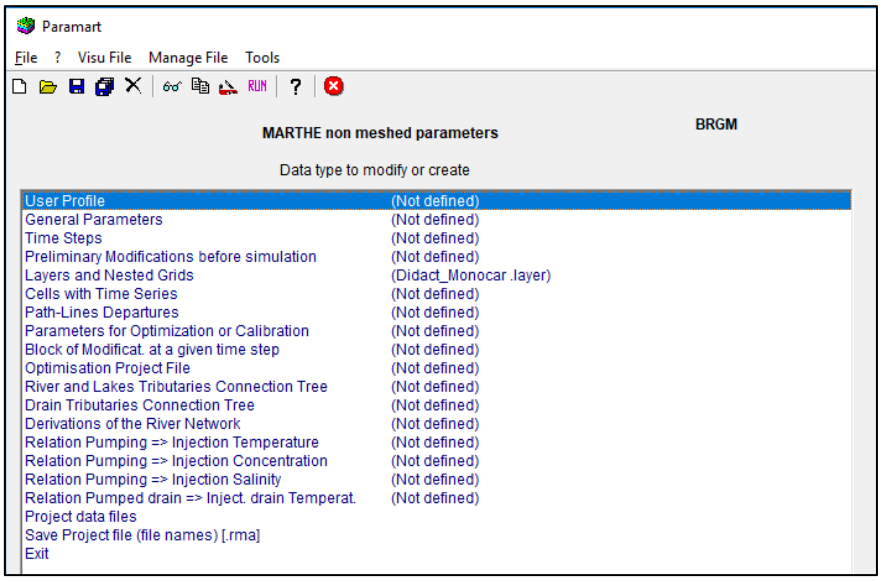


Figure 27 –General menu for defining non-meshed parameters.

4.5.1 User profile

Double-click on the first line: "User Profile". Select “Pre-processor” then “Create a new ‘User Profile’ file (as no ‘Profile’ has been defined yet): Figure 28.

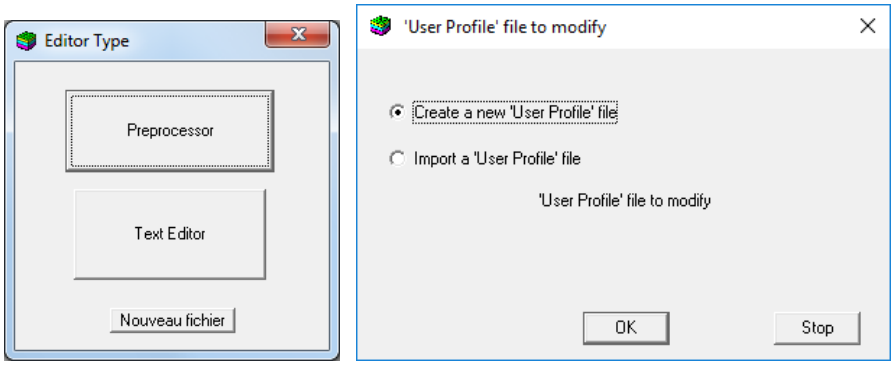


Figure 28 – Creation of a new "User Profile".

In the definition window that appears, select only (giving value 1): "Transient state" (Figure 29).

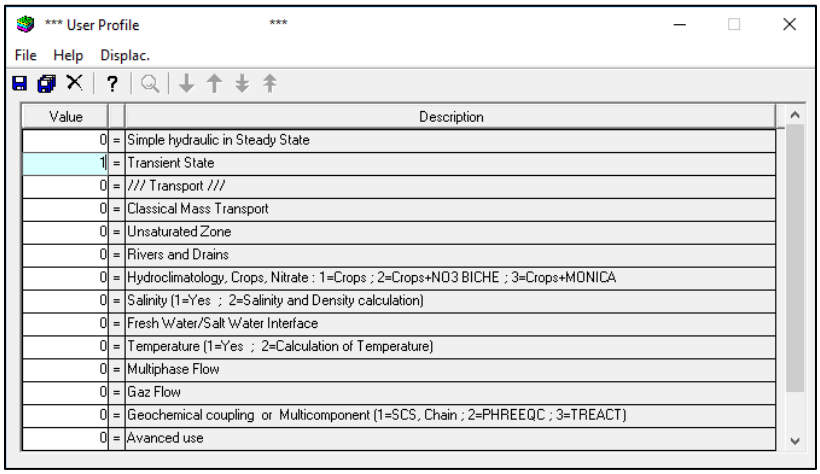


Figure 29 – Selecting options of the "User Profile".

4.5.2 "General Parameters" File

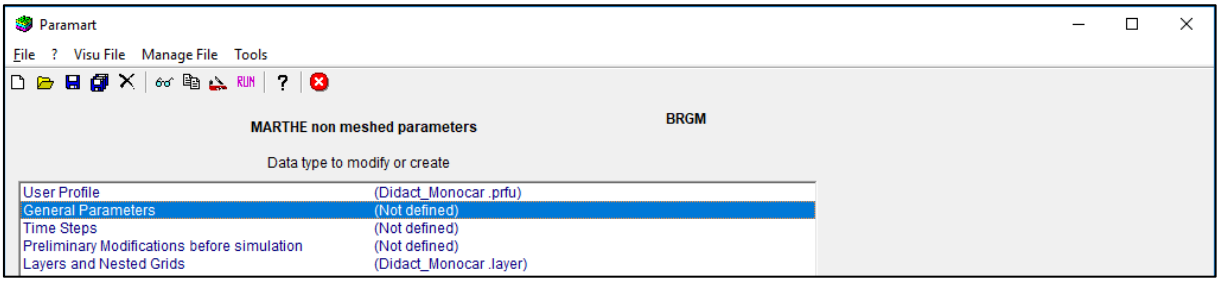


Figure 30 – Selecting the "General Parameters" file.

In the general definition menu of MARTHE's "Non-meshed parameters", select line "General Parameters" (Figure 30). As before, create a new file. Only a few options are defined in the paragraphs "Backup and Controls", "Control of hydraulic resolution of groundwater" (only three parameters to be defined), "Data Units" and "Initialization before simulation".

Figure 31 presents an excerpt from the "General Parameters" file resulting from a definition of parameters with the pre-processor.

To perform "Change Data Before Simulation", in the General Parameters file, for instance to set a point value of "Well Radius" equal to 0.2 m in the pumping cell (the cell of column 26, row 26), proceed as shown in Figure 32 to Figure 34.

N.B.: One could have simply created the "Well Radius" field and introduced the value 0.2 into the appropriate cell of the grid pre-processor, but another method was used here to show how to introduce "point changes".

```
Monocar
 #<V7.8># --- End of Header lines --- ; Do not modify/delete this line
 *** Outputs and controls                                    ***
       1 = Detailed listing (1=Yes; 0=No)
       1 = Listing of all cells data read
 *** Control of Aquifer Hydraulic solving process ***
      20 = Maxi number of iterations for time steps after time step #°0 (transient)
    5e-6 = Average hydraulic head deviation between 2 iterations for convergence
       0 = Coefficient of sub-relaxation of calculation [Def=0 => Sub-relaxation step]
Transient = Hydrodynamic state [0= Transient ; 1=Steady]
 *** Data units                                              ***
    1e-4 = Aquifer Hydraulic Conductivity   unit in m/s (or m2)
    m3/h = Flow (Discharge, Yield)        unit in m3/s (Kg/s for Gas flow)
    1e-4 = Confined storage coefficient   unit in [-] or [m-1]
       % = Specific yield                 unit in [-] ['%' when in %]
    hour = Time unit (for model time steps)
       % = Porosity unit = Water content in [-] ['%' if in %]
 *** Initialization before simulation                        ***
  /WELL_RADIUS/CELL        C=     26R=     26L=      1V=       0.2;
  /*****/***** End of Initialization
 *** End of General Parameters file        ***
```

Figure 31 –"General Parameters" file of the detailed application example.

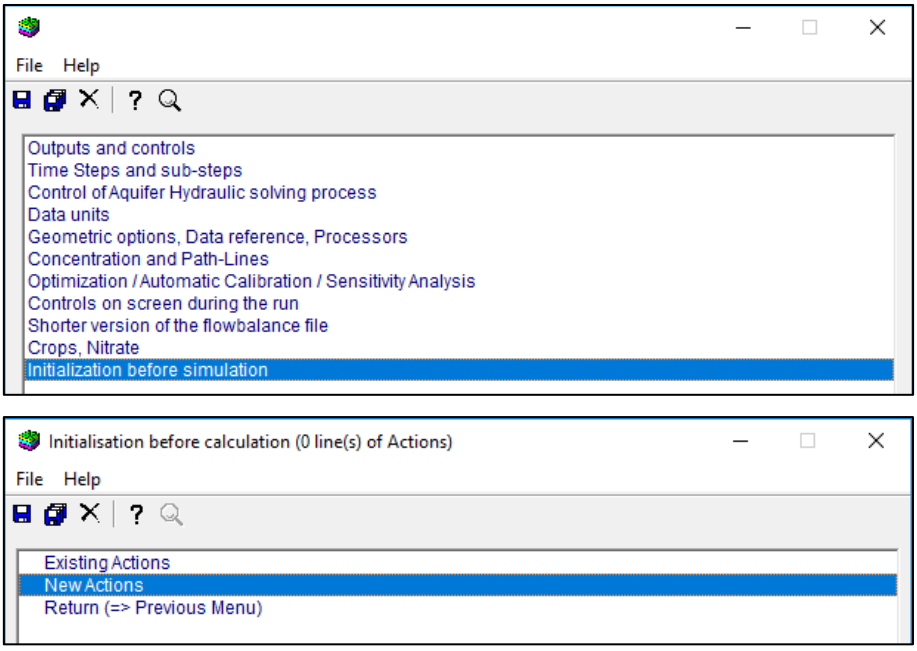


Figure 32 – Selecting the paragraph "Initialization before simulation", choose "New action".

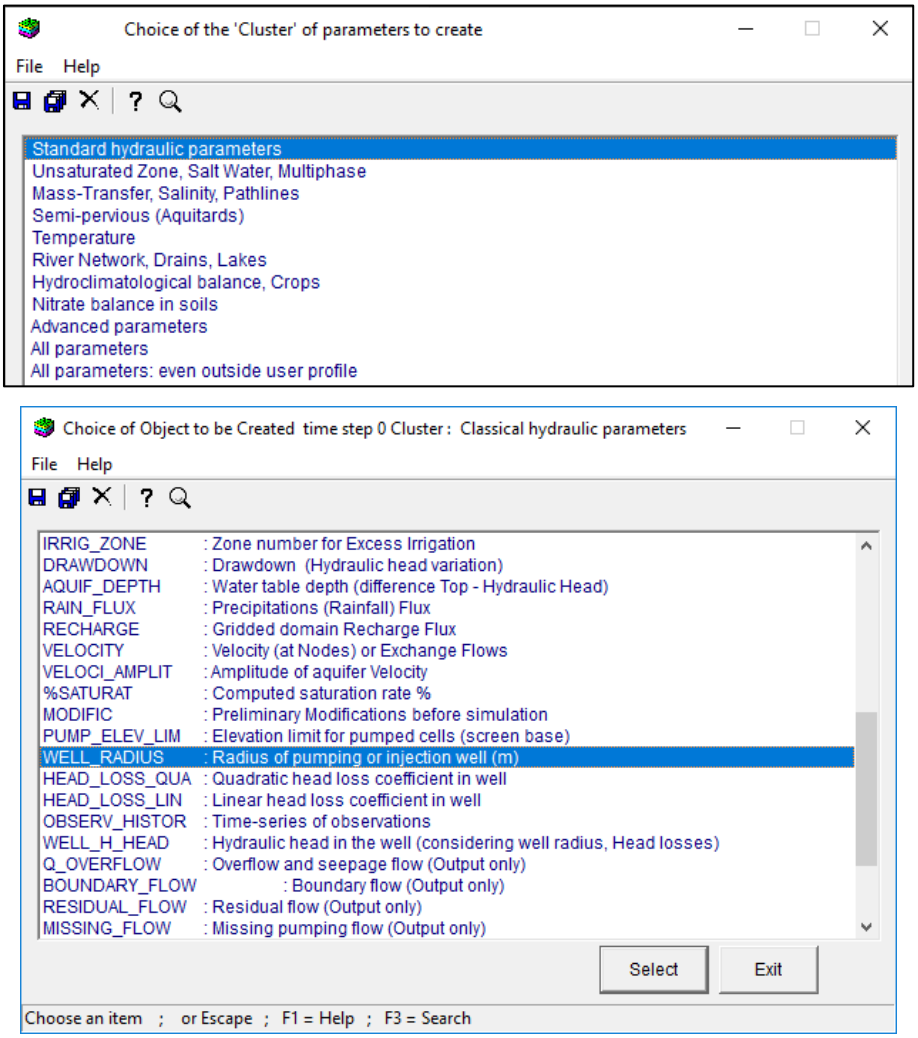


Figure 33 – Selection of the cluster "Standard hydraulic parameters", followed by selection of the field "Well radius".

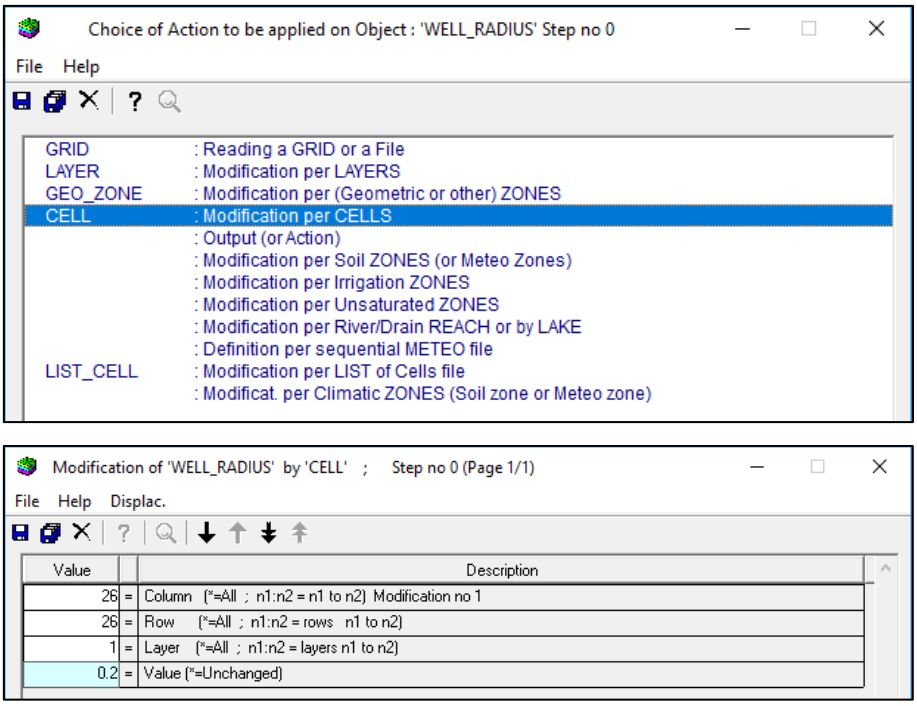


Figure 34 – Selection of a "Modification by Cells"
and introduction of the value 0.2 m in the cell of column 26, row 26, layer 1.

4.5.3 "Time step" file

In the general menu for defining "Non-meshed parameters", select "Time steps" (Figure 35).

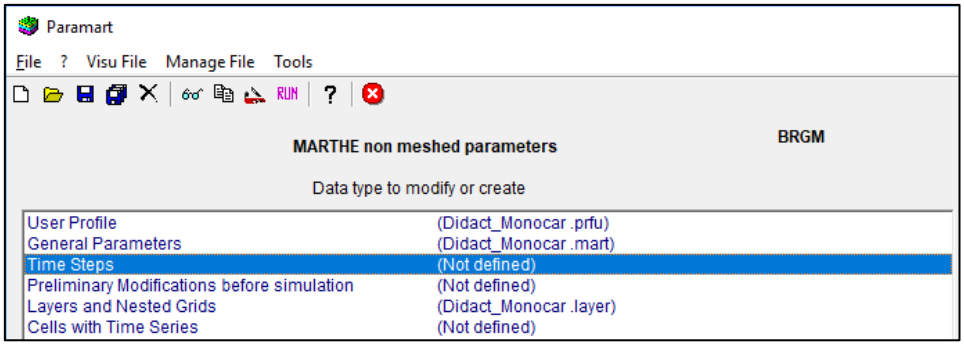


Figure 35 – Selection of the "Time step" file.

As before, create a new file. Accept default value ***0*** as starting date of the simulation. Then request Automatic creation of 15 time steps for the model (Figure 36). Indicate that time steps have a non-uniform duration and define the end of the time steps with the integrated spreadsheet (Figure 37 and Figure 38).

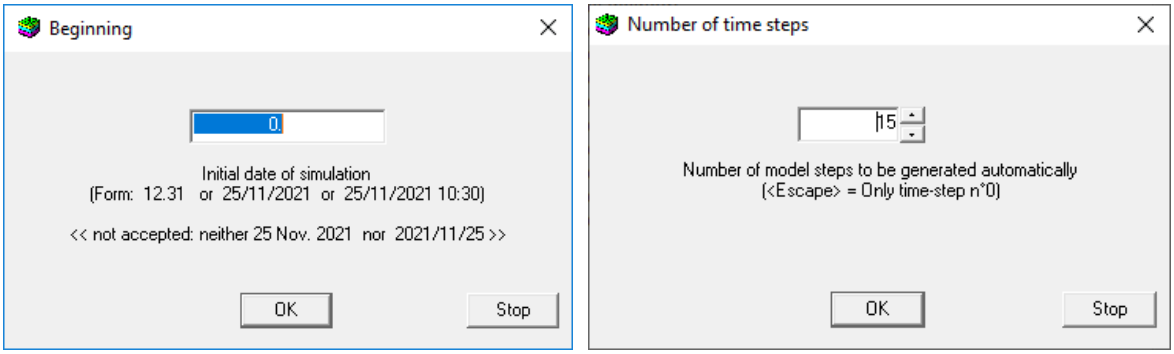


Figure 36 – Definition of the simulation start date and Automatic Creation of 15 time steps.

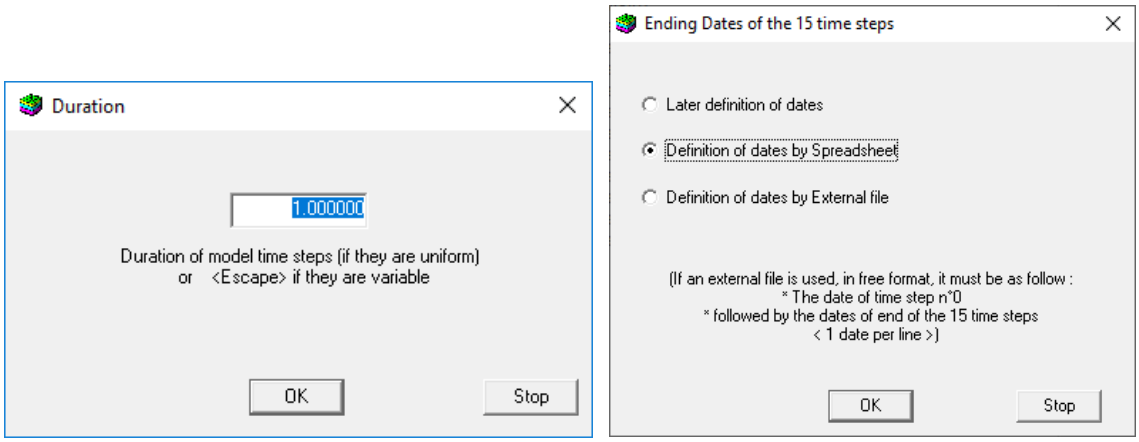


Figure 37 – Definition of the duration of time steps ("Esc." as the duration is not uniform) Define the end-of-time-step dates with the integrated spreadsheet.

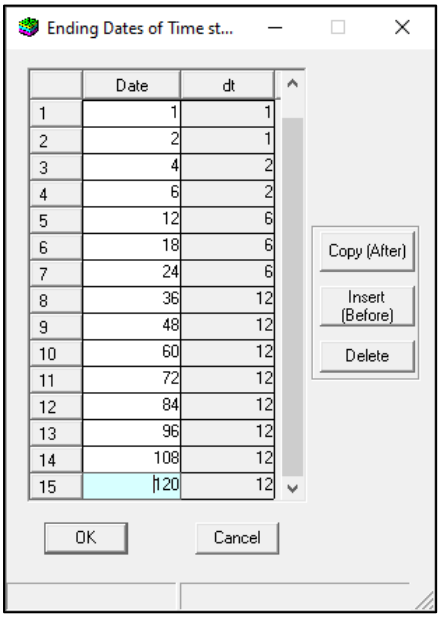


Figure 38 – Define the end dates of the 15 time steps with the integrated spreadsheet.

Introduction of pumping discharge:

Proceed as follows for introducing the pumping rate in the cell of column 26, row 26, layer 1, starting with time step 1: Select time step 1: Figure 39, then "New Actions".

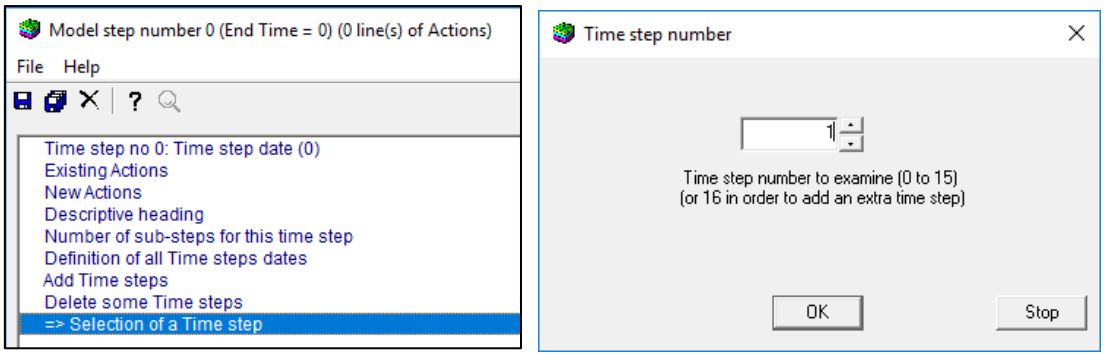


Figure 39 – Selection of the time step 1.

Select the subject "Standard hydraulic parameters", then the field "Discharge", then select modification per "Cell". Then introduce the value -100 in the appropriate cell (Figure 40).

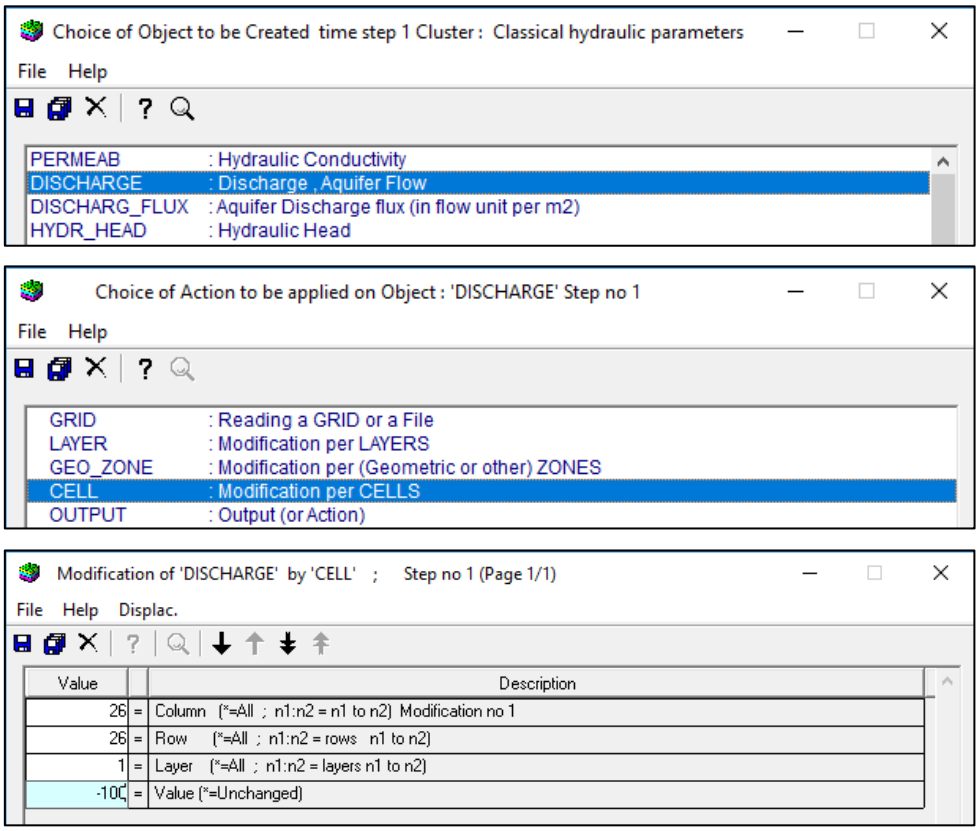


Figure 40 – Select "discharge" field, then modify per "Cell" and introduce the value -100 in the appropriate cell.

At time step 15, save the field of "Simulated hydraulic head".

As before, select time step 15, then "New Actions". Then select the *cluster* "Standard hydraulic parameters", then the field "HYDR_HEAD", then the action "OUTPUT", and then set the output index to 1 (that is to say, standard output): Figure 41.

In the same way, it is possible to request the output of other fields, such as the calculated flow rate (“DISCHARGE”), boundary flow, etc.

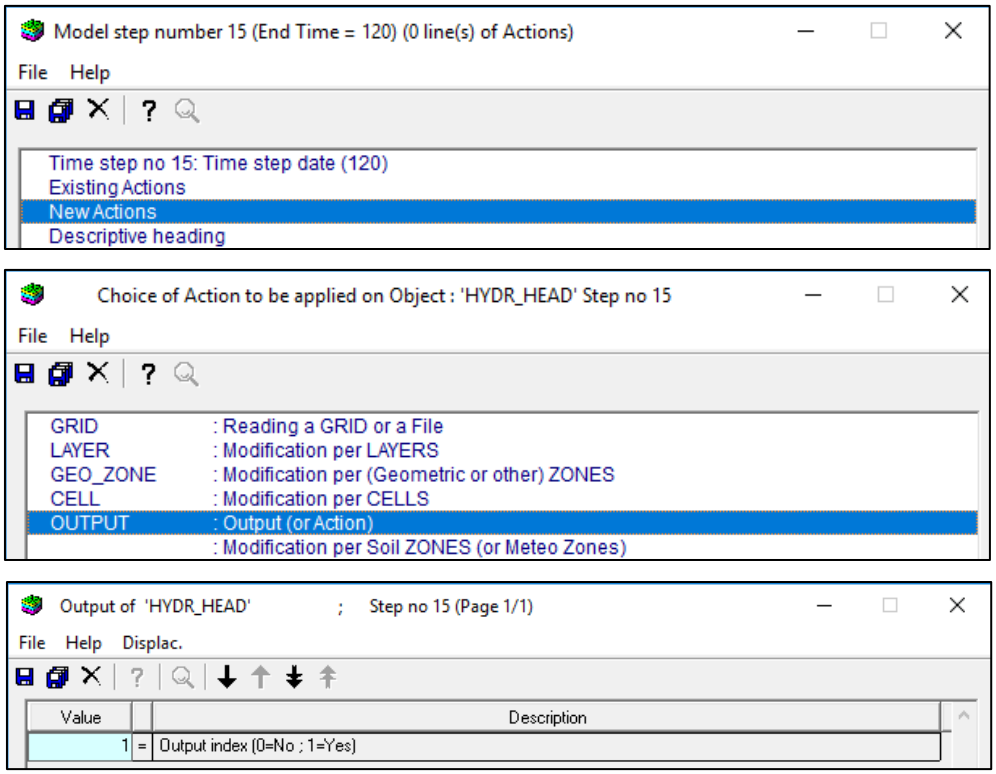


Figure 41 – Introduce "New action", for the field "HYDR_HEAD". Select action "Edit", then the backup index value 1.

4.5.4 "Cells with Time Series" file

In the general menu definition for "Non-meshed parameters", select line "Cell with time series" (Figure 42).

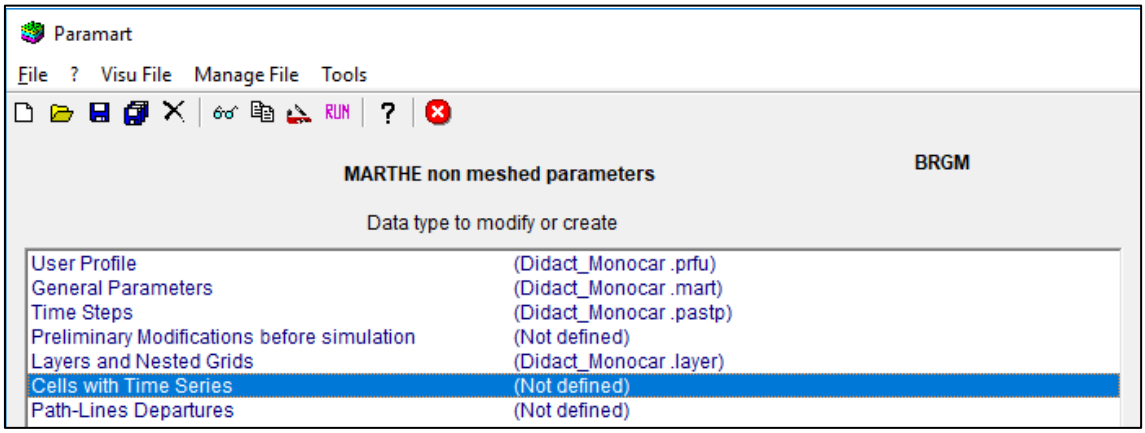


Figure 42 – Selecting the "Cells with Time Series" file.

As before, create a new file. Then select the desired type of Time series: "Hydraulic head". Choose to add a new “Cell with Time Series”, and define this cell by its column number, row, and layer. The number of pumped cells is introduced (column 26, row 26, layer 1) (Figure 43).

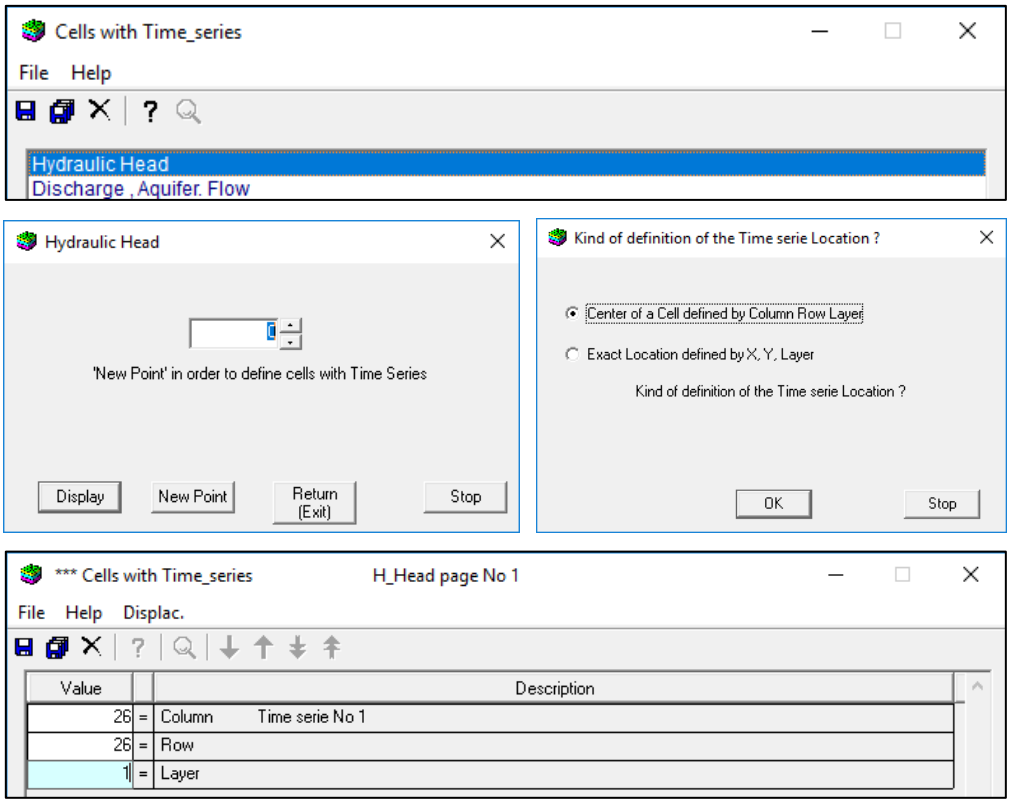


Figure 43 – Selection of the type of Time Series, the method for defining the cell, and definition of a cell whose Time Series should be saved.

Other cells are selected whose Time Series should be saved. This then results in the file of “Cells with Time Series” (Figure 44).

```
Monocar
  /H_Head       /HISTO/    =   /CELL:C=     26R=     26L=      1;
  /H_Head       /HISTO/    =   /CELL:C=     27R=     26L=      1;
  /H_Head       /HISTO/    =   /CELL:C=     51R=     26L=      1;
  /Discharge    /HISTO/    =   /CELL:C=      1R=     26L=      1;
  /Well_H_Head  /HISTO/    =   /CELL:C=     26R=     26L=      1; Name=Well
*** End of file: 'Cells with Time Series'            ***
```

Figure 44 – File of obtained "Cells with Time Series".

4.5.5 Running the calculation and visualization of the results

To run the simulation, click on button 

on the first row of the lower toolbar, and validate the running of the calculation with the file project *Didact_Monocar.rma* (Figure 45). The calculation is completed in a fraction of a second.

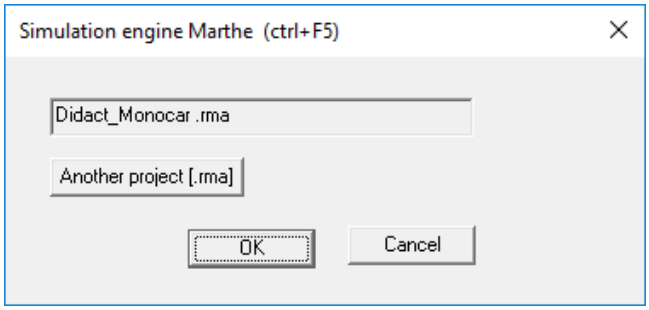


Figure 45 – Running the calculation.

Examining the flow rate balance:

Start by examining the "*flowbalance.txt*" file. For this, use the eyeglass button on the lower toolbar of WinMarthe, and select the file called *flowbalance.txt*.

Figure 46 shows the progress of the calculation during time step 1. The average variation of hydraulic head becomes less than 10^{-6} m in three external iterations. The pumped flow rate of 100 m^3/h is 100% aquifer dewatering, indicating that the imposed hydraulic head limits are not reached. The internal convergence is obtained with an excellent difference of 3.3 10^{-4} %. The overall convergence (between input and output) is obtained with an insignificant difference of 6.4 10^{-5} %.

Figure 47 shows the progress of the calculation during time step 15. The average hydraulic head variation becomes less than 10^{-6} m in three external iterations. The flow balance shows that 16.85 m^3/h come from the imposed hydraulic head limits, which are therefore reached at this time, and 83.2 m^3/h come from groundwater release from storage. The convergence is also excellent (10^{-3}% divergence on the internal convergence, and a 10^{-4}% gap on the overall convergence)

Visualization of the evolution over time of the flow rate balance:

Use the automatically generated file "histobil_debit.prn", (water balance flow history). This file can be immediately imported into Excel ®, or an equivalent spreadsheet software, and shows the changes over time of the flow rate balance terms and their convergence (Figure 48); the limit is almost reached after about 50 hours. It also verifies that the calculation has perfectly converged at all time steps.

Examining the calculated hydraulic head grid:

Import in WinMarthe the "*gridsimul.out*" file results. For this, use the menu "File" ➔ "File Simulated Grids (open)", or, more rapidly, use the shortcut "Control + R" ("R" as "Results"). The calculated hydraulic heads grid appears immediately on-screen.

Superimpose the design of hydraulic head isovalues using the menu "Tools" ➔ "Isovalues" ➔ "Simple" (or the shortcut "Control + I", with "I" as "Isovalues") (Figure 49). We see that, logically, the drawdown is less important in the north-east area which has a lower hydraulic conductivity.

```
------------------------------------------------------------------------------
 $ Model time step nb 1
------------------------------------------------------------------------------

    Start of Step :      0.000  (=   0.00     seconds =      0.000 day(s))
    Duration      :      1.000  (=  3.600E+03 seconds =      0.042 day(s))
    End   of Step :      1.000  (=  3.600E+03 seconds =      0.042 day(s))
=============================================================
 Summary of Hydraulic Head Convergence
 Sub   Iter  Mean Var   Max var    Resid_Q  Nb_Internal
 Step                  Iterat 1   Iterat 1  iterat.
    1    1  1.999E-03 -1.359E+00  1.000E+02     6
    1    2  1.062E-05 -1.327E-02  2.492E+00     4
    1    3  7.697E-08 -9.592E-05  2.013E-02     2
=============================================================

     Max. deviation / Mean deviation = 1246.3

 Under-relaxation could possibly reduce this ratio
   (this ratio doesn't prejudge the convergence quality)
 especially if the maximum accuracy is obtained

 - Balance in Flow unit : Time step    Nb 1 - t= 1.000 -------------

 Inflow  in Prescribed Heads    =  2.121E-09
 Outflow in Prescribed Heads    =                    0.000
 Flow into the cells            =  1.014E-04
 Flow out of the cells          =                 -100.000 (-100.000 Prescribed)
 ------------------------------------------------------------------------------
    Storage                     =   -100.000  (  3.677E-11    -100.000)
    Control Balance             = -4.547E-13               (Sum of all flows)
 Residual Flow Error            =  3.316E-04               (Sum of absolute value
                                                            of residual flows)
 Significant Internal Flow      =      0.000       -100.000 (computed in cells with
                                                            pumping or injection)
                 Lumped Balance=  6.439E-05


 Maximum Residual flow               =  6.439E-05 Col: 26 , Row: 26
 corresponding to a Head deviation of :  9.100E-07
 Maximum Residual Head Error         =  9.100E-07 Col: 26 , Row: 26

 Abs sum (residual flows)       =  3.316E-04 Maxi Total Flow = 100.000
 then internal converg. within  :  3.316E-04 %   of error
 Deviation in Lumped Balance    =  6.439E-05    (Input/output balance using
                                                 computed pumping/injection flow rates)
 then a Lumped convergence with :  6.439E-05 %   of error

 ======================================== Time step    Nb 1 - t= 1.000

 --Aquifer--- Cumulated Volumes  Water --- Time step    Since start of simulation
 Inflow  volume through Prescribed Heads = 2.1208E-09         2.1208E-09
      Prescribed Internal Outflow volume = -100.0             -100.0
       Positive volume Storage  (Inflow) = 3.6771E-11         3.6771E-11
      Negative volume Storage  (Outflow) = -100.0             -100.0
        Aquifer Volume Balance deviation =-4.2704E-11        -4.2704E-11
                                     (%) = 4.2704E-11         4.2704E-11
```

Figure 46 – Flow rate balance for Time step 1.

```
 ------------------------------------------------------------------------------
  $ Model time step nb 15
 ------------------------------------------------------------------------------

     Start of Step :    108.000  (=  3.888E+05 seconds =      4.500 day(s))
     Duration      :     12.000  (=  4.320E+04 seconds =      0.500 day(s))
     End   of Step :    120.000  (=  4.320E+05 seconds =      5.000 day(s))
=============================================================
 Summary of Hydraulic Head Convergence
 Sub   Iter  Mean Var   Max var    Resid_Q  Nb_Internal
 Step                  Iterat 1   Iterat 1  iterat.
    1    1  1.987E-02 -5.746E-02  8.566E+01     7
    1    2  2.905E-05 -3.057E-03  2.390E-01     5
    1    3  2.203E-07 -8.375E-05  1.189E-02     3
=============================================================

      Max. deviation / Mean deviation = 380.1

 Under-relaxation could possibly reduce this ratio
   (this ratio doesn't prejudge the convergence quality)
 especially if the maximum accuracy is obtained

 - Balance in Flow unit : Time step    Nb 15 - t= 120.000 -------------

 Inflow  in Prescribed Heads    =     17.166
 Outflow in Prescribed Heads    =                    0.000
 Flow into the cells            =  4.363E-04
 Flow out of the cells          =                 -100.000 (-100.000 Prescribed)
 ------------------------------------------------------------------------------
     Storage                    =    -82.834  (      0.000     -82.834)
     Control Balance            = -1.705E-13               (Sum of all flows)
 Residual Flow Error            =  1.088E-03               (Sum of absolute value
                                                            of residual flows)
 Significant Internal Flow      =      0.000       -100.000 (computed in cells with
                                                            pumping or injection)
                 Lumped Balance=  1.078E-04


 Maximum Residual flow               =  1.080E-04 Col: 26 , Row: 26
 corresponding to a Head deviation of :  1.607E-06
 Maximum Residual Head Error         =  1.607E-06 Col: 26 , Row: 26

 Abs sum (residual flows)       =  1.088E-03 Maxi Total Flow = 100.000
 then internal converg. within  :  1.088E-03 %   of error
 Deviation in Lumped Balance    =  1.078E-04    (Input/output balance using computed
                                                 pumping/injection flow rates)
 then a Lumped convergence with :  1.078E-04 %   of error

 ========================================= Time step    Nb 15 - t= 120.000

 --Aquifer--- Cumulated Volumes  Water --- Time step    Since start of simulation
 Inflow  volume through Prescribed Heads =  206.0             789.2
      Prescribed Internal Outflow volume = -1200.           -1.2000E+04
       Positive volume Storage  (Inflow) =  0.000            2.2894E-09
      Negative volume Storage  (Outflow) = -994.0           -1.1211E+04
        Aquifer Volume Balance deviation =-1.8337E-06       -4.4172E-06
                                     (%) = 1.5281E-07        3.6810E-08
```

Figure 47 – Flow rate balance for Time step 15.

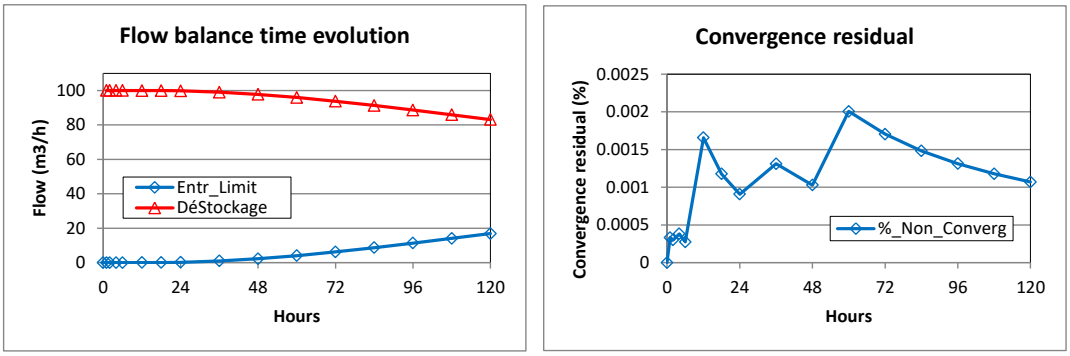


Figure 48 – Temporal evolution of the terms of the flow rate balance and of the percentage of non-convergence.

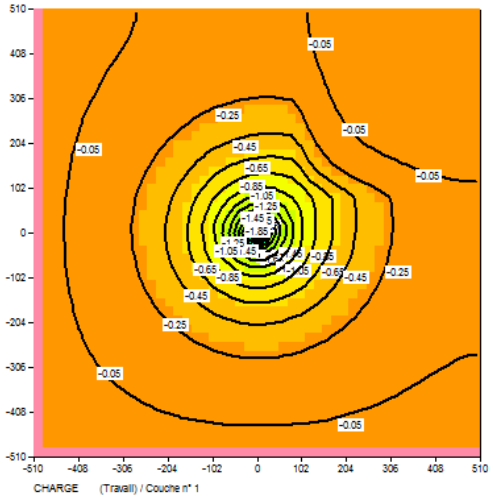


Figure 49 – Grid of the calculated hydraulic head. Isovalues are drawn every 0.2 metres.

Visualization of the evolution of hydraulic head in cells with Time series:

Use the automatically generated file "historiq.prn". This file is immediately imported into Excel ® or an equivalent spreadsheet software, providing immediate visualization of the temporal evolution of the hydraulic head in the aquifer at two points and in the pumping well. Given the size and radius of the well, the hydraulic head in the well is 4.4 m below the average head in the 20 x 20 m cell where it is located (Figure 50).

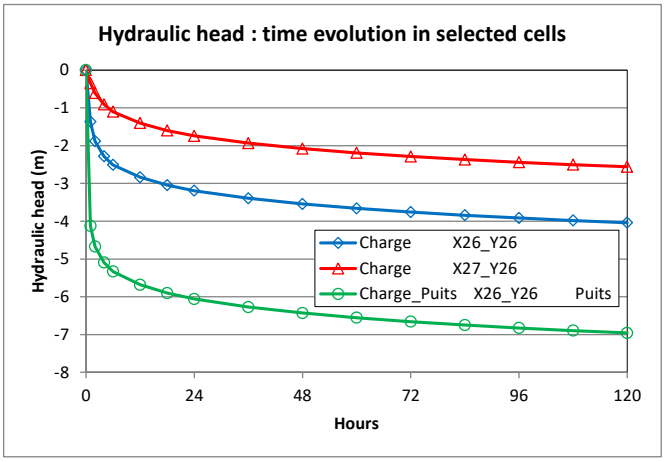


Figure 50 – Evolution of the hydraulic head calculated in three points.

5 Application example 1

This example corresponds to the project ***Didact2.rma***.

The example to be modelled corresponds to an aquifer system composed of two superimposed geological formations. The north and south boundaries are impermeable and the west and east ones each correspond to a river that imposes its potential on the aquifer. The prescribed heads on the west and east boundaries are 9 m and 8 m, respectively, above a reference level (for instance sea level). The distances are 600 m from north to south and 580 m from west to east between the two rivers. The aquifer is unconfined and both formations are assumed to be homogeneous.

The (horizontal) hydraulic conductivities of the two formations are, respectively and from top to bottom, $1.\ 10^{-4}$ m/s and $5.\ 10^{-4}$ m/s. Each formation is anisotropic, the vertical hydraulic conductivity being the different from the horizontal one. The effective porosity is 25%. The two formations are, respectively and from top to bottom, 4 m and 6 m thick, the top of the first formation being horizontal at an elevation of 10 m. The aquifer is fed by uniform recharge of 252 mm/year, or $8.\ 10^{-9}$ m/s, from atmospheric precipitation. A contaminated zone occurs in the upper aquifer near the west boundary, in a rectangle between abscissae 100 m and 220 m, and ordinates 240 m and 380 m. The aim of the model is to isolate the contaminated zone by using a well at coordinates (490 m, 310 m), that completely intersects the two formations. (Figure 51).

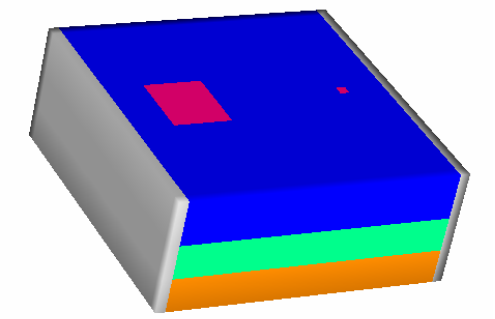


Figure 51 – 3D view of the aquifer system to be modelled, the red square being the contaminated zone and the red dot the well
(NB: The lower formation is modelled by two layers).

The pollution transport parameters are the following: the pollution release is $1.\ 10^{-4}$ μg/s/m^2, (or $1.05\ 10^5$ μg/month per 400 m^2 cell). Given that recharge from rainfall is $8.\ 10^{-9}$ m/s, this corresponds to a concentration of $1.\ 10^{-4}$ [μg/s/m^2] / $8.\ 10^{-9}$ m/s = $1.25\ 10^{+4}$ [μg/m^3]. Longitudinal and transverse dispersivity values are 10 m and 1 m, respectively, and the retardation coefficient is 2. The molecular diffusion coefficient and the half-life degradation constant are equal to 0. The initial contaminant concentration in the aquifer is 0, as is that from recharge and rivers. Evolution of the contaminant concentration is calculated over 3 years, and any changes in concentrations will be examined in the two points P1 and P2, respectively located at coordinates (290 m, 310 m) and (390 m, 310 m) in each formation.

In summary, the characteristics of the site are the following:

Geometry

- Two formations, 4 m (top) and 6 m (bottom) thick.
- Lateral extension: 580 m from west to east and 600 m from south to north.
- Southern and northern limits are impermeable.

- Western limit: fixed hydraulic head at +9 m; eastern limit: fixed hydraulic head at +8 m.

Hydraulic characteristics and recharge

- Hydraulic conductivity of the two formations: 1. 10^{-4} m/s (top) and 5. 10^{-4} m/s (bottom).
- Vertical anisotropy of the hydraulic conductivity (Kv / Kh): 1/10.
- Effective porosity: 25%.
- Recharge from precipitation: 252 mm/year, or 8. 10^{-9} m/s.
- Pumping well intersects both formations (at 490 m and 310 m).
- Hydraulic regime: steady-state.

Transport characteristics

- Contaminated zone in the rectangle: [100 m < x < 220 m], and [240 m < y < 380 m].
- Concentration of the contamination: 1.25 10^{+4} µg/m^3, or a mass flux of 1.10^{-4} µg/s/m^2 (or 1.05 10^5 µg/month per cell of 400 m^2).
- Longitudinal and transversal dispersivity: 10 m and 1 m.
- Retardation coefficient: 2.
- Calculation of the pollution concentration over 3 years and checking its evolution at coordinate points (290, 310) and (390, 310).

Discretization

For the simulation of this example we will consider a grid of 20-m-square cells. The lower formation, 6 metres thick, is divided into two identical model layers of 3 metres thickness, for a better representation of vertical flow. The system will be modelled by a set of three aquifer layers.

5.1 DEFINITION OF THE GRID

5.1.1 Grid creation

Double-click on the button  to run the WinMarthe pre-processor, then click on the button  or on "File ➔ New" to create a new model.

In the window "Definition of the Marthe project file" that opens (Figure 52), click the button  to select the folder where the model will be saved. The button  then creates a specific sub-folder (for instance, the Didactic folder) where all model files will be saved.

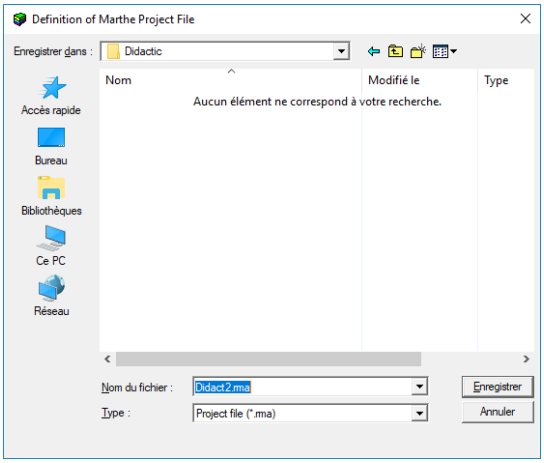


Figure 52 – Dialog box for creating a working folder.

WinMarthe then asks a file name for the model to be created (automatic extension .rma), enter for instance the name **Didact2** (in the **Didactic** folder**)**, which then opens a dialog box for definition of the grid to be created (Figure 53).

Enter the following data:

- Project title: **Example_2** (box "Miscellaneous", lower right);
- Hydraulic conductivity by default = **1** [i.e. uniform **hydraulic conductivity** = 1].

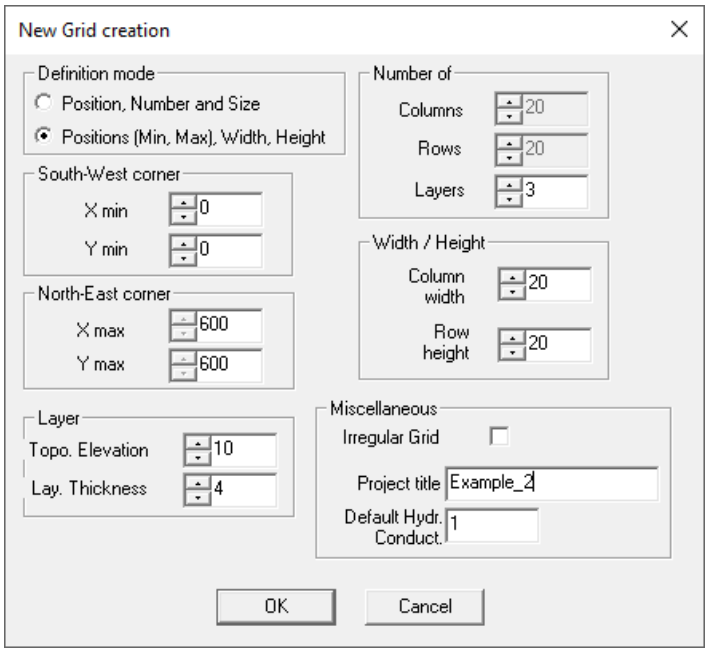


Figure 53 – Dialog box for creating the grid.

The box "Definition mode", upper left, proposes two options for defining the grid:

Either check: "Positions (Min, Max), Width, Height" and give the horizontal grid extension, the width of the columns and the width of the rows:

- Southwest corner: X = **0**; Y = **0**;
- Northeast corner: X = **+600**; Y = **+600**;
- Width of columns = **20**; Width of rows = **20**;

Or check "Position, Number and Size" and indicate the number of columns and of rows, with their width or height:

- Southwest corner: X = **0**; Y = **0**;
- Number of columns = **30**; Number of rows = **30**; Number of layers = **3**;
- Width of columns = **20;** Width of rows = **20**;

Then, in the "Layer" box, set the two parameters that might be modified later:

- Topo. Elevation = **10** [i.e. “Uniform topographic elevation" = 10 m];
- Lay. Thickness = **4** [The thickness of each layer is 4 (metres), the bottom of the first layer will thus be at an elevation of 6 (metres)].

Click on **OK**: the regular grid has been generated and is shown on screen.

To create an irregular grid, we should check "Irregular Grid" in the "Miscellaneous" box and define one by one the successive column widths from left to right, and row widths from top to bottom.

Remarks:

- In the grid, each cell is defined by its column number (increasing from left to right), its row number (increasing from top to bottom), and its layer number (increasing downward). The cell in the top left-hand corner of the grid thus has coordinates (1, 1, 1).
- At this stage, it is recommended to save the data entered in the model, by clicking on the button  . The Windows Explorer shows that several files have been created in the folder

Didactic: *Didact2.rma* (MARTHE project file), *Didact2.permh* (hydraulic conductivity file), *Didact2.hsubs* (bottom file), *Didact2.layer* (aquifer layers file) and *Didact2.wmi* (WinMarthe configuration file).

- All files created and used by MARTHE are text files that can be read and modified with a text editor, for instance the one accessible with button  on the bottom toolbar. Still, any modification of a data-entry file with a text editor must be done very carefully and only by well-informed users.
- The file [.rma] (Marthe) contains a list of all files that constitute the model, and is updated every time the project file is saved by clicking on  . Figure 54 shows the first lines of this file, mentioning the *Didact2.permh* and *Didact2.hsubs* files. However, the topography file (*Didact2.topog*) has not been created as, being uniform, it can be simply defined with a single value. Hence its condensed formulation "=10" in the *Didact2.rma* project file.

```
Tutorial 2: Steady state hydraulics [Project title]
Didact2.permh                          = Hydraulic conductivity
                                       = Discharge , Aquifer Flow
                                       = Hydraulic Head
                                       = Confined Storage Coefficient
                                       = Specific yield
                                       = Geometry Zone number
Didact2.hsubs                          = Substratum elevation
                                       = Equipotential Zone number
=10                                    = Topographic elevation
```

Figure 54 – First lines of the Didact2.rma project file.

- The models generated by MARTHE are geo-referenced, which allows exchanges with third-party Geographic Information Systems (GIS). The latter are used for preparing model-input data, as well as for visualizing simulation results.

5.1.2 Definition of layer thickness

The first layer is well defined: top ("Topography") at +10 m, and bottom at +6 m. To define the parameters of the other layers, select the field "Bottom elevation". For this we choose a field ("Select field F3", top toolbar), which brings up the dialog box of Figure 55.

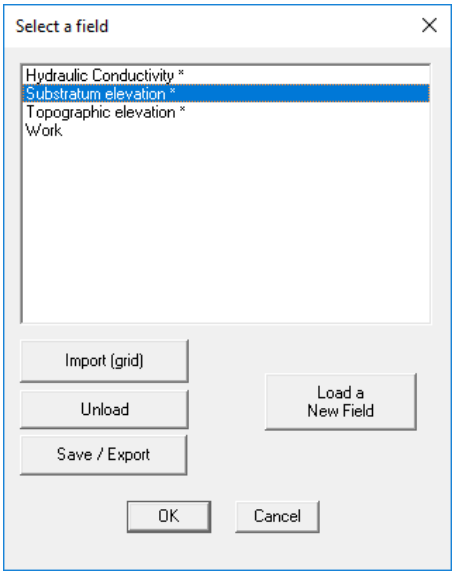


Figure 55 – Dialog box for selecting data fields.

Select the field "Substratum elevation", and click the button  "Select by layer" (bottom toolbar). Then use the arrow keys  on the same toolbar to switch to layer **2**. Double-click in the grid. As the button  was clicked, all cells of this layer are selected and appear in red. Then use the button  "Assign value to selected cells" and enter the value **3**, which is the elevation of the bottom of the 2nd layer (the cells are automatically deselected). Now select layer **3** with the arrow keys, and in the same manner select all cells and assign to them a null value (i.e. **0**) that is the substratum elevation of this 3rd layer. Click on the button  (column shape) "Visualize Model Style in Cross- section" of the left toolbar, and verify in the cross-section shown in Figure 56 that the geometry is well defined. (Exit to plan view with the button  = "Plan View").

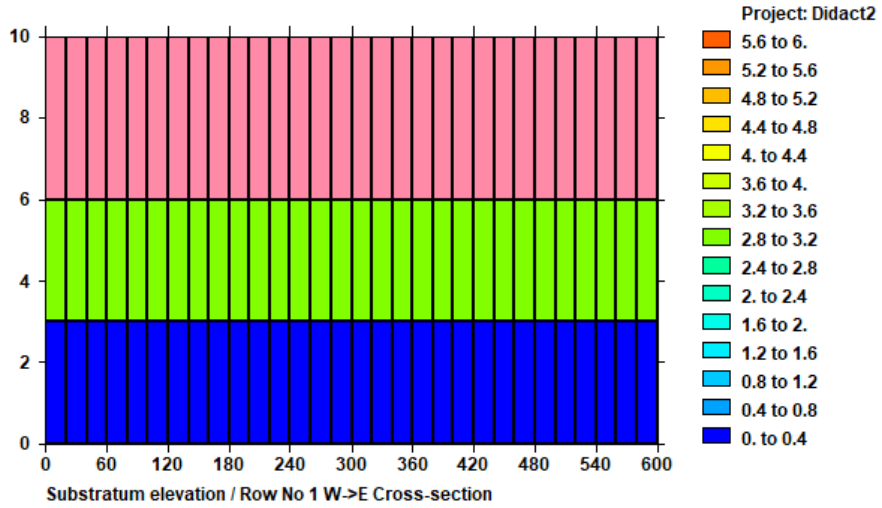


Figure 56 – Visualization of the thickness in vertical cross-section.

It should be noted that in the MARTHE code, unlike other groundwater modelling software, there is no concept of “confined layer”, "unconfined layer” or “convertible layer”. At any time, any cell can become confined, unconfined or dewatered, depending upon the current hydraulic head. The status of each cell is integrally managed by the software algorithms.

5.2 PARAMETER DEFINITION FOR HYDRAULIC CALCULATION

5.2.1 Definition of boundaries with a prescribed hydraulic head

To define an impervious boundary on the edge of the model, nothing has to be done as it is the default option.

To define a prescribed hydraulic head boundary (also known as “prescribed potential boundary"), the concerned cells must be assigned a “discharge” equal to a value code 9999; the fixed hydraulic head then is equal to the declared hydraulic head in the field "Hydraulic head" (see hereafter).

We proceed as follows:

Select the field of Water Flow ("Select Field F3", upper toolbar), then click on the button "Load New Field", designate "Discharge, Aquifer Flow" and accept the creation of this new field. To

affect the 9999 values, use button  "Selection by column" (lower toolbar) and double-click on column 1 (to the left). The column is selected (in all layers) and becomes red. With button  it is assigned value 9999, which colours this column grey as value 9999 is a "code" value. The same is done for the column on the right (column 30).

Now the hydraulic head values must be assigned. For this, the hydraulic head field is created ("Select Field F3" ➔ "Load New Field", designate "Hydraulic Head" and accept the creation). An initial value of 8 metres is assigned, using the button  "Select All" and double-click in the domain => All cells are selected (and coloured red). With the button  it is assigned a value 8. Then select column 1 and assign it a value of 9 metres.

5.2.2 Definition of the pumping rate

The pumping rate (negative because it is abstracted) is 12 10^{-4} m^3/s at the point of coordinate 490 m, 310 m. Start by assigning this rate only in layer 3, and we will show later how to ensure that this flow is distributed correctly in all 3 layers.

The discharge field is re-selected ("Select Field F3" ➔ "Discharge, Aquifer Flow"), and select the cell coordinates (490 m, 310 m) in layer 3. Use for this, on the upper toolbar, the menu "Tools" ➔ "Go to x/y/layer" and set X= 490, Y= 310, Layer= 3. Validate the cell (Column=25, Row=15, Layer=3) that colours red. Give it value -12 with the button  . Enter -12, and ***not*** -0.0012, as it will be more readable to work with flow rates expressed in 10^{-4} m^3/s (the flow rate unit will later be set at 10^{-4}).

5.2.3 Definition of hydraulic conductivity

Select the hydraulic conductivity field ("Select Field F3" ➔ "Permeability"). Then select layer 1, the upper one, in the same way the bottom elevation was defined. For this, click the button  of "Selection by Layer", double-click in the domain => All Cells (of the layer). With the button  assign value = 1. Enter "1", and ***not*** 0.0001, as it will be more readable to express the hydraulic conductivity in 10^{-4} m/s (the hydraulic conductivity unit = 10^{-4}, see above).

N.B.: MARTHE offers great flexibility for defining units of flow rates, hydraulic conductivity, hydraulic head, recharge, time, horizontal coordinates, etc., without the need for a coherent system. For instance, the hydraulic conductivity can be expressed in 10^{-4} m/s, the flow in m^3/h, the hydraulic head in cm, the horizontal coordinates in km, and the time in days.

Then select layer 2 by using the button "  " on the bottom toolbar. Double-click in the domain => All Cells, which selects all of layer 2. Assign value = 5 to them. Then select layer 3 and assign it value 5 in the same way.

5.2.4 Definition of uniform porosity and recharge-zone fields

Proceed as before to define these uniform fields. ("Select Field F3" ➔ "Load New Field" ➔ "Porosity = Saturation Water Content") and define a value of 25 (%) for the entire domain. Then create the field "Soil Zone Number" and assign value 1 to the entire domain. In fact, only the cells that are exposed, here the cells of layer 1, will be affected. Please note that MARTHE offers the very important flexibility of allowing layers to disappear, such as layers that wedge out, creating “short-circuits” between any layers, and allowing other layers to be exposed.

The value of the recharge to be assigned to this zone 1 will be defined later, as the “Recharge” field—under standard conditions—cannot be assigned on a cell-by cell basis, but only by groups of cells (called “Meteo zones”).

5.2.5 Saving the model

At this stage it is recommended to save the data entered in the model with the button  . Repeat this operation regularly, as there is no "Undo" function for cancelling a wrong operation. When saving the data, the "*" symbols—placed next to the modified fields—as well as the symbol "*" in the title bar, disappear.

The imposed-potential (*Didact2.debit*) and initial-hydraulic head (*Didact2.charg*) files are created. However, the porosity (*Didact2.poros*) and recharge-zone (*Didact2.zonep*) files are not created as they are uniform. Their names appear, respectively, as "=25" and "=1" in the *Didact2.rma* project file.

5.2.6 Definition of Non-meshed parameters

The “Non-meshed parameters” are accessible via the button  on the first lower toolbar. This brings up the general menu shown on Figure 57.

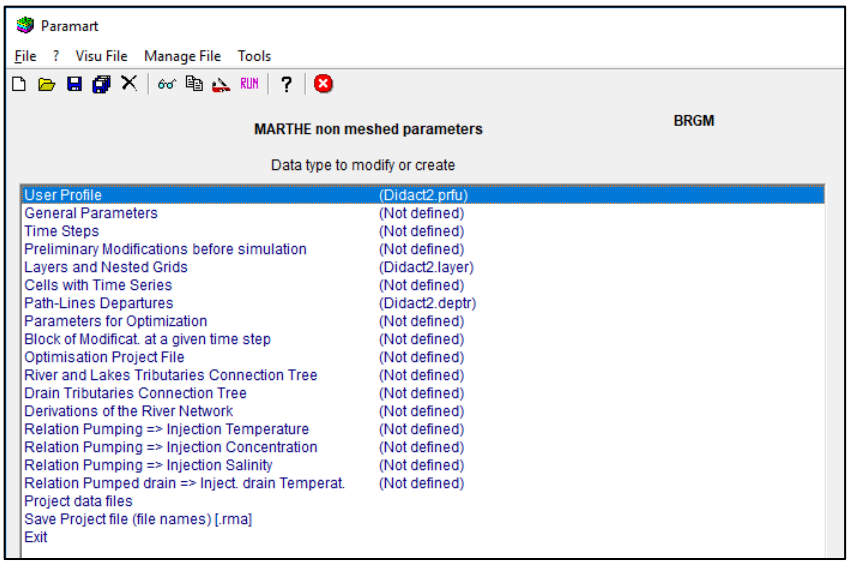


Figure 57 –"Non-meshed parameters" menu.

5.2.6.1 User profile

The "User Profile" file allows to set the type of modelling to apply a mask on the parameters and files that will not need to be defined by the user at later stages. This "User Profile" file is optional; if it is not given, all parameters and files will be visible. There is however an exception to this rule: when geochemical reaction are considered, this should selected in the "User Profile" file.

The definition of this profile allows finding the parameters more rapidly and especially facilitates the software use by non-expert users. The "User Profile" file is not used by the computational engine but it is used by the “Non-meshed parameters” module, activated by the button  , and by WinMarthe *sensu stricto*.

In our example, we double-click on "User Profile" and then on "Load a New User Profile". Then select (giving the value "1") the lines: "Transient State" and " Standard mass transport", validate by OK and confirm. Save this file by the proposed default name.

5.2.6.2 General Parameters

In the module of "Non-meshed parameters", double-click on the first line "General Parameters", then on "Pre-processor", then on "Load a New Parameter File". This brings up 12 lines that each allow selecting a General Parameters paragraph (Figure 58). If no User Profile is defined, there will be 22 paragraphs, each with far more parameters.

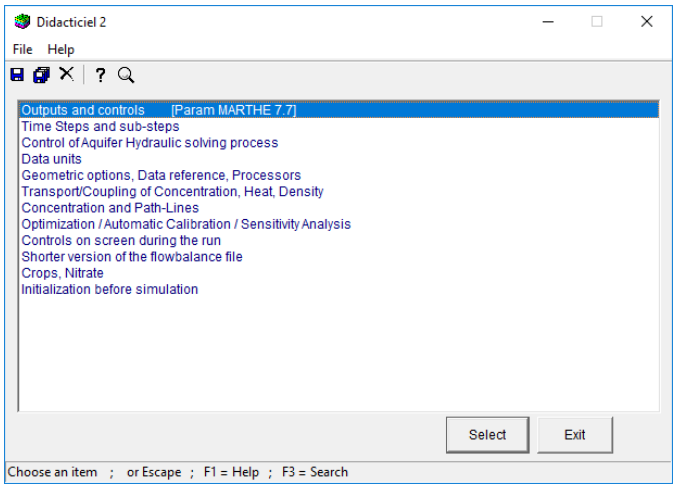


Figure 58 – The menu of the "General Parameters" file.

Only few parameters must be defined, the others can be left at their default value ("space" or "0"). In all cases, "space" or **0** means "**No**", **1** indicates "**Yes**", and other options are also possible.

Paragraph: "Outputs and Controls":

Select:

```
       1 = Detailed listing
       1 = Output Time Series of Aquifer Flow Balance (-1=No ; 1=Yes ; 0=Automatic)
```

Paragraph "Control of Aquifer Hydraulic solving process"

```
    20 = Maximum number of hydraulic iterations for time step 0 (Initial Steady State)
Steady = Hydraulic Flow Regime [[0=Transient state; 1=Steady State]
```

Paragraph "Data Units"

```
1e-4 = Aquifer Hydraulic conductivity unit in m/s (or m2)
1e-4 = Flow (Discharge, Yield) unit in m3/s (kg/s for Gas flow)
Year = Duration unit for hydro-climatic data (sec, min, hr, day, decade, month, year)
 Day = Time unit (for model time steps) (sec, min, hour, day, decade, month, year)
 0.1 = Vertical Anisotropy coefficient Kv/Kh for Permeability
   % = Porosity = Water Content unit [dimensionless] ['%' when in %]
```

The units left “empty” or equal to 0 are in the International System, except for the “Hydro-climatic (Rainfall, PET, Infiltration, Recharge)" units in mm: hydraulic head and horizontal coordinates in metres, and water storage in m^3. The hydro-climatic units are left in mm, the hydro-climatic duration is in "years", and recharge is in mm/year. The vertical anisotropy coefficient Kv / Kh is set at 0.1.

Paragraph "Control of screen during the run"

```
1 = Control of external resolution iterations
```

Paragraph "Initialization before simulation" (last line in the list of paragraphs)

In this paragraph any occasional modifications of the grid can be defined. As this paragraph corresponds to time step 0, any outputs of the fields simulated during time step 0 can be requested here, but it is more logical to request them in the “Time Steps” file.

5.2.6.3 Infiltration flux

After having selected the paragraph "Initialization before simulation", select "New Actions", then choose the *Cluster:* "Standard hydraulic parameters", then the *object* "INFILTR_FLUX" (or the *object* "RECHARGE"), and the *action* "CLIM_ZONE = Modification per Climatic zone (Soil zone or Meteo zone)". Then set (Figure 59) Zone Number = **1**, value (of recharge) = **252.46** (mm/year).

5.2.6.4 Output of the simulated hydraulic head and of the calculated flow rates and discharges

The outputs of simulated fields can be requested in paragraph "Initialization before simulation", as illustrated here. More logically, they can also be requested in a “Time Step” file at time step 0, as described later under Transient State Simulation.

Select the *cluster* "Standard hydraulic parameters", then the *object* "HYDR_HEAD" and *action* "OUTPUT = Output”, and the option “**1** = Output index (0=No ; 1=Yes)”.

In same cluster “"Standard hydraulic parameters", select the *object* "DISCHARGE", the *action* "OUTPUT = Output", and the option "**1** = Output index".

Figure 60 shows that the Output request of the hydraulic head field appears as:

" / HYDR_HEAD / OUTPUT I = 1".

The Output request for the Discharge field appears in a similar format, though with a few more options.

Then click three times on "Exit" for saving the entered data. These are recorded in the file *Didact2.mart*, called the MARTHE parameters file; this is a fundamental component of a MARTHE model, combining all choices made for simulation options, data units, outputs, controls, etc.

Figure 60 shows the end of the *Didact2.mart* file, where the paragraph "Initialization before simulation" combines the data supplied on infiltration flux and the requests for outputs of the hydraulic head and discharge fields.

At the end of the simulation, the hydraulic head field will be output in text format in a file with the generic name *gridsimul.out*, and the flow rate field (discharge field) in a file called *flowsimul.out*.

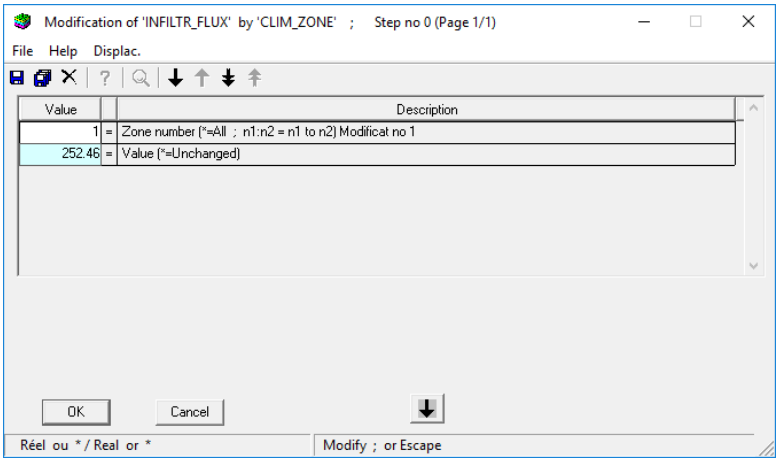


Figure 59 – Assigning a recharge of 252.46 mm/year in Climatic zone 1 (here in Soil zone 1).

```
*** Initialization before simulation                    ***
  /INFILTR_FLUX/CLIM_ZONE  Z=   1V=  252.46;
  /HYDR_HEAD/OUTPUT        I= 1;
  /HYDR_HEAD/OUTPUT        I= 1;
  /DISCHARGE/OUTPUT        *= 1;V=  ;L=  ;S=  ;Z=  ;
  /*****/***** End of Initialisation
```

Figure 60 – Last lines of the 'Didact2.mart' parameter file.

It should be noted that, unlike in other modelling software, the choice was made in MARTHE not to save all fields at every time step. In fact, there are many fields that can be saved (water content, temperature, density, pressure head, etc.), representing a considerable amount of computer storage. Such a storage volume may not be manageable for large grids with many time steps and is mostly useless. It is up to the user to choose which fields he wants to save and to indicate at which time step he wishes to do so.

5.3 RUNNING THE SIMULATION AND EXAMINATION OF THE RESULTS

To run the simulation, click on the button 

on the first row of the lower toolbar, then validate the running of the simulation with file *Didact2.rma*. The simulation takes place in a fraction of a second.

5.3.1 Preliminary verification of the groundwater budget

First, before any examination of the simulated hydraulic head and the groundwater discharge, and especially during the first "run", one should check that the iterative calculations has converged properly. To that end, the "flowbalance.txt" file must be rapidly checked. Use the  (eyeglasses) button on the lower toolbar for this, and select the file named *flowbalance.txt*. A rapid check shows that the simulation stopped after four (external) iterations. The "lumped convergence", i.e. the difference between incoming and outgoing flow rates, is $1.1\ 10^{-3}$ % (compared to the largest term). The "internal convergence", a more severe criterion that is the sum of the absolute values of the differences between inflow and outflow in each cell, is $1.1\ 10^{-2}$ % (Figure 61). This convergence is very good, since in practice it is generally enough to have an internal convergence in the order of 1%.

```
================================================================================
                            Total Flow Balance: Time step # 0
================================================================================

 - Balance in Flow unit : Time step    Nb 0 - t= 0.000 -------------

 Inflow  in Prescribed Heads    =     21.290
 Outflow in Prescribed Heads    =                    -38.089
 Flow into the cells            =  5.054E-03
 Flow out of the cells          =                    -12.006 (-12.000 Prescribed)
 Recharge/Evaporation flow      =     28.800
 --------------------------------------------------------------------------------
     Control Balance            =  2.311E-10                (Sum of all flows)
 Residual Flow Error            =  1.076E-02                (Sum of absolute value
                                                             of residual flows)
 Significant Internal Flow      =      0.000        -12.000 (computed in cells with
                                                             pumping or injection)
                  Lumped Balance=  5.736E-04
```

Figure 61 – Flow balance for the three layers

Figure 62 shows the net balance of flow in the three layers, expressed in 10^{-4} m^3/s that is the unit selected for flow.

Figure 63 presents the exchanges between layers. For instance, layer 1 receives a recharge of 28.8 flow units of which 26.3 pass into layer 2. Layer 2 receives 26.3 flow units (from layer 1), 19.1 of which pass into layer 3, the rest being the outflow balance via the fixed hydraulic head boundaries. Layer 3 receives 19.1, 12 of which are outflow through pumping and the rest through the boundaries.

```
================================================================================
                            Total Flow Balance: Time step # 0
================================================================================

 - Balance in Flow unit : Time step    Nb 0 - t= 0.000 -------------

 Inflow  in Prescribed Heads    =     21.290
 Outflow in Prescribed Heads    =                    -38.089
 Flow into the cells            =  5.054E-03
 Flow out of the cells          =                    -12.006 (-12.000 Prescribed)
 Recharge/Evaporation flow      =     28.800
 --------------------------------------------------------------------------------
     Control Balance            =  2.311E-10                (Sum of all flows)
 Residual Flow Error            =  1.076E-02                (Sum of absolute value
                                                             of residual flows)
 Significant Internal Flow      =      0.000        -12.000 (computed in cells with
                                                             pumping or injection)
                  Lumped Balance=  5.736E-04
```

Figure 62 – Net balance for the 3 layers of the domain.

Flow exchanged between the 3 layers

Num Lay	Contribution of layers (> 0 if layer exports ; < 0 if layer receives) 1	2	3	Recharg	Total
1	*	-26.28	0	28.8	2.523
2	26.277	*	-19.06	0	7.22
3	0	19.057	*	0	19.057

Figure 63 – Flow exchanged between the three layers of the domain.

5.3.2 Examining the obtained results

Quit the text editor, which had been activated by the eye glasses button , and now you are back in WinMarthe.

5.3.2.1 Hydraulic head simulated in steady-state mode

Activate the menu "File" ➔ "Simulated Grids (Open)" , or, easier, type Control+R ("R" for Results), and select the *gridsimul.out* file. The field of the simulated hydraulic head, the only one requested with that of flow, is copied in the "Work" field and appears on screen for the current layer (Figure 64).

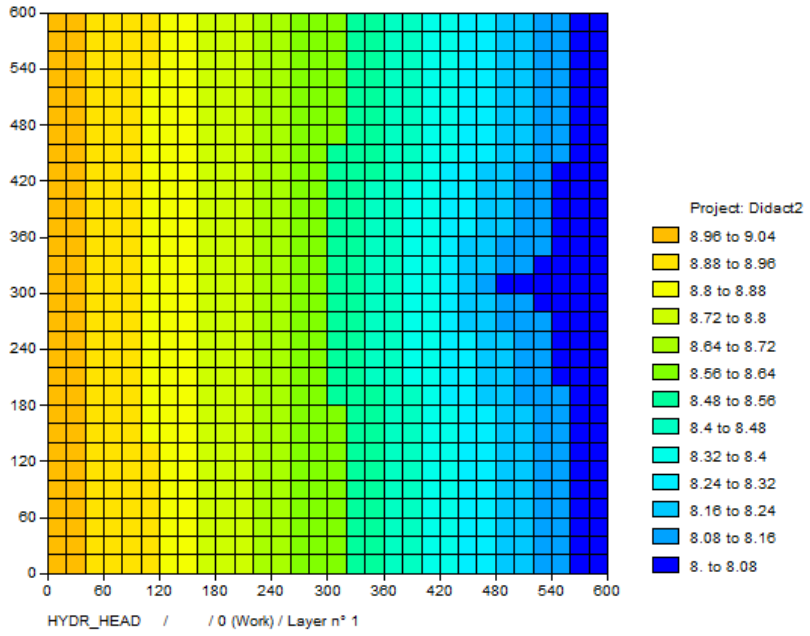


Figure 64 – Field of the simulated hydraulic head (layer 1).

It is possible to scroll the layers with the arrows (,), for examining a vertical cross-section, changing the distribution of coloured fields (eQui-distributed = Control+Q, or Linears = Control+L, or logariThme = Control+T), masking the cell contours (View => Draw cell contours), superimposing polygons, or for placing identification points (boreholes, etc.)

5.3.2.2 Isovalues of simulated hydraulic head

To trace the isovalues, use the menu "Tools" ➔ "Isovalues" ➔ "Simple", or type directly Control+I ("I" for Isovalues), and accept or modify the default values (Figure 65).

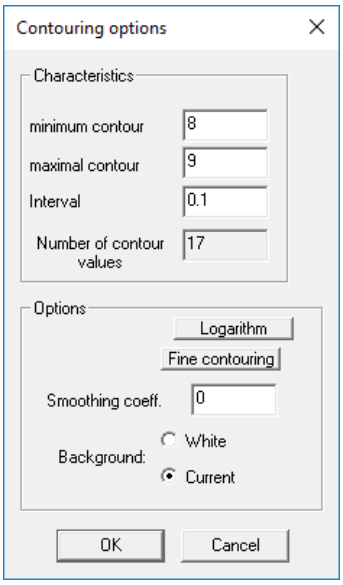


Figure 65 – Dialog box to setup the isovalues of a simulated hydraulic head field.

We now obtain a plot of the simulated hydraulic head isovalues (Figure 66), the colours, line thickness and visibility of which can be selected in the menu "Polygons management" (button ).

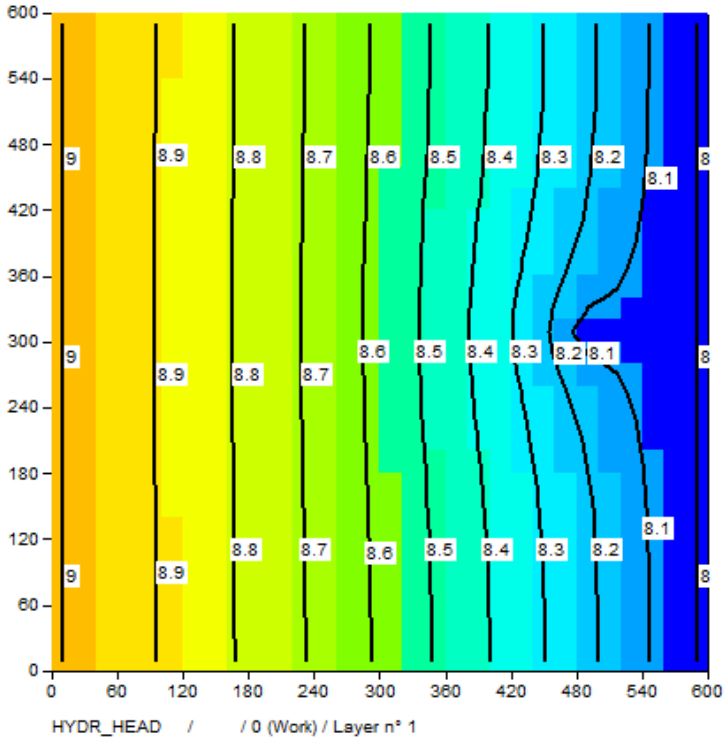


Figure 66 – Isovalues plot of the simulated hydraulic head (layer 1).

5.3.3 Pathlines

To improve this plot, we can add some flow pathlines, especially those converging towards the pumping well. This operation takes four steps: 1) Selecting the option for simulating pathlines in the backward flow direction (arriving at the well); 2) Designating the cell of the pumping well as the origin of the backward pathlines; 3) Re-start the simulation with outputs of the pathline, 4) Draw the pathlines in superimposition on top of the potentiometric map.

5.3.3.1 Optional simulation of pathlines

Click on the button 

to open the menu of "Non-meshed parameters", double-click on the first line "General Parameters", click on "Pre-processor", and select the Paragraph "Concentration and Pathlines". Select the option "Inverse Pathlines":

```
    -1 = Path-Lines calculation (1 = Yes  ;  -1 = Inverse Path-lines)
```

or

```
Invers = Path-Lines calculation (1 = Yes  ;  -1 = Inverse Path-lines)
```

Click on "Exit" and save the modified “General parameters” file.

5.3.3.2 Pathlines origins

Now select the "Pathline Departures" line, click on "Pre-processor" and "Create New File Pathline Departure".

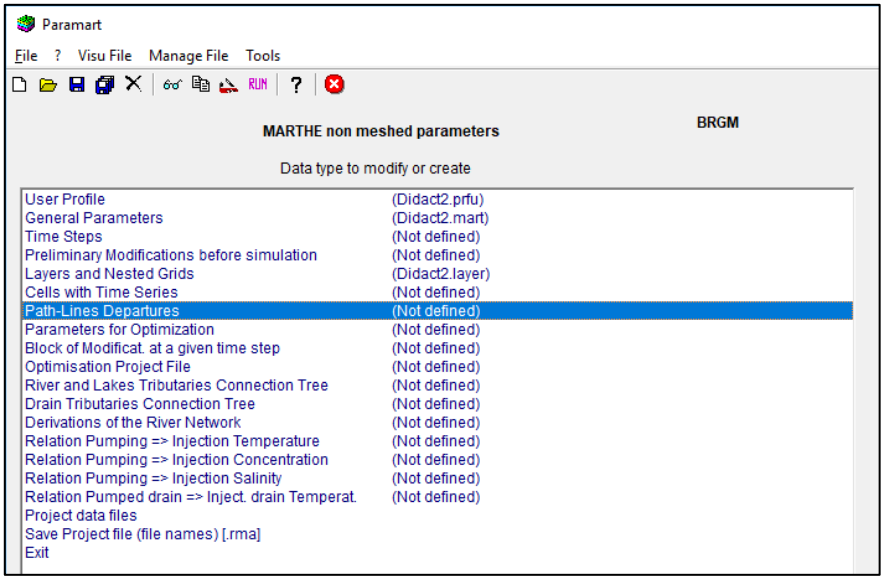
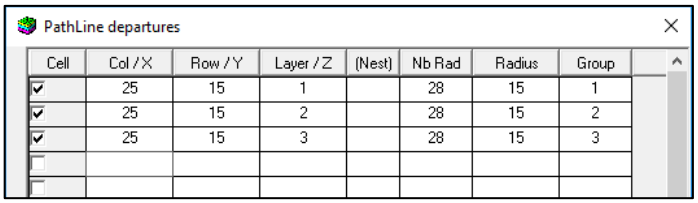


Figure 67 – Selection of the ‘Pathline departures’ file.

Position the pathline departures on circles in the centres of the three pumping cells (column 25, row 15, layers 1 to 3). The circles have a radius of 15 m (falling slightly outside the pumping cell) with 28 departure points distributed over each circle. Tick the column "Grid" (Figure 68) to indicate that the given values are column, row and layer, and not x, y and z coordinates. The optional group number serves to group the pathlines into sub-groups (here a group of pathlines per model layer).



Cell	Col / X	Row / Y	Layer / Z	(Nest)	Nb Rad	Radius	Group
☑	25	15	1		28	15	1
☑	25	15	2		28	15	2
☑	25	15	3		28	15	3
☐							
☐							

Figure 68 – Definition of the starting points of the pathlines.

We now leave the spreadsheet for defining pathline departures and leave the “Non-meshed parameters” menu, after saving the project file. A file named "*Didact2.deptr*", containing the pathline departures has been created, and its name was added to the "*Didact2.rma*" project file.

5.3.3.3 Calculating pathlines

Re-run the simulation with the button 

.

5.3.3.4 Visualization of pathlines

The pathlines are saved in two files: "*pathline.out*" (coordinates, layer number and time) and "*pathline.bln*"; this file is a pointwise (x, y) file that is directly visualized with WinMarthe as a “polygon”.

To view the pathlines, click the button  "Polygons management", then click "Load [.bln] Polygons" and select the "*pathline.bln*" file. The pathlines appear, plotted for an infinite duration since the hydraulic calculation is performed in a steady-state regime (Figure 69).

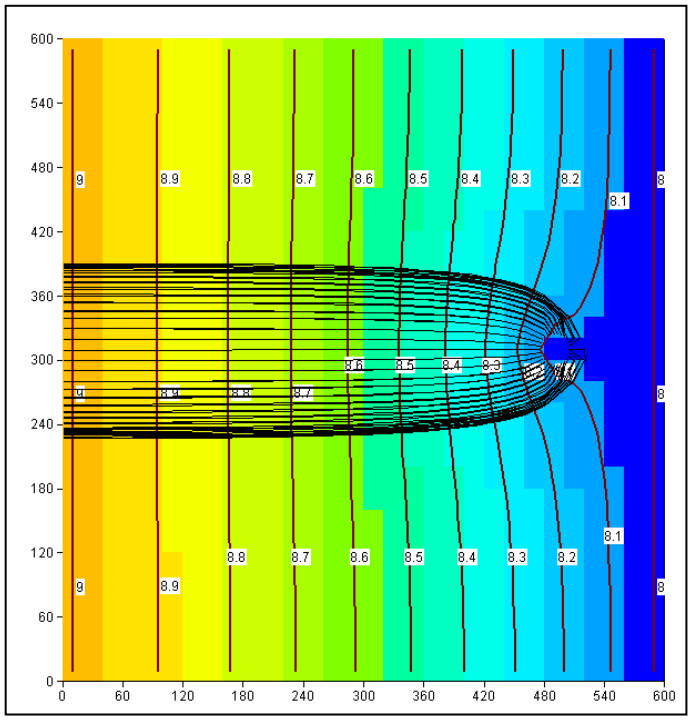


Figure 69 – Simlated pathlines in a steady-state regime.

To view the pathlines for a given duration, e.g. 100 days, which would correspond to a protection zone for 100 days, carry out a transient state simulation (not described here) while maintaining a steady-state hydraulic calculation. For instance, define a time step of 100 days. The pathlines are then calculated in a transient state until the end date of the simulation. It is also possible to draw

the isochrones (Figure 70), which are the arrival points of the pathlines (in red in layer 1, less permeable thus slower, and in blue in layer 2).

MARTHE also allows simulating and visualizing the pathlines corresponding to a transient groundwater flow simulation.

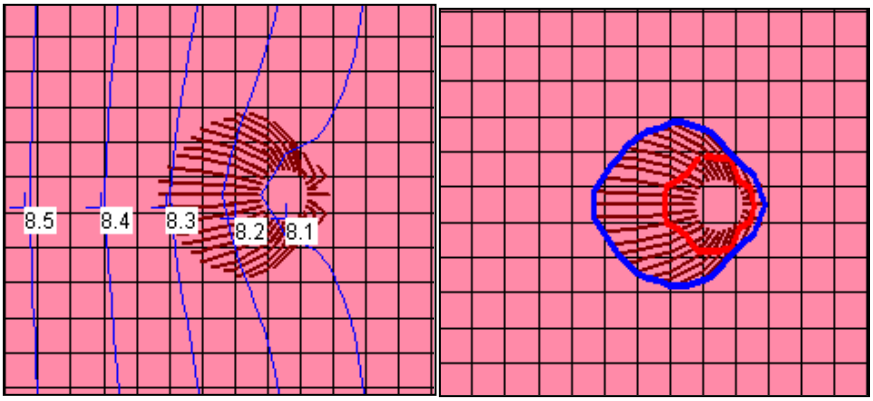


Figure 70 – Pathlines simulated over a duration of 100 days.

5.3.4 Vertical anisotropy of the hydraulic conductivity in a pumping well

The pumping well is screened in the three layers. For an accurate simulation, we need the same hydraulic head (unknown) for the three cells of the three layers corresponding to column 25, row 15. To this end, we define a strong vertical anisotropy, 500 for instance, in the three cells. The vertical hydraulic conductivity will thus be equal to 500 times the horizontal one.

Click the button PAR to activate the “Non-meshed parameters” module, double-click on "General Parameters", "Pre-processor", "Initialization before simulation", "New Actions", and select " Standard hydraulic parameters"; this contains 40 objects and "Vertical Anisotropy" is not immediately visible. Click the "Help" button or key "F3", which opens the window shown on Figure 71. Now type "Vertical Anisotropy" without accounting for capitals. Click "Select". No answer is found ("Not Found"). When no answer is found, click twice on "Esc" key and select "All Parameters" or even "All Parameters: even outside user profile" which brings up over 200 objects.

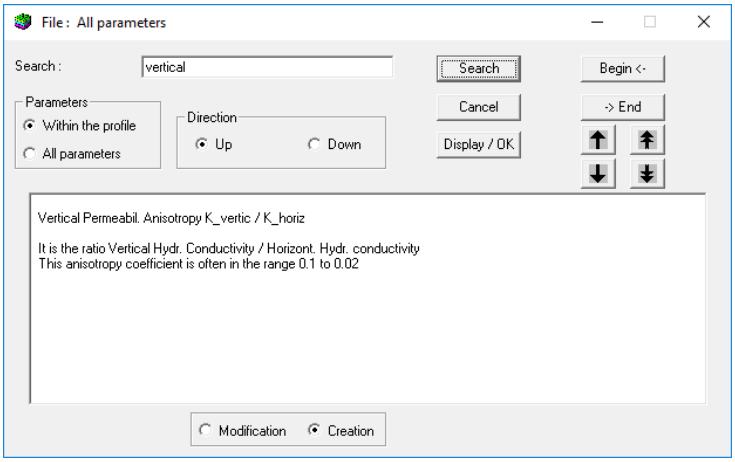


Figure 71 – Search for object "Vertical Anisotropy".

Now click again on the button  to look for "Anisotropy", then on "S  t", and immediately find the answer "Horizontal Permeability Anisotropy Kx / Ky". Button then gives access to "Vertical Permeability Anisotropy K_vertic. / K_horizont.". Press "OK" and we arrive on the object "VERTIC_ANISOT = Vertical Anisotropy …". Select this object and choose the action "CELL = Modification by Cell". In the window of Figure 72, set the numbers column = 25, row = 15, and layer = 1:3 for "1 to 3", or "*" for "all", and set the value to 500.

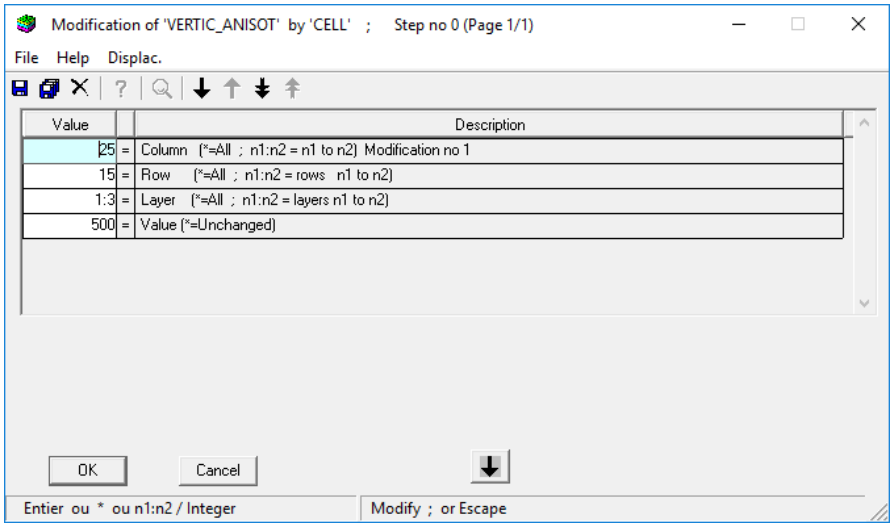


Figure 72 – Setting a vertical anisotropy of 500 in the 3 cells of the pumping cell.

This modification is shown at the end of file *Didact2.mart* as:

/**VERTIC_ANISOT**/CELL C= **25**R= **15**L= **1:3** V= **500**;

("C=" is Column, "R=" is Row, "L=" is Layer, "V=" is the assigned value).

Re-run the simulation with the button  . The results show that in this example they are almost unchanged. In the well, the hydraulic heads are now almost the same in all three layers, whereas before they differed by a dozen centimetres.

5.4 SIMULATION OF THE HYDRAULIC HEAD IN TRANSIENT REGIME

This example is project ***Didact2_Transi.rma***, where a hydraulic simulation is run in a transient regime.

First, additional parameters must be defined for a transient groundwater flow simulation. For safety reasons, conserve the project *Didact2.rma* unchanged by making an automatic copy named *Didact2_Transi* that will be the new project in transient state. For this, use the menu "File" ➔ "Make a Copy of the Project", and choose the name *Didact2_Transi*. Then close the project *Didact2.rma* and open project *Didact2_Transi.rma*.

Now add two new pumping wells to the existing one. The new ones are in layer 3, at coordinates x = 450 m, y = 370 m and x = 450 m, y = 250 m, respectively, (or in the cell of column = 23, row = 12 and in the cell of column = 23, row = 18, respectively). We assume that both new wells are screened only in layer 3. Each well will be pumped at a rate of -130 (10^{-4} m^3/s).

The simulation starts in the steady-state without any pumping, after which the pumping yield will be introduced in time step 1. The pumping will continue for 500 days after which it will stop, and the simulation will then continue for another 500 days.

Two new fields now must be defined:

- The specific yield (i.e. the storage coefficient in an unconfined state).
- The storage coefficient in a confined state.

Via the menu "Select-Field F3" ➔ "Load a New Field", load the new field of the "Specific yield" coefficient, then select the cells of the entire domain, and assign them the value 25 (in % as the specific yield coefficient unit is in percent). Then load the field of the "Confined Storage " coefficient and assign the value of 1e-5 (in m^{-1}) to all cells of the domain.

5.4.1 Definition of the Non- meshed parameters

Click the button 

to bring up the general menu of "Non-meshed parameters".

5.4.1.1 General Parameters

Double-click on the first line "General Parameters", then "Preprocessor". As shown below, make some modifications in the paragraphs "Control of the Hydraulic Resolution of Groundwater" and "Data Units"

Paragraph "Control of the Hydraulic Resolution of Groundwater"

```
       20 = Maxi number of iterations for time steps after time step #°0 (transient)
       20 = Maxi number of iterations for time step #0 (Initial Steady State)
Transient = Hydraulic flow Regime [0=Transient state ; 1=Steady state]
```

Paragraph "Data units"

```
     0 = Confined storage coefficient unit in [-] or [m-1]
     % = Specific yield               unit in [-] ['%' when in %]
   Day = Time unit (for model step) (second, min, hour, day, decade, month, year)
Specif = Input Confined Storage Coeff. (0=Hydrogeol. ; 1=Specif. ; 2=Compressibilit.)
```

5.4.1.2 Cells with time series

We define the places where we wish to memorize the changes over time of the values simulated during this period.

In the general "Non-meshed parameters" menu, click on the line "Cells with Time Series". Then on "Preprocessor", then on "Create a new 'Time Series' file".

A list of fields, corresponding to the User Profile, appears where it is possible to memorize the time evolution in some points of the domain. Select the field "Hydraulic Head". Then click on "New Point" to add points for this field. Now select the three cells of layer 1 located above the pumping.

Select "Cell Centre Defined by Column, Row, Layer" and type in the coordinates of the first point for which the hydraulic head evolution should be memorized: Column = 25, Row = 15, Layer = 1, then Column = 23, Row = 12, Layer = 1, and finally Column = 23, Row = 18, Layer = 1.

5.4.1.3 Definition of time steps

To simulate the two periods of 500 days, we use of 36 model time steps whose final dates, in days, are given in Table 1 (durations increase from left to right and from the first to the last row).

0.1	0.2	0.5	1	2	5	10	20	50
100	150	200	250	300	350	400	450	500
500.1	500.2	500.5	501	502	505	510	520	550
600	650	700	750	800	850	900	950	1000

Table 1 - Dates of the 36 time steps of the hydraulic simulation in transient a regime.

The definition of these time steps is shown on Figure 73 to Figure 77.

In the general "Non-meshed parameters" menu, double-click on the line "Time Steps" (Figure 73). Click on "Pre-processor" then "Create a new 'Time steps' file" (Figure 74).

Accept "0." as starting date of the simulation (the date of time step 0) and request Automatic generation of 36 time steps. (Figure 75)

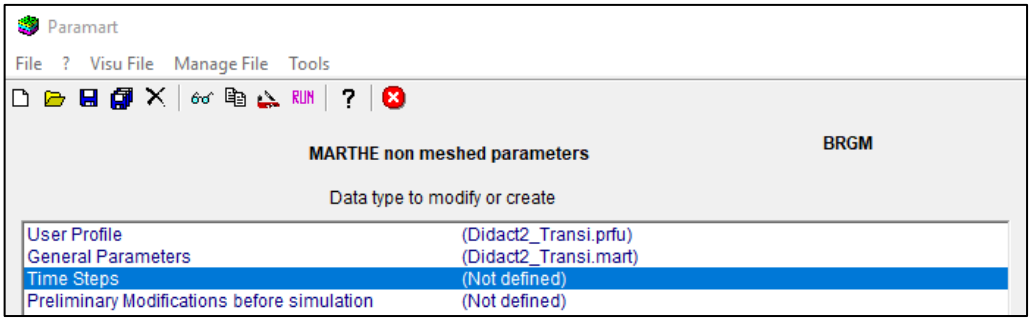


Figure 73 – Selection of the "Time steps" file.

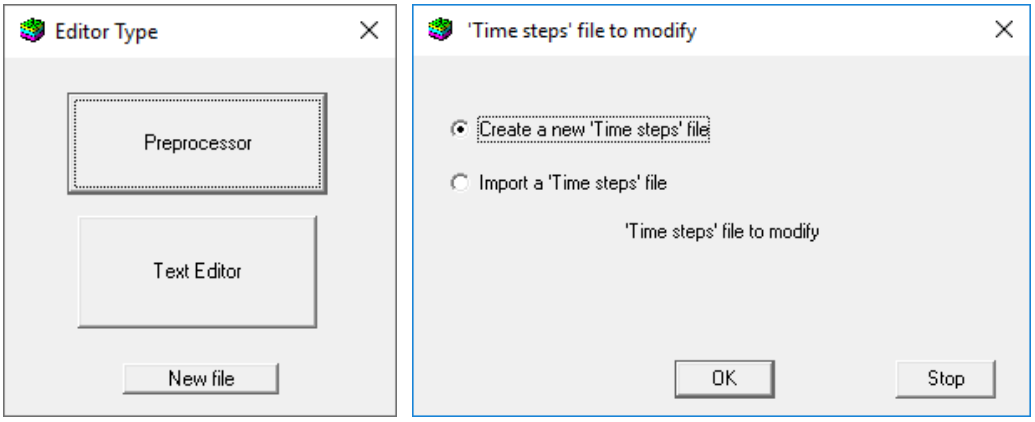


Figure 74 – Selection of the "Pre-processor" mode and "Creation of a New "Time Steps" file.

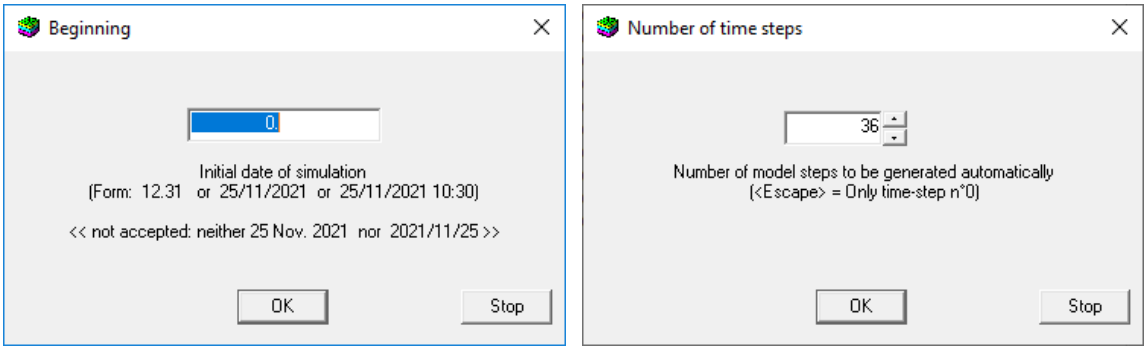


Figure 75 – Definition de the starting date of the simulation and automatic creation of the 36 time steps.

Accept the (fictitious) value 1 (day) as "Duration of Time Steps if Uniform", key "Esc" as the duration is not uniform, click on "Definition of Dates of All Time Steps" then on "Definition by Integrated Spreadsheet" (Figure 76). Then define the end dates of time steps 1 to 36 by giving them the values of Table 1. (Figure 77)

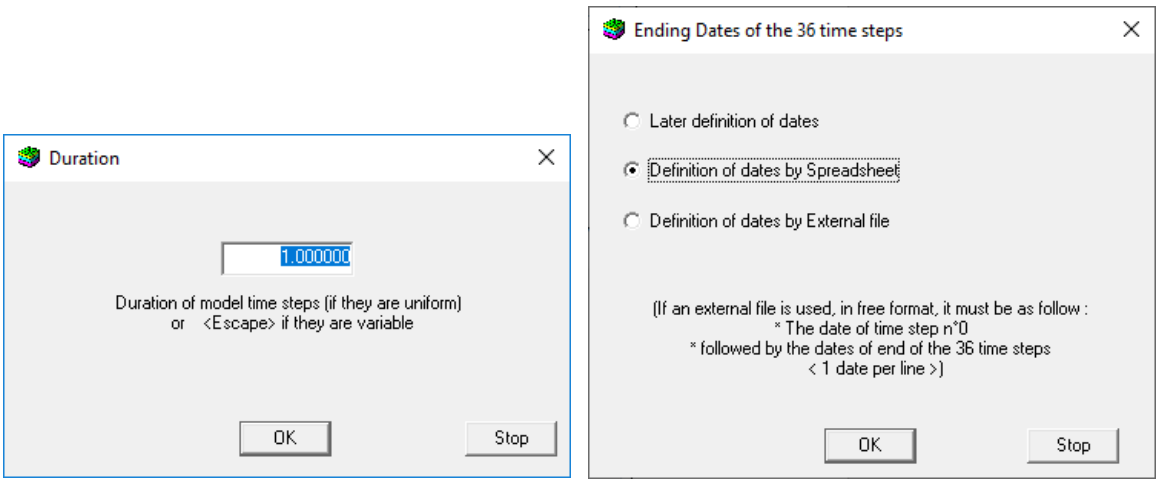


Figure 76 – Definition of the duration of the time steps ("Esc" as the duration is not uniform) Select "Definition by Integrated Spreadsheet" of the end dates of the time steps.

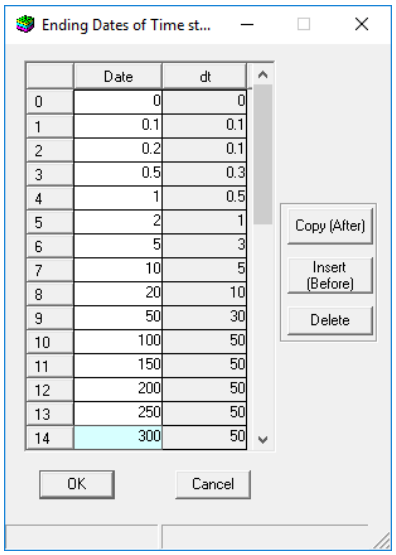


Figure 77 – Definition of the end dates of the 36 time steps with the integrated spreadsheet.

Time step number zero

Time step 0, corresponding to the steady-state or initialization, is selected by default.

- Annul the pumping discharge rate (initially set at -12). Click on "New Actions" then ➔ "Standard hydraulic parameters" ➔ "DISCHARGE" ➔ "CELL" and in the cell of the well, assign value **0** to column = 25, Row = 15, Layer = 3.
- Now output the field of the simulated hydraulic head. Click on ➔ "Standard hydraulic parameters" ➔ "HYDR_HEAD" ➔ "OUTPUT", and set the value "1" for obtaining an output.

Then click "Exit".

Time step number 1 (date = 0.1 day)

This is the start of the transient regime. We introduce three pumping flow rates of -130 10^{-4} m^3/s.

Now request the selection of time step 1:

- Selection of a time step ➔ *Number 1*.
- "New Actions" then ➔ "Standard hydraulic parameters" ➔ "DISCHARGE" ➔ "CELL" and in the cell of column = 25, row = 15, layer = 3 assign the value -130. We repeat the same operation in cell column = 23, row = 12, layer = 3, and then in cell column = 23, row = 18, layer = 3.

Time step number 18 (date = 500 days)

Request an output of the fields "HYDR_HEAD" , "%SATURAT" and "AQUIF_DEPTH".

Time step number 19 (date = 500.1 days)

Stop the pumping for observing the recovery. For this, introduce a "DISCHARGE" of 0 in the three pumping cells where a flow rate of -130 was introduced.

Time step number 36 (date = 1000 days)

Request an output of the field of simulated hydraulic head.

5.4.2 Running the simulation

The simulation takes place a fraction of a second. Examination of the file "*histobil_debit.prn*" (water balance flow history), with Excel ® or its equivalent, shows a very good convergence: the internal rate of non-convergence is always less than 10^{-4} %, except during the start of recovery when it reaches 4 %. This due to the hydraulic shock resulting from the sudden stop of pumping and to the resulting strong hydraulic head variations. The file also shows that at the end of pumping there were 56 saturated cells.

To try and improve the convergence, we can introduce an under-relaxation coefficient of 0.3, at the same time increasing the maximum number of iterations.

Paragraph "Control of the Hydraulic Resolution of Groundwater"

```
 90 = Maximum number of iterations for time steps after time step #°0 (transient)
 50 = Maximum number of iterations for time step #0 (Initial steady state)
0.3 = Relaxation coefficient for resolution [Def=1]
```

After re-running of the simulation, a check of the file "*histobil_debit.prn*" shows a very good convergence: the internal rate of non-convergence is always less than 10^{-3} %, except during the start of recovery when it reaches 0.3% (over a very short time).

5.4.3 Results

Figure 78 shows the field of the simulated hydraulic head in layer 3, after the initial steady state and after 500 days of pumping. After 500 days of pumping (Figure 79), we observe that:

- In layer 1, a large zone of the domain is dewatered;
- In layer 2, the central pumping cell is dewatered.

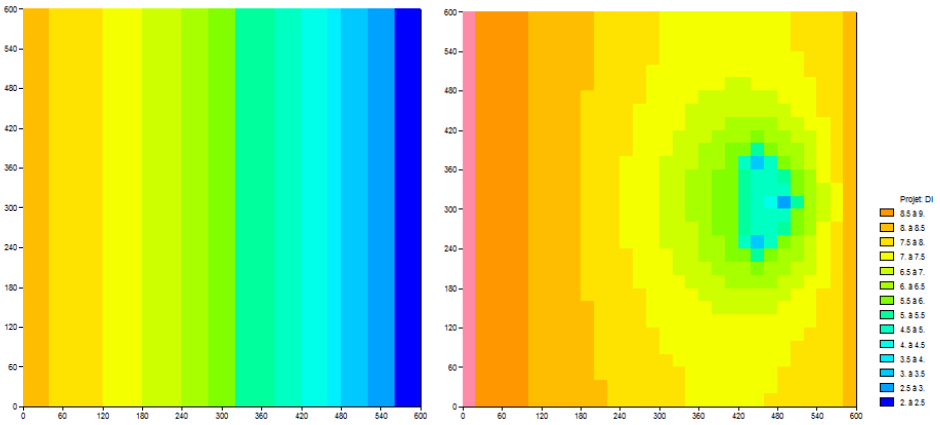


Figure 78 – Hydraulic head in layer 3:
Left: Steady-state without pumping; Right: After 500 days of pumping.

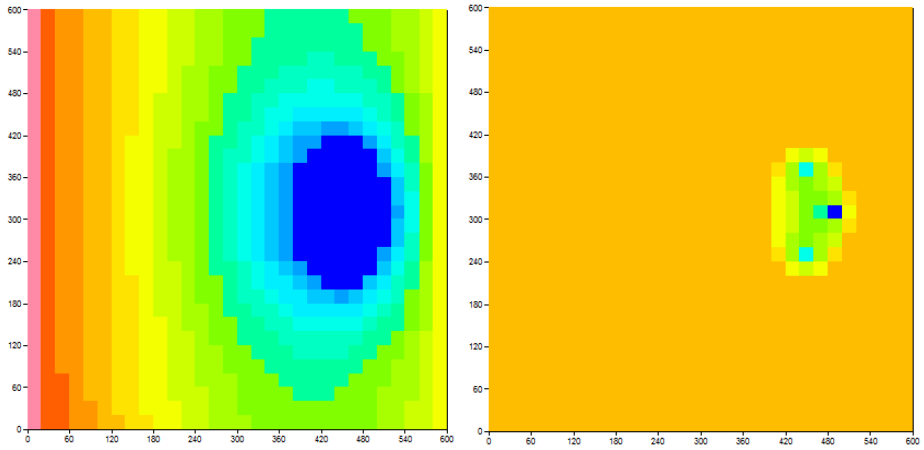


Figure 79 – Percentage of water saturation after 500 days of pumping.
Left: layer 1; Right: layer 2.
The deep-blue colour indicates cells that are (almost) dewatered.

Figure 80, based on the "*histobil_debit.prn*" file, shows the evolution of destorage flow in the groundwater, which becomes almost nil after 250 days when a steady-state regime is almost reached. (The “destorage flow” is the rate of aquifer storage decrease).

Figure 81, based on the "*historiq.prn*" file, shows the hydraulic head evolution in layer 1 below the central well and in one of the neighbouring wells. The evolution is regular, notwithstanding the dewatering of layers 1 and 2 in the central well. We saw that the convergence of flow rates was very good, with the default "Pseudo-Non-Saturated" scheme.

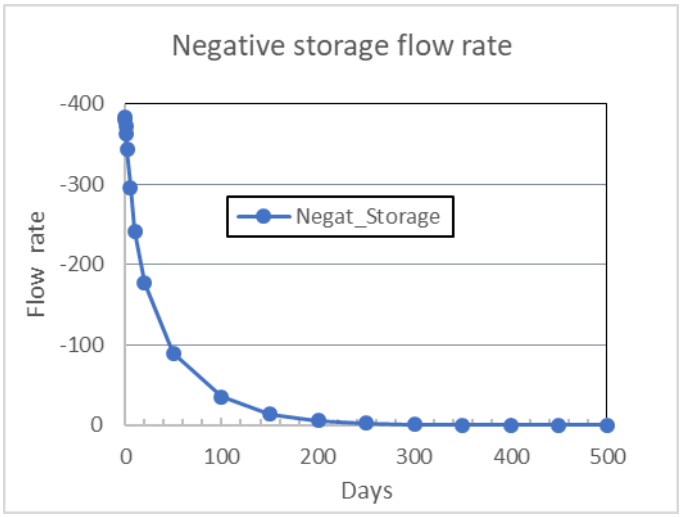


Figure 80 – Evolution of groundwater destorage flow.

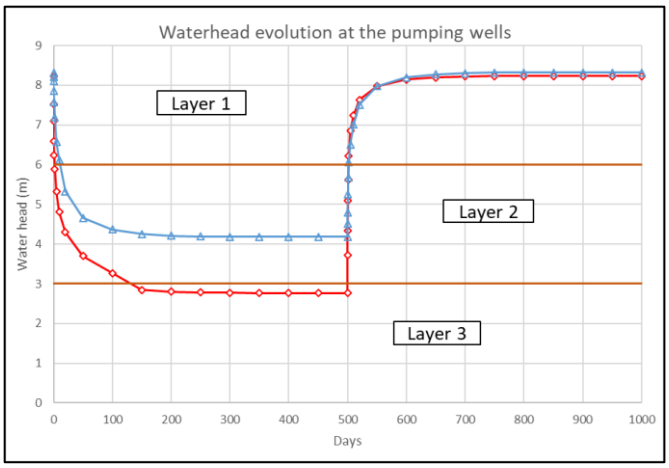


Figure 81 –Hydraulic-head evolution in layer 1 in the central well (in red) and in a neighbouring well.

5.5 SIMULATION OF MASS TRANSPORT

This example corresponds to the project ***Didact3.rma***.

Contrary to other modelling software, the MARTHE code enables a coupled simulation of flow and mass transport, which is optimal for complex settings. Such settings include unconfined groundwater with dewatering or the unsaturated zone, especially in case of interaction between transport and the flow-velocity field, when the fluid density is modified by salinity and/or temperature, or when viscosity is influenced by temperature and concentration, etc.

Implementation of the simulation of mass transport with the MARTHE code is described by Thiéry (2015b) in an individual report BRGM/RP-64765-FR.

Starting from the simulation example of groundwater flow in the steady-state regime: project *Didact2.rma*. Close the current project (*Didact2_Transi.rma*) and open the project *Didact2.rma* that was saved.

First, define additional parameters for continuing the hydraulic simulation by a mass transport calculation in a transient mode. For security reasons, keep the project *Didact2.rma* unchanged,

and automatically make a copy under the name *Didact3* that will be the new project with transport. To do this, use the "File" menu ➔ "Make Backup Copy of the Project" and choose the name *Didact3*. We could have chosen to create the copy in a different folder, but this is not necessary.

All files in the project "*Didact2.rma*" are copied “as is” under the name "*Didact3*". However, any other included files, for instance in a time-step file [.pastp], are not copied.

This copying operation is also handy for keeping a project in a given state for archiving, or for exporting all files related to a project to another modeller, or to another computer.

Close the current project and open the project ***Didact3.rma***.

5.5.1 Definition of Non-meshed parameters

Click on the button 

to bring up the general menu of "Non-meshed parameters".

5.5.1.1 General Parameters

Double-click on the first line "General Parameters", then "Pre-processor". Then modify the four paragraphs as shown below.

Paragraph "Time Steps and Sub-Steps"

```
12 = Number of sub-time steps of model              [Default=1]
```

To simplify, we will later create three model time steps of 12 months, each subdivided into 12 sub-time-steps of one-month duration.

Paragraph "Data Units"

```
 Month = Time unit (for model time steps) (sec, min, hour, day, decade, month, year)
mug/m3 = Concentration unit in kg/m3
   mug = Mass Unit in kg
```

As the "mug" units correspond to "µg", they might be replaced by 1 10^{-9} kg.

Paragraph "Transport/Coupling of Concentration, Heat, Salinity"

```
TVD = Transport method (0=Finite Diff. ; 1=Random-W ; 2=Characteristics=MOC ; 3=TVD)
 10 = Longitudinal Dispersivity (m) [* = Spatialized Field]
  1 = Transverse   Dispersivity (m) [* = Spatialized Field]
```

We use the more accurate TVD transport method and keep the maximum default number of iterations at 20.

Paragraph "Concentration and Pathlines"

```
        1 = Concentration Calculation
Transient = Transport scheme for Concentration [0=Transient ; 1=Steady state]
        2 = Retardation coefficient (except with Unsaturated Zone scheme) [Def=1
```

The default transport scheme is in transient mode, but it is clearer to re-state this.

Click twice on “Exit” to save the modifications of the “General Parameters”.

5.5.1.2 Definition of time steps

We want to define 36 time steps of the model as 3 "model time steps" of 12 months (each subdivided into 12 equal sub-time steps). A ‘***model time step***’, contrary to an ‘internal simulation time step’, is a time step during which actions can be introduced, such as modification of pumping flow rate, or output of simulation results.

In the general menu of "Non-meshed parameters", double-click on the line "Time steps". Click on "Pre-processor" and then on "Create a new 'Time steps' file". Accept 0 as starting date of the simulation (the date of time step 0). Request the automatic creation of 3 time steps, and assign the value 12 (months) as "Duration of time steps if uniform".

Then request the consultation of time step 1 to introduce the mass flux in the contaminated zone: select "=> Selection of a time step" and increment to 1 the "Number of Time Steps to Consult". Then choose "New Actions" (Figure 82), and then ➔ *Cluster* "Mass-Transfer, Salinity, Pathlines".

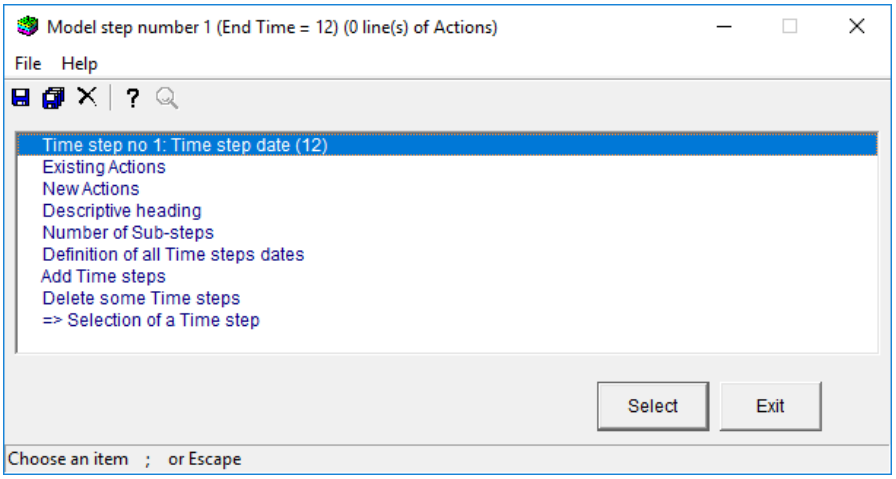


Figure 82 – Creation of an "Action" or "Modification" for time step 1.

After this, the *object* "CONC_MASS_FL = Concentration mass flux" (Figure 83) ➔"Modification per cell". Set the value 1.0519 10^5 (µg/month per cell of 400 m^2) in the block "Columns 6 to 11, Rows 12 to 18, Layer 1" (Figure 84) and click OK. This modification will be considered from the start of the first sub-time step of this model time step 1.

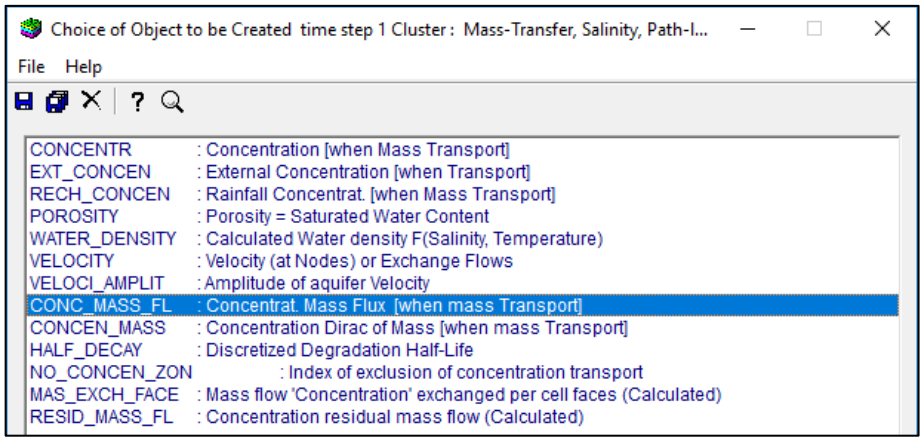


Figure 83 – Selection of object "Concentration" mass flux" for time step 1.

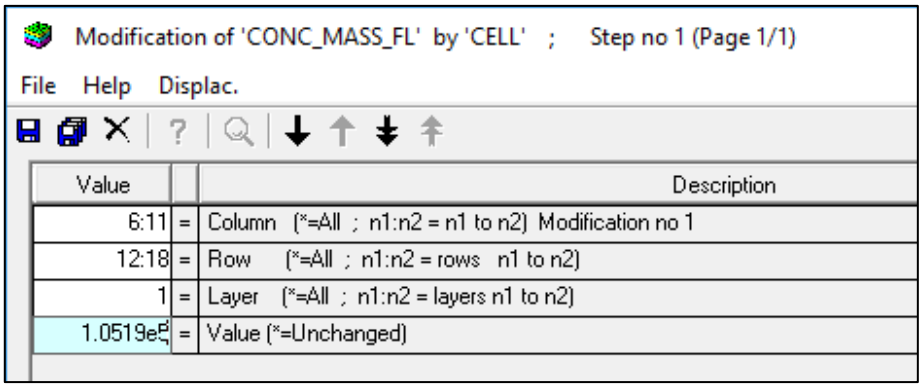


Figure 84 – Definition of the value of "Concentration" mass flux in time step 1.

Also request an output of the concentration field simulated during time steps 1, 2 and 3, after 12, 24 and 36 months, respectively. The concentration will be output in text format, in a file with the generic name "*gridsimul.out*". Click again on the *cluster* "Mass-Transfer …" and choose the *object* "CONCENTR = Concentration", then select the *action* "OUTPUT" and assign "1" as the output index value, leaving the other fields unchanged.

This operation of requesting an output of the simulated concentration field will now be repeated for time steps 2 and 3; "CONC_MASS_FL = Concentration mass flux" will not be redefined for these time steps, as, in MARTHE, all assignments remain valid until (renewed) modification.

To select another time step, press the "Exit" button, then in the menu that appears (Figure 85) select option "=> Selection of a Time step".

Choose time step 2, introduce the same request for output of the field "CONCENTR", and then repeat the same operation for time step 3.

After that, press "Exit" twice and output the description of the time steps that appears in clear in the file "*Didact3.pastp*".

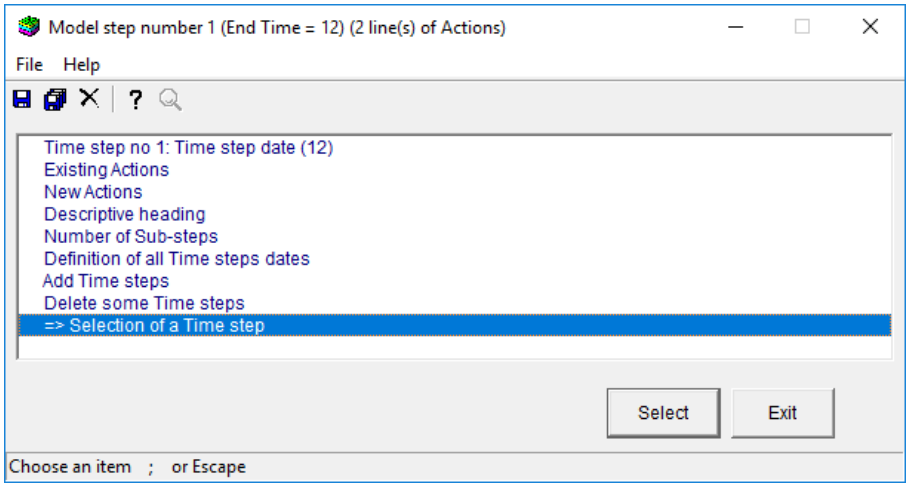


Figure 85 – Selection of a time step.

5.5.1.3 Definition of cells with time series

We now define the places where the evolution over time of the simulated values will be memorized.

In the general menu of "Non-meshed parameters", click on the line "Cells with Time series" (Figure 86) and click on "Pre-processor" and then on "Create a new Time Series File".

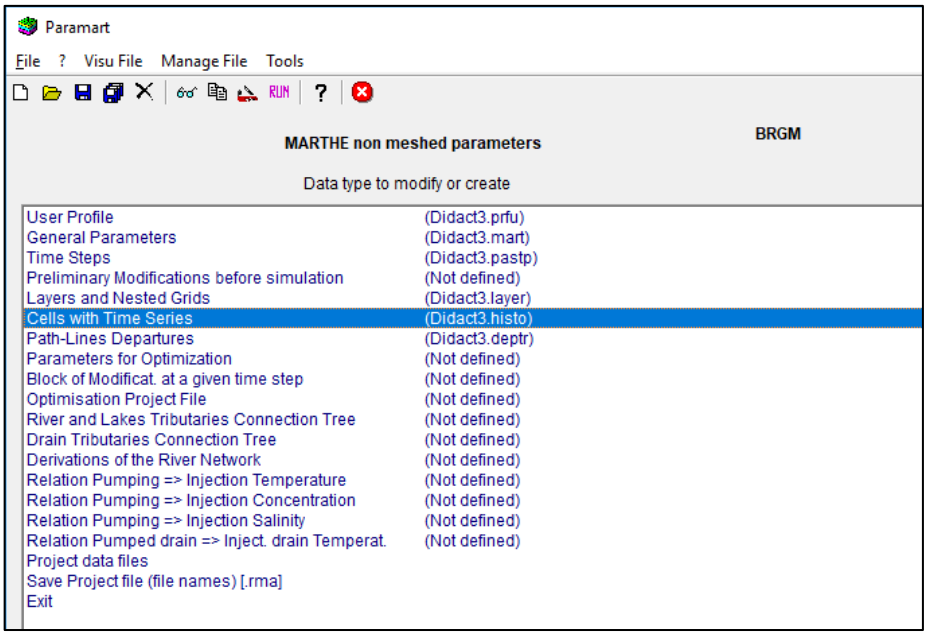


Figure 86 – Definition of the cells with time series.

A list of fields appears, corresponding to the user profile for which we can request a time series in certain points of the domain. Select "Concentration" and click "Add" to add points for this field.

Then select "Exact Point defined by X, Y, Layer", as the selected points are not located in the exact centre of a cell (Figure 87).

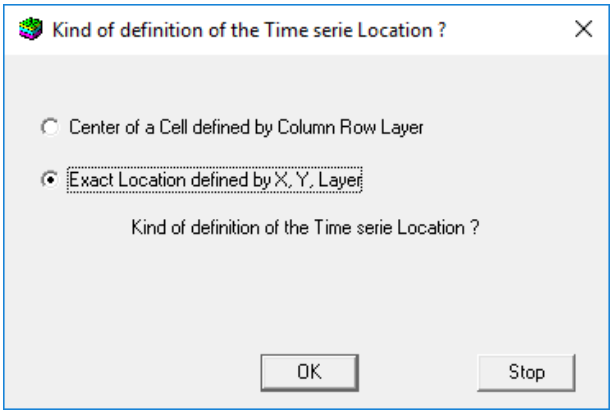


Figure 87 – Type of definition of a time series.

Then introduce the coordinates of the first point for which one wishes to memorize the time evolution of the concentration, giving it the identifier "P1" (Figure 88).

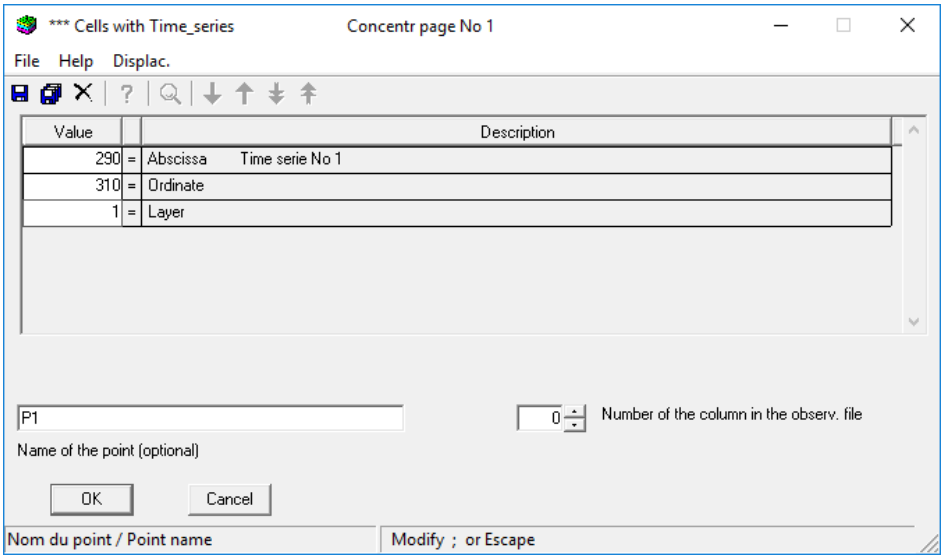


Figure 88 – Definition of the coordinates of a time series place.

Repeat the same operation "New Point" and "Exact Location" followed by (390, 310 Layer 1) for point P2, and continue by setting the same coordinates but for layer 2 (P3 and P4), and then for layer 3 (P5 and P6). Click on "Exit" twice and save. The cell coordinates with time series now are output, in clear, in the file "*Didact3.histo*" (Figure 89).

```
  /Concentr     /HISTO/    =    /XCOO:X= 290Y= 310L=    1; Name=P1
  /Concentr     /HISTO/    =    /XCOO:X= 390Y= 310L=    1; Name=P2
  /Concentr     /HISTO/    =    /XCOO:X= 290Y= 310L=    2; Name=P3
  /Concentr     /HISTO/    =    /XCOO:X= 390Y= 310L=    2; Name=P4
  /Concentr     /HISTO/    =    /XCOO:X= 290Y= 310L=    3; Name=P5
  /Concentr     /HISTO/    =    /XCOO:X= 390Y= 310L=    3; Name=P6
*** End of file: 'Cells with Time Series'              ***
```

Figure 89 – File of "Cells with Time Series".

After having saved the project file, double-click on “Exit” in the main menu of “Non-meshed parameters”. You are now back in WinMarthe *sensu stricto*.

5.5.2 Running the transport simulation and examination of the results

To start the simulation, click on the button 

located on the first row of the bottom toolbar. The simulation is done in a few seconds.

5.5.3 Preliminary verification of the balance values

As before, examine the "flowbalance.txt" file using the button  . A quick review shows that the calculation is done correctly. To comply with the TVD method (Courant number not exceeding 1), each of the 36 model time steps was automatically subdivided into 3, resulting in 108 calculation time steps. At the end of the calculation the overall input flow - output flow is balanced to within 1/1000th of a percent (Figure 90). We also see that the steady-state regime is far from being reached, as during the last step only 0.5 % of the mass from the contaminated area (4.4181e+06) is captured by the well (-2.5538e+04).

```
======================================== Time step    Nb 36 - t= 36.000

 ----- Cumulated Concentration mass        Time step    Since start of simulation
              Outflow through the Limits = -6.041             -18.75
               Inflow  in Internal cells = 4.4181E+06         1.5905E+08
               Outflow in Internal cells =-2.5701E+04        -1.1570E+05
                                 Storage = 4.3926E+06         1.5894E+08
            [Positive Storage (Inflow)] = 4.3926E+06         1.5894E+08
           [Negative Storage (Outflow)] =-1.1349E-03        -3.4954E-02
         Mass or Heat Balance deviation = -206.0             -1296.
                                    (%) = 4.6617E-03          8.1512E-04

              Total Mass (mobile phase) = 1.5894E+08
```

Figure 90 – Cumulative mass balance after three years.

5.5.4 Examining the simulated concentration

Quit the text editor (run by the eye glasses button ) and you are now back in WinMarthe.

5.5.4.1 Simulated concentration field

Activate the menu "File" ➔ "Simulated Grids (Open)", or simply type Control+R, and select the file *gridsimul.out*. This file contains the hydraulic head grid calculated at time step 0 and the concentration grids at time steps 12, 24 and 36. Choose the field "CONCENTR", then time step 36, at date 36 months, by double-clicking on that date, or by pressing the "Visualize" button (Figure 91). The concentration grid is then placed in the "Work" field and appears on screen for the current layer, which can be changed by selecting, for instance, layer 3 (Figure 92).

One can immediately draw the concentration contour lines with the menu "Tools" ➔ "Isovalues" ➔ "Single Field", or using the shortcut "Control+I", of which Figure 93 shows a partial view.

It is also possible in two mouse clicks to examine the concentration field in vertical cross-section. Use button  to select a row, and double-click the row in the well axis ➔ Click on button  to turn into a vertical cross-section (Figure 94). Use button  to return to a 2D plan view.

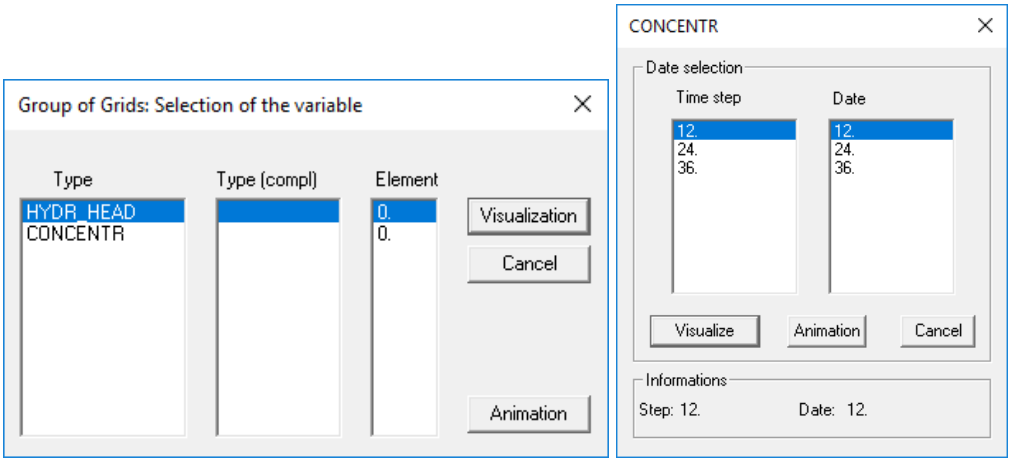


Figure 91 – Selecting the grid and the time steps to be visualized.

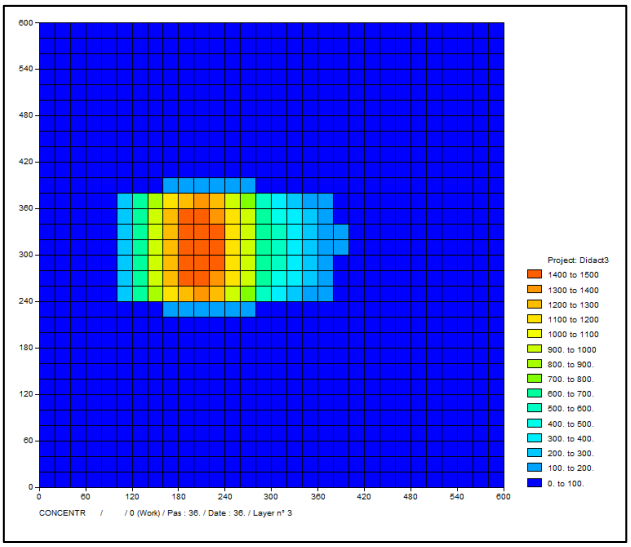


Figure 92 – Concentration after 3 years in layer 3.

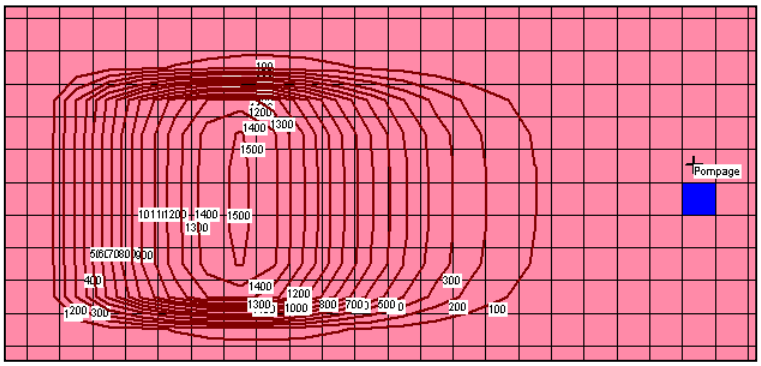


Figure 93 – Concentration contours after 3 years in layer 3.

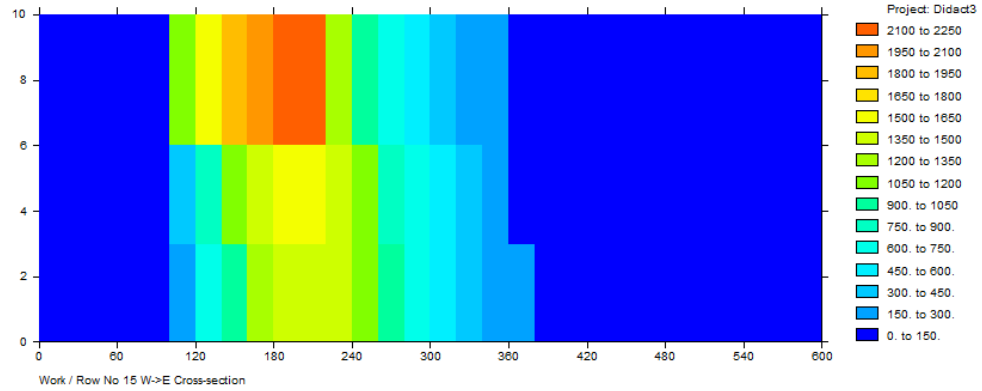


Figure 94 – Concentration after 3 years in vertical cross-section in the well axis.

5.5.4.2 Concentration variation in cells with time series

The simulation has generated a file with a generic name *historiq.prn* that is directly compatible with Excel ® or an equivalent spreadsheet. Simply double-click on it (or *open it* with Excel), and you automatically obtain a diagram in 3 or 4 mouse clicks (Figure 95). The TVD transport method

provides a fast simulation with very little numerical dispersion, and with no oscillations. Simply changing the selection (method 0, 1 or 2 instead of method 3), MARTHE can also simulate the transport with the finite-difference method, the "Random Walk" method, or the MOC method.

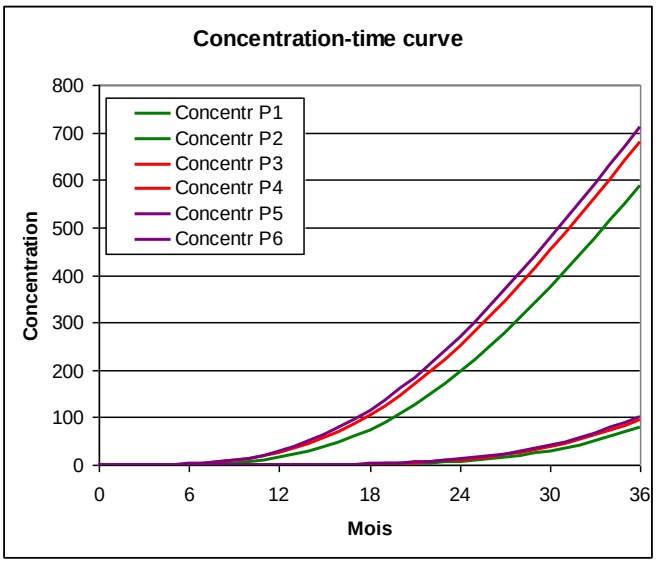


Figure 95 – Evolution of the concentration over time in six cells with time series.

5.5.5 Transport by the Method of Characteristics (MOC)

Use the button 

to display the main "Non-meshed parameters" menu, then "General Parameters", then "Transport/Coupling of Concentration, Heat, Salinity", and select the MOC transport method.

Paragraph "Transport/Coupling of Concentration, Heat, Salinity"

```
MOC = Transport method (0=Finite Diff. ; 1=Random-Walk ; 2=Charact.=MOC ; 3=TVD)
```

Paragraph "Concentration and Pathlines"

Then, in the "Concentration and Pathlines" paragraph, attribute to each particle a mass of 500 μg, and set, for safety, a maximum number of particles equal to 200,000.

```
   500 = Mass of each salinity particle (when particles)
200000 = Maximum possible number of salinity particles (MOC or R.W.)
```

As before, the simulation takes a few seconds, and gives comparable results (Figure 96 and Figure 97). We note that the time evolution is very regular, almost without oscillations.

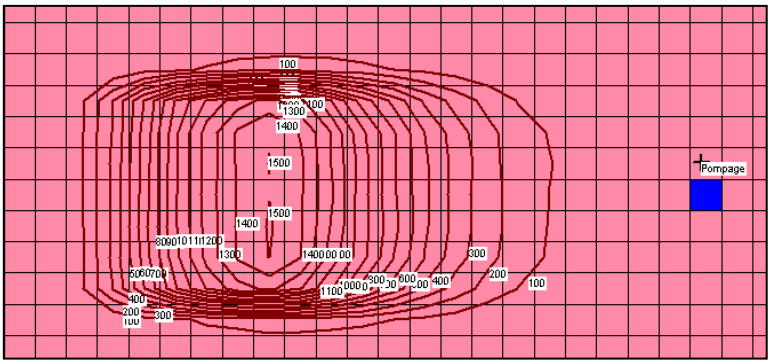


Figure 96 – Contour lines of the concentration after three years in layer 3, MOC transport method.

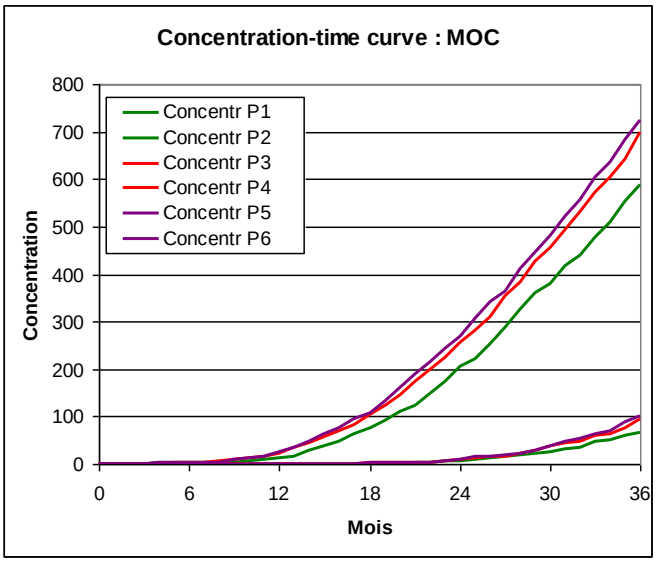


Figure 97 – Time evolution of concentration in six control points using the MOC transport method.

5.5.6 Variation in the definition of a contaminated area

Instead of introducing a mass flux equal to 1.0519 10^5 (µg/month per 400 m^2 cell), we could have introduced a concentration equal to 12,500 (µg/m^3) in the recharge over the cells concerned, proceeding as follows.

5.5.6.1 Definition of the contaminated area

The contaminated area lies in the rectangle [100 m < x < 220 m], and [240 m < y < 380 m]. To view this area for didactic purposes, draw the rectangle with the button located on the top bar. Click on button "Field Selection" and select the field "Zones for Soil, Rainfall, PET" that appears in blue. For more visibility, choose “equidistributed” colour ranges through the menu "View" ➔ "Colour Class Types" ➔ "E**Q**uidistributed", or more directly by the shortcut "Control+**Q**".

The background now becomes pale pink. Click again on button , and draw a rectangle bounding the area: x = 100 to 220 m, y = 240 to 380 m (or columns 6 to 11, rows 12 to 18). End by double-clicking on the last point to close the boundary. Drawn over the grid, give it the name "Zone_Contam". Accessing the menu "Polygons management" with the button , we see that this contour is a "*Polygon layer*" called "Drawing". Use the "Save" button on the far right to save

this polygon as "Zone_Contam.bln". We can change its colour, e.g. red, and its thickness, e.g. 6 units.
Now assign the zone number 2 to the inside of the contaminated area, because we will set a concentration equal to 12500 µg/m^3 to the recharge in this zone. Select the button  "Selection of cells contained in the closed contour" and double-click close to the contour. Confirm that it is inside the polygon "Zone_Contam". All cells inside the rectangle now are selected (in red). Using the button  , assign them zone number 2. Now type Control+L to return to the linear colour classes.

A 252.46 mm/year infiltration flux was defined in zone 1. Now there are two recharge zones and this flux must be defined in both zones, which can be done in the General Parameters file.

Click on the button 

to bring up the main "Non-meshed parameters" menu. Double-click on the first line "General Parameters" and on "Preprocessor". Then select the paragraph "Initialization before simulation". Select "Existing Actions" and "Hydroclimatological Balance, Crops". Then replace the number of zone "1" by the number "*" (all zones) or "1:2" (zone numbers 1 to 2).

5.5.6.2 Defining the recharge concentration

In the main "Non-meshed parameters" menu, double-click on the line "Time Steps" and "Preprocessor" and "Select a Time Step". Then select time step 1 and "New Actions" and *cluster* "Mass-Transfert, Salinity, Pathlines" and *object* "RECH_CONCEN" = Recharge Concentration (Figure 98). Then set the value 12500 in soil zone 2 and click "OK".

It is necessary to remove the mass flux 1.0519 10^5 µg/month that had been introduced: for this, after clicking on "Exit" select "Existing Actions" and *cluster* "Mass-Transfer Salinity, Pathlines" and *object* "CONC_MASS_FL = Concentration Mass Flux". Replace value 1.0519 10^5 by value 0.

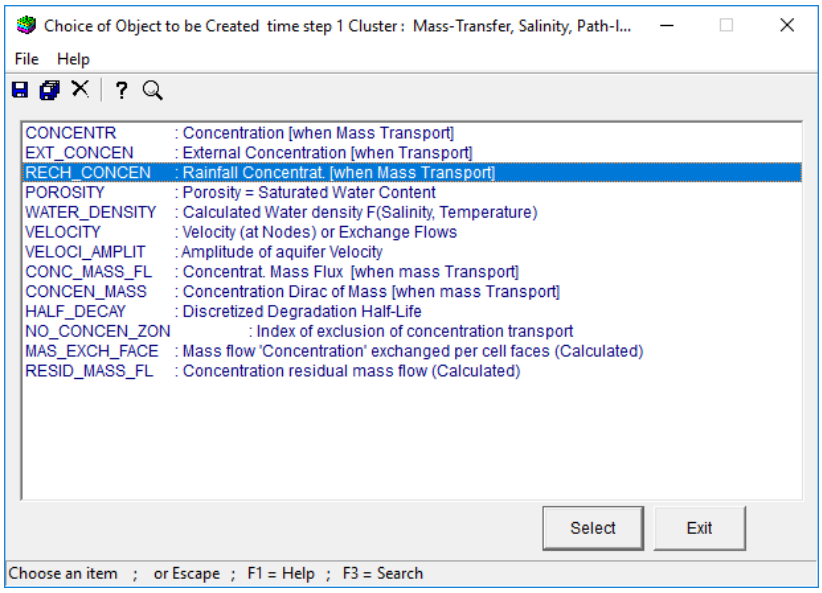


Figure 98 – Definition of the Recharge Concentration at time step 1.

6 Example 4: Simulation of a water table rise resulting from local recharge through the unsaturated zone - Radial coordinates

Project: ***Didact_Rad_Vert_1.rma*** (steady-state regime).

Project: ***Didact_Rad_Vert_2.rma*** (transient regime).

This example shows how to use a radial model for a simulation of a water table (or free surface) rise of groundwater resulting from local recharge through the unsaturated zone. It is modelled with the standard "Pseudo-UZ" scheme (and ***not*** with an unsaturated zone scheme).

The system characteristics are the following (Figure 99):

- Aquifer thickness = 70 feet (bottom = 0, topography = 70 feet)
- Lateral extension = 5000 feet
- Horizontal hydraulic conductivity = 5 feet/day = 5 x 3.57278 10^{-6} m/s
- Vertical anisotropy of the hydraulic conductivity = 0.05
- Imposed on the lateral boundary = 25 feet (up to an elevation of 25 feet).
- Specific yield coefficient = 20% (negligible confined storage coefficient at 0.001 m^{-1}).
- Recharge flux = 254 m^3/day over a surface of about 24,281 m^2.
- Transient simulation.

(N.B.: 1 foot = 0.3048 metres).

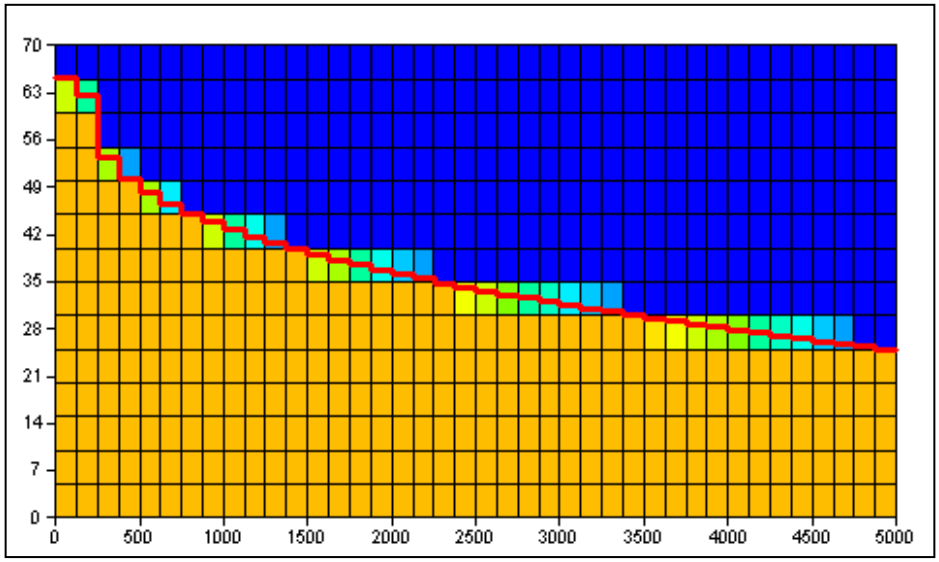


Figure 99 – Field of the saturation rate and rise of the steady-state free surface profile (in red). Totally saturated in yellow/orange.

6.1 MODELLING SETUP

We discretize the system into 14 layers of 5 feet thickness, with cells of a lateral extension of 125 feet. For efficient modelling of this system due to its symmetry, we setup the MARTHE model on a radial grid, where the:

- Abscissae correspond to the radial distance from the origin, the columns thus corresponding to a crown whose radius is the abscissa; and the

- Ordinates correspond to an angle (in degrees), the rows corresponding to an angle quadrant.

In view of symmetry, each layer can be represented as a row of a width of 360° and a length of 5000 feet, divided into 40 columns of 125 feet. This gives 14 layers, each composed of a row of 40 columns.

In fact, it is much easier to create a "radial vertical cross-section". The grid then is composed of 40 columns of 125 feet width, and 14 rows of 5 feet that represent the 14 layers. We indicate that the cross-section sector angle (“slice”) is 360°.

WinMarthe creates a regular grid with 40 columns, 14 rows and a single layer. We retain the default values of the "Topo. Elevation" at 0 metre, and of the thickness at 10 m as these data will not be used, but calculated from the grid.

6.1.1 General Parameters

Paragraph "Data units"

```
3.57278e-6 = Aquifer Hydraulic conductivity   unit in m/s (or m2)
      m3/j = Flow (Discharge, Yield)        unit in m3/s (Kg/s for Gas flow)
    0.3048 = Hydraulic Head, Elevation, Pressure   unit in meter
      1e-3 = Confined   Storage Coefficient unit in [-] or [m-1]
         % = Specific yield                 unit in [-] ['%' when in %]
    0.3048 = Grid horizontal coordinate unit in m
      5e-2 = Uniform Vertical Anisotropy coefficient Kv/Kh for Hydraulic Conductivity
         % = Porosity = Water Content unit [dimensionless] ['%' when in %]
```

Paragraph "Geometric options, Data reference, Processors"

```
 Vertic = Grid orientation: 0=Standard ; 1=Vertical Cross-section: gravity along Oy
    360 = Vertical slice width (Grid coordinate unit or Degrees) [Def=1]
```

6.1.2 Definition of the radial grid type

Use the button 

to bring up the general menu of "Non-meshed parameters", then "Layers and Nested Grid" and "Pre-processor" and Paragraph "Nested Grids, Cross-section, Radial" (layer description file [.layer]).

Paragraph "Nested Grids, Cross-section, Radial"

```
 0 = Number of included Nested Grids
 0 = Vertical cross-section with Irregular Substratums (0=No ; 1=Yes)
 1 = Radial grid [Radius , Angle] (0=No ; 1=Yes)
```

6.1.3 Percolation flow rate

We assign a percolation flow rate of 254 m^3/day distributed over the first two cells, i.e. over a disc with a radius of 125 feet (a crown with a diameter of 250 feet), or a total surface of about 18,240 m^2. Introduce a quarter of the flow into cell 1 and three-quarters into cell 2 that has a three times larger surface area.

6.2 STEADY-STATE MODELLING

Carry out a first simulation in steady-state with the following resolution parameters:

Paragraph "Control of Aquifer Hydraulic solving process"

```
    60 = Maxi number of hydraulic iterations for time step n°0 (Initial Steady State)
  1e-7 = Average hydraulic head deviation between 2 iterations for convergence
     0 = Relaxation coefficient for resolution [Def=1]
Steady = Hydraulic flow Regime [0=Transient state ; 1=Steady state]
     1 = Full vertical hydraulic conduct. when Pseudo-USZ [1=Yes ; 0=Funct(saturat)]
```

N.B.: The last parameter “Full vertical hydraulic conductivity when Pseudo-USZ" allows a more efficient management of the percolation through dewatered layers.

6.3 RESULTS OF STEADY-STATE MODELLING

In the time steps file [.pastp], request an output of the hydraulic head field and of the saturation rate field "%SATURAT/OUTPUT I= 1;"; The simulation is performed quickly, in 16 iterations, 1/10th of a second, with no difficulty and a good convergence:

- Overall convergence difference = 1 10^{-4}%
- Internal convergence difference = 2 10^{-10}%

As we are dealing with a vertical cross-section, we obtain a "free_surf.bln" file containing the profile of the calculated free surface. We also generate a "free_surf.prn" file in a format compatible with Excel ® or an equivalent spreadsheet software. The field "Saturation Rate" is output in the "gridsimul.out" file.

Figure 99 shows the field of the saturation rate (totally saturated in yellow/orange) with superposition of the calculated free-surface profile (i.e. the red line) of the "free_surf.bln" file.

6.4 TRANSIENT MODELLING

This example corresponds to the project ***Didact_Rad_Vert_2.rma***.

Start from a horizontal uniform potentiometric level at an elevation of 25 feet and calculate the evolution of the free surface over time. Model a total period of 498,000 days, using time steps whose duration follows a geometrically increasing rate of 1.3. The first time-step lasts 0.3 day, the 2nd 0.39 day and the 50th 114,906 days.

Paragraph "Data Units"

Add:

```
   Day = Time unit (for model time steps) (second, day, decade, month, year, etc.)
Specif = Input Confined Storage Coeff. (0=Hydrogeol. ; 1=Specific ; 2=Compressibil.)
```

The transient simulation is carried out with following solution parameters:

Paragraph "Control of Aquifer Hydraulic solving process"

```
     100 = Maxi number of iterations for time steps after time step #°0 (transient)
       0 = Maxi number of hydraulic iterat. for time step n°0 (Initial Steady State)
    1e-7 = Average hydraulic head deviation between 2 iterations for convergence
     0.2 = Relaxation coefficient for resolution [Def=1]
Transient = Hydraulic flow Regime [0=Transient state ; 1=Steady state]
       1 = Full vertical hydraulic conductivity when Pseudo-Usz [1=Yes]
```

In transient mode, because of the resulting system non-linearities, we must use an under-relaxation coefficient for the calculation at each new external iteration. With these parameters, the 50 time steps of the model are calculated in a few seconds. The convergence of the simulation is very good. In the [.pastp], time steps file with the pre-processor, request the output of the

hydraulic head field after 12, 50, 111, 190, 700, 2600, 9700 and 36000 days. This gives the hydraulic head profiles for these dates in the "free_surf.bln" file.

Figure 100 shows the field of the saturation rate at the last time step, as well as the changing profiles of the free surface after 12, 50, 111, 190, 700, 2600, 9700 and 36000 days, from bottom to top. For a better visualization, use a text editor for extracting the profiles at the different dates of the "free_surf.bln" file and put them in separate files for giving them different colours in the "Polygons" menu of WinMarthe.

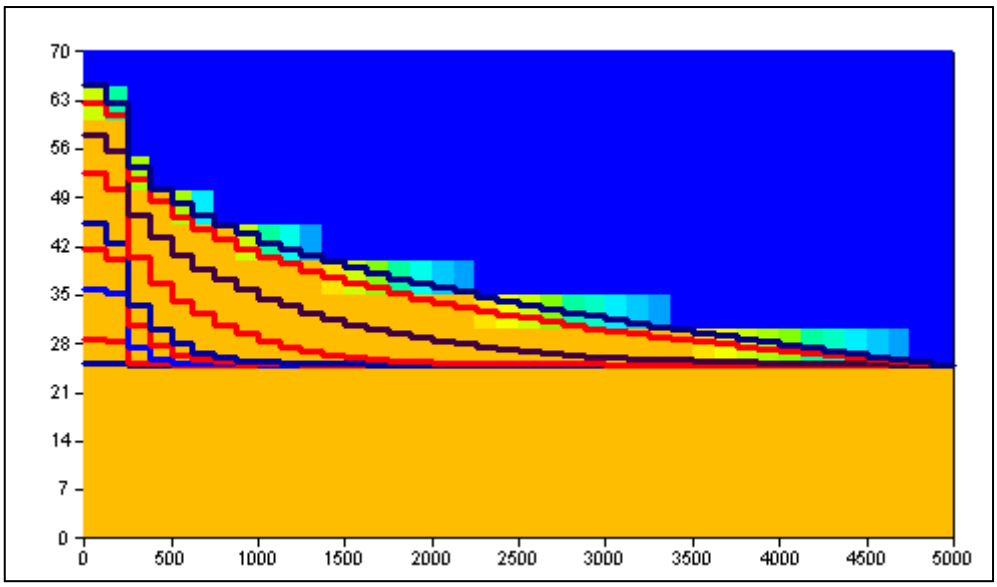


Figure 100 – Transient rise of a water table. Field of the saturation rate at the end of the simulation and successive profiles of the water table from bottom to top.

N.B.: For simplicity, this example was processed in a 2D radial configuration, but MARTHE also allows processing it in full 3D.

7 Example 5: Flow with density effects near the sea: The Henry saltwater wedge problem

Project ***Henry_Perma.rma*** (steady-state).
Project ***Henry_Perma_Loin.rma*** (steady-state, integrating the sea-coast).
Project ***Henry_Transi.rma*** (transient mode).

This classic benchmark from the literature shows how to consider in a simple manner the density effects related to salinity variations in a coastal aquifer. Implementation of how to account for density effects is described by Thiéry (2015b) in a dedicated report BRGM/RP-64765-FR.

The aquifer system of 200 cm width by 100 cm height, will be modelled in a vertical cross-section. The sea boundary is located at the right-hand side, and fresh-water inflow of 660 10^{-7} m^3/s per metre thickness of the cross-section, comes in at the left boundary (Figure 101).

The characteristics of this system are:

Hydraulic and hydrodispersive parameters:

- Hydraulic conductivity : K = 1. 10^{-2} m/s,
- Porosity : ω = 35%,
- Diffusion coefficient : D = 6.6 10^{-6} m^2/s,
- Dispersivity : α = 0,
- Density law = Schlumberger relationship (described by Vandenbeusch 1976).

Boundary conditions:

- Western boundary: external salinity = 0, fresh-water flow rate = 660 10^{-7} m^3/s distributed over 20 cells,
- Eastern boundary: imposed salinity 35 kg/m^3 (external salinity = 9999), prescribed hydraulic head = 0 in each cell.

Initial state:

- Salinity = 0 in the entire domain (except 35 kg/m^3 at the eastern boundary),
- Hydrodynamics: Uniform hydraulic head = 0 in the entire domain.

Grid:

- Adopt a vertical-section layout. The grid consists of 40 columns of 5 cm width, and 20 rows of 5 cm width, corresponding to 20 layers of 5 cm thickness.

7.1 STEADY-STATE MODELLING

Project ***Henry_Perma.rma***.

The first modelling of this system poses no problems with the hydraulic head simulation and the transport simulation in steady-state. In view of the steady-state, we set a maximum of 25 iterations of coupling between the hydrodynamics and the transport of salinity. For the hydrodynamics, a maximum of three external iterations was set at each coupling iteration. As the groundwater is confined, 1 or 2 external iterations are effectively enough, provided there are enough internal iterations (here set at 50).

In view of the strong diffusion coefficient (6.6 10^{-6} m^2/s), we opt for calculating the transport with the "finite-difference method", which is the default method.

In summary, the parameters are:

Coupling:

- Number of coupling iterations = 25.

Hydrodynamics:
- Regime = Steady-state,
- Method = Simulation in “real hydraulic head”,
- Maximum number of iterations = 3 (and 50 internal iterations at most).

Transport:
- Regime = Steady-state,
- Method = Finite differences.

7.1.1 Grid definition:

Create a new project with a regular grid of 40 columns of 5 cm and 20 columns of 5 cm, with as origin the point (x=0, y=-100).

7.1.2 Definition of gridded data

As in the preceding examples, we define:
- A porosity equal to 35 (%) in the entire domain.
- A "DISCHARGE" field with +33 (10^{-7} m^3/s) for each of the 20 rows of column 1, and "9999" for the 20 rows of column 40.
- A "Fluid Salinity" field with only values equal to 35 (kg/m^3) for column 40.
- An "External Salinity" field, again with only values equal to 9999 for column 40.

We see that it is also possible to define all these data as "Initialization before simulation" with the "Non-meshed parameters" management module. This second approach, though slightly less “visual”, is perfectly suited to a Single Field case. Its advantage is that it only generates a single gridded field, that of hydraulic conductivity, which much facilitates any later modification of the grid, as well as providing an easy way of visually checking all the data.

7.1.3 Definition of the Non-meshed parameters

We proceed as for the earlier examples.

Press the button 

to bring up the general menu of "Non-meshed parameters", and then a "User Profile". Then select:

```
  1 = Transient State
  2 = Salinity (1=Yes  ;  2=Salinity and Density calculation)
```

Choose the option "Transient State" of the user profile, as we will later make a transient simulation.

After saving, return to the general menu "Non-meshed parameters", and select "General Parameters". Then define the following parameters:

Paragraph "Control of Aquifer Hydraulic solving process"

```
      3 = Maxi number of hydraulic iterat. for time step n°0 (Initial Steady State)
   5e-6 = Average hydraulic head deviation between 2 iterations for convergence
     50 = Maximal number of internal iterations in the solver [Def=10]
 Steady = Hydraulic flow Regime [0=Transient state ; 1=Steady state]
```

Paragraph "Data units"

```
  cm/s = Aquifer Hydraulic Conductivity      unit in m/s (or m2)
  1e-7 = Flow (Discharge, Yield)             unit in m3/s (Kg/s for Gas flow)
    cm = Hydraulic Head, Elevation, Pressure unit in meter
     % = Specific yield                      unit in [-] ['%' when in %]
    cm = Grid horizontal coordinate          unit in m
     % = Porosity = Water Content unit [dimensionless] ['%' when in %]
  1e-6 = Mass unit in kg
```

Paragraph "Geometric options, Data reference, Processors"

```
   100=Vertical slice width (Grid coordinate unit or Degrees) [Def=1]
Vertic=Grid orientation: 0=Standard ; 1=Vertical Cross-section: gravity along Oy
```

Paragraph "Transport/Coupling of Concentration, Heat, Density":

```
    25 = Maximum number of iterations for Density/Pressure *Coupling*
6.6e-6 = Molecular Diffusion (m2/s)    [ *=Spatialized Field ]
```

Paragraph "Salinity, Density":

```
  Head = Taking into account Density (0=No ; 1=Hydr_Head ; 2=Pressure ; etc.)
Schlum = Density(Salinity) relation (0=no ; 1=Linear ; 3=Schlumberger_VDB[Salinity])
     0 = Derivative of Density = F(Salinity) when Linear relationship [Def=0.7]
 1.e-4 = Average Salinity variation between 2 iterations for convergence
Steady = Salinity transport scheme [0=Transient ; 1=Steady state]
     1 = Calculation (Transport) of Salinity
```

It is indispensable to select "**1**=Calculation (Transport) of Salinity"; if not, the salinity is only "taken into account", but not "simulated" from the coupled transport features.

Paragraph "Initialization before simulation"

As explained before, this is the paragraph for defining point modifications in the grid before the simulation. Here, too, we can request an output of the calculated fields for time step 0, i.e. in steady-state. Instead of graphically defining the fields of "Discharge, Aquifer Flow", "Salinity", and "External Salinity", we can define them here in the following manner:

- Select the Paragraph "Initialization before simulation", then "New Actions" and *cluster* "Mass-Transfer, Salinity, Pathlines" and *object* "**POROSITY**" and *action* "**GRID**" to which we assign value "=35" (do not forget the "**=**" sign!).
- Then, in the same *cluster*: *object* "**SALINITY**" and *action* "**CELL**" and select: *Col* **41**, *Row* **1***, Layer* *****, *value* **35**. (seawater salinity in kg/m^3), then *object* "**EXT_SALIN**" and *action* "**CELL**" and select: *Col* **40**, *Row *, Layer* *****, *value* **9999**.
- Then, in the *cluster* "Standard hydraulic parameters", *object* "**HYDR_HEAD**" and *action* "GRID", we assign the value "**0**" (which is in any case the default value).
- Then, *object* "**DISCHARGE**" and *action* "CELL", and select: *Col* **1**, *Row* **1***, Layer* *****, *value* **33**.
- Then, *object* "**DISCHARGE**" and *action* "CELL", and select: *Col* **40**, *Row* **1***, Layer* *****, *value* **9999**.

N.B.: It is important to define the initial hydraulic heads "/HYDR_HEAD /GRID N: =0" *after* having defined the initial salinity values.

For the outputs, we select:

- *object* "**HYDR_HEAD**" and *action* "Output index " *index* **1,**
- *object* "**SALINITY**" and *action* " Output index " *index* **1,**
- *object* "**VELOCITY**" and *output* **1** = "Velocity at nodes",
- *object* "**SALIN_MASS_FL**" and *action* " Output index " *index* **1** = "Salinity Mass Flux".

If one wishes to check the field of the residual mass balance, we can also request:

- *Object* "RESI_SALIN_FL" and output **1** = "Residual Mass Flow of Salinity".

N.B.: It is recommended, as being more logical, to create a time-steps file for introducing these three output requests at time step 0, rather than introducing them in the paragraph "Initialization before simulation" of the "General Parameters" file.

7.2 RESULTS

The simulation is ready after a second and converges very well.

Figure 101 shows the iso-salinity (kg/m^3) contours that form a saltwater wedge with a mixing strip due to diffusion. The arrows indicate the direction and intensity of the local velocity. The fresh water, coming from the left and being lighter, flows over the wedge. A saltwater circulation enters lower right and mixes with fresh water. Figure 102 presents the real hydraulic head (in cm), clearly showing that the velocities are *not* perpendicular to the iso-hydraulic head contours. The real hydraulic head on the right-hand boundary is equal to 0 (as the resolution takes place in "real hydraulic head").

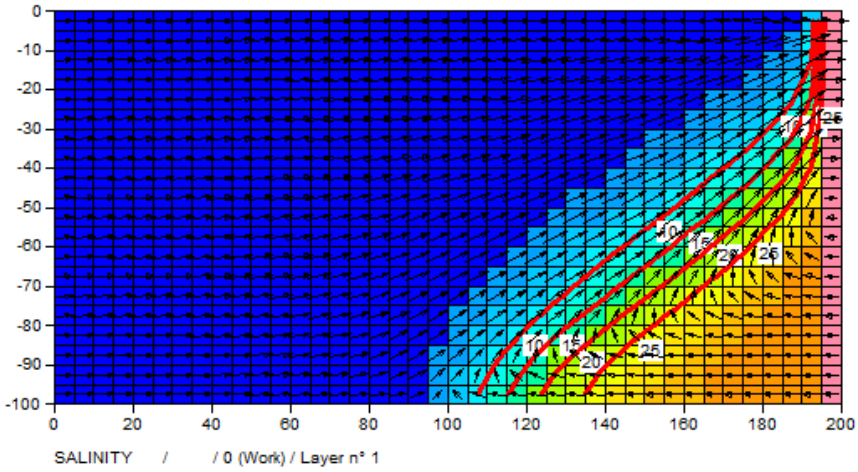


Figure 101 – Salinity field simulated in steady-state.

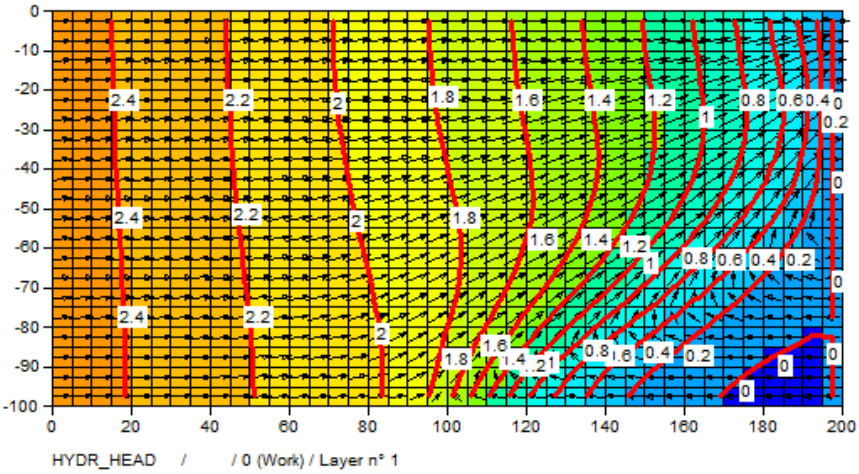


Figure 102 –Real hydraulic head field.

7.3 STEADY STATE MODELLING BY INTEGRATING THE SEA

Project ***Henry_Perma_Loin.rma***.

For the modelling of this system, the choice of a boundary condition is not easy. Figure 101 shows that it is unrealistic to set the salinity at 35 kg/m^3 as brackish water flows to the sea in the upper part of this boundary and might decrease the salinity. We thus ran a new simulation by considering that the sea was represented by abscissa 150 to abscissa 200, i.e. by columns 31 to 40.

To account for the sea, we made the following modifications in this zone formed by columns 31 to 40:

- Hydraulic conductivity = 100 10^{-2} m/s
  (multiplied by 100 as there is 100% water without porous medium);
- Porosity = 100% (as there is 100% water without porous medium);
- Initial salinity = 35 (kg/m^3)

We also set the relaxation coefficient for “Density/Pressure coupling" at 0.5 to obtain a good convergence notwithstanding the high hydraulic conductivity contrast.

Figure 103 shows the simulated salinity field and Figure 104 the simulated real-hydraulic head field. The black vertical line is the coastline. The isovalues are very close to those of the preceding simulation, but the velocity and salinity fields clearly show that brackish water flows to the sea.

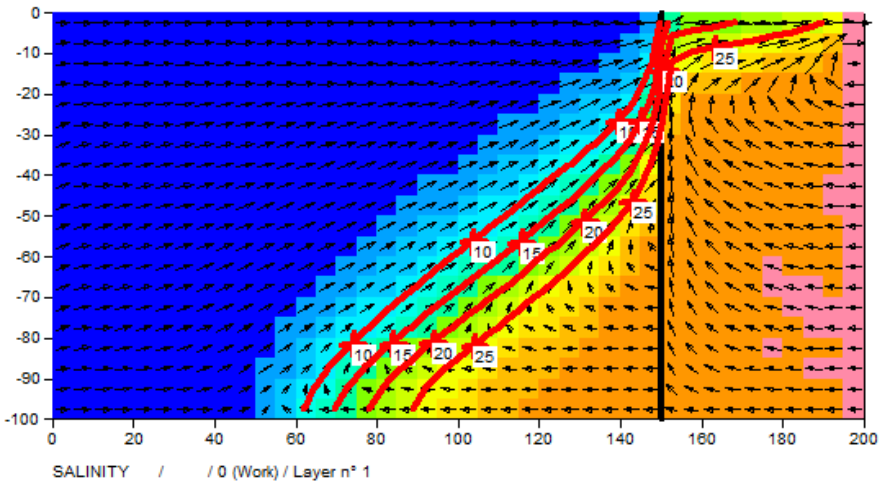


Figure 103 – Salinity field simulated in steady-state, by integrating the sea.

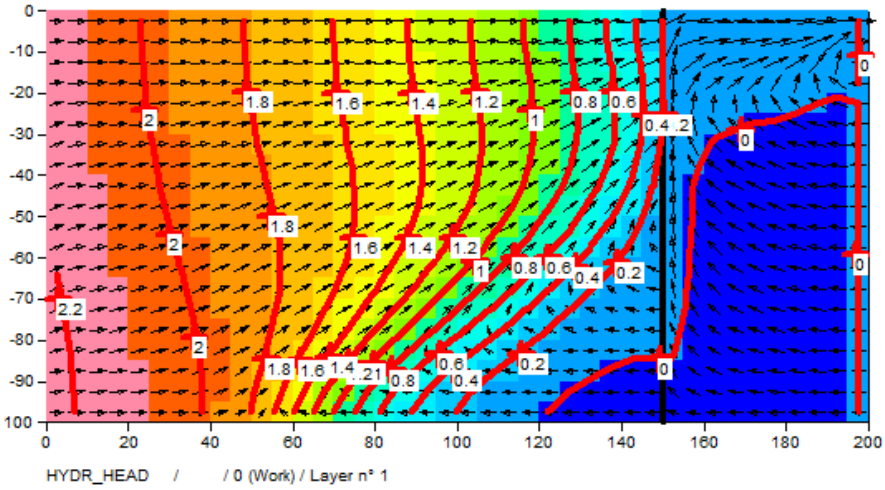


Figure 104 –Real hydraulic head field by integrating the sea

7.4 TRANSIENT MODELLING, WITHOUT DIFFUSION OR DISPERSION

Project ***Henry_Transi.rma***.

The third modelling exercise of this system is made in transient conditions and without diffusion or dispersion, which would generate an abrupt interface. For simulating a system without diffusion with an abrupt interface, we use the TVD transport method. Transport is simulated in transient state, but flow is simulated in a steady-state regime as—the system being confined—the confined storage coefficient is negligible, and the velocity field is very rapidly established. The simulation covers 15 time steps of increasing duration, from 1 mn at the start to 10 mn at the end, for a cumulative duration of 80 minutes. For a better understanding of how the wedge evolves, each of the 15 model time-steps was automatically cut up into 5 sub-time steps. The hydrodynamic parameters and the boundary conditions are the same as those of the steady-state, as the system is initially filled with fresh water, and the saltwater wedge gradually develops to the left. As the transport is in transient state, we set a maximum of 10 coupling iterations between the hydrodynamics and the salinity transport.

In summary, the parameters are:

Coupling:

- Maximum number of coupling iterations = 10,
- Under-relaxation Coefficient = 0.7 (but without under-relaxation we also obtain correct results).

Hydrodynamics:

- Regime = Steady-state,
- Method = Simulation with a real hydraulic head scheme,
- Maximum number of iterations at each time step = 3 (and 50 internal iterations at most).

Transport:

- Regime = Transient,
- Method = TVD ("**T**otal **V**ariation **D**iminishing"),
- Diffusion = 0,
- Dispersivity = 0.

Note that the interface is quite abrupt, without numerical dispersion.

Paragraph "Time Steps and sub-steps"

```
      = Maximum possible number of model time steps     [Def = All]
    5 = Number of model time sub-steps                  [Default=1]
```

Paragraph "Transport/Coupling of Concentration, Heat, Salinity"

```
     10 = Maximum number of iterations for Density/Pressure *Coupling*
    0.7 = Relaxation coefficient for Density/Pressure coupling [Def=1]
    TVD = Transport method (0=Finite Diff. ; 1=Random-Walk ; 2=Charact=MOC ; 3=TVD)
      0 = Molecular Diffusion (m2/s)     [ *=Spatialized Field ]
```

Paragraph "Salinity, Density"

```
     Head = Taking into account Density (0=No ; 1=Hydr_Head ; 2=Pressure ; etc.)
   Schlum = Density(Salinity) relation (0=no; 1=Linea; 3=Schlumberger_VDB[Salinity])
Transient = Salinity transport scheme [0=Transient ; 1=Steady state]
```

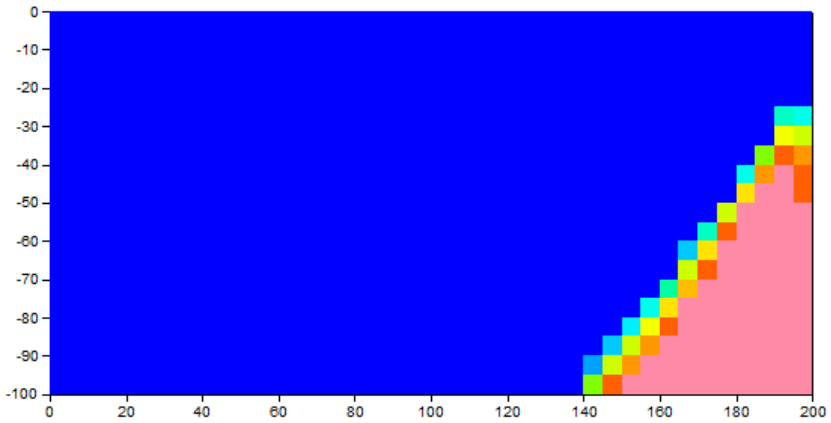


Figure 105 – Simulated salinity field after 15 minutes.

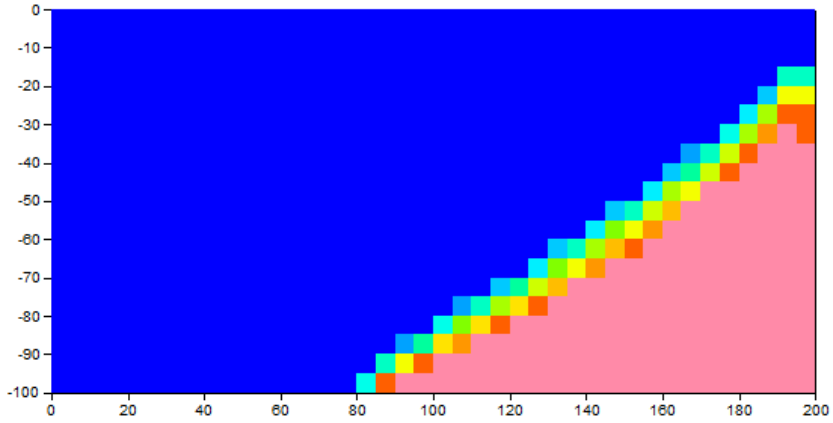


Figure 106 – Simulated salinity field after 80 minutes.

8 Principles of simulation in the unsaturated zone

Modelling the transfer of water and solutes through the unsaturated zone overlying saturated groundwater is a fundamental part of studies of how to protect against pollution and for depollution projects. In view of the heterogeneity of the natural soil, it is generally necessary to model such flow in two or three dimensions (2D or 3D), especially near recharge sites, waste-storage sites, or landfills.

Using the algorithms described by Thiéry (1993), the BRGM MARTHE ® software (Thiéry, 2015b) was adapted for modelling, in 2D or 3D, the flow in both the saturated zone and the unsaturated zone (UZ). For more detailed information, please consult the document by Thiéry (2015c).

8.1 DEFINITION OF VARIABLES AND HYDRAULIC PROPERTIES OF THE POROUS MEDIUM

In a standard simulation of confined or unconfined aquifer, a porous medium is characterized by two properties:

- A hydraulic conductivity for water (hydraulic conductivity) "$\mathbf{K_s}$" that is invariant (m/s);
- A specific storage coefficient $\mathbf{S_s}$ that is also invariant (m^{-1}).

For a standard simulation of unconfined groundwater, the specific storage coefficient $\mathbf{S_s}$ is replaced by the “specific yield” $\mathbf{S_L}$ (dimensionless), that is invariant as well.

For simulation with an unsaturated zone scheme, the porous medium is again defined by two properties:

- A hydraulic conductivity;
- A storage factor (equivalent to a storage coefficient) that links a variation of the water content to a pressure head variation. This coefficient is close to the capillary capacity. *There is use of a “specific yield”*.

The main difference is that, in a simulation with an unsaturated zone scheme:

- The hydraulic conductivity depends upon the condition of the soil—the more the soil is saturated, the higher will be the hydraulic conductivity—by means of a "relative permeability law";
- The storage factor also depends upon the soil condition by means of a "retention law". *There is use of a “specific yield”*.

8.1.1 Hydraulic head

The hydraulic head has the same definition as in standard modelling, but the notion of dewatering does not exist in a simulation in the unsaturated zone. The default expression of hydraulic head is in metres water and is noted "H". In practice the "hydraulic head" may be sometime referred in the text as “head”

8.1.2 Cell elevation

This is the elevation of the cell centre. It is expressed in the same unit as the vertical height (hydraulic head, and ‘Top’ and ‘Bottom’ elevation).

8.1.3 Fluid density

This is the mass of the fluid unit volume (kg/m^3). It is noted “ρ”, “ρ_0” being the fresh water density at a reference temperature (generally 20 °C):

$$\rho_0 = 1000 \text{ kg/m}^3 \text{ (approximately)}$$

8.1.4 Relative density (compared to water)

This is the ratio (dimensionless) of the fluid density to the pure water density:

$$d = \rho / \rho_0 \qquad (1)$$

For pure water at a reference temperature, d = 1. For seawater (Atlantic Ocean) the approximate value is d = 1.025.

8.1.5 Pressure, pressure head

Pressure, noted **p**, is expressed in pascals. In MARTHE, we use the "pressure head" noted **h**, which is the fresh-water height equivalent to the pressure:

$$h = p / \rho.g \qquad (2)$$

With g = gravity acceleration = 9.81 m/s^2.

In practice, in the MARTHE software and its documentation, “pressure head” is occasionally replaced by just “pressure".

We note that:

h_w = water pressure ("w" for water)
h_g = gas pressure (air)
h_c = capillary pressure = $h_w - h_g$ (3)
h_{atm} = atmospheric pressure

In a simulation in the unsaturated zone with MARTHE, we opt by convention for expressing pressure with respect to atmospheric pressure:

$$h_{atm} = 0$$

We also consider that the hydraulic conductivity to air is infinite. Air is thus always at the atmospheric pressure, which gives:

$$h_g = h_{atm} = 0$$

or: $h_c = h_w - h_g$ which gives:

$$h = h_w = h_c \qquad (4)$$

The water pressure head is equal to the capillary pressure.

8.1.6 Suction

- In the unsaturated zone, suction is the opposite of capillary pressure;
- In the saturated zone, the suction is null.

Suction is thus always positive or null.

In summary:
- Suction = -h if h ≤ 0
- Suction = 0 if h > 0

The suction, like the pressure head, is expressed in fresh-water height.

The MARTHE software does not use suction, but only pressure head. For numerical reasons, however, the user must define a maximum suction (or maximum depression) corresponding to the driest soil possible. For a soil covered by vegetation, such a maximum suction (around 100 to 500 metres) physically corresponds to the wilting point of vegetation: the pF = 4.2 of agronomists corresponds to a suction equal to 158.48 m.

The maximum suction also serves to avoid numerical problems with a pressure head that would tend towards minus infinity, for instance when applying evaporation to an extremely dry soil, i.e. with an almost null hydraulic conductivity.

N.B.: The pF, by analogy with the pH of chemistry, is the suction expressed by the decimal logarithm of its value in cm. For instance, a suction of 1000 cm corresponds to a pF of 3.

8.1.7 Hydraulic head - Pressure head relationship

Taking into account the definitions of elevation "z" and (real) hydraulic head "H" we have the relation:

$$p = \rho \cdot g \cdot (H - z) \qquad (5)$$

or, by using the relations (1) and (2):

$$h = d \cdot (H - z) \qquad (6)$$

or again:

$$H = h/d + z \qquad (7)$$

8.1.8 Free surface

In fact, this is not a "free surface" but a "saturation limit", the combined points where the water pressure is equal to the atmospheric pressure (that is taken as 0):

$$\text{or:} \quad h = 0 \quad \text{and} \quad H = z \qquad (8)$$

which is the saturation limit:

- $h > 0$ (or $H > z$) where the porous medium is (locally) confined (Saturated Zone);
- $h < 0$ (or $H < z$) where the porous medium is (locally) in an Unsaturated Zone

8.1.9 Volumetric water content

This is the ratio of the water volume in a ground volume. The water volume is noted $\boldsymbol{\theta}$. To express that it is a dimensionless variable, it can be noted on graphs as m^3/m^3.

The "water content at saturation" is noted $\boldsymbol{\theta_s}$. This is the water content corresponding to a higher, or equal, pressure than the atmospheric pressure ($h \geq 0$).

In the MARTHE software, the water content at saturation is represented by the POROSITY variable with the file extension [.poros]. This variable represents the total porosity. Like all variables of the MARTHE software, it can be defined by grid, by layer, by zone or by cell.

8.1.10 Water saturation rate

The water saturation rate, noted "$\boldsymbol{S_w}$", is the ratio of water content to the maximum water content. It is based on the "residual (irreducible) water content", "$\boldsymbol{\theta_r}$":

$$S_w = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

where:

- $S_w = 100$ % when $\theta = \theta_s$ (saturation);
- $S_w = 0$ % when $\theta = \theta_r$ (total desaturation).

8.1.11 Retention law

For a given unsaturated soil, we need a relationship, called "retention law", between the pressure head **h** and the water content **θ**:

$$h = h(\theta) \qquad \text{if } \theta < \theta_s \qquad (\text{or } h \leq 0) \qquad (9)$$

The dryer the soil (low water content), the more negative will be the pressure head (strong suction).

Conversely:

$$\text{If } h \leq 0 \Rightarrow \theta = \theta(h) \qquad (10)$$

$$\text{If } h > 0 \Rightarrow \theta = \theta_s \qquad (11)$$

We can thus always deduce **θ** from **h**, but we can deduce **h** (or **H**) from **θ**, only if **θ** < $\boldsymbol{\theta}_s$.

In practice, the relation h(θ) is not perfectly one-to-one and is affected by a hysteresis phenomenon (Figure 107 and Figure 108), which will be the stronger with a more heterogeneous grainsize distribution of the porous medium, being very strong for sandy or gravelly materials. This hysteresis effect is difficult to account for and is ignored in the MARTHE software, as in most standard simulation codes.

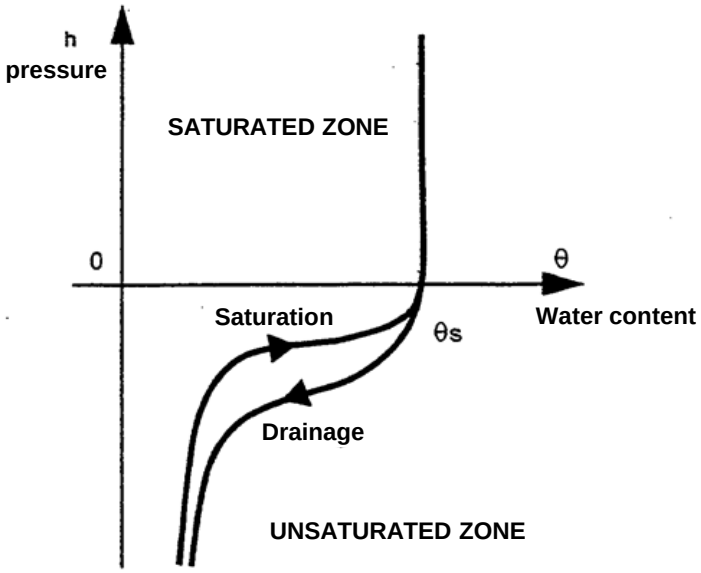


Figure 107 – Relationship between pressure head and water content.

N.B.: To avoid negative signs, retention curves are generally represented as a suction graph = f(θ).

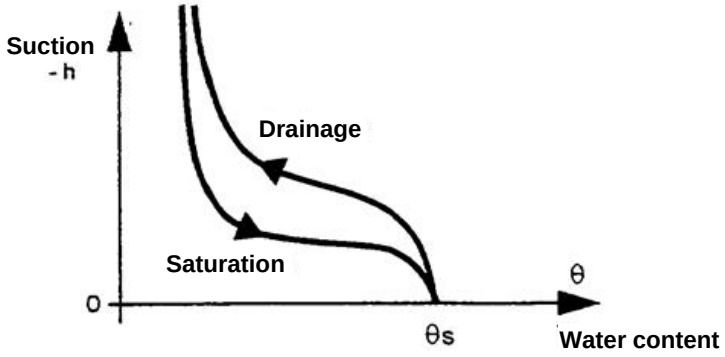


Figure 108 – Relationship suction – water content.

For a given saturation state **θ**, we can define a specific equivalent storage coefficient S_{eq}; this is equal to the water volume V_{WATER} obtained per volume of ground V_{GROUND} for a decrease of one unit of hydraulic head:

$$S_{eq} = \frac{1}{V_{GROUND}} \cdot \frac{\Delta V_{WATER}}{\Delta h} \text{ (in } m^{-1} \text{ if h is in m)} \qquad (12)$$

As a first approximation $\Delta V_{WATER} = V_{GROUND} .\Delta\theta$. More exactly, when considering the compressibility of the ground and the water, proportionately to the water saturation:

$$\Delta V_{WATER} = -V_{GROUND} . [\Delta\theta + (\theta/\theta_s) . S_s .\Delta h]$$

with S_s = specific storage coefficient (in confined groundwater),

This can be written as:

$$S_{eq} = \frac{\Delta\theta}{\Delta h} + (\theta / \theta_s). S_s \qquad (13)$$

This results in the representations of Figure 109:

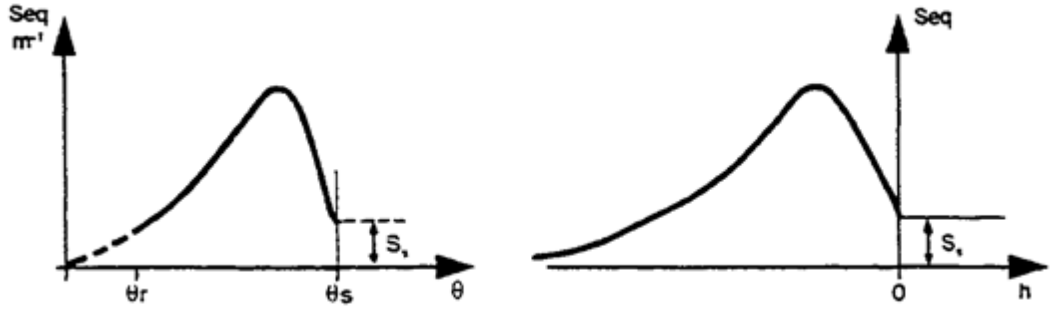


Figure 109 – Capillary capacity:
On the left depending on water content; on the right depending on pressure head.

N.B.: We call “capillary capacity”, noted **C_a**, the derivative dθ / dh:

$$C_a = d\theta / dh$$

8.1.12 Permeability law

Darcy’s law, valid for flow in the saturated zone, can be extended to the unsaturated zone:

$$q = -K . dH / dx \qquad (14)$$

With: q = flow rate per surface unit (q = "Darcy velocity"),
K = hydraulic conductivity to water (or hydraulic conductivity)
(has the dimension of a velocity),
dx = distance between two points.

Contrary to flow in the saturated zone, the hydraulic conductivity **K** is not a constant, but strongly depends upon the saturation state:

$K = K(\theta)$

or: $K = K(h)$ for $h < 0$

This second expression will be less affected by hysteresis.

The lower the water content (or the more negative the pressure head), the lower will be the hydraulic conductivity. At saturation ($\theta = \theta_s$, $h > 0$), we obtain a hydraulic conductivity at saturation that is constant and maximum:

$K = K_s$.

N.B.: In steady state, the simulation is independent of the storage coefficient and it suffices to know the relation K(h). The retention curve will no longer be useful. If we only know the relation K(θ), which is the general case, the retention law h(θ) is only used for obtaining the relation K(h) = K[h(θ)]. In MARTHE, however, one must always introduce a retention law for calculating the range of water-content values.

8.2 DIFFERENT TYPES OF RETENTION LAWS IN THE MARTHE SOFTWARE

There are several options in the MARTHE software for defining and choosing among different types of retention laws:

- In the parameters file [.mart] in paragraph "Initialization before simulation";
- In a file of "Unsaturated Zones constitutive laws", of file extension [.unsat];
  - If there is only one type of soil (a single law): in the parameters [.mart] file in paragraph "*Unsaturated zone*", by means of an index.

The main available retention laws are:

"Homog" or "1" = Homographic law (or Brutsaert's law, 1966)
"Puiss" or "2" = Power law (or Polynomial) or Brooks & Corey (1964)
"Logar" or "3" = Logarithmic law
"Van-Gen" or "4" = Retention law of Van Genuchten
"Pseudo" or "9" = Retention law "Pseudo Unsaturated"

In very specific cases we can also choose a linear law (code "Linear" or 7), or a "capacity effect" law (code "Capaci" or 10). All these laws can be described depending on the following reduced variables:

- The reduced pressure: $\mathbf{h_{rt}} = h / h_t$
  h_t being a parameter representing a reference pressure head (given positively in the software);
- The water saturation rate $\mathbf{S_w}$:

$$S_w = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right) \qquad (15)$$

With:

θ_s = Water content at saturation.
This parameter can be measured in the laboratory, but we can also consider this as a calibration parameter, the maximum laboratory value generally being higher than that obtained under natural conditions.

θ_r = "residual water content" or "irreducible water content", corresponding to a quasi-infinite suction.
In practice, it is a calibration parameter, as a quasi-infinite suction cannot be applied.

Each of these retention laws depends, as reduced variable, upon a single parameter, an exponent noted **b_t**. Only the logarithmic law (little used) depends upon no parameter. The formulation of the retention laws is given in Table 2.

Type of law	Pressure	Saturation
Homographic	$h_{rt} = [S_w^{-1} - 1]^{b_t}$	$S_w = 1/\left[1 + h_{rt}^{\ 1/b_t}\right]$
Power (Brooks & Corey)	$h_{rt} = S_w^{-b_t}$	$S_w = h_{rt}^{\ -1/b_t}$
Van Genuchten (b_t = 1/n ; m = 1-1/n)	$h_{rt} = \left[S_w^{-1/m} - 1\right]^{1/n}$	$S_w = [1 + (h_{rt})^n]^{-m}$
Logarithmic	h_{rt} = -Ln(S_w)	S_w = exp(-h_{rt})
Pseudo Unsaturated	h/dz = S_w - 0.5	S_w = 0.5 + h/dz

Table 2 - Mathematical expression of the retention laws implemented in the MARTHE software.

8.2.1 Homographic retention law

This law, also called Brutsaert's law (1966), has the advantage of being simple and well reproducing most observed retention curves.

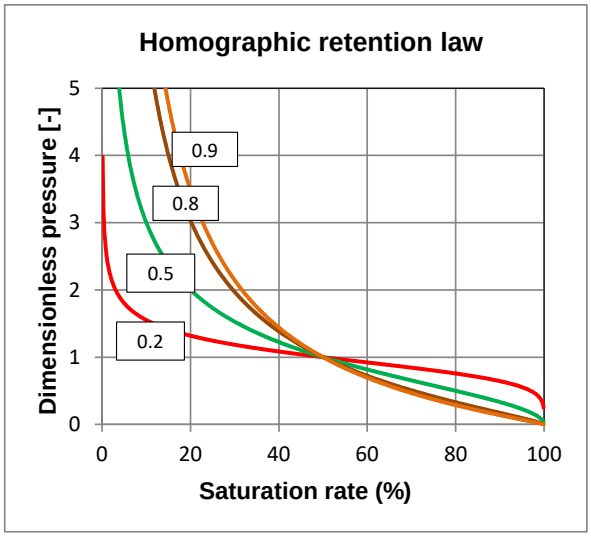


Figure 110 –"Homographic" retention laws: based on the value of exponent "b_t".

Using the water saturation rate "S_w", this retention law is written:

$h / h_t = [S_w^{-1} - 1]^{b_t}$ b_t being an exponent ≤ 1

We see that when **S_w** = 0.50, i.e. for a saturation rate of 50%, we obtain a reduced pressure head equal to 1. The pressure head then is equal to **h_t**. The reference pressure head h_t thus corresponds to a saturation rate of 50%, hence its name in MARTHE of "half-saturation" pressure (head).

Using the water content variables, this retention law is written:

$$\frac{h}{h_t} = \left(\frac{\theta_s - \theta}{\theta - \theta_r}\right)^{b_t}$$

which clearly is a homographic relation depending on θ.

8.2.2 Power retention law

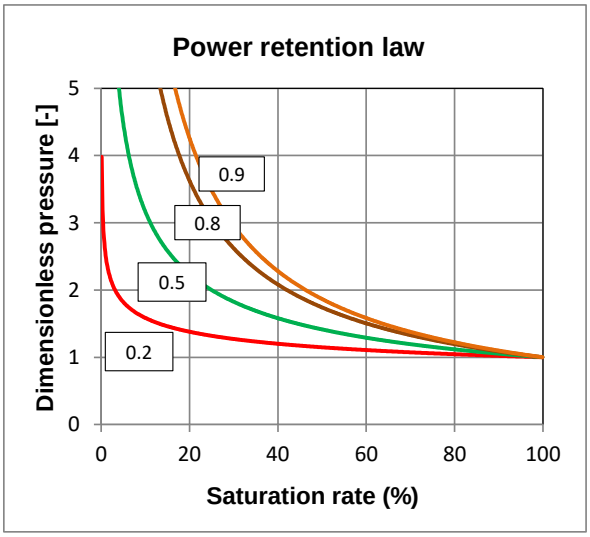


Figure 111 – "Power" retention law according to the value of exponent "b_t".

This is a very simple law, derived from the by Brooks & Corey (1964) retention law:

$h / h_t = S_w^{-b_t}$ b_t being an exponent < 1

or, using the water content variables:

$$\frac{h}{h_t} = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{-b_t}$$

or again:

$$\frac{h}{h_t} = \left(\frac{\theta_s - \theta_r}{\theta - \theta_r}\right)^{b_t}$$

This should not be confused with the homographic law: $\frac{h}{h_t} = \left(\frac{\theta_s - \theta}{\theta - \theta_r}\right)^{b_t}$

The "Brooks & Corey" retention law has two major drawbacks:

- The pressure head at saturation is *not* null: h_{rt} (100%) = 1, or h = h_t
- The derivative of the function $h_{rt}(S_w)$ for S_w = 100% is incorrect: it is *not* infinite as it has no vertical tangent).

To correct these shortcomings in the MARTHE code, we modify in the "Power" retention law the formulation of the Brooks & Corey" retention law near saturation. When the saturation rate "S_w" reaches or exceeds 98%, we replace the function by a parabolic arc that ensures continuity and presents the required properties:

S_w = 100% → h_{rt} = 0, with a vertical tangent (infinite derivative).

With the "power" retention law, the parameter h_t is ***not*** exactly the pressure head corresponding to a saturation rate of 50%, but its value is of the order of magnitude of this pressure.

For instance, based on the value of b_t, we obtain:

- $b_t = 0.5 \Rightarrow h_t = 0.70$ x pressure (saturation 50 %)
- $b_t = 0.8 \Rightarrow h_t = 0.57$ x pressure (saturation 50 %)

This "power" retention law generally can be replaced by the homographic retention law; its interest is to be close to the "Brooks & Corey" law that is often cited in the literature.

8.2.3 Brooks & Corey (1964) retention law

This law is the same as the "Power" retention law, but without the correction introduced by the latter near saturation. It thus presents a discontinuity near saturation as the reduced pressure abruptly passes from 1 to 0.

$h / h_t = S_w^{-b_t}$ b_t being an exponent < 1,

Or using the water content variables:

$$\boxed{\frac{h}{h_t} = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{-b_t}}$$

In the literature, this law generally appears as:

$h / h_t = S_w^{1/\lambda}$

With:

λ = pore-distribution parameter,
$\lambda = 1 / b_t$,

h_t being called the air-entry pressure head.

8.2.4 Van Genuchten (1980) retention law

This law, described by Van Genuchten (1980), is much used in the scientific literature. Its expression is more complicated than that of the homographic law, but its interest is that it allows a simple expression of the prediction of the permeability law relative to Mualem's (1976) method. The Van Genuchten retention law is represented for various values of the parameters on Figure 112.

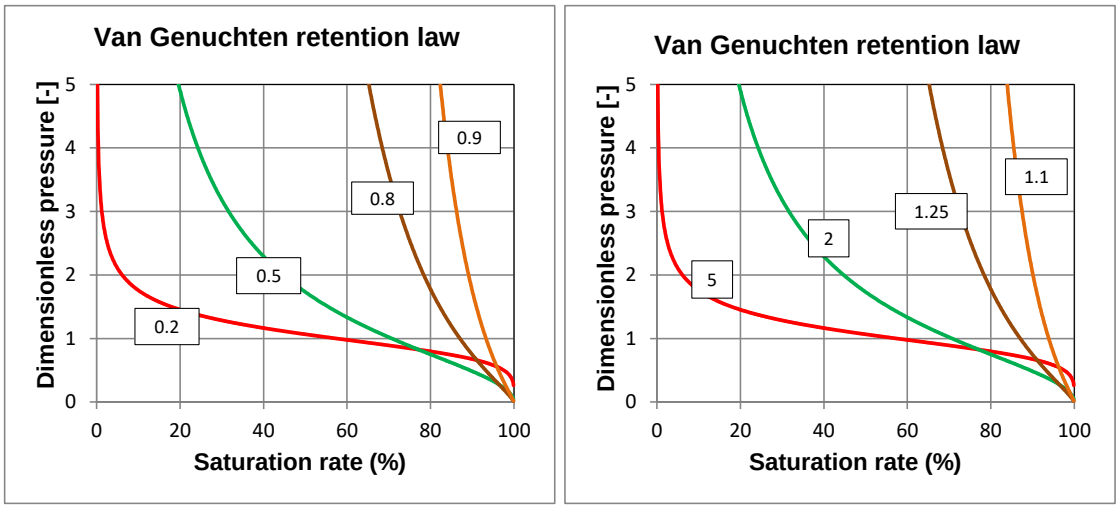


Figure 112 –Van Genuchten retention laws:
left, according to the value of the "bt" exponent;
right, according to the value of the "n = 1/b_t" parameter.

In the literature, the Van Genuchten relation generally appears as:

$h_{rt} = \left[S_w^{-1/m} - 1\right]^{1/n}$	=>	$S_w = [1 + (h_{rt})^n]^{-m}$
with: m = 1 – 1 / n	(n > 1)	

The Van Genuchten law has the following required properties:

- $h_{rt}(0) = \infty$
- $h_{rt}(100\%) = 0$
- $dh_{rt} / dS_w\ (100\%) = \infty$

In the literature on this law, the reduced pressure head or suction is generally given as:
h_{rt} = alpha x h, "alpha" being a constant with a dimension in [L^{-1}].

In MARTHE, as was explained before for the retention law, the reduced pressure head, or suction, is defined as:

$$h_{rt} = h / h_t$$

"h_t" being a dimensional parameter: the reference pressure head with the dimension [L], called "half-saturation pressure" by analogy with the "homographic" law, even though this pressure does not correspond with a 50 % saturation rate.

We have thus: alpha = 1 / h_t h_t = 1 / alpha

By analogy with the "homographic" and "Power" laws, we use an exponent (< 1) on the saturation rate S_w, of the $S_w^{-b_t}$ type.

In MARTHE, we now have: b_t = 1 / n and h_t = 1 / alpha

With the Van Genuchten retention law, the reference pressure "h_t" corresponds to:

- A saturation rate of 87% if **b_t** = 0.8 (or **n** = 1.25)
- A saturation rate of 70% if **b_t** = 0.5 (or **n** = 2)

After verification on a very large sample of Van Genuchten retention laws in the literature, we have adjusted these laws with a "homographic law" with a correlation coefficient above 0.99 and

even mostly above 0.999 (at least in the suction range of 0 to 20 m). The values obtained for θ_r, h_t and b_t are obviously not the same for both laws.

Table 4 to Table 7 give the parameters of the Van Genuchten law for 12 USDA soil classes. It should, however, be understood that the values in these tables are only orders of magnitude. It may be necessary to divide or multiply the saturation hydraulic conductivity K_s in these tables by a factor over 5.

In Table 4 and Table 6, the "**h_t**" parameter is equal to "1/alpha" and the "**b_t**" parameter is "1/n" ("alpha" and "n" being the “traditional” parameters of the Van Genuchten formulation). Table 5 and Table 7 use the "traditional" literature notation with "**alpha**" of dimension [L^{-1}] and "**n**" > 1.

Some databases and programs allow to have a first order of magnitude of parameters based on present soil: the UNSODA (Schaap and Leij, 1998) database, the GRIZZLY (Haverkamp et al., 1998) database, and the ROSETTA program on the basis of UNSODA (Schaap et al., 2001).

8.2.5 "Pseudo unsaturated" retention law

This law allows reproducing the "pseudo unsaturated" simulation scheme of MARTHE or, in practice, the simulation of an "unconfined aquifer". This law is written as:

h / dz = S_w - 0.5 dz being the vertical cell thickness.

We have the following properties that correspond exactly to an unconfined aquifer:
- $S_w = 0$ => h = -dz/2 => H = z – dz/2 (= elevation of the cell bottom),
- $S_w = 1$ => h = +dz/2 => H = z + dz/2 (= elevation of the cell roof).

We see that, in this law, the "h_t" parameter is replaced (automatically in MARTHE) by "dz", which is the vertical thickness of the cell (that may be different for each cell).

For simulating an unconfined groundwater, we generally choose:
- $\theta_r = 0$,
- θ_s = Specific yield coefficient.

The interest of using this retention law is that we can make a simulation identical to the standard "pseudo unsaturated" one, though benefiting from the advantages of a simulation with an unsaturated zone scheme. Of especial interest are the:
- Possibility of simulating a vertical cross-section that integrates nested grids;
- Progressive calculation with time-step durations that are automatically dependent on the saturation variations and on the convergence rate.

To carry out a simulation identical to a "pseudo unsaturated" one, we use a “Power” permeability law with an exponent equal to 1. We then get:

A hydraulic conductivity $K = K_s \cdot S_w$,
⇨ A transmissivity $T = K \cdot dz = K_s \cdot dz \cdot S_w$,

which effectively corresponds to an unconfined aquifer.

8.2.6 Logarithmic retention law

The logarithmic retention law is represented on Figure 113.

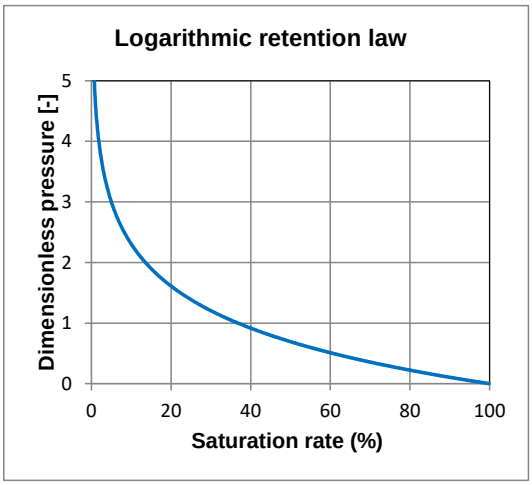


Figure 113 –"Logarithmic" retention law.

This law is little used. For given θ_r and θ_s values it does not depend upon any parameter:

$h_{rt} = -Ln(S_w)$.

The required properties are verified:

- $h_{rt}(0) = \infty$,
- $h_{rt}(100\%) = 0$,

However, the derivative for $S_w = 100\%$ is ***not*** infinite, but equal to +1.

With the logarithmic retention law, parameter h_t is ***not*** exactly the pressure corresponding to a saturation rate of 50%, but it is in the order of magnitude range of this pressure:

$h_t = 1.44 \times h\ (50\%)$.

Reciprocally, the pressure h_t corresponds to a saturation rate of 36.8%

8.3 DIFFERENT TYPES OF RELATIVE PERMEABILITY LAWS

In the MARTHE software, we can choose among several types of relative permeability laws. As for the retention laws, they can be defined:

- In the parameters [.mart] file in paragraph "Initialization before simulation";
- In a "Unsaturated Zones constitutive laws" file, of file extension [.unsat];
- If there is only one soil type (a single law): in the [.mart] parameter file in the paragraph "Unsaturated Zone and Multiphase flow", by means of an index.

The main available permeability laws are:

"Power" or "2" = Power (or Polynomial) law.
"Van-Gen" or "5" = Permeability law of Van Genuchten and Mualem.
"Brooks" or "6" = Permeability law of Burdine Brooks & Corey.
"Homog" or "1" = Homographic permeability law in terms of pressure (*not recommended*).
"Expon" or "4" = Exponential law depending on pressure (*not recommended*).

These permeability laws can be used with a "double permeability" scheme to account for the presence of macropores or fractures.

Please note:

K_s = Hydraulic conductivity at saturation. It is the maximum hydraulic conductivity obtained when saturation reaches 100% (i.e. when pressure head is positive or null).

$K_r = K / K_s$: is the relative permeability (dimensionless).

- The "Power", "Van_Gen" and "Brooks" permeability laws give the relative permeability **K_r** = K / K_s depending on the saturation rate **S_w**.
- The "Power" law involves a single parameter, the exponent **b_k**.
- The "Van_Gen" and "Brooks" laws do not involve any additional parameter, as it is assumed (but not always verified) that they derive from their retention law.
- The "Homog" and "Expon" permeability laws (*not recommended*) involve the parameter **h_k**, which is a reference suction or pressure. The "Homog" permeability law involve a second parameter: exponent **b_k**.

Table 3 summarizes the characteristics of the main permeability laws of MARTHE.

Type of law	Permeability depending on saturation	Permeability depending on pressure
Power	$K_r = S_w^{b_k}$	
Van Genuchten **(m = 1 - b_t ; m = 1-1/n)**	$K_r = \sqrt{S_w} \cdot \left[1 - \left(1 - S_e^{\frac{1}{m}}\right)^m\right]^2$	
Brooks & Corey	$K_r = (S_w)^{3+2 \cdot b_t}$	
Homographic (versus pressure)		$K_r = 1/\left[1 + {h_{rk}}^{b_{kt}}\right]$
Exponential (versus pressure)		$K_r = \exp(-h_{rk})$

Table 3 - Mathematical expression of the permeability laws implemented in the MARTHE code.

8.3.1 Power permeability law

The power relative permeability law is represented for various values of the parameters on Figure 114.

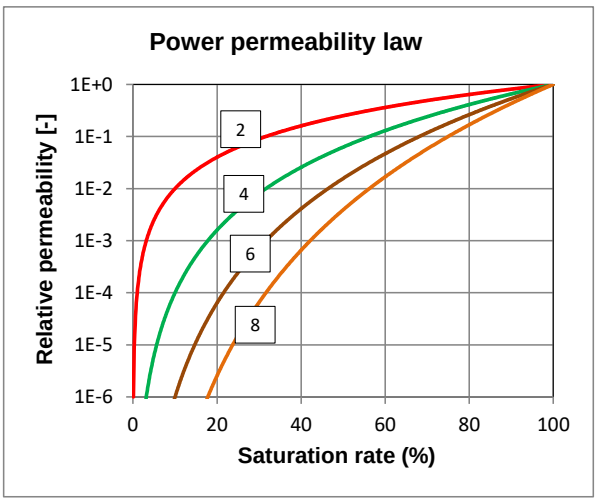


Figure 114 – Power permeability laws, according to the value of exponent "b_K".

The Power law is very classic and is written as:

$K_r = S_w^{b_k}$

Using the water content variables, this relative permeability law is then written as:

$$K_r = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{b_K}$$

b_k being a dimensionless exponent

8.3.2 Van Genuchten permeability law

The expression giving K_r is obtained by Mualem's (1976) formula based on the retention law of Van Genuchten (1980). This expression $K_r(S_w)$ does not call upon any other parameter, which is the interest of the Van Genuchten law. If Mualem's (1976) law applies, which is sometimes—but not always—the case, it suffices to know the hydraulic conductivity at saturation K_s for a direct determination of the permeability law, without any other measurement. In practice, one should be cautious when applying Mualem's formula, especially when using field data.

The Van Genuchten relative permeability law is represented for various values of the parameters on Figure 115.

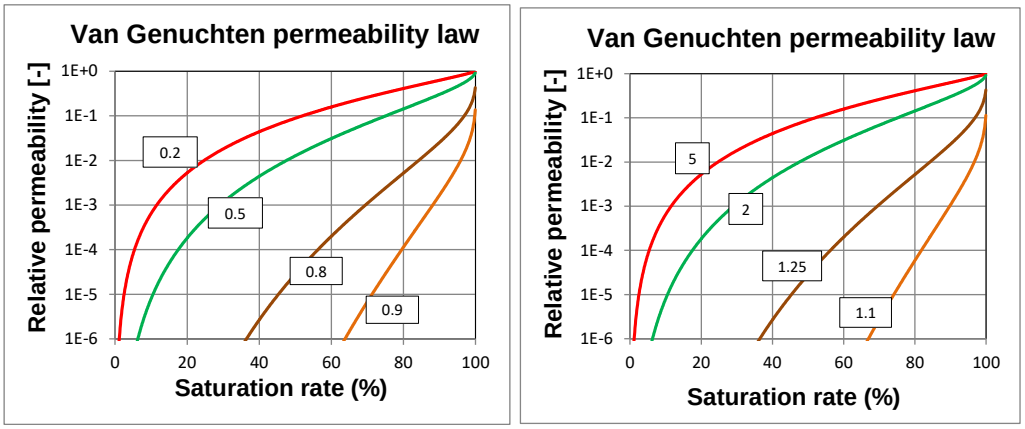


Figure 115 –Van Genuchten permeability laws;
left, according to the value of exponent "b_t"; right, according to the value of parameter "n".

The Van Genuchten relative permeability law is written as:

$$K_r = \sqrt{S_w} \cdot \left[1 - \left(1 - S_w^{1/m}\right)^m\right]^2$$

where $m = 1 - b_t$.

With necessary, after the Van Genuchten retention law:

$S_w = [1 + (h_{rt})^n]^{-m}$ or $S_w = \left[1 + (h_{rt})^{1/b_t}\right]^{b_t - 1}$

(as: $n = 1/b_t$ and $m = 1 - b_t$)

8.3.3 Brooks & Corey permeability law

The expression giving K_r is obtained by the formula of Burdine (1953), based on the retention law of Brooks & Corey (1964). Its expression is the same as the "Power" permeability law, but with exponent $b_k = 2\ b_t + 3$. Its expression is thus written as:

$K_r = (S_w)^{3+2 \cdot b_t}$

8.3.4 Homographic permeability law as a function of pressure

This homographic relative permeability law is represented for various values of the parameter on Figure 116.

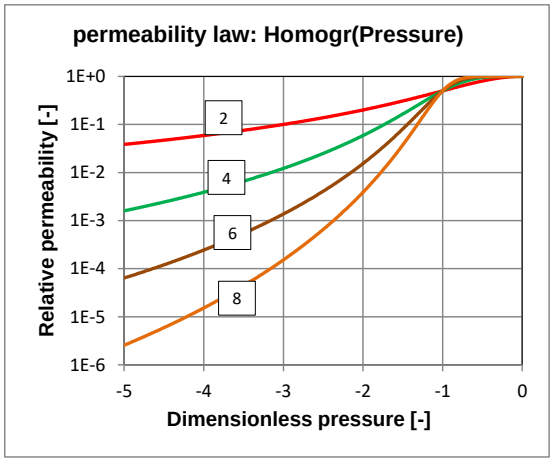


Figure 116 – "Homographic" permeability as a function of pressure.

N.B.: This is a relative permeability law versus a reduced pressure, and *not* versus the saturation rate.

The homographic permeability law is written as:

$$K_r = 1/[1 + (h/h_k)^{b_k}]$$

It depends upon the exponent $\mathbf{b_k}$ and a reference pressure $\mathbf{h_k}$ called “half-permeability suction”. In fact, when $h = h_k$ we have $K_r = ½$ and thus $K = K_s / 2$

8.3.5 Exponential permeability law as a function of pressure

This law allows establishing analytical single-field steady-state solutions and is quite often used to this end. Sometimes also called "Gardner’s law" (1958), it is a relative permeability law based on a reduced pressure and *not* on the saturation rate (Figure 117).

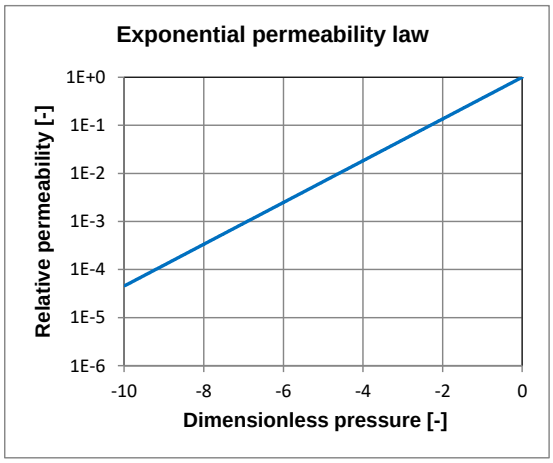


Figure 117 –"Exponential" permeability law as a function of the pressure.

The exponential permeability law is written as:

$K_r = \exp(-h / h_K)$

It does not depend on exponent b_k, but on a reference pressure h_k, called "capillary attenuation".

8.4 NECESSARY PARAMETERS FOR DEFINING THE RETENTION AND PERMEABILITY LAWS

To determine the two characteristic soil laws for simulating flow in the unsaturated zone, the following parameters must generally be defined:

θ_r, θ_s, h_t, b_t**:** for the retention law,
K_s and b_k**:** for the permeability law,
h_k**:** in addition, for the homographic permeability law.

Parameter **h_t** is a reference pressure head; **b_t** and **b_k** are exponents.

- If one chooses the Van Genuchten (1980) formulation with the Mualem (1976) formula, the b_k parameter is ***not*** needed for determining the permeability law.

  The Van Genuchten permeability law depends on the five parameters: θ_r, θ_s, h_t, b_t and K_s.

- If one chooses a Brooks & Corey (1964) retention law with the Burdine (1953) formula, it is also possible to predetermine the permeability law in the form of a power law:

  $K/K_S = (S_w)^{3+2 \cdot b_t}$ or: $b_k = 3 + 2\ b_t$.

  The Brooks & Corey permeability law thus depends on the five parameters: θ_r, θ_s, h_t, b_t and K_s.

The homographic retention law is very little different from the power retention law, even though it is better suited to our purpose. We can thus apply it with the same first estimate of exponent b_k of the permeability law: $b_k = 3 + 2\ b_t$. Having chosen the Burdine model, we thus retain the following two approximations:

b_t = 0.25 at 0.75 ➔ $K_r = S_w^{b_k}$ with b_k = 3 to 5

For a sandy soil, if no other information is available, we can set a half-saturation suction h_t of 20 to 50 cm with a homographic retention law.

For a more clayey soil, we can set a half-saturation pressure h_t of around 1 metre with a homographic retention law.

We can also use a Van Genuchten law by means of Table 4 to Table 7 that give the parameters of the Van Genuchten law for 12 USDA soil classes. It should be noted, however, that the values in these tables are only orders of magnitude. It may sometimes be necessary to divide or multiply by a factor over 5 the hydraulic conductivity at a given saturation K_s in these tables

In Table 4 and Table 6, the parameter "**h_t**" is equal to "1/alpha" and the parameter "**b_t**" is equal to "1/n" ("alpha" and "n" being the "traditional" parameters of the Van Genuchten formulation). Table 5 and Table 7 use the "traditional" literature notation for "**alpha**" of dimension [L^{-1}] and "**n**" > 1.

Soil type	Type de sol	θr	θs	h_t	b_t	Ks
(English)	(French)	[L^3L^{-3}]	[L^3L^{-3}]	[cm]	[-]	[cm/j]
Sand	**Sable**	0.045	0.43	6.90	0.37	712.8
Loamy_Sand	**Sable limoneux**	0.057	0.41	8.06	0.44	350.2
Sandy_Loam	**Loam sableux**	0.065	0.41	13.3	0.53	106.1
Loam	**Loam**	0.078	0.43	27.8	0.64	24.96
Silt	**Limon**	0.034	0.46	62.5	0.73	6
Silty_Loam	**Loam limoneux**	0.067	0.45	50	0.71	10.8
Sandy_Clay_Loam	**Loam sablo-argileux**	0.1	0.39	16.9	0.68	31.44
Clay_Loam	**Loam argileux**	0.095	0.41	52.6	0.76	6.24
Silty_Clay_Loam	**Loam limono-argileux**	0.089	0.43	100	0.81	1.68
Sandy_Clay	**Argile sableuse**	0.1	0.38	37.0	0.81	2.88
Silty_Clay	**Argile limoneuse**	0.07	0.36	200	0.92	0.48
Clay	**Argile**	0.068	0.38	125	0.92	4.8

Table 4 - Parameters for the van Genuchten [1980] formulation for 12 soil types of the USDA classification, after Carsel and Parrish [1988], cited by Šimůnek et al. [2006].
*In the table "**h_t**" is equal to "1/alpha" and the exponent "**b_t**" is equal to "1/n".*

Soil type	Type de soil	θr	θs	a	n	Ks
(English)	(French)	[L^3L^{-3}]	[L^3L^{-3}]	[cm^{-1}]	[-]	[cm/j]
Sand	**Sable**	0.045	0.43	0.145	2.68	712.8
Loamy_Sand	**Sable limoneux**	0.057	0.41	0.124	2.28	350.2
Sandy_Loam	**Loam sableux**	0.065	0.41	0.075	1.89	106.1
Loam	**Loam**	0.078	0.43	0.036	1.56	24.96
Silt	**Limon**	0.034	0.46	0.016	1.37	6
Silty_Loam	**Loam limoneux**	0.067	0.45	0.02	1.41	10.8
Sandy_Clay_Loam	**Loam sablo-argileux**	0.1	0.39	0.059	1.48	31.44
Clay_Loam	**Loam argileux**	0.095	0.41	0.019	1.31	6.24
Silty_Clay_Loam	**Loam limono-argileux**	0.089	0.43	0.01	1.23	1.68
Sandy_Clay	**Argile sableuse**	0.1	0.38	0.027	1.23	2.88
Silty_Clay	**Argile limoneuse**	0.07	0.36	0.005	1.09	0.48
Clay	**Argile**	0.068	0.38	0.008	1.09	4.8

Table 5 - Parameters for the van Genuchten [1980] formulation for 12 soil types of the USDA classification, after Carsel and Parrish [1988], cited by Šimůnek et al. [2006].
*This table uses the "traditional" literature notation: "**alpha**" [L^{-1}] and "**n**" > 1.*

Soil type	Type de soil	θr	θs	h_t	b_t	Ks
(English)	(French)	[L^3L^{-3}]	[L^3L^{-3}]	[cm]	[-]	[cm/j]
Sand	**Sable**	0.053	0.375	28.57	0.31	643
Loamy_Sand	**Sable limoneux**	0.049	0.39	28.57	0.57	105
Sandy_Loam	**Loam sableux**	0.039	0.387	37.0	0.69	38.2
Loam	**Loam**	0.061	0.399	90.9	0.68	12
Silt	**Limon**	0.05	0.489	143	0.60	43.7
Silty_Loam	**Loam limoneux**	0.065	0.439	200	0.60	18.3
Sandy_Clay_Loam	**Loam sablo-argileux**	0.063	0.384	47.6	0.75	13.2
Clay_Loam	**Loam argileux**	0.079	0.442	62.5	0.71	8.18
Silty_Clay_Loam	**Loam limono-argileux**	0.09	0.482	125	0.66	11.1
Sandy_Clay	**Argile sableuse**	0.117	0.385	30.3	0.83	11.4
Silty_Clay	**Argile limoneuse**	0.111	0.481	62.5	0.76	9.61
Clay	**Argile**	0.098	0.459	66.7	0.80	14.8

*Table 6 - Parameters for the van Genuchten [1980] formulation for 12 soil types of the USDA classification obtained with "Rosetta Lite" software [Schaap et al., 2001], cited by Šimůnek et al. [2006]. In the table "**h_t**" is equal to "1/alpha" and the exponent "**b_t**" is equal to "1/n".*

Soil type	Type de soil	θr	θs	a	n	Ks
(English)	(French)	[L^3L^{-3}]	[L^3L^{-3}]	[cm^{-1}]	[-]	[cm/j]
Sand	**Sable**	0.053	0.375	0.035	3.18	643
Loamy_Sand	**Sable limoneux**	0.049	0.39	0.035	1.75	105
Sandy_Loam	**Loam sableux**	0.039	0.387	0.027	1.45	38.2
Loam	**Loam**	0.061	0.399	0.011	1.47	12
Silt	**Limon**	0.05	0.489	0.007	1.68	43.7
Silty_Loam	**Loam limoneux**	0.065	0.439	0.005	1.66	18.3
Sandy_Clay_Loam	**Loam sablo-argileux**	0.063	0.384	0.021	1.33	13.2
Clay_Loam	**Loam argileux**	0.079	0.442	0.016	1.41	8.18
Silty_Clay_Loam	**Loam limono-argileux**	0.09	0.482	0.008	1.52	11.1
Sandy_Clay	**Argile sableuse**	0.117	0.385	0.033	1.21	11.4
Silty_Clay	**Argile limoneuse**	0.111	0.481	0.016	1.32	9.61
Clay	**Argile**	0.098	0.459	0.015	1.25	14.8

*Table 7 - Parameters for the van Genuchten [1980] formulation for 12 soil types of the USDA classification obtained with "Rosetta Lite" software [Schaap et al., 2001], cited by Šimůnek et al. [2006]. This table uses the "traditional" literature notation: "**alpha**" [L^{-1}] and "**n**" > 1.*

8.5 MODELLING WITH THE MARTHE CODE

The following chapters describe how to use the unsaturated scheme with the MARTHE code.

8.6 EQUATION SOLUTION SCHEME WITH THE MARTHE CODE

To have a formulation that is valid for both the unsaturated and saturated zones, we use Richards' equation (1931):

$$div[K \cdot Grad(H)] = S_{eq} \cdot \frac{\partial H}{\partial t} + q \qquad (16)$$

With:

- H: hydraulic head at point x, y, z [L],
- q: volumetric density of inflow (infiltration, injection) or outflow (pumping) (dimension [T^{-1}]),
- S_{eq}: equivalent storage term, dimension [L^{-1}]; "S_{eq}" is close to the capillary capacity "Ca",
- K: hydraulic conductivity water tensor (diagonalized) of dimension [LT^{-1}].

This equation is discretized in finite differences with a formulation close to that of the MARTHE code in the saturated zone (Thiéry, 2015b). The algorithm used is the one described by Thiéry (1993):

$$\sum_v K(H_v, H_v) \cdot A_v \cdot (H_v - H_c)/dx_v + Q_c = STO \qquad (17)$$

with:

- c: index of the simulation cell (centre);
- v: one of the six directions north, south, east, west, up and down;
- A_v: exchange area [L^2];
- H: hydraulic head [L];
- Q_c: source term = inflow (positive) or outflow (negative) in the cell [L^3T^{-1}];
- dx_v: distance between neighbour cell centre v and simulation cell centre c [L];
- STO: storage term [L^3T^{-1}].

The storage term is given by:

$$STO = dx \cdot dy \cdot dz \cdot \left[\Delta\theta + \left(\frac{\theta}{\theta_s}\right) \cdot S_s \cdot \left(h_c - h_{prec}\right)\right]/dt$$

This term can be discretized as:

$$STO = dx \cdot dy \cdot dz \cdot \left[\frac{\Delta\theta}{H_c - H_{prec}} + \left(\frac{\theta}{\theta_s}\right) \cdot S_s \cdot d\right] \cdot \left(H_c - H_{prec}\right)/dt \qquad (18)$$

With:

- H_{prec}: hydraulic head at the start of the time steps,
- d: relative density of the fluid,
- S_s : specific confined storage coefficient [L^{-1}],
- Δθ: variation of water content during the time steps "dt",
- h : pressure head expressed in fresh-water height [L].

We note that this expression does not refer to any "specific yield", but only on the specific (confined) storage coefficient "S_s".

In steady state, we have: STO = 0

The combination of equations (17) and (18) produces a system of non-linear equations. This system is solved by an iterative manner that updates the saturation state at each time step. For a given saturation state, we obtain a linear symmetrical system that is efficiently solved by a preconditioned conjugate gradients solver with a specially adapted pre-conditioning scheme for a sparse matrix, which is optimal for computer storage. To consider the strongly non-linear character of the equation system, we apply, after each new iterate, an under-relaxation coefficient to guarantee the stability of the calculations.

8.7 BOUNDARY CONDITIONS

Four types of boundary conditions are supported:

- Impervious boundary;
- Prescribed hydraulic head;
- Unit-hydraulic head gradient;
- Seepage (or overflow) face.

Impervious boundary

This is the standard condition for a contact with an impermeable environment.

Prescribed hydraulic head

In view of the relations between hydraulic head, pressure head and water content, it is equivalent to fixing a hydraulic head, a pressure head or a water content. In all cases, we use the standard MARTHE code method by affecting to the cell in question a flow with code value "9999".

Unit-hydraulic head gradient

This is a boundary condition specific to the unsaturated zone that is generally observed under natural conditions below a certain depth in soil. It corresponds to:

- A non-fixed hydraulic head;
- A non-fixed flow rate;
- But the vertical gradient of the hydraulic head is equal to +1:

$$dH / dz = +1 \qquad (19)$$

After Darcy's law (12): $q = -K \cdot dH/dz$

$$\text{or: } \boxed{q = -K(h)} \qquad (20)$$

For pure water, we have: $H = h + z$. As $dH / dz = +1$, this results in: $dh/dz = 0$, or h = locally constant (unknown) on the vertical, hence: θ = constant on the vertical.

In the MARTHE software, to prescribe a unit-gradient in a cell, it suffices to introduce a "seepage index" with a code value "9".

Seepage face

This is a boundary through which water can only exit, by gravity, from the modelled domain if the hydraulic head "H" is higher than the cell elevation "z", but into which it can never enter:

- if H > z: H is fixed at z and water seeps out.
- if H <= z: the boundary becomes impervious.

This boundary, equivalent to an "overflow limit" (or an imposed half-potential), plays a role like a "diode" as the outside depends on the inside, but the inside does not depend on outside conditions. This boundary condition corresponds for instance to a drain or a domain boundary in contact with air.

In practice, we can define in the software a "seepage index" file (0 = No: no seepage possible; 1 = Yes: seepage possible). The default extension of this file is [.suint] and its code is "IND_SUINTEM". Each cell (regardless of the layer) can receive a seepage index, especially the lateral cells of a vertical wall. It should be clearly understood that the seepage, i.e. the overflow, occurs as soon as the hydraulic head exceeds the cell centre elevation and *not* when it surpasses the cell top elevation, as when using an "unconfined scheme". If seepage is not allowed ("seepage index = 0"), the porous medium becomes locally "confined" as soon as the hydraulic head exceeds the cell-top elevation.

Independently of the boundary conditions, one can assign an injected (positive) or pumped (negative) flow to any cell that does not have a prescribed potential (or unit-gradient).

8.8 INITIAL STATE AND INITIALIZATION

In view of the retention laws, the three variables hydraulic head, pressure and water content, at least in the UZ, are three aspects of the same phenomenon as they are linked by one-to-one relations. Considering that one can give a file name to each of these three variables in the MARTHE project file, there is a risk of redundancy, which might lead to values that are incoherent with the retention law. It should thus be indicated to MARTHE which one is the initial variable selected for defining the initial state of the modelled domain. This choice is made in the [.mart] parameters file by using the parameter "Initial State Read: Head, Pressure or Water Content" in paragraph "Geometric options, Data reference, Processors".

The three variables hydraulic head, pressure head and water content, then are on par, and we can introduce point modifications (per cell, zone or layer) of a variable. The other variables then are immediately put on par as well. It is also possible to change the parameters of the retention law; the variables then are modified by conserving the (most important) hydraulic head value, but readjusting the other two variables. Such "modifications" can be made at the start of the simulation or later, after certain time steps of the simulation.

It should be noted that if the domain is initialized in water content, one cannot have a “confined” initial state but, at most, at the saturation limit. We have the same effect if the water content is modified. For example, the initial state is pressure head = + 5 m, hydraulic head = 55 m (i.e. elevation = 50 m), water content = 30% which is the water content at saturation.

If the water content later is set at 30% (= water content at saturation), MARTHE will set a pressure head corresponding to the saturation, or 0 m, hence a hydraulic head of 50 m.

8.9 DURATION OF THE SIMULATION TIME STEPS (IN TRANSIENT STATE)

Normally, the user sets the "Model Time Steps" in the "Time Steps" file. Such model time steps correspond to the dates when modifications are made, or when intermediate results become known. For a simulation in the UZ, the software uses a minimum time step "dtmin" and a maximum time step "dtmax", set by the user. The simulation time step "dt" depends upon the variation in water content and the convergence rate, thus remaining between "dtmin" and "dtmax".

At the start of simulation and at each model time step when there are parameter modifications, the duration of the simulation time steps start with the minimum value "dtmin"; then, provided the constraints of convergence are respected, they can increase, but not more than at a ratio of 1.414, until reaching the maximum value "dtmax". If at a certain moment the constraints are no longer respected, the time-step duration can decrease.

This time-step control follows the following rules:

- During a time step, the variation in water content "VarSat" of any cell should not exceed a value "VarSatMax" set by the user. VarSatMax is expressed in water-content units. For instance, if the water content passes from 0.20 to 0.23, the variation is 0.03; if it passes from 30% to 35%, the variation is 5%:

  VarSat < VarSatMax

- A maximum error of the "ErrBilMax" balance must be respected:

  ErrBil < ErrBilMax.

The user assigns by means of an "Index" the type of balance error "ErrBil":

Index = 0 The error percentage of convergence (internal) during the time steps, expressed in percent.
Index = 1 The error of the overall balance for the time steps, expressed in user units of water volume.
Index = 2 The error of the overall balance for the time steps, expressed in percent.

The recommended index value is 0 or 2.

- Index = 0, the safest, can be too severe, especially when the time steps are very small.
- Index = 2 uses a balance error ErrBilMax expressed in per cent (for instance 5%). It can be too severe as well, especially when there are very few variations during the time steps. For instance, an error of 30% over 1 millilitre of water flow during the time steps represents a volume error that may be insignificant.
- Index = 1 allows fixing the maximum balance error as a given water volume, rather than as a percentage. However, the user can have difficulties in setting an acceptable order for such volumetric errors.

Examples:

Index = 0,	ErrBilMax = 2 %	of (internal) convergence,
or Index = 1,	ErrBilMax = 1 Litre	for instance,
or Index = 2,	ErrBilMax = 2 %	of an overall balance.

Based on the obtained results, the software reacts as follows:

- If the balance is not accepted: the simulation restarts from the beginning of the time steps with a new duration planned for respecting the balance constraints;
- If the balance is accepted: the duration of the following time steps is increased or decreased, provided it stays within 80% of the authorized saturation variation;
- If the balance is not accepted but it is impossible to go back (in case of coupling with particle transport), the duration of the next time steps is decreased, at most with a ratio of 2, to respect the constraints of saturation variation and of the balance.

N.B. 1: If one wishes to simulate with a constant time step, it suffices to set dtmin = dtmax.

N.B. 2: In the steady state, the values of dtmin, dtmax, VarSatMax, ErrBilMax are not used.

8.10 SUPPLEMENTARY DATA FILES FOR MAKING A SIMULATION IN THE UZ

Up to three supplementary files can be used:

Description	Default extension	Code
Water content	.satur	SATURAT
Pressure head	.press	PRESSURE
Retention law Permeability law	.unsat	UNSAT_PARAM

8.11 DEFINITION OF RETENTION AND PERMEABILITY LAWS

Retention and permeability laws are defined per geometric zone of the modelled domain (a geometric zone is a unit of cells with common properties). First define in the parameters file, at paragraph “Unsaturated zone”, a default retention law and permeability law. These laws are valid for all zones for which no specific laws were defined, and for the cells of zone number zero.

In addition, we can define Particular Characteristics laws for given (geometric) zones. This definition can be made:

- In the parameters file at paragraph "Initialization before simulation", i.e. the general case;
- Or, possibly, in an "Initial Modifications" file;
- Or in the time steps file (at any time step).

We proceed as follows:

- Select the object: "UNSAT_PARAM" (parameters of the unsaturated zone laws);
- Then select the action:

FILE = Reading a file

or:

GEOM_ZONE = Modification by zone

If the action: "GEOM_ZONE" was chosen, one must define the following 7 or 8 parameters for each selected (geometric) zone:

θ_s, θ_r, h_t, b_t, K_s, b_k, (possibly h_k) and the type of retention law and permeability law.

For a given zone, all parameters (explained below) must be defined. Only the number of the retention law can be left at 0 to maintain the law defined by default in the “Unsaturated Zone and Multiphase flow” paragraph of the “General parameters” file.

Example: Definition of the cells of zone 1 and zone 2, then definition of the characteristic laws of zones 1 and 2. (Figure 118)

Paragraph "Initialization before simulation":

```
*** Initialization before simulation                *** 
      Default: All the cells belong to Zone 2
  /GEOM_ZONE/GRID          N: =2
      Definition of the geometrical zone 2
  /GEOM_ZONE/CELL          C=      *R=  1:16 L=      1V=         1;
  /GEOM_ZONE/CELL          C=      *R= 57:72 L=      1V=         1;
      Definition of hydraulic conductivity in the 2 zones: 1000 and 1 permeab unit
      Definition of porosity in the 2 zones: 18.5% and 10%
      Definition of water residual content in the 2 zones: 3.75% and 5%
  /PERMEAB/GEO_ZONE        Z=      1V=      1000;
  /PERMEAB/GEO_ZONE        Z=      1V=         1;
  /POROSITY/GEO_ZONE       Z=      1V=      18.5;
  /POROSITY/GEO_ZONE       Z=      1V=        10;
  /RESID_SATUR/GEO_ZONE    Z=      1V=      3.75;
  /RESID_SATUR/GEO_ZONE    Z=      1V=         5;
      Definition of the UZ parameters in zone 1
  /UNSAT_PARAM/GEO_ZONE Zon= 1; Retent_Law= HOMOG; Succ_Reten=  2.115; Expon_Reten= 0.25; &
  /UNSAT_PARAM/GEO_ZONE         Permea_Law= Power; Expon_Perm=      4; Succ_Permea=    0;
      Definition of the UZ parameters in zone 2
  /UNSAT_PARAM/GEO_ZONE Zon= 2; Retent_Law= HOMOG; Succ_Reten= 4.4721; Expon_Reten=  0.5; &
  /UNSAT_PARAM/GEO_ZONE         Permea_Law= Power; Expon_Perm=      4; Succ_Permea=    0;
```

Figure 118 – Definition by zone of the parameters for the UZ laws.

When defining the retention and relative permeability laws for "Geometric zones", we can also define supplementary parameters "Double hydraulic conductivity" laws. This allows representing unsaturated porous environments containing "macropores" or fractures.

The parameters concerning macropores (or fractures) are:

- Cut-off water content: *the hydraulic conductivity increases above this water content threshold.*
- Factor of hydraulic conductivity increase at saturation above the threshold: *the hydraulic conductivity at saturation increases when the water content exceeds this threshold.*
- Exponent of the macropore permeability law: *when the water content exceeds the threshold*.
- Water content at saturation in the matrix.
- Residual water content in the macropore.

Moreover, when requesting a data output at the end of the simulation, we obtain an "Unsaturated Zones constitutive laws" file with the file extension [.unsat] that recapitulates the retention and relative permeability laws. A file of this type may be re-used as input file for MARTHE:

- Its name can be given in the MARTHE project file at line "Unsaturated Zones constitutive laws";
- It can also be introduced in the [.mart] parameters file at paragraph "Initialization before simulation", or at any time step by using the syntax:

  Object = UNSAT_PARAM
  Action = FILE: Reading a file.

Contrary to other data, the parameters of characteristic laws always remain defined by zone. From a computational viewpoint, they are not assigned to cells, i.e. when the zones extensions are changed at a later stage, the characteristic laws will be assigned to these new zones.

8.12 DEFINITION OF RETENTION AND PERMEABILITY LAWS

The hydraulic conductivity "PERMEAB" in the hydraulic conductivity file is the "Hydraulic conductivity at Saturation". In MARTHE, this hydraulic conductivity file also serves as a "presence" file:

- Hydraulic conductivity = 0 or 9999 => cell outside the domain to be modelled.
- Hydraulic conductivity = value different from 0 and 9999 => cell of the porous medium.

The relative hydraulic conductivity of each cell is calculated in terms of its saturation state, by the permeability law that is defined for each (geometrical) zone.

The hydraulic conductivity used in the simulation is the product of the "Hydraulic conductivity at Saturation" by the relative hydraulic conductivity. It also considers the anisotropy coefficients and the possible presence of impervious links that prohibit any flow between two cells.

8.13 WEIGHTING OF THE HYDRAULIC CONDUCTIVITY BETWEEN TWO ADJACENT CELLS

In a software for the saturated zone, we normally use harmonic weighting between the transmissivity values of two adjacent cells. In the unsaturated zone, the hydraulic conductivity contrasts that are strongly dependent upon the saturation state, can be extremely large. A harmonic weighting usually is unsuitable, especially in transient simulations with a propagation of abrupt fronts.

Therefore, MARTHE can use using other weighting schemes, which can be selected by a parameter of the paragraph "Control of Hydrodynamic Groundwater Resolution" of the parameters file:

"GEOMET" Geometric average of adjacent hydraulic conductivity values. This is the recommended value that generally is the most efficient in the UZ. It is the default value for a simulation in the unsaturated zone.

"UPSTREAM" "Upstream" weighting: the hydraulic conductivity of the upstream cell is used, i.e. the hydraulic conductivity of the cell with the highest hydraulic head. In transient state calculation, this weighting tends to propagate the abrupt fronts a bit too rapidly.

"HARMON" Harmonic weighting is used standard simulations that do not consider the unsaturated zone. In a transient simulations with an unsaturated zone scheme, the weighting is often ill suited, especially in the presence of abrupt saturation fronts.

"ARITHM" Arithmetic weighting (rarely used).

8.14 FREE INFILTRATION

It is common, for instance during internal drainage, that runoff is left freely to infiltrate on a soil surface. In that case:

- There is no prescribed flow rate, as it is unknown at what velocity the runoff will infiltrate;
- There is no prescribed hydraulic head, as this will decrease over time. This hydraulic head variation will be conditioned by the initial state of the soil and its characteristic laws.

To simulate such runoff, we consider that this water is identical to a very permeable porous medium, located above the soil surface. Here, the water content is proportional to the water stage. For modelling runoff with a maximum stage of water "L", we create above the soil surface a cell of dimension "dz" with:

$$dz \geq 2 \, . \, L$$

We then create a specific zone for this cell, and we assign it a retention law of the "CAPACI" type. This is a retention law that automatically manages:

- The porosity = 100%;
- The residual water content = 0%;
- The suction at half-saturation = dz;
- The retention law: $h = -dz. (50\% - \theta)$ (equivalent to $H = Subst + \theta \, . \, dz$).

We also assign a high value to the hydraulic conductivity at saturation, such as 100 times more than the cells in contact with overlying one. The permeability law then can be summarized as $K = K_s$.

For instance, a cell with a height dz = 500 mm will allow the infiltration 200 mm runoff maximum. This implies an initial state (or at a given date):

$$\theta = 200 / 500 = 40\%$$

or:

$$h = 50 \text{ mm (i.e. } H = 200 \text{ mm if the bottom is at level 0)}$$

N.B.: As the height dz is used as a parameter of this retention law, one should, in the case of a 2D simulation, assign the same height "dz" to all cells that represent this runoff.

8.15 SAVING THE RESULTS

Cells with time series

It is possible to save the evolution over time of certain fields in specific cells. The selected fields and cells are specified in a "Cells with time series" file, with the file extension [.histo].

We can save the time series of:

○ Hydraulic head:	Variable: H_Head
○ Aquifer flow rate (Discharge):	Variable: Discharge
○ Overflow or seepage flow rate:	Variable: Q_Overflow
○ Pressure head	Variable: Pressure
○ Water content	Variable: Saturat
○ Permeability (under saturation)	Variable: Unsat_Permeab

The time series of the selected cells are saved in the "historiq.prn" file (and possibly the "historiq.out" file).

When "Variance analysis" is selected, the simulated and observed time series are also saved in the "historiq_sim_obs.prn" file.

Fields (Grids) of the simulated states

At any time step, we can save the "grids" of simulated water content or pressure head. The selection method is the same as that used for the hydraulic head, flow rate, concentration, etc., fields:

Select the object:

SATURAT = Water content (for instance)

Then the action:

OUTPUT

We can save the fields of:

- Hydraulic head
- Hydraulic head in a well
- Aquifer flow rate
- Overflow or seepage flow rate
- Pressure head
- Water content
- Saturation rate
- Permeability (during saturation)
- Amplitude of the real velocity

The selected simulated grids are saved as text or binary files in the "gridsimul.out" file. Moreover, if the domain is one-dimensional, the values appear in free format in the sequential "gridsimul_sq.prn" file (and in the " gridsimul_sq.out" file).

In the case of vertical 1D or 2D flow, when saving the field of simulated hydraulic head, the position of the "saturation boundary" (wrongly referred to as "free surface") is also saved in the following files:

- "free_surf.prn" for visualization in Excel ® or an equivalent spreadsheet;
- "free_surf.bln" for visualization with WinMarthe;
- "free_surf.out" for processing.

The saturation boundary is defined as the curve where the pressure head is zero. If there are several saturation boundaries on the vertical, only the first one (nearest the soil surface) is saved.

The state at the end of simulation

At the end of simulation, if requested via an option in the parameters file, the software saves all modified files and, especially, the grids of hydraulic head, pressure head and water content. This allows continuing the simulation at a later stage, if required.

8.16 EXAMPLE 7: FLOW BELOW A RIVER, THROUGH THE UNSATURATED ZONE

This example corresponds to the project ***ZNS_Sous_Riv.rma***.

This is adapted from Example 6 of simulation in the unsaturated zone, as cited by Cooley (1983). It shows how to carry out a simulation with a UZ calculation scheme, for calculating the changes in a saturation profile below a river and the groundwater response. Implementation of a simulation in the UZ with the MARTHE code is described by Thiéry (2015c), report BRGM/RP-64495-FR. The system to be modelled consists of groundwater and a 12-m-wide river whose bed lies 14 m above the free surface of the groundwater (Figure 121).

Initially, the whole system of saturated and unsaturated zones has a uniform hydraulic head equal to +2 metres. The river then is instantly filled to a water height of 2 metres above the bed and

maintained at this height. We now simulate in vertical cross-section the evolution of the humidification front. The system characteristics are:

Geometry:

- Elevation of the bottom of the groundwater = 0 m
- Elevation de the initial free surface of the groundwater = +2 m
- Elevation of the river bed = +16 m
- Width of the river = 12 m
- Thickness of the cross-section slice = 1 m

Initial state:

- Uniform hydraulic head in the entire domain = 2 m
- Hydraulic head in the river bottom and in the banks (up to a height of 18 m) initialized at 8 m.

Boundary conditions:

- Imposed hydraulic head in the groundwater (at 2 m) at the abscissa 17 metres from the axis of the river, from an elevation of 0 m up to 2 m.
- Imposed hydraulic head of 18 m in the river.

Hydrodynamic parameters:

- Hydraulic conductivity at saturation: K_S = 1 10^{-2} m/h (or 2.778 10^{-6} m/s)
- Specific confined storage coefficient = 1 10^{-4} m^{-1}.
- Water content at saturation (efficient porosity) θ_S = 25 %
- Residual water content θ_R = 5%
- Retention law = Homographic $\frac{h}{h_t} = \left[\frac{(\theta_S - \theta)}{(\theta - \theta_R)}\right]^{b_t}$ (h is the pressure head and θ the water content).
- Suction at half-saturation h_t = 1.778 m
- Exponent of the retention law b_t = 0.25
- Relative permeability law = Power $Kr = \left[\frac{(\theta - \theta_R)}{(\theta_S - \theta_R)}\right]^{b_K}$
- Exponent of relative permeability law b_k = 4
- Transient state simulation

8.16.1 Modelling

The modelling of this system poses no problems. After adopting a "Pseudo-vertical cross-section" geometry and in view of the symmetry of the system, only the right-hand part of the domain is modelled, counting from the middle of the river. The grid consists of 34 columns of 0.5 m width and 40 rows 0.5 m wide that represent 40 model layers. The modelled vertical extension thus extends from 0 to 20 m and the lateral extension is from 0 to 17 m.

To arrive at a thickness of 1 meter, we must set up in WinMarthe "Topographic elevation = 0" and "Thickness = 1". It is also possible to define later a "Topographic elevation" = 0, and a "Substratum elevation" = -1 m, (or even Topography = -10 m and Substratum = -11 m.

User profile

Create a "User Profile", selecting:

- "Transient state"
- "Unsaturated zone"
- (and "Standard mass transport")

The hydraulic is supposed to be in transient state during a period of 400 hours, and the simulated water content and pressure head fields are saved every 10 hours.

Numerical parameters

In view of the highly non-linear character of the system, we set a maximum number of external iterations equal to **150** and an under-relaxation coefficient initially equal to 0.7. In fact, for a correct convergence, this under-relaxation coefficient should be lower and set at **0.5**.

As the initial relative hydraulic conductivity is extremely low, an "Upstream" weighting should be selected, but an equivalent simulation will be obtained with an "Arithmetic" weighting.

"General Parameters" File

In the parameters [.mart] file we define with the pre-processor:

Paragraph "Control of Aquifer Hydraulic solving process"

```
     150 = Maxi number of iterations for time steps after time step #°0 (transient)
       0 = Maxi number of hydraulic iterations for time step n°0
    2e-5 = Average hydraulic head deviation between 2 iterations for convergence
     0.5 = Relaxation coefficient for resolution [Def=1]
Upstream = Weighting for neigh. Hydraul. Conductiv. (1=Geom ; 3=Upstream ; 4=Harmon)
```

Paragraph: "Data units":

```
    m/h = Aquifer Hydraulic conductivity   unit in m/s (or m2)
   1e-8 = Flow (Discharge, Yield)        unit in m3/s (Kg/s for Gas flow)
   Hour = Time unit (for model time steps)
 Specif = Input Confined Storage Coeff. (0=Hydrogeol. ; 1=Specific ; 2=Compress.)
      % = Porosity = Water Content unit [dimensionless] ['%' when in %]
```

Paragraph: "Geometric options, Data reference, Processors":

```
 Vertic = Grid orientation: 0=Standard ; 1=Vertical Cross-section: gravity along Oy
```

Paragraph: "Unsaturated Zone and Multiphase flow":

```
     1 = Unsaturated Zone calculation [0=No ; 1=Yes]
   0.1 = Minimum internal time-step
    20 = Maximum internal time-step
     5 = Maximum water content variation during the time step
   0.5 = Maximum balance error during a time-step [in % or in water Volume unit]
     0 = Type of balance error [0=% Intern_CVG ; 1=Net Bal. (vol.) ; 2=Net Bal.in %]
    50 = Maximum suction <==> Maximal dryness (in hydraulic head unit)
  1e-8 = Minimum hydraulic conductivity or permeability (numerical security)
Homogr = Retention law [1=Homogr. ; 2=Power ; 3=Logarithm ; 4=Van-Gen. ; 5=B&C etc]
 Power = Permeability law [1=Homogr(press) ; 2=Power(Saturat) ; 5=V.G. etc.]
 1.778 = Suction at 'half-saturation'
  0.25 = Exponent of retention law (> 0)
     4 = Exponent of relative permeability law (except when V.G., or B&C law)
```

8.16.2 Results

The simulation finishes in a few seconds and converges perfectly (balance deviation of 10^{-3} % or 10^{-5}). Figure 119 shows the evolution of the simulated saturation below the river. For verification, a simulation with cells that are four times smaller (0.125 m instead of 0.5 m, or 16 times more cells) was run as well (Figure 120). This simulation is longer, taking several minutes, but the results are extremely close, which shows that the 0.5 m grid was suitable. Figure 121 shows the evolution of the free surface (pressure head = 0). The groundwater rises after 160 hours and the saturation front catches up with the groundwater after 170 hours.

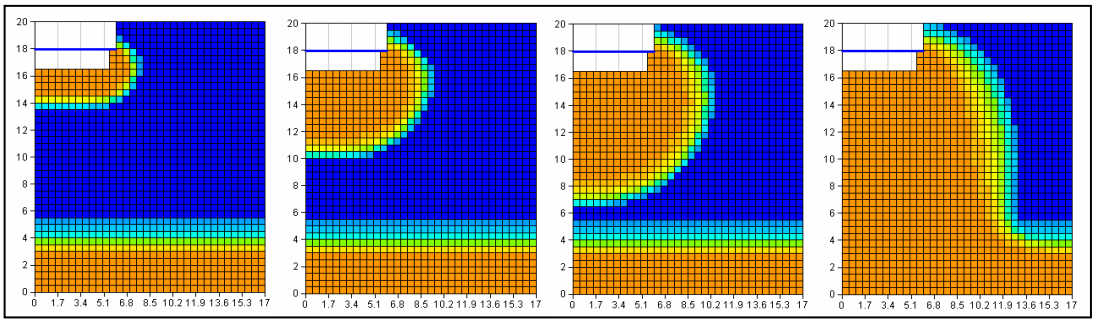


Figure 119 – Water content profiles after 10, 50, 100 and 300 hours (grid of 0.5 m).

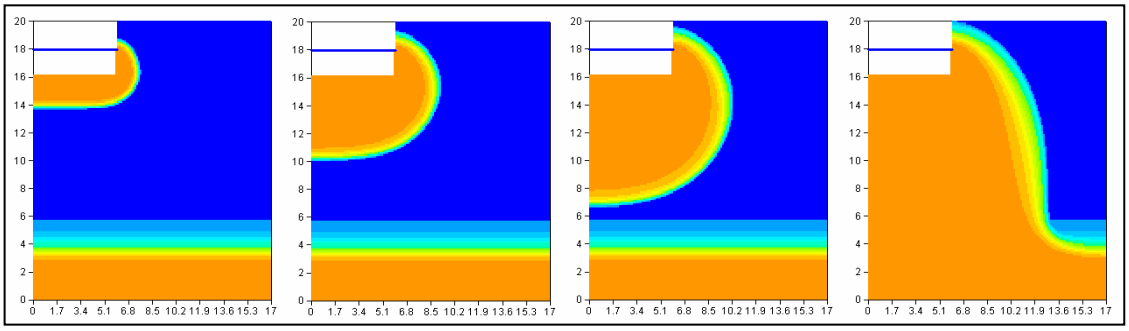


Figure 120 – Water content profiles after 10, 50, 100 and 300 hours (grid of 0.125 m).

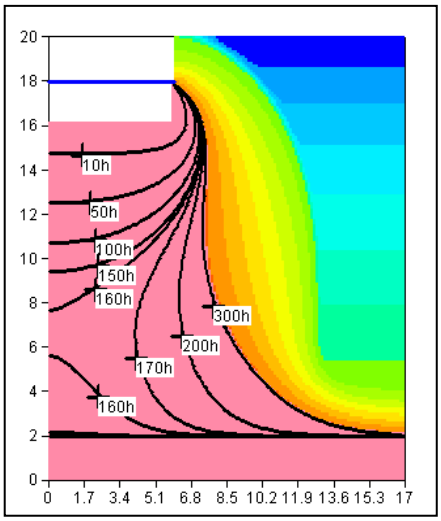


Figure 121 – Evolution over time of the position of the free surface (pressure head = 0).

8.16.3 Simulation in a radial grid

Project: ***ZNS_Sous_Riv_Rad.rma***.

The preceding simulation can be re-run almost immediately in radial coordinates, i.e. simulating the infiltration front below a circular basin of 12-m diameter. As before, it suffices to select "radial grid" in the layers file [.layer]. A few seconds later, we obtain the corresponding simulation. The results are little different, as is shown by Figure 122. The saturation "bubble" is just a little smaller as it diffuses in a radial manner, in two directions rather than only perpendicular to the river axis.

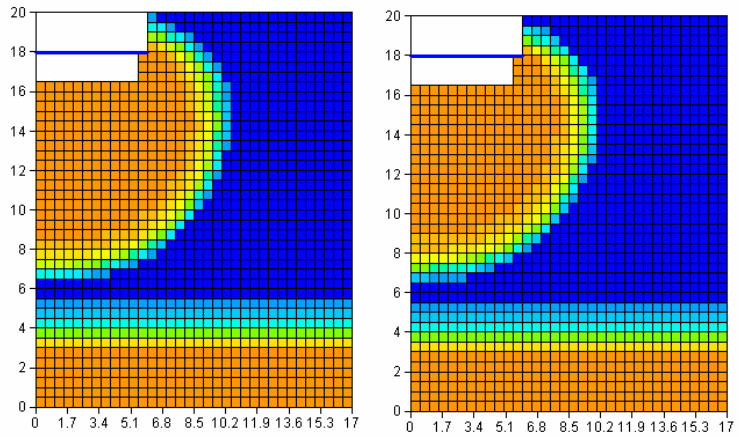


Figure 122 – Water content profile after 100 hours: left: River, right: Circular basin.

8.16.4 Mass transport in the unsaturated zone

Project: ***ZNS_Sous_Riv_Transport.rma***.

A transport simulation in the unsaturated zone under a transient hydraulic regime can be run in a few clicks. Proceed as in the earlier examples of transport simulation. First, the user profile [.prfu] file is modified by selecting "Standard mass transport". Then, the following parameters are defined:

Paragraph "Transport/Coupling of Concentration, Heat, Salinity"

```
TVD = Transport method (0=Finite Diff. ; 1=Random-W ; 2=Characteristics=MOC ; 3=TVD)
1.5 = Longitudinal Dispersivity (m) [*=Spatialized Field]
0.2 = Transverse   Dispersivity (m) [*=Spatialized Field]
```

We use the powerful TVD transport method, keeping the default number of iterations = 20.

Paragraph "Concentration and Pathlines"

```
 1 = Concentration Calculation
(The default transport regime is in transient state)
```

Also, remember:

- To set an initial concentration of 1000 units in the cells representing the bottom and the banks of the river (the cells with an imposed hydraulic head of 18 metres), and to set an "external concentration" equal to 1000 in the same cells.
- To request, with the pre-processor, in the time steps [.pastp] file, the output of concentration fields simulated at specific dates.

Then run the simulation that takes a few seconds. Figure 123 shows the simulated concentration field after 300 hours.

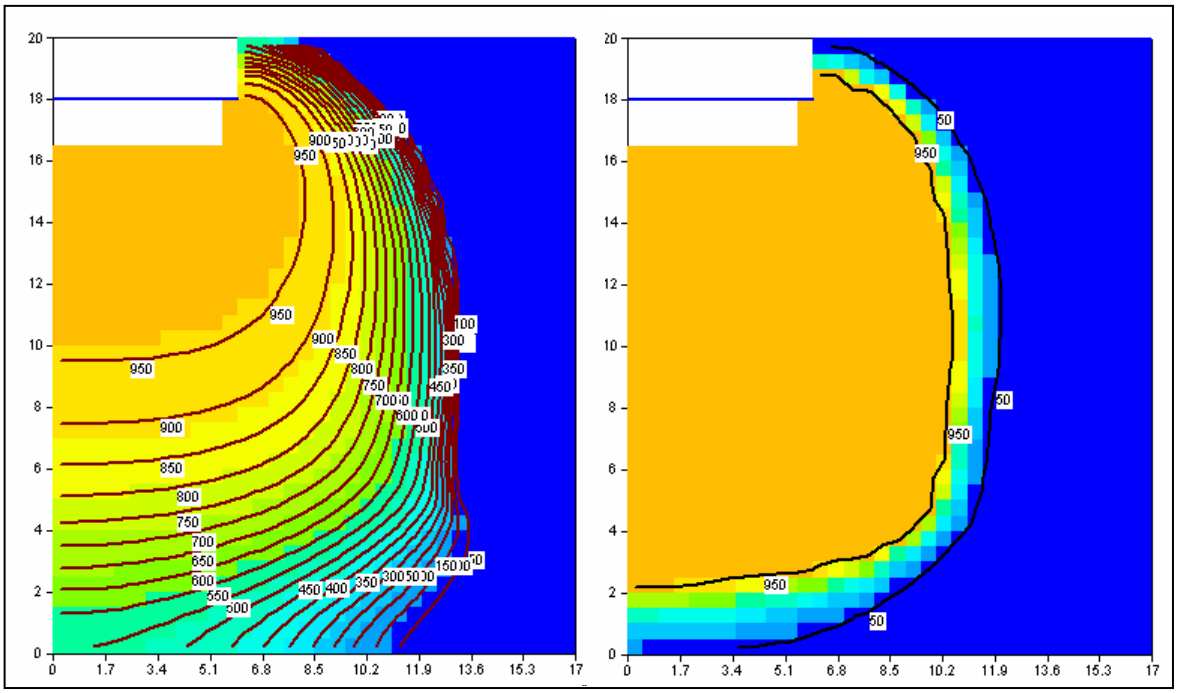


Figure 123 – Concentration after 300 hours: left, with dispersivity; right, without dispersivity.

8.16.5 Considering infiltration flux

Here we explain the procedure for introducing an infiltration or a recharge flux in a "Pseudo-vertical section" scheme.

Soil and Meteorological zones

In MARTHE, the "Soil zones" and "Meteo zones" are defined in "layer 0". In a "Pseudo-vertical cross-section" grid used with a UZ simulation scheme, row 1 corresponding to layer 0. It is in row 1 that the numbers of the "Soil zones" and the "Meteo zones" are defined (Figure 124)

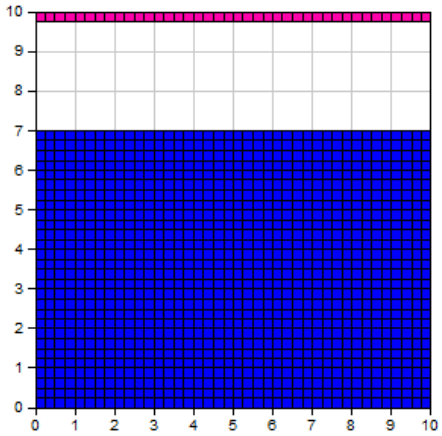


Figure 124 –"Pseudo-vertical cross-section" grid: Row 1, in pink, corresponds to layer 0. This is the row where the numbers of the Soil zones and the Meteo zones must be defined.

Recharge flux

A recharge flux can be defined per "Climatic zone", but it can also be defined per "Grid", per "Layer", per "Geometric zone" or per "Cell". If a recharge flux is defined per cell (or group of cells), only the values defined in the outcropping cells will be considered (Figure 125).

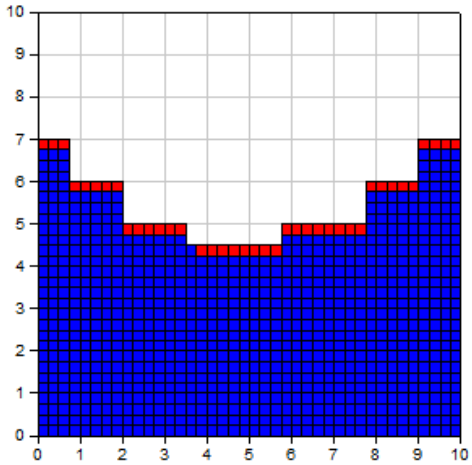


Figure 125 –"Pseudo-vertical cross-section" grid: Definition of recharge flux per "cell". Only recharge flux defined in outcropping cells (in red) are considered.

8.17 TRANSPORT EXAMPLE 8: SOLUTE INFILTRATION IN A VERTICAL UNSATURATED COLUMN

8.17.1 Aim of Example 8

This example allows verifying transport in the unsaturated zone, in a transient hydrodynamic regime, compared to reference simulations in the scientific literature.

8.17.2 Description of Example 8

Water containing chlorine is injected in a vertical semi-infinite column whose initial hydraulic state is defined by a saturation profile. This example, a reference since 1973, is described by Van Genuchten (1982), by Voss (1984) and by Warrick *et al.* (1971).

Characteristic soil laws

Characteristic soil laws are given by Van Genuchten (1982); based on his values, Thiéry (2015c) adjusted the following characteristic soil laws by means of automatic calibration with a correlation coefficient of 0.999:

- A homographic retention law:
  θ_r = 10%
  θ_s = 40%

  $$\frac{h}{h_t} = \left(\frac{\theta_s - \theta}{\theta - \theta_r}\right)^{b_t}$$

  h_t = 95.21 cm
  b_t = 0.699
- A homographic permeability law:

  K_S = 5.531 10^{-6} m/s
  h_k = 23.3 cm
  b_k = 3.473

  $$K/K_S = 1/[1 + (h/h_k)^{3.473}]$$

Transport parameters

The dispersivity is equal to 1.0 cm and there is no delay coefficient.

Initial and boundary conditions

The initial water content profile varies in linear fashion from 15% to 20%, from 0 to 60 cm depth, and is 20% below 60 cm depth. The initial concentration is equal to zero.

Upper boundary

At the start of simulation, a hydraulic "saturation" (θ = 38%) condition is imposed. The concentration is imposed at a value of 209 meq/litre during 168 mn (2 h 48 mn), after which it becomes 0.0 (meq/litre).

Lower boundary

This boundary will not be reached during simulation. We thus impose an initial water content of 20% and an external concentration equal to 0.

Reference solution

There is no analytical solution, but a "numerical solution" was defined (see Van Genuchten, 1982) by using several simulation codes with very fine space and time steps. Figure 126 presents the reference profiles of water content and concentrations, 2 hours and 9 hours after the start of infiltration. Note that, even in the absence of a delay coefficient, the concentration front moves slower than the humidity front as after 2 h they have reached depths of 40 cm and 90 cm, respectively. This is due to the water contained in the initial humidity profile.

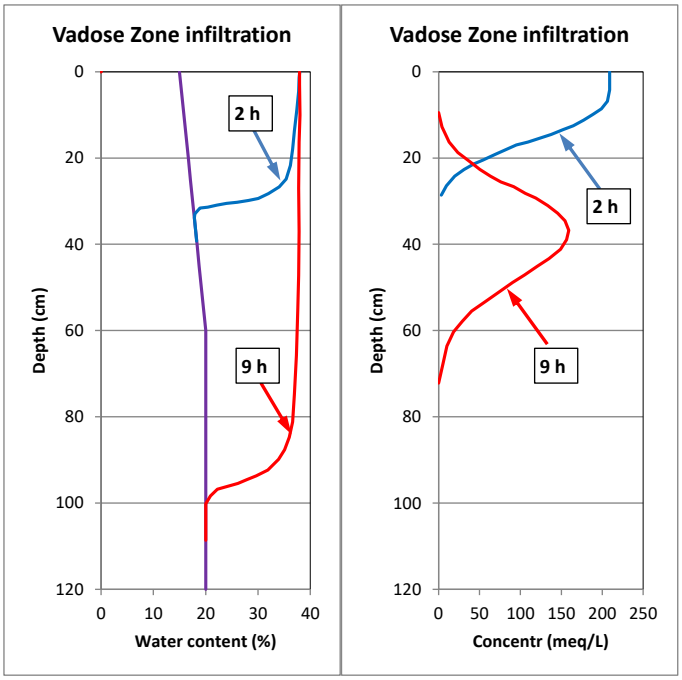


Figure 126 – Transient infiltration in a vertical unsaturated column. Reference profiles of water content and concentration.

8.17.3 Simulation with the MARTHE software of Example 8

The aim is to simulate the concentration profile 2 hours and 9 hours after the start of infiltration. Choose simulation time steps between 2 s and 500 s, which are determined automatically by MARTHE to ensure a good water flow convergence. Then select a vertical one-dimensional grid of 61 cells of 2 cm high by 100 cm wide, for a total modelled height of 122 cm.

Successively simulate the mass transport in the UZ with the TVD, MOC, FD and RW methods. For the simulations that handle particles (MOC and RW methods), we assumed that the concentrations were in kg/m^3. The unit mass of the particles was then set at 0.002 kg to have 8000 particles at the end of simulation.

8.17.4 Results obtained for Example 8

Figure 127 shows that simulation with the TVD method is more accurate. The simulated concentrations are, however, slightly higher than for the reference simulation. This is caused by the saturation hydraulic conductivity used in the homographic law that is slightly higher than the reference hydraulic conductivity.

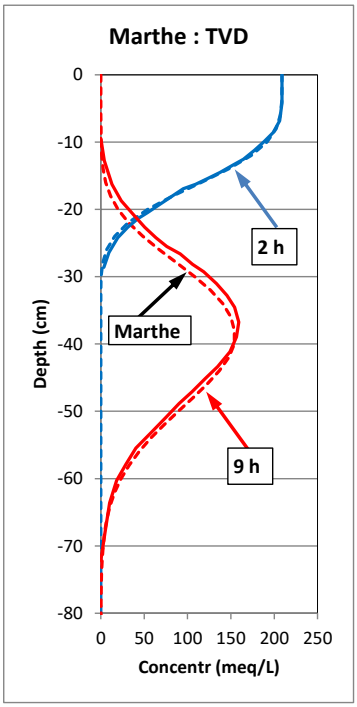


Figure 127 – Transient state infiltration in a vertical UZ column.
Concentrations simulated with the TVD method are reference profiles as a continuous line.

Figure 128 shows the simulations obtained with the MOC, RW, FD and FD methods in cells of 0.25 cm.

- Simulation with the MOC method is very close to the TVD simulation, presenting only a few small fluctuations.
- Simulation with the RW method is acceptable, but presents strong fluctuations.
- Simulation with the FD method (“DF” on the graph) with a grid of 2 cm shows a strong numerical dispersion, which is logical as the Péclet number is equal to 2.
- Simulation with the FD method, with a grid of 0.25 cm (Péclet = 0.25) and with simulation time steps limited to 125 s, is very close to the TVD simulation, and very fast.

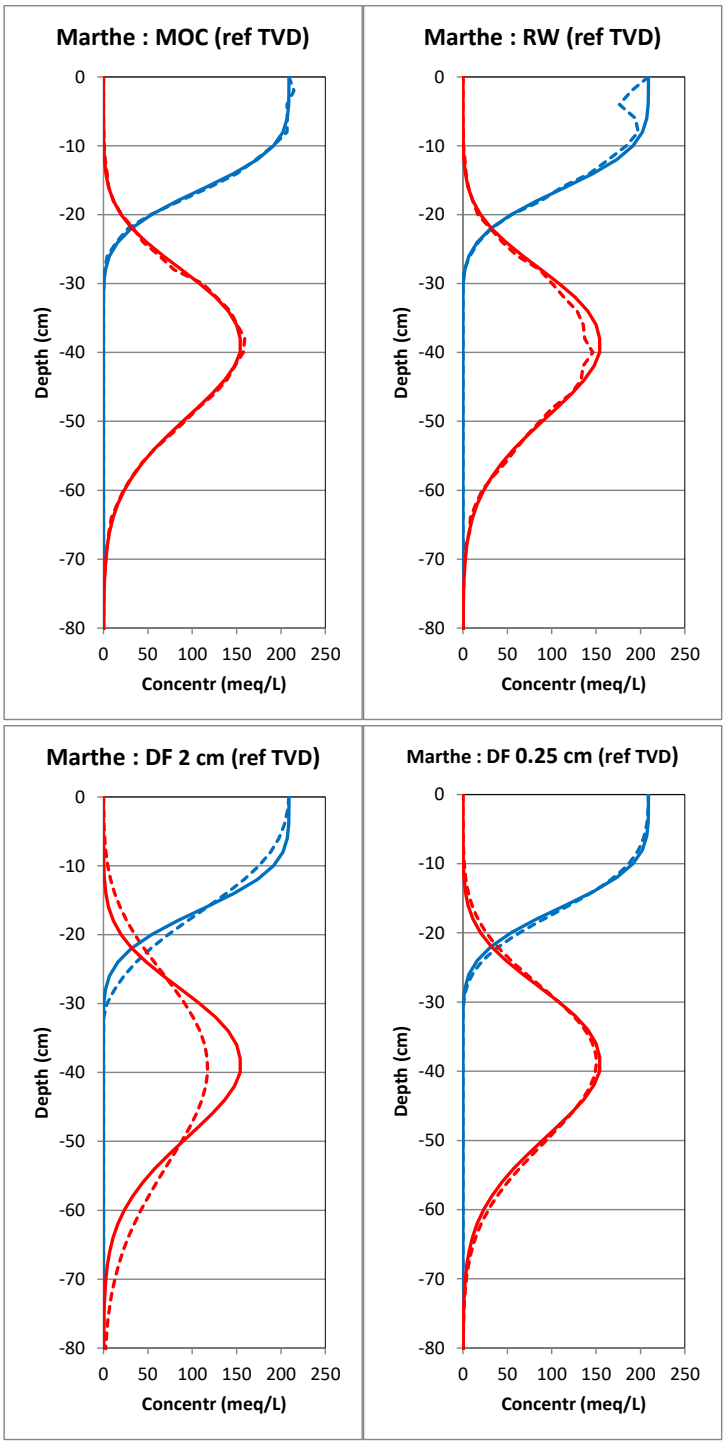


Figure 128 – Transient infiltration in a vertical UZ column.
Concentrations simulated with the TVD, MOC, RW, DF_2 cm and DF_0.25 cm methods
TVD solutions in solid line.

9 Principles of the river network and drain network

This chapter presents the features of a river network that are considered when modelling hydrosystems. Such networks are coupled to groundwater for simulations of flow, mass transport and heat transfer in rivers. A river network is also coupled to a hydro-climatic balance to which runoff is directed.

9.1 PRINCIPLE OF THE RIVER NETWORK

9.1.1 Presentation of the river network

The river network that is superimposed on the surface grid, is composed of a branching system of river reaches (or sections), organized in tributaries (Figure 129).

It is only in contact with the locally outcrop layers.

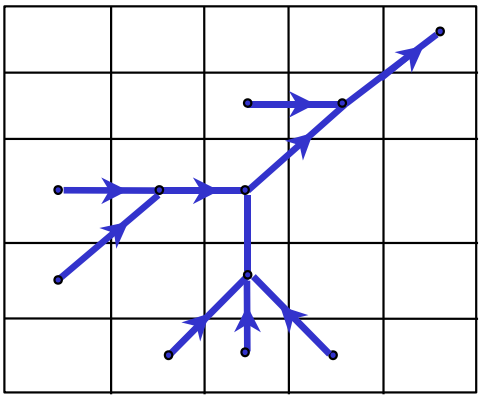


Figure 129 – River network connected to the domain grid.

Each river reach has:

- A single downstream reach.
- Up to **five** upstream reaches.

A reach is described (Figure 130) by its:

- Geometry:
  - Length,
  - Width,
  - Elevation of the river bed,
- Physical properties,
  - Roughness of the river bed and river banks,
  - Slope of the river bed,
  - Thickness of the bed and the banks,
  - Permeability of the bed and the banks,
  - If the reach has a sill at its downstream end:
    - Sill flow factor,
    - Sill height above the river bed
    - Exponent of the river flow versus water height above the river bed
- Source term,
  - Pumping from or injection into the reach,
- Condition,
  - Water level (absolute) in the river.

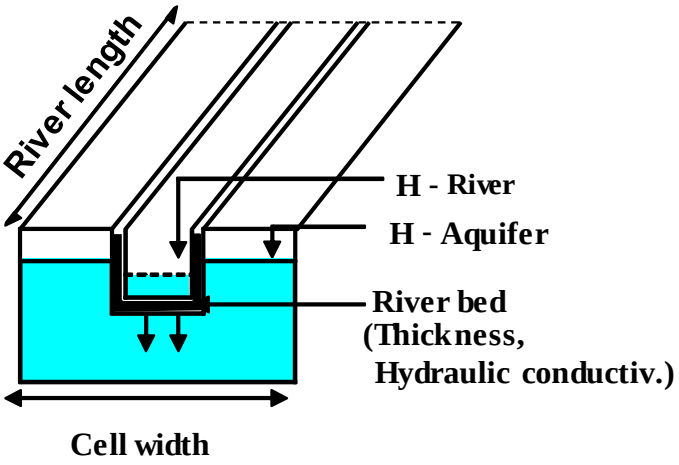


Figure 130 – Geometry of a river reach.

9.1.2 Flow propagation in a river reach

The flow in a river reach results from the equilibrium between all flow terms (Figure 131):

- Upstream flow (Q_{AM}),
- Downstream flow (Q_{AV}),
- Flow exchange with the aquifer (Q_{ECH}),
- Runoff flow and groundwater overflow (Q_{RUIS}),
- Inflow into or outflow from the reach (Q_{INJ})

And, when transient state routing is considered:

- Storage flow (STO).

The flow equation is written as:

$$Q_{AV} = Q_{AM} + Q_{ECH} + Q_{RUIS} + Q_{INJ} - \frac{dSTO}{dt} \qquad (1)$$

where "dt" is the duration of the time steps.

In the case of a rectangular section, the storage term "STO" is the product of reach width and water stage in the river "H_{RL}".

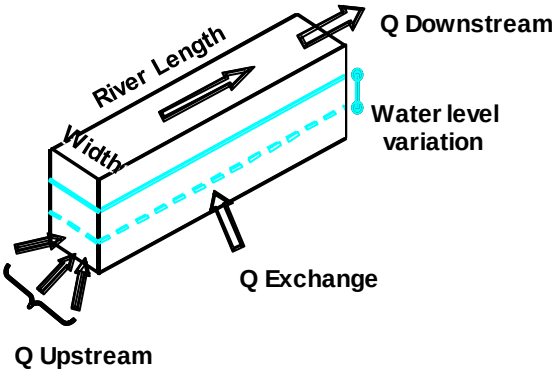


Figure 131 – Flow balance in a river stretch.

The water stage "H_{RL}" in the reach is related to the downstream flow "Q_{AV}" of the reach by the Manning-Strickler formula:

$$Q_{AV} = \frac{1}{n} \cdot A \cdot R^{2/3} \cdot \sqrt{Slope} \qquad (2)$$

where:

A = Cross-section area of the reach

R = Hydraulic radius =

$$(\text{Width} \cdot H_{RL}) / (\text{Width} + 2\, H_{RL}) \qquad (3)$$

n = Manning-Strickler coefficient (translating the "roughness")

Slope= Slope of the river bed

H_{RL} = Water height above the river bed ("Water stage")

If one introduces a sill—such as a small dam—downstream of the stretch, we no longer use a Manning-Strickler law, but a sill law as follows:

$$Q_{AV} = \text{Width} \cdot \text{FactQ} \cdot \sqrt{2g} \cdot (H_{Riv} - H_{Sill})^{Expon}$$

with:

FactQ = Factor (no unit) with a default value of 0.40

g = Gravity acceleration = 9.81 m/s^2 (in Paris).

Width = Width of the reach (m).

H_{Riv} = Water stage above the river bed in the reach considered (m).

H_{Sill} = Height above the river bed, of the sill downstream of the reach considered (m).

Expon = Exponent: generally equal to 1.5 (no dimension).

Combining equations (1), (2) and (3), we obtain an implicit equation that gives the flow downstream of the reach in terms of the flow in the upstream reaches. The flow in the whole river network then is optimally obtained by an iterative process, using the Strahler order of each reach. This routing scheme is very efficient and has been successfully compared with a quasi-analytical solution of flood-wave propagation in a canal, as well as with observed data on flood propagation in the Haute-Loire (France). As the simulation method assumes that in each reach the free surface has the same slope as the river bed, the approximation is even better if the river bed slope is not too small and if the water-height variations in the river are not too rapid, which is generally the case in natural systems.

9.1.3 Flow exchange between a river reach and the underlying aquifer

Depending upon the relative position of the water level in the river and of the aquifer level, water flow can be from the river reach to the aquifer, or, inversely, from aquifer to river. Such flow exchange is controlled, in a non-linear manner, by the bed and banks of the river, based on their surface, thickness and hydraulic conductivity (Figure 132).

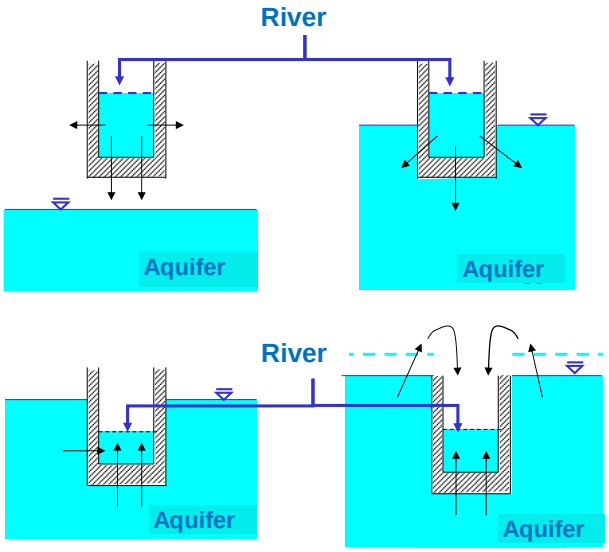


Figure 132 – Different configurations of exchanges between an aquifer and a river.

Three situations are possible:

- When the aquifer level is below the bottom of the river bed, the exchange flow to the aquifer is a percolation term independent of this level. In fact, the groundwater is "disconnected". The environment is no longer under pressure, no longer saturated, but the bottom of the riverbed is at the limit of saturation, with a quasi-null suction. The hydraulic head at the base of the bed is equal to the elevation "H_f". This situation is embodied in equation (5).
- When the aquifer level is located above the riverbed bottom, the exchange flow is the product of the hydraulic conductivity of bed and banks by the exchange surface. The latter integrates the river banks multiplied by the difference between the water-surface height in the river and the hydraulic head in the aquifer, divided by the thickness of the bed; equation (6).
- When the hydraulic head of the aquifer is higher than the soil level (i.e. “topographic elevation”) and also higher than the water level in the river, the exchange flow (of groundwater to the river) is increased by a complementary term of groundwater overflow. This term is applied to the complementary cell surface of the underground domain; see equation (7).

$$AREA_{Exch} = L \cdot [W + 2 \cdot (H_R - H_b)] \quad (4)$$

$$Q_{Percol} = AREA_{Exch} \cdot K_R \cdot \frac{(H_R - H_b)}{Thickn} \quad (5)$$

$$Q_{Exch} = AREA_{Exch} \cdot K_R \cdot \frac{(H_R - H_G)}{Thickn} \quad (6)$$

$$Q_{Overfl} = (AREA_{Cell} - L \cdot W) \cdot K_R \cdot \frac{(H_G - H_{Topo})}{Thickn} \quad (7)$$

With: L = Length of the river reach,
W = Width of the river reach,
K_R = Hydraulic conductivity of the river bed and river banks,
Thickn = Thickness of the river bed (and the river banks),
H_R = Absolute elevation of the free water surface in the river,
H_G = Hydraulic head in the underlying groundwater,
H_b = Elevation of the bottom of the river bed,
H_{Topo} = Elevation of the topographic surface of the cell containing the reach,
$AREA_{Cell}$ = Horizontal area of the cell in which the reach is located,
$AREA_{Exch}$ = Area of the groundwater-river exchange,
Q_{Exch} = Flow of the river exchange towards groundwater,

Q_{Percol} = Flow of the river percolation towards “disconnected” groundwater,
Q_{Overfl} = Complementary overflow of groundwater to the river.

Generally, the exchange flow depends upon water variations in the river. Considering a given level in the aquifer, the exchange flow is higher when the river flow—and thus the water height in the river—is higher. The model can be verified or calibrated based on observed variations in water height, or water level.

9.1.4 Detailed organization of the river network and terminology

In MARTHE, the river network is organised in "tributaries", each divided in “reaches” (*or "sections"*):

- A "tributary" is a serial group of reaches, without confluences; a "tributary" can thus only be plugged in downstream in the upstream reach of another "tributary". It can never be plugged into the middle of a "tributary".
  For convenience’s sake, a real tributary can be divided into several tributaries "in the MARTHE sense".
- Each tributary can have up to **5** upstream tributaries, but each has at most one downstream tributary.
- If a tributary has no downstream tributary, its downstream extremity is an "outlet".
- If a tributary has no upstream tributary, its upstream extremity is a "spring".
  An upstream tributary can be fed by a (river) flow from outside the modelled domain. This "upstream flow" can be set by the user, or it is automatically calculated with a hydro-climatic balance.
- There can be as many outlets and springs as required. There can be several completely independent river networks (such as the Seine and Loire river networks in a regional French model).
- Each cell of the domain can contain at most one element of a river network.
- A modelled aquifer domain can be monolayer or multilayer.
- A river network only concerns outcropping layers. This is not necessarily layer 1 but can be any exposed layer.
- In the current layer, the neighbouring reaches or tributaries can be located in **8** neighbouring cells (N, S, E, W, NE, NW, SE, SW) thus including oblique cells.
  In a multilayer system, the neighbouring reaches can be in the under- or overlying layer, provided it is outcropping. The following **8** directions are possible: HN, HS, HE, HW for overlying layers, and LN, LS, LE, LW for the lower layer (N = north; S = south; E = east; W = west; H = Higher; L = Lower).
  In all, there are thus **16** possible directions.

9.1.5 Numbering the elements of a river network

A river reach is defined by its "tributary number" and its "reach number". In MARTHE, for a given tributary, the reaches have increasing numbers from upstream to downstream. The reach numbers do not have to be continuous, but must be increasing in the same tributary. However, different tributaries can have elements with the same reach number.

A tributary number must be at most 1000, as from 1001 a tributary number corresponds to a "Lake" and not a river.

For convenience of modelling, a (real) tributary can be divided into several consecutive tributaries.

The number of reaches in a same tributary is limited at 999,998.

The total number of reaches is unlimited.

To designate a "river element" in this document, we generally use the term "river reach". A "river element" is thus defined by its "tributary number" and its "reach number".

9.1.6 Branching tree of river tributaries

The "Branching tree of river tributaries" fixes the relations between river tributaries. For each tributary, it gives the number of its downstream tributary. If downstream there is no tributary but an outlet, by convention the downstream tributary has the number "0".

There can be several downstream tributaries, if there are several independent rivers.

At most **5 river** tributaries can have the same downstream tributary, hence a river tributary cannot have more than **5** upstream tributaries.

9.1.7 External upstream tributary

This is a river outside the simulated grid domain that branches into the upstream reach of a tributary (that has no upstream reach within the grid domain).

The flow coming from this "external upstream tributary" is automatically calculated by a hydro-climatic balance. For simulating this flow by such a balance, the following fields must be defined:

- Surface of the catchment basin of this upstream tributary outside the simulated domain;
- Number of the soil zone for the outside river (for the hydro-climatic parameters),
- List of Meteo Zones and their associated weighting, for meteorological data concerning the catchment of the "external upstream tributary". Such data (atmospheric precipitation, PET, air temperature) must be in sequential files.

9.1.8 Options for simulation

If required, the software can calculate the water height in each river reach from the flow rate, using the complete (or simplified) Manning-Strickler law. Reciprocally, this law gives the discharge flow from the water height in the river reach. For a given reach (and a given shape) the "stage-discharge" relation depends upon two parameters:

- The slope of the reach,
- The roughness of the river.

Downstream of certain reaches, a sill—or small dam—can be introduced. The flow downstream of the reach, i.e. the flow over the sill, is ***not*** given by the Manning-Strickler law, but depends on the water height with respect to the sill height, as well as on two other parameters:

- The flow factor given by the flow-over-the-sill law.
- The exponent of the flow-over-the-sill law.

In transient state, if a relation between height and flow (a “stage-discharge” relation) has been defined, it is possible to take into consideration the variation in water volume in the river that causes “routing", i.e. a delay in propagation.

If a stage-discharge relation (a relation between water height and flow) has been defined, the water level in the river can be imposed in certain reaches (certain cells); after setting an injected flux equal to 9999; the software determines the flow to inject (or abstract) in the river reach for maintaining this water level.

Coupling with the simulation of hydraulic head in the groundwater:

Generally, the simulation of flow in a river is done at each time step of the model. In order to streamline the simulation, it is possible not to refresh the hydraulic head simulation of the aquifer at each time step, but this option can create instability when the coupling is strong.

It is thus recommended to carry out the simulation of the river and that of the hydraulic head in the groundwater during the same time steps. This is the default option, but another one can be selected.

Mass and heat transfer in the river network and exchange with groundwater can be considered as well.

9.1.9 Data fields to be defined in each cell containing a river reach

- Length of the river reach.
- Width of the river reach.
- Elevation of the river bottom (when dry).
- Thickness of the river-bed sediments.
- Hydraulic conductivity of the river bed.
- Elevation (absolute) of the river water.
- Injection (or pumping) flow in the river, negative when it is injected, negative when pumped. An injection flow equal to the value 9999 is used for imposing the water level in the river (only if a scheme with a Stage-Discharge relation was selected).
- Upstream (spring) flow in the river (in the "spring reaches").
  Such upstream tributary flow from outside the modelled domain:
  - can be set by the user,
  - or can be calculated automatically by a hydro-climatic balance.

If the simulation is carried out in transient state, the field of the initial flow downstream of the reach must be defined as well.

If a Stage-Discharge relation is set with the Manning-Strickler relation, it is necessary to define the:

- Roughness of the river bed (around 0.02 $m^{-1/3}$.s]);
- Slope of the river bed (dimensionless; around 1:100 to 1:1000).

If a sill is introduced downstream of the reach, the Height-Flow relation (Stage-Discharge relation) will depend upon the following fields that must be defined:

- Height above the bottom, of the sill located downstream of the reach (in user units of hydraulic head and elevation).
- Flow factor of the flow-over-the-sill: default value 0.4 (unitless).
- Exponent of the flow-over-the-sill: default value 1.5 (unitless).

If mass transfer in the river is considered, the field of mass flux in the river, whether injected or abstracted, must be defined.

N.B.: It is also possible to define such data (reach length, reach width, thickness, roughness, etc.) outside the drainage network. MARTHE does not consider this as an error but ignores such data. If the "section lengths" or "roughness" are uniform throughout the domain, it is possible, and easier, to define such values with the "MARTHE grid".

The data-user units are the following:

- Lengths and widths of reaches, in coordinate-user units.
- Water level, depth, elevation of the river bottom, sediment thickness: in user units of hydraulic head and elevation.
- Flow in user units of river flow (or, by default, in user discharge units if no river-flow unit was defined.
- Hydraulic conductivity of the river bed and banks in user units of hydraulic conductivity
- Roughness in $m^{-1/3}$.s
- Slope: no unit.

9.1.10 Global data that define the whole network

- The "branching tree" of river tributaries is a file that, for each tributary, gives the number of its downstream reach.
  If a tributary has no downstream reach as it is an outlet, it is given "0" as downstream tributary number.

  At most **5 river** tributaries can have the same downstream tributary
  (A river tributary can have at most **5** upstream tributaries).
- The optional file of flow derivations is a file that defines for each derivation the spring reach, the percentage of derived flow and the targeted reach.
- The diffusion coefficient of the concentration in the drainage network (m^2/s), if mass transfer is considered.

9.1.11 Assigning or modifying the fields of river data

All data fields (number, water level, length, width, hydraulic conductivity, etc.) can be defined in the cells with the WinMarthe graphic preprocessor.

The data can also, like the other MARTHE fields, be defined or modified:

- by "Grid",
- by "Zone",
- by "Layer",
- by "Cell".

In addition, the river data can be defined or modified by "section**",** i.e. by the couple "tributary-section".

9.1.12 Initial state

- If the Stage-Discharge relation is not defined (the simplest case), absolute water levels must be set for each river reach. These water levels remain unchanged during the simulation.
- If the Stage-Discharge relation is defined, one must set *either*:
  - The initial water level in all river reaches, *or*
  - The initial flow in all river reaches. MARTHE then calculates the corresponding water level. The initial flow option is recommended for initializing, as the use of an approximate water level can lead to instability.

    At each time step, the code then calculates the flow and the water level in each reach.

- If mass transfer is considered, the initial concentration in all reaches of the network must be considered as well.

9.1.13 Numerical parameters for a relative simulation of the drainage network

For simulation of the river network, it is necessary to define specific options and parameters. Among these parameters are:

- The maximum number of simulation iterations (for the river).
- The maximum flow variation between two successive iterations for considering that the simulation has converged.
- The (potential) under-relaxation coefficient.

9.1.14 Results of the simulation

Time series for rivers in selected cells

- Flow in a river reach, is the *flow downstream of the reach.*
- River-Groundwater exchange flow, *is positive when the river 'feeds' the groundwater*.
- Injection flow (or "outside flow") calculated in a river reach.
    - If the flow is injected (i.e. > 0), the simulation converges when the calculated injection flow is the same as the imposed injection flow.
    - If the imposed injection flow is < 0, it is an abstraction. The calculated abstraction may be less that the imposed one if the river flow is insufficient.

  In reaches with a set water level, the calculated "outside flow" is that needed for imposing this level.
- Upstream tributary flow is calculated by hydro-climatic balance.
- Water level in a river reach (*if a Stage-Discharge relation was defined*).
- Water depth in the river, or the height of water over the reach bottom. In surface hydrology, this is commonly called "draught".
- Concentration in a river reach (*if mass transport is considered*).

Calculated field grids

- Flow in the river cells.
- River-Groundwater exchange flow with the groundwater is *positive when the river 'feeds' the groundwater*.
- Calculated injection flow (or calculated outside flow):
    - In the reaches where flow is injected (i.e. > 0), the simulation converges when the calculated injection flow is the same as the imposed injection flow.
    - If the imposed injection flow is < 0, we are dealing with abstraction. The calculated abstraction may be less that the imposed one if the river flow is insufficient.

  In the reaches where the water level is set, the calculated injection flow is the "outside flow" necessary for imposing this level.
- Water level in the river reaches (*if a Stage-Discharge relation was defined*).
- Concentration in the reaches of the drainage (*if mass transport simulation is made*).

9.2 EXAMPLE 10: MULTILAYER HYDROSYSTEM WITH RIVERS

- Project: ***Didact_Riv_3D.rma***
  Steady state without stage-discharge relation.
- Project: ***Didact_Riv_3D_Mann.rma***
  Steady state with Manning-Strickler stage discharge relation.
- Project: ***Didact_Riv_3D_Mann_Rout_Transi.rma***
  Transient regime (with routing).
- Project: ***Didact_Riv_3D_Transport.rma***
  Transport in groundwater and in river over 5 years.

This example shows how to simulate a multilayer system with a river network formed by several river tributaries. Start by modelling with a fixed water height in the river. The simulation of the water level, and of the groundwater and river flow, takes place in the steady state. Then model the transport couple in the groundwater and in the river network, for simulating the consequences of pollutant injection in a river reach.

The characteristics of the system are the following:

***Geometry*:**

- The modelled system consists of three aquifer layers.
- Layer 1 is exposed in the north, layer 2 is exposed in the central part and layer 3 is exposed in the south (Figure 133 and Figure 134).
- In plan, the hydrosystem is a rectangle of 102 km in the east-west direction (abscissae -51 to +51) by 300 km north-south (ordinates 0 to 300).
- Total aquifer thickness is 200 m (from elevation -100 to +100 m).
- The bottom of layer 1, when existing, is at elevation -33.33 m, that of layer 2, when existing, at elevation -66.66 m and that of layer 3 at elevation -100 m.
- The topographic elevation is uniform, at +100 m.

***Boundary conditions*:**

- The only boundary condition is an imposed hydraulic head of 0 m in the farthest downstream cell, in the third layer at coordinate point x = -2 km, y = +1 km.

Hydraulic parameters in the aquifer:

- Aquifer hydraulic conductivity = 10^{-4} to 10^{-3} m/s depending on the simulation.
- Specific storage coefficient = 1 10^{-5} m^{-1}.
- Specific yield coefficient = 5%
- Porosity = 5%

River network:

- The drainage system consists of six tributaries numbered 10, 20, 30, 40, 50 and 60. Flow is globally north-south (Figure 135).
- The coordinates of the tributary extremities are given in Table 8.
  - River widths are given in Table 8.
  - Elevation of the river bed bottom = 0 m.
  - Elevation (initial) of the river water = 4 m.
  - Thickness of river bed and -banks = 0.1 m
  - Permeability of river bed and -banks = 10^{-6} m/s
  - Roughness of river bed ("n" of Manning-Strickler) = 0.04
  - Slope of the river bed (for Manning-Strickler) = 10^{-4}.
- The outcrops show three soil zones: zone 5 in the upper third (ordinates 200 to 300 km), zone 10 in the middle (ordinates 100 to 200 km) and zone 15 in the lower third (ordinates 0 to 100 km).

Grid:

- A regular grid is chosen, with 51 columns of 2 km width and 150 rows of 2 km width.
- Three layers of variable thickness.

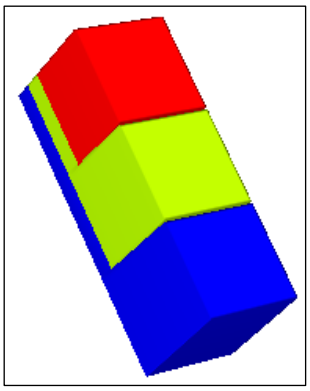


Figure 133 –Multilayer hydrosystem with rivers.

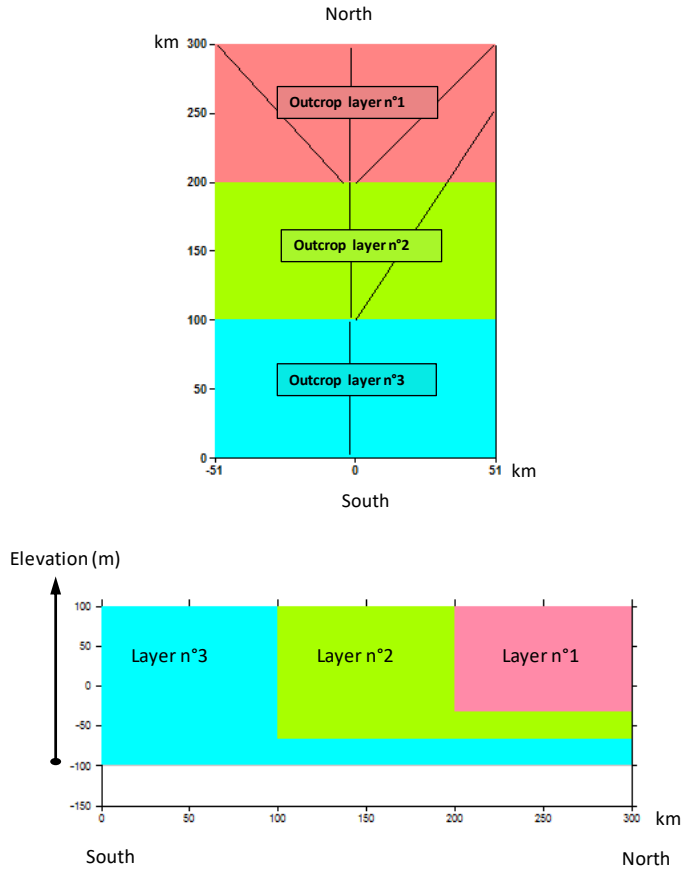


Figure 134 – Geometry of the multilayer hydrosystem with rivers.
Above: Plan view; Below: Vertical cross-section view.

Tributary:	**10**		**20**		**30**		**40**		**50**		**60**	
Start (km)	-2	297	-2	199	-2	99	50	299	-50	299	50	251
End (km)	-2	201	-2	101	-2	3	0	199	-4	199	0	99
Width (m)	50		100		100		50		50		50	

Table 8 - Coordinates in km of the extremities of the six tributaries, and widths of the tributaries in metres.

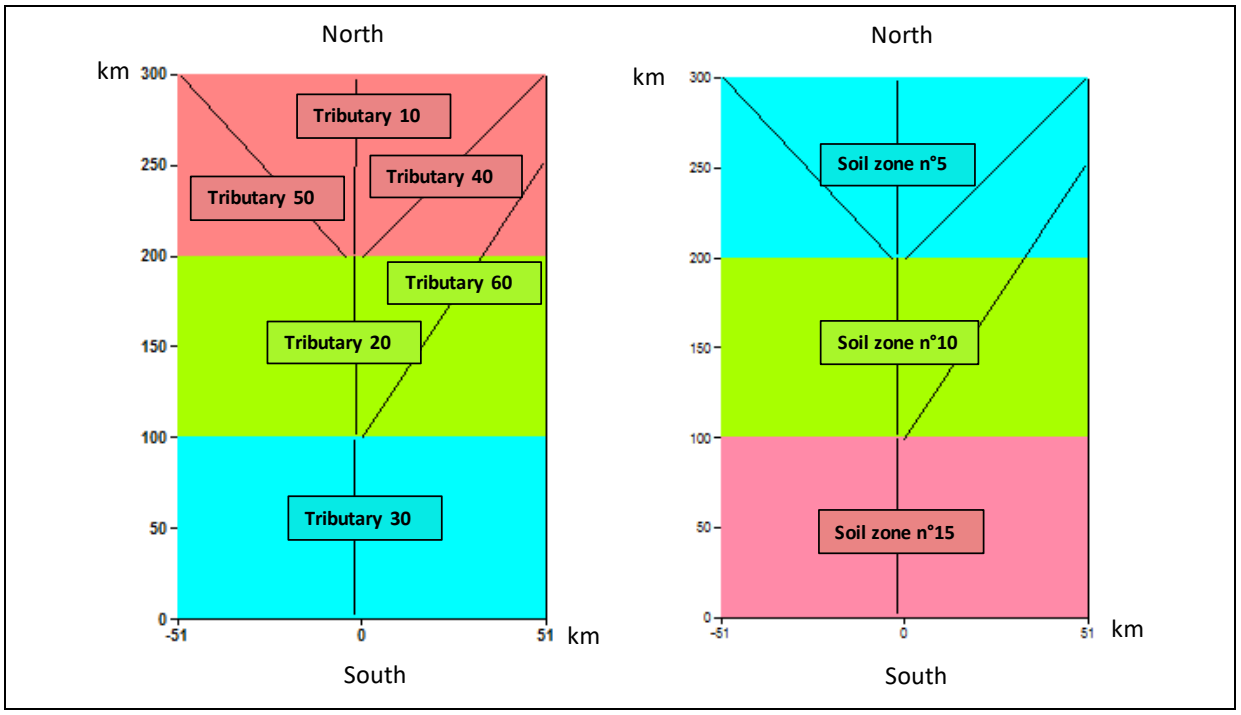


Figure 135 – Description of the river network and the soil zones.

9.2.1 Creation of the Grid

Project name: **Didact_Riv_3D;**

- Southwest angle: X = **-51;** Y = **0** (km)
- Northeast angle: X = **+51;** Y = **300** (km)
- Column width = **2;** Row width = **2** (km)
- Number of layers = **3;**
- Default hydraulic conductivity = 1;
- Topographic elevation = **100** (m)
- Thickness (of each layer) = **60** (m)

To have a more agreeable representation, with a slightly less elongate rectangle, use button  "Y/X Distortion in plane view" and set a factor of 0.5.

Then select the bottom field and assign it the following elevation values:

- Layer 1: **-33.33**
- Layer 2: **-66.66**
- Layer 3: **-100**

Defining the extension of layers 1 and 2:

Even though it would have been more practical to set the layer extensions at a later stage, it is done here for didactic purposes.

To expose layer 2 and layer 3 where they should outcrop, proceed as follows:

- Select the hydraulic conductivity field.
- Layer 1: select the rows of the lower two-thirds of the domain (rows 51 to 150) and assign them a hydraulic conductivity value of 0.
- Layer 2: select the rows of lower third of the domain (rows 101 to 150) and assign them a hydraulic conductivity of 0.

9.2.2 Defining the river network

Defining the tributary numbers:

Create the new field "**River Tributary Number**" in the *cluster* "River Network, Drains, Lakes" and select layer 1 as the river network is defined in surface layer 1.

Then choose option "**Cells of the entire lateral extension of the model**" (or “All cells of the layer") in the “View” menu, to show all cells of this layer, including the non-aquifer cells that have a hydraulic conductivity of 0.

Then select button  "Create a line (open)" and successively draw the tributaries:

- Tributary 10: from point (x=-2, y=297) to point (x=-2, y=201),
  (from point (col. = 25, row = 2) to point (col. = 25, row = 50).
- Tributary 20: from point (col. = 25, row = 51) to point (col. = 25, row = 100).
- Tributary 30: from point (col. = 25, row = 101) to point (col. = 25, row = 149).
- Tributary 40: from point (col. = 51, row = 1) to point (col. = 26, row = 51).
- Tributary 50: from point (col. = 1, row = 1) to point (col. = 24, row = 51).
- Tributary 60: from point (col. = 51, row = 25) to point (col. = 26, row = 101).

To make this drawing, the easiest is to select beforehand the cells containing the start and end points. They appear in red and it is easy to trace the segment. For each tributary, click on the starting point, double-click on the end point, and watch lines appearing that represent the tributaries. These are successively given the polygon names "Tributary_10", "Tributary_20", etc.

The drawing appears in the graphic layer called "Drawing" in the menu "Polygons management", accessed with button  . This drawing is then saved for later visualization: in the menu "Polygons management", to the right of the "Drawing" polygon, click on the button "Record" that saves the tributary drawings in a file called "Didact_Riv_3D_Rivieres.bln". Before starting, deselect all cells that may have been selected earlier by clicking on button  .

To assign the tributary numbers, use button  "Select cells located on a Line or a Closed Boundary". Click on the drawing of a tributary (or close to the drawing). Start for instance with tributary 10. All cells traversed by this tributary are selected and assigned the value 10.

Carry out the same operation with tributary 20, but the cells of layer 1 that are traversed by this tributary 20 are not selected, as they are not aquifer cells. In fact, it is layer 2 that is exposed in this zone.

It is thus necessary to "Give access to cells outside the (aquifer) domain" by clicking on button  , on the right toolbar. Now select the cells traversed by tributary 20, and proceed in the same manner for tributaries 30 to 60.

Defining reach numbers:

"Reach numbers" are the sequential numbers of river reaches of a tributary. Such numbers must be increasing in each tributary, from upstream to downstream.

Create the new field "**River Reach Numbers**", in the *cluster* "River network, Drains, Lakes" and select layer 1.

To assign the tributary numbers, we use button  "Interpolate or number values along a(n) (open) line”, on the upper toolbar. Click on the drawing of a tributary that is now shown in red. Select "Numbering" then "Numbering increment", i.e. numbering "step". The default incremental

value is 1, but 2 can be chosen as well, for instance if intermediate points have to be added later. Select "Number from the first point" as the coordinates shown on screen are effectively those of the upstream reach (if not, choose “Last point"). Click "OK" and the cells located on the tributary in question are selected and automatically numbered. For instance for tributary 10, the numbers increase two-by-two from 1 to 97. Successively repeat the same operation for all tributaries.

Don’t forget to regularly save the work!

Defining the branching tree of tributaries:

The branching of the tributaries is defined by the "Branching tree of river tributaries". For each tributary, the unique number of its downstream tributary is given. When there is no ‘downstream’ as the reach is an outlet, the ‘downstream tributary’ by convention is given the number "0".

To create the branching tree, use button 

to access the "Non-meshed parameters" menu. Then select "Branching tree of river tributaries" (Figure 136).

Click on "Preprocessor" and then "Create a new file "Tree of Rivers/Lakes Tributaries". Then define the downstream numbers of the six tributaries (Figure 137).

Save this file under the name "Didact_Riv_3D.arb_r"

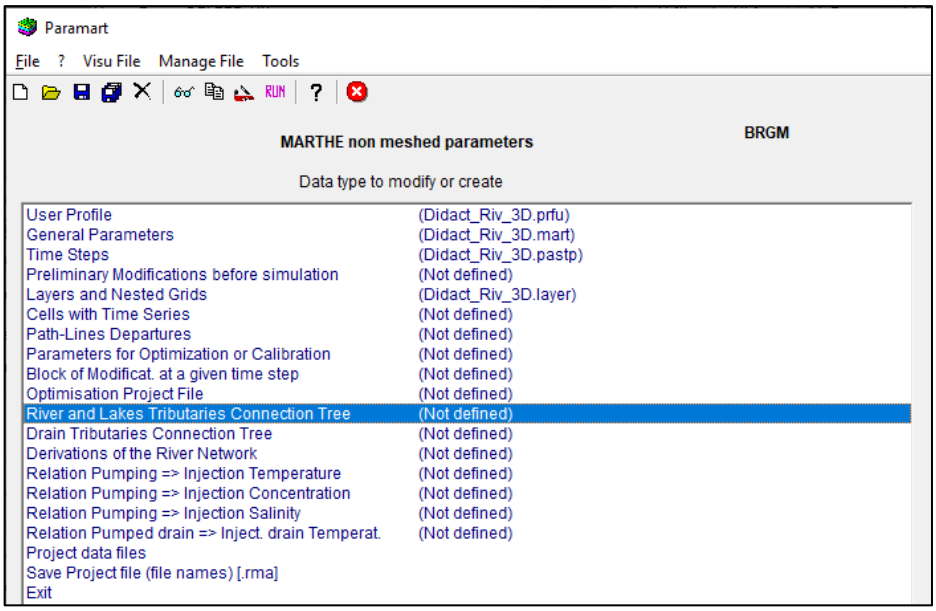


Figure 136 – Creation of a “Branching tree of river tributaries” file.

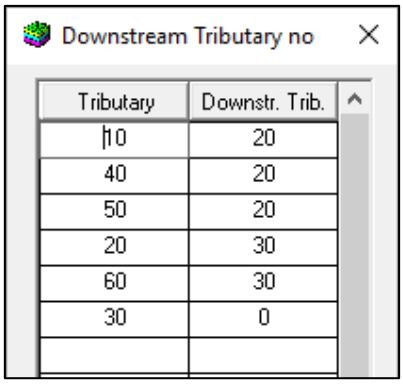


Figure 137 – Definition of the Branching Tree of river tributaries.

Defining the user profile.

As, after a first steady-state simulation, there will later be transient-state and mass-transport simulations, the "User profile" is defined by giving the value "1" to the following options:

- 1 = Transient state.
- 1 = Standard mass transport.
- 1 = Rivers, Drains, Lakes (1=Rivers and Lakes; 2=Drains; 3=All three).

Save this profile as "Didact_Riv_3D.prfu" and return to WinMarthe *sensu stricto*.

9.2.3 Definition of the other fields

Defining "Soil Zone numbers":

"Soil Zones" are zones wherein the hydro-climatic parameters ("soil capacity", "1/2 percolation duration", etc.) are uniform. In a Single Field case, a Soil Zone can be used for introducing rainfall or infiltration flux. We saw in our example that zone number 5 must be assigned to rows 1 to 50, number 10 to rows 51 to 100, and number 15 to rows 101 to 150.

In WinMarthe, create the new field "**Soil Zone number**" and select layer 1 as soil data, like topographic or river-network data, are defined in the surface layer, i.e. layer 1.

Verify that the option "***Cells of the entire lateral extension of the model***" is selected in the menu "View", and that button "**Access to cells outside of the (aquifer) domain**" is activated.

Then select the rows 1 to 50 with the elastic rectangle, and assign the value 5 to the selected cells. Assign in the same way value 10 to rows 51 at 100 and value 15 to rows 101 to 150.

Defining "Overflow Index":

Exposed cells can all overflow, as there is no impermeable cover over the aquifer. All of layer 1 must therefore be assigned an "Overflow Index".

Create the new field "**Overflow Index**" and select layer 1 as overflow-index data, like those of the topography or the river network, are defined in the surface layer, or layer 1.

Verify that button "**Give access to cells outside the (aquifer) domain**" is activated. Then select all cells of this layer by clicking button  of "Selection by layer", and by double-clicking in a spot of the layer. All cells are selected => Assign them value 1.

Defining "Geometric Zones":

To easily assign hydraulic conductivity values, define the same numbers for "Geometric Zones" as the aquifer grid-layer numbers. To this end, create the new field "Geometric Zones".

Remove "**Access to cells outside the (aquifer) domain**" by clicking on the corresponding button. Now select the cells of layer 1 with button  , and assign them the value 1, then the cells of layer 2 that are assigned the value 2, and finally the cells of layer 3 that get the value 3.

Defining cells with imposed hydraulic head:

The hydraulic head is imposed at 0 metres in the farthest downstream cell, i.e. in the third layer, at coordinate point x = -2 km, y = +1 km. Select the field "Discharge, Aquifer flow" and choose the option "Go to x/y/layer" in the menu "Tools". Set the coordinates x = -2, y = 1 and layer = 3, and arrive at the corresponding cell in which a flow value of 9999 is set for imposing the hydraulic head.

9.2.4 Simulation in the steady state without a Stage-Discharge relation

Project: ***Didact_Riv_3D.rma***

Start a simulation in the steady state, first with constant water heights in the river, ***without*** a relation between the water level in the river and its flow. For this steady state, consider an infiltration equal to 20 mm/month (or 240 mm/year).

Defining the General Parameters.

Use button 

for access to the "Non-meshed parameters" menu. Select "General Parameters" and create a new file.

Paragraph: **Control Aquifer Hydraulic solving process**

```
     0 = Maxi number of iterations for time steps after time step #°0 (transient)
    50 = Maxi number of hydraulic iterat. for time step n°0 (Initial Steady State)
    20 = Maximal number of internal iterations in the solver [Def=10]
Steady = Hydraulic flow Regime [0=Transient state ; 1=Steady state]
```

Paragraph: **Data Units**

```
       = Hydroclimatic (Rainfall, PET, Infiltration, Recharge) Height unit in mm
Month  = Duration unit for hydroclimatic data (second, hour, day,month, year, etc.)
   km  = Grid horizontal coordinate unit in m
       = River Flow unit (Def = General 'Flow and Yield' unit)
```

Paragraph: **River network, Drains, Lakes**

```
    1 = Coupling with a River Network [0=No ; 1=Yes]
   15 = Maximum number of iterations for River flow calculation
```

The uniform fields, whether by zone or by tributary, are simply defined by the preprocessor in the paragraph "Initialization before simulation":

- Aquifer hydraulic conductivity: 10^{-4} m/s in zones 1 to 3, i.e. in the aquifer cells of layers 1 to 3.
- Length of river reach = 2 km in the entire domain. (This poses no problem in defining lengths where there are no rivers; such data are ignored).
- Widths of river reaches of 50 m in the tributaries 10, 40, 50 and 60, and widths of 100 m in the reaches 20 and 30. Attention: the widths, like the lengths, are in horizontal cell-coordinate units, here 0.05 and 0.1 km, respectively.
- Absolute height of the water in the river reaches: 4 metres in all reaches ("T = *****") of tributaries 1 to 60 "A = 1:60").
- Absolute elevation of the river bottom: 0 m in all reaches.
- Thickness of the bed: 0.1 metre in all reaches.

- Hydraulic conductivity of the bed and the banks of the river: 10^{-6} m/s in all reaches.

  Paragraph: "**Initialization before simulation"**:

```
/PERMEAB/GEOM_ZONE        Z=  1:3  V=      1e-4;
/RIVER_LENGTH/GRID        N: =2
/RIVER_WIDTH/TRIBUTAR     A=     10T=      *V=      5e-2;
/RIVER_WIDTH/TRIBUTAR     A=     40T=      *V=      5e-2;
/RIVER_WIDTH/TRIBUTAR     A=     50T=      *V=      5e-2;
/RIVER_WIDTH/TRIBUTAR     A=     60T=      *V=      5e-2;
/RIVER_WIDTH/TRIBUTAR     A=     20T=      *V=       0.1;
/RIVER_WIDTH/TRIBUTAR     A=     30T=      *V=       0.1;
/RIVER_STAGE/TRIBUTAR     A=  1:60 T=      *V=         4;
/RIVER_BOTTOM/TRIBUTAR    A=  1:60 T=      *V=         0;
/RIV_BED_THICK/GRID       N: =0.1
/RIV_BED_PERM /GRID       N: =1e-6
```

Defining infiltration flux and fields to be saved

After saving the "General Parameters" file, select the line "Time Steps" and create a new file. With the preprocessor define only time step 0 in the steady state.

In the "Time steps" file, define an infiltration flux of 20 mm/month in <u>all</u> "Climatic zones". (***** = Zone number). The flux is in mm/month as, in the paragraph "Data Units" of the "General Parameters" file, the unit of hydro-climatic heights is by default in mm, and the unit of hydro-climatic duration was set at "Month".

The "Climatic zones" are by default "Soil zones", as in the paragraph "Hydroclimatology" of the "General Parameters" file we left by default the value at 0:

"**0 = Type of Zones for Rain, PET, Recharge etc. [0=Soil Zones ; 1=Meteo Zones]** ".

At the end of the simulation request the output of:

- The field of the simulated hydraulic head,
- The field of aquifer flow at the boundaries,
- The field of river flow.

```
*** Beginning of simulation  at date    :         0; ***
  /INFILTR_FLUX/CLIM_ZONE  Z=      *V=        20;
  /HYDR_HEAD/OUTPUT        I= 1;
  /Q_OVERFLOW/OUTPUT       I= 1;
  /BOUNDARY_FLOW/OUTPUT    I= 1;
  /RIVER_FLOW/OUTPUT       I= 1;L= 0;F= 0;B= 0;
  /*****/***** End of this Time Step
 ***        :     : End of simulation    :            ; ***
```

Running the simulation

Now launch the simulation that finishes in a few seconds.

The river network is described in the "*riv_drains_lakes_network.txt*" file, which contains more details if one requests the “Detailed listing” and "Listing of all cells data read" in the “General parameters”. This is the file that must be checked for errors in the river network.

Results of the steady state simulation at a fixed water level in the river

The “flow balance.txt” file shows that the simulation has perfectly converged.

The aquifer flow balance (in flow units, here in m^3/s):

```
- Balance in Flow unit: Time step    Nb 0 - t= 0.000 -------------

 Outflow in Prescribed Heads    =                   -0.6816
 Recharge/Evaporation flow      =    232.717
 Overflow or Seepage            =                   -85.120
 Flow River -> Aquifer          =      0.000       -146.916 (   -146.916 )
 ---------------------------------------------------------------------

 hence internal converg. within :  3.098E-06 %   of error
```

The recharge is equal to 232.7 m^3/s (77.6 m^3/s for each layer), 85.1 m^3/s of which is overflow and runoff to the river network and 146.9 m^3/s of which are drained by the rivers. The rest of 0.7 m^3/s flows downstream of the groundwater, through the cell with imposed hydraulic head.

The river network flow balance (in flow units):

```
                   ========================================================
                    River network flow balance: Lumped balance
                   ========================================================
   Balance in flow unit                    : Time step    Nb 0 - t= 0.000
                               Inflow         Outflow         Net
 Aquifer Exchange          =    146.916          0.000         146.916
 Aquifer Overflow          =     85.120
(Residual Flow             =  3.973E-08     -5.563E-06     -5.523E-06 )
 Outlet(s)                 =                  -232.036
 ---------------------------------------------------------------------
 deviation in Lumped Balance =  5.523E-06    (Input/output balance)
```

9.2.5 Simulation with consideration of drainage directions

Project: ***Didact_Riv_3D_Dir_Aval.rma***

For precisely directing runoff flow to the rivers, one needs the "Drainage Directions", or the “Downstream Direction for Runoff". The rivers flows will then be simulated more precisely, respecting the surface extensions of the catchment areas.

The "Downstream Direction" of each cell is defined by a number. The simplest manner to define it is with a number from 1001 to 1008: 1001 to 1004 = north, east, south, west (clockwise); 1005 to 1008 = NE, SE, SW, NW (clockwise).

The "Downstream Directions" are defined in the surface layer, i.e. in layer 1.

A steady-state simulation, without Stage-Discharge relation and without mass transport, is run. The modifications to be made to project "Didact_Riv_3D.rma" are the following:

- As no downstream directions file is available for this theoretical example, a simplified one is created in the paragraph "Initialization before simulation”. Give the direction south-east, or 1006, to all cells of the western part of the domain, in columns 1 to 24 of all rows, and the direction south-west, or 1007, to the cells of the eastern part of the domain, in columns 26 to 51 of all rows. In the next to last row, row 149, set the direction east (or 1002) to the columns of the western part (columns 1 to 24), and set the direction west (or 1004) to the columns of the eastern part (columns 26 to 51).
- To produce runoff: define in each soil zone:
  - A height of ‘equi’-runoff equal to 1 (mm)
  - A half-percolation time equal to 5 (months)

The lines added to paragraph: "**Initialization before simulation**" are:

```
/DOWNSTR_DIREC/CELL  C=  1:24 R=   *L=   1V=      1006;
/DOWNSTR_DIREC/CELL  C= 26:51 R=   *L=   1V=      1007;
/DOWNSTR_DIREC/CELL  C=  1:24 R= 149L=   1V=      1002;
/DOWNSTR_DIREC/CELL  C= 26:51 R= 149L=   1V=      1004;
/EQU_RUNO_PERC/SOIL_ZONE Z=  *V=   1;
/PERCOL_HALF_T/SOIL_ZONE Z=  *V=   5;
```

The simulation thus obtained is locally rather different from that which would have been obtained if no “Downstream Directions” would have been defined. In the absence of "Downstream Directions" the runoff flow in a cell is automatically directed towards the nearest river reach, without considering the slope effects of the topography.

10 Principles of groundwater recharge and runoff calculations

At each model time step, a groundwater recharge flux and a runoff flux can be introduced at the surface of the domain, or directly calculated from climate data.

In the simplest case we can directly introduce:

- A (calculated) recharge flux;
- A runoff flux.

10.1 PRINCIPLE OF THE HYDRO-CLIMATIC BALANCE BY ZONES

In most MARTHE applications, the calculation of recharge and runoff is based on:

- Climatic data:
  - The flux of liquid atmospheric precipitation,
  - The flux of snowy precipitation (snowfall),
  - The flux of Potential Evapotranspiration (PET)
  - The air temperature (if snowmelt is considered).
- Parameters of the hydro-climatic balance:
  - A retention capacity of the soil that may be a “progressive soil reserve" or a "maximum soil deficit" of the “useful reserve” type,
  - A parameter for distributing the rain surplus in runoff and infiltration,
  - The half-percolation infiltration time toward groundwater => Groundwater recharge.

Generally, this recharge is not calculated on a cell basis in the domain extension, and we proceed as follows:

- Define "Meteorological zones" in which the climatic data (rain, PET, etc.) are uniform. Such Meteorological zones are generally selected on the basis of:
  - The local climate that depends on the relief, the distance to the sea, etc.;
  - The availability of climatic data.

- Define "Soil zones" in which the hydro-climatic balance parameters are uniform. Such Soil zones (should) depend upon:
  - The soil type,
  - Land use, crops and vegetation,
  - The average slope angle,
  - etc.

The "Meteorological zones" and the "Soil zones" are only defined in the cells of layer 0. They can be defined in zones where there are no aquifers, mountain slopes or impermeable zones.

All surface cells in the same "Meteorological zones" and the same "Soil zone" will thus have the same hydro-climatic balance, which considerably decreases the number of calculated balances. For instance, with 10 Meteorological zones and 7 Soil zones, there are at most 70 climatic balances to calculate, even if there are 500,000 active cells.

N.B.: If we use "Meteorological zones", the meteorological data will be considered only in the cells for which a "Soil zone" was defined (i.e. a number of "Soil zones" different from 0).

In the simplest cases, we can opt for defining the climatic data (rain and PET flux, air temperature) by "Soil zone" rather than by "Meteo zone". This, however, is *not recommended* for regional

models, as climatic data and parameters of the hydro-climatic balance generally do not have the same spatialization.

In small domains, or in the absence of precise data, we can adopt a uniform value for recharge and runoff over the entire domain.

10.2 THE FATE OF RECHARGE, RUNOFF AND OVERFLOW

10.2.1 The fate of recharge

Recharge (or infiltration) flows into the groundwater, whether the cell is flooded or dewatered. However, if the hydro-climatic balance produces recharge in a non-aquifer cell (with zero or 9999 hydraulic conductivity) => this recharge is converted into runoff and transferred to the drainage network.

10.2.2 The fate of runoff

Where a river network exists, the runoff occurring during a model time step generally is transferred to this network during the same time step (without propagation time on the soil surface). It is directed to the river reach downstream of the cell. Based on the available data, the downstream tributary reach is defined by the software:

- By using the surface downstream-flow directions, which may have been calculated from precise data of the elevation field of the topographic surface.
- Or as the closest river reach, if no surface downstream-flow directions are available.

The runoff is *not* transferred to a drain network.

If there is *no* river network, the runoff is transferred to groundwater, as if it were recharge.

10.2.3 The fate of groundwater overflow

In case there is a river network, if the groundwater overflows in a point outside the network, the overflow is transferred to the downstream tributary reach, like runoff (see above).

Specific case: If the overflow index of the cell is equal to 99 (instead of being 1), the overflow is not directed to the river network, but exits the hydrosystem.

If there is no river network, the overflow exits the hydrosystem.

10.2.4 Evaporation applied to the grid domain

When the maximum deficit of the soil is reached and when PET exceeds rainfall, a complementary evaporation applied to the grid domain is calculated by default, but there are several options to limit or suppress this complementary evaporation.

When a standard aquifer system is modelled with a hydro-climatic balance and a soil capacity, it is strongly recommended to suppress this evaporation applied to the grid domain.

Please note that, in the case of mass transport, the evaporation applied to the grid domain only removes water and no solutes, and, logically, can lead to (over-) concentration of pollutants.

10.3 THE GARDENIA HYDRO-CLIMATIC BALANCE

The Rain—Evapotranspiration hydro-climatic balance is mostly carried out with the **GARDENIA** module (Thiéry, 2009b, 2010a, 2014b, 2015a). The results of this balance are identical in all cells of the domain belonging to the same "Meteo zone" and the same "Soil zone".

10.3.1 Principle of the GARDENIA module

For a detailed description, please consult BRGM/RP-62797-FR (Thiéry, 2014b), and BRGM/RP-64500-FR (Thiéry, 2015e) for validation of the GARDENIA scheme.

The standard GARDENIA module (Figure 138) calls upon three compartments (reservoirs):

- A "soil" compartment: (the "superficial" RU reservoir submitted to evapotranspiration.
- An intermediate compartment (or Unsaturated Zone): The H reservoir (H for Hypodermic) that produces runoff.
- An underground compartment: The G reservoir, corresponding to groundwater.

When the GARDENIA module is coupled to an aquifer system, there is no underground compartment in GARDENIA as this compartment is replaced by MARTHE's aquifer cells (Figure 139).

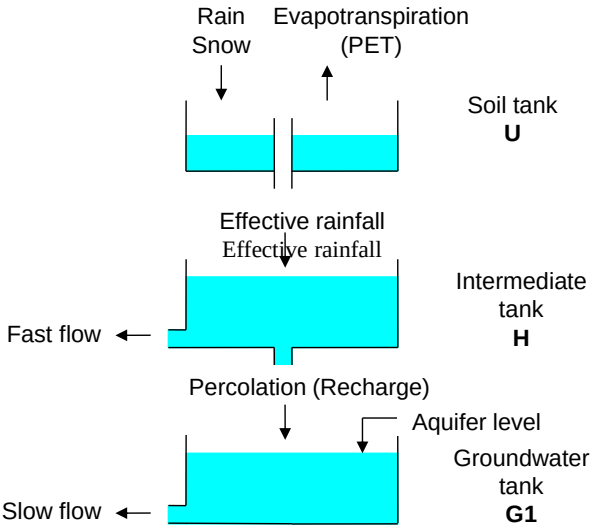


Figure 138 – Complete GARDENIA hydro-climatic balance scheme.

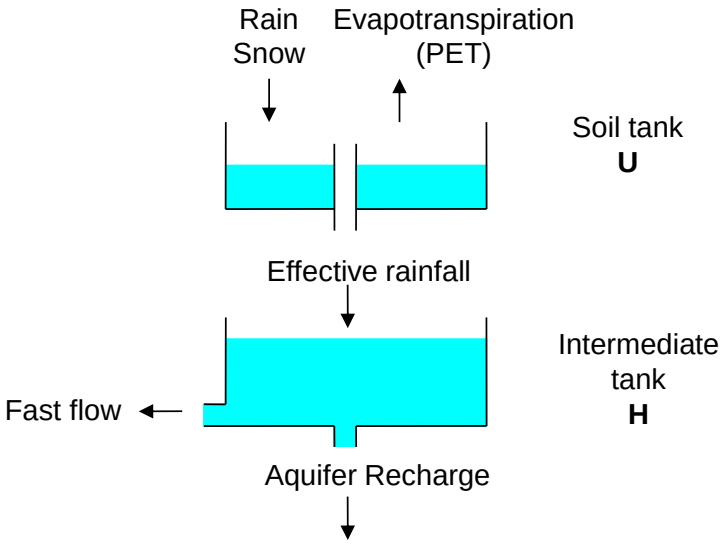


Figure 139 – GARDENIA hydro-climatic balance module integrated in MARTHE.

The GARDENIA module coupled to MARTHE simulates the water cycle with a two-reservoir system representing respectively:

- The first tens of centimetres of the soil in which evapotranspiration occurs (zone of root influence);
- An intermediate reservoir that produces rapid flow.

The first reservoir ensures the "production" function: it determines the evaporated part (AET = Actual Evapo-Transpiration) and the "Net Rainfall" (or "Effective Rainfall"). The "Net Rainfall" is the part of atmospheric precipitation remaining after the action of evapotranspiration.

The second reservoir ensures the "transfer" function by distributing the "Net Rainfall" into runoff and recharge, and by considering the time of percolation down to the groundwater.

10.3.2 The stock in the near-surface reservoir

The near-surface reservoir, or "soil reservoir", represents the first tens of centimetres of soil that undergo the action of vegetation roots and of evaporation (Figure 140).

The "Production" function exists only in the near-surface reservoir. The capacity of this reservoir is the "available reserve for evapotranspiration" or the "retention capacity", not counting fixed water. It also integrates the capacity of interception by the aerial part of the vegetation, as well as the water volumes in potential surface depressions (puddles, furrows, etc.).

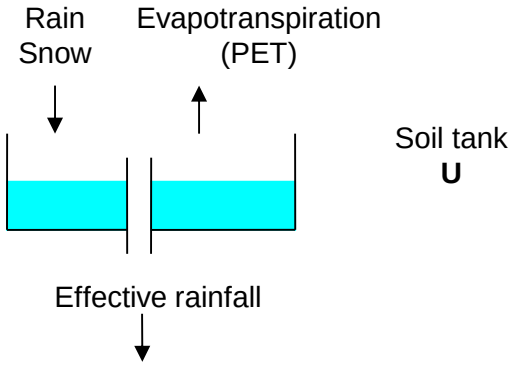


Figure 140 - The GARDENIA near-surface reservoir.

Two types of near-surface reservoirs are possible:

- A "progressive soil reservoir", with quadratic laws in terms of the saturation rate of the reservoir: This is the recommended scheme.
- A Thornthwaite type soil reservoir, that function in an “all-or-nothing” manner.

The soil reservoir is fed by rain (and snowmelt in winter). It is subject to PET (Potential Evapo-Transpiration) and allows calculating the actual evapotranspiration AET and the "Net Rainfall" (Figure 141).

"Progressive" soil reservoir:

Satur = Filling of the reservoir / Capacity of the reservoir:

- If rainfall exceeds PET:
  Net Rainfall = (rainfall - PET) x $Satur^2$
- If PET exceeds rainfall:
  AET = (PET - rainfall) x Satur x (2 - Satur).

Soil reservoir of "all-or-nothing" type (Thornthwaite type):

- If rainfall exceeds PET:
  Net Rainfall = 0 if the reservoir is not full,
  Net Rainfall = Rainfall – PET when the soil reservoir is full.
- If PET exceeds rainfall:
  AET = (PET – rainfall) if the soil reservoir is not totally empty,
  AET = 0 when the soil reservoir is empty. Net Rainfall = 0

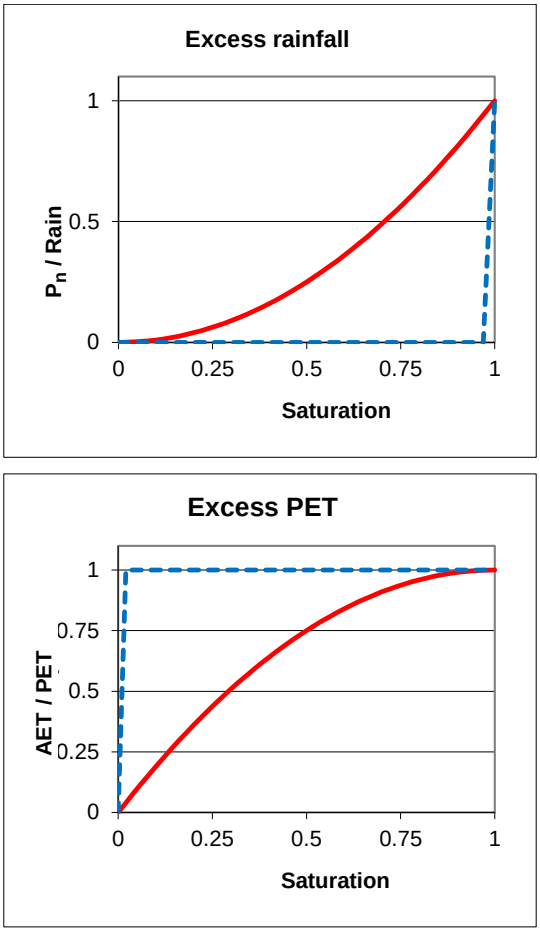


Figure 141 – Net Precipitation Pn and real evapotranspiration RET in the soil reservoir.
Dashed blue line: reservoir of the "all-or-nothing" type; in red: "progressive reservoir".

It is possible to associate in series: a soil reservoir of the Thornthwaite type and a "progressive" soil reservoir, but in practice this generally does not lead to a better simulation.

10.3.3 The intermediate reservoir H

Reservoir H (Figure 142) represents the Unsaturated Zone. The water height it contains at a given moment is noted H. It is fed by "Net Rainfall" water coming from the near-surface reservoir, and it is emptied by two components:

- Percolation towards groundwater following a linear law (exponential draining) of a temporal constant THG:

$$ALIMG = H \cdot dt / THG \qquad (dt = \text{duration of time step})$$

- Runoff QH, following a non-linear law controlled by the RUIPER parameter; this parameter (RUIPER for "Runoff-PERcolation") is the water height in reservoir H, for which the percolation ALIMG is equal to runoff QH:

$$QH = H \cdot dt / (THG \,.\, RUIPER / H)$$

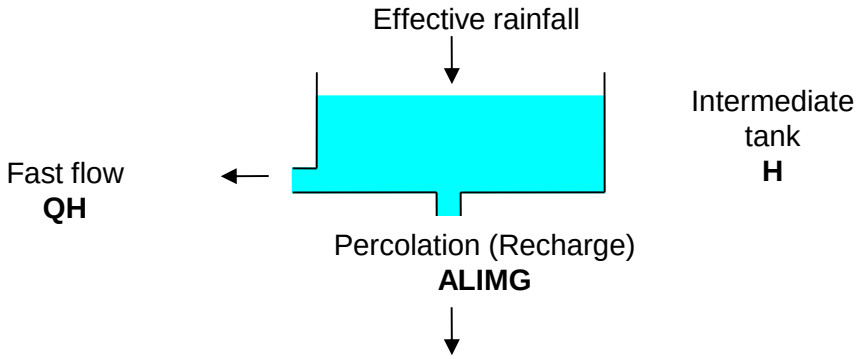


Figure 142 - Scheme of the intermediate GARDENIA reservoir H.

Runoff QH predominates when reservoir H has a high filling ratio. However, the percolation ALIMG predominates when the reservoir H has a low filling ratio. The ratio QH / ALIMG is equal to the H / RUIPER ratio. The functioning of reservoir H thus resembles that of a progressive overflow sill at an average RUIPER height, but with a more realistic representation of the flow, in two components that are not mutually exclusive.

(If the RUIPER parameter is assigned a code value of 9999 mm, there will be *no* runoff).

Reservoir H only serves for transferring water. It determines the distribution of net rainfall, coming from the near-surface reservoir, into runoff and recharge.

10.4 EXAMPLE 11: SIMPLE HYDROSYSTEM WITH THE GARDENIA HYDRO-CLIMATIC SCHEME, ANALYSIS OF SIMULATION DIFFERENCES

This example is project: ***Didact_Chennetr.rma***.

This example shows how to simulate a hydrosystem whose variations over time are conditioned by the hydro-climatic processes in its catchment area. The modelled hydrosystem is a simplification of a real catchment area. A river, the Voulzie at Jutigny, drains a catchment area of 280 km^2 near the town of Provins in France. The Saint Martin-Chennetron observation well, located in the Champigny Limestone aquifer, shows the changes in groundwater level at a point of the basin. We model the domain as a single layer aquifer, traversed from north to south by a straight river (Figure 143).

Runoff and infiltration are calculated by MARTHE by means of a water balance made with the GARDENIA algorithm (Thiéry, 2013, 2014, 2015e). This software is described in the report BRGM/RP-62797-FR and validated in the report BRGM/RP-64500-FR

Example 11 also shows how to use an "**Observations time Series**" [.obs_his] file for **analysing simulation discrepancies**, and for easy comparison between observed and simulated time series. The functionality of "Analysing simulation discrepancies" is described in report BRGM/RP-69210-FR (Thiéry, 2020c).

The following hydro-climatic data are available:

- The average monthly rainfall on the basin in mm/month, from 1962 to 2004. This is a uniform water surface over the basin, calculated by arithmetic weighting of data from surrounding weather stations.
- The potential evapotranspiration (PET) at Melun from 1962 to 2004, in mm/month.

- The values of average monthly flow in the Voulzie at Jutigny, in m^3/s from 1974 to 2004.
- The monthly water-level records in the well at St Martin-Chennetron, in m NGF, from 1973 to 2004, read around each 15th of the month.

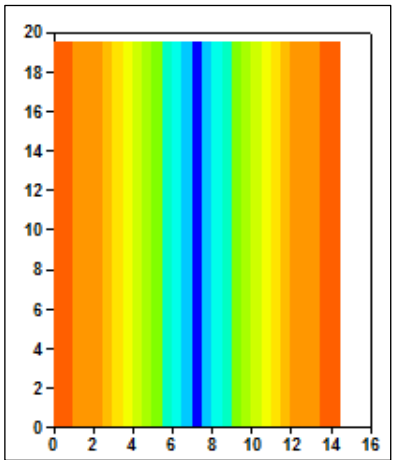


Figure 143 – Geometry of the hydrosystem,
with a river oriented north-south in the middle of the domain.

The characteristics of the system are as follows:

Geometry:

- The domain is a rectangle of 14.5 km east-west by 19.5 km north-south, or 282.75 km^2.
- A regular grid is selected, with 29 columns of 0.5 km width and 39 rows of 0.5 km width. The origin of the grid is located at coordinate point (0, 0)
- The topographic elevation is arbitrarily set at +200 m NGF.
- The bottom is set at an elevation 0 m NGF.

Boundary conditions:

- No imposed hydraulic head.

Hydraulic parameters:

- Aquifer hydraulic conductivity = 4.594 10^{-5} m/s
- Specific yield coefficient = 1.07 %

River network: The drainage consists of a single north-south oriented tributary in the middle of the domain (at abscissa 7.25 km). To simplify, we consider that its bed is horizontal, like the elevation of the free water surface.

- Width of the river = 0.015 km (or 15 m).
- Length of the river reaches = 0.5 km (in each concerned cell).
- Elevation of the river bottom = 107 m NGF.
- Water elevation in the river = 107.62 m NGF.
- Thickness of the riverbed and the banks = 0.1 m
- Riverbed and banks Hydraulic conductivity = 10^{-6} m/s

Parameters of the hydro-climatic balance: The following parameters are set in the domain:

- Progressive capacity of the reservoir soil = 103 mm
- Equi-runoff height = 405 mm
- Half-percolation time = 4.4 months

10.4.1 Creation of the grid

Project title: **Didact_Chennetr;**

- Southwest angle: X = **0;** Y = **0** (km)
- Northeast angle: X = **14.5;** Y = **19.5** (km)
- Column width **0.5;** Row width = **0.5** (km)
- Number of layers **1;**
- Default hydraulic conductivity value **1** (true value is defined later);
- Topographic elevation = **200** (m);
- Thickness (of each layer) = **200** (m).

10.4.2 Definition of the user profile

As the simulation will be in transient mode, with a drainage network and a hydro-climatic balance, a "user profile" is defined by giving the value "1" to the following options:

- 1 = Transient state;
- 1 = Rivers, Drains, Lakes (1=Rivers and Lakes ; 2=Drains ; 3=all three);
- 1 = Hydroclimatology, Crops, Nitrate.

Save this user profile under the name "Didact_Chennetr.prfu" and return to WinMarthe *sensu stricto*.

10.4.3 Definition of other fields

As the domain is very simple, all grid-data fields are defined in the "Initialization before simulation" at the end of the parameters file [.mart].

Defining "Soil Zones"

"Soil Zones" are zones with uniform hydrologic parameters ("Soil capacity", "Percolation time", etc.). In this simple example, we also use "Soil Zones" for introducing rainfall and PET (potential evapotranspiration) data. In fact, we define a single zone number equal to 1 for the whole domain. There will thus be a single soil zone.

Defining the Branching Tree of Tributaries

As there is only one river, there is no branching, and no "Drain tributaries connection tree" file will have to be defined.

Defining General Parameters

Press the button 

, to open the "Non-meshed parameters" menu, select "General Parameters" and create a new file.

Paragraph: **Outputs and Controls**

```
Flux = Output Time-Series of Hydroclimatic Balance (0=No ; 1=Flux ; 2=Flow)
   0 = Output of full calendar dates (0=dd/mm/yyyy ; -1=dd/mm/yyyy hh:mm)
       [Hence by default calendar dates are in the form: jj/mm/aaaa, without hh:mm]
       [Note that the form: aaaa/mm/dd is not supported]
```

Paragraph: **Control of Aquifer Hydraulic solving process**

```
      20 = Maxi number of iterations for time steps after time step #°0 (transient)
      20 = Maxi number of hydraulic iterat. for time step n°0 (Initial Steady State)
Transient = Hydraulic flow Regime [0=Transient state ; 1=Steady state]
```

Paragraph: **Data units**

```
  1e-6 = Aquifer Hydraulic conductivity unit in m/s (or m2)
       = Hydroclimatic (Rainfall, PET, Infiltration, Recharge) Height unit in mm
Month = Duration unit for hydroclimatic data (hour, day, month, year, etc.)
  Day = Time unit (for model time steps) (minute, hour, day, month, year, etc.)
   km = Grid horizontal coordinate unit in m
      = River Flow unit (Def = General 'Flow and Yield' unit)
```

N.B.: Even though the simulation will use a time step of 1 month, we select a "*Time Unit (for model time steps)*" in "Days" as we will use in the "*Time steps*" file calendar dates in days as "dd/mm/yyyy". However, this is not a critical choice, as the resulting time series are given in calendar dates.

Paragraph: **Optimization / Automatic calibration / Sensitivity analysis**

```
    1 = Analysis of simulation discrepancies [0=No ; 1=Yes]
```

Paragraph: **River network, Drains, Lakes**

```
    1 = Coupling with a River Network [0=No ; 1=Yes]
```

Paragraph: **Hydroclimatology**

```
    2 = Limitation of evaporation from the gridded domain
        [0=No ; 1=Limitation ; 2=Cancelation]
           [Important: 2 => No evaporation applied directly to the gridded domain]
    0 = Hydroclimatic balance [0=GARDENIA]
        [Hence, by default, selection of a Gardenia hydro-climatic balance]
    0 = Type of Zones for Rain, PET, Recharge etc. [0=Soil Zones ; 1=Meteo Zones]
```

With the pre-processor, it will be easy to define the uniform fields, generally by zone or by tributary, in paragraph "Initialization before simulation":

- Aquifer hydraulic conductivity is 4.594 10^{-5} m/s, or 45.94 as a hydraulic conductivity unit of 10^{-6} m/s was selected.
- Specific yield is 1.07 10^{-2} (or 1.07%).
- Head for initializing the simulation is 109 m NGF.
- Definition of the river network:
  - Tributary **1**, in column **15**, for all rows (note "*****").
  - Reach number = row number, or shortcut "**-2**", in column **15** and for all rows (note "*****").

    N.B. It was possible to use the row number as reach number because the row number increases from upstream to downstream along the tributary.
- Length of the river reach is **0.5** km in the entire domain. (There is no problem when such lengths are defined in cells without rivers, as these data will be ignored by MARTHE).
- Width of river reach is 15 m.

  N.B.: The river widths, like reaches lengths, are “horizontal cell coordinate units”, here in km. This gives a width of 0.015 km and a length of 0.5 km.
- Absolute water elevation in the river reaches is 107.62 metres NGF in all reaches.
- Absolute elevation of the river bottom is 107 m in all reaches.
- Thickness of the bed is 0.1 metre in all reaches.
- Hydraulic conductivity of bed and banks of the river is 10^{-6} m/s in all reaches.
- "Soil Zone" number is 1 for all cells of the domain.
- Parameters of the GARDENIA hydro-climatic balance:
  - Progressive soil tank capacity: 103 mm, in soil zone 1.

- Equi-runoff height: 405 mm in soil zone 1.
- Half-percolation time: 4.4 months in soil zone 1 (in months, as this is the unit chosen for hydro-climatic duration.)

Paragraph: **Initialization before simulation**

```
/PERMEAB/GRID              N: =45.94
/UNCONF_STORAG/GRID        N: =1.07e-2
/TOPOGR_ELEV/GRID          N: =200
/SUBSTRATUM/GRID           N: =0
/HYDR_HEAD/GRID            N: =109
/RIVER_TRIB/CELL           C=  15R=    *L=    1V=     1;
/RIVER_REACH/CELL          C=  15R=    *L=    1V=    -2;
/RIV_BED_THICK/GRID        N: =0.1
/RIV_BED_PERM/GRID         N: =1
/RIVER_WIDTH/GRID          N: =0.015
/RIVER_LENGTH/GRID         N: =0.5
/RIVER_BOTTOM/GRID         N: =107
/RIVER_STAGE/GRID          N: =107.62
/SOIL_ZONE/GRID            N: =1
/PROG_SOIL_CAP/SOIL_ZONE Z=       1V=    103;
/EQU_RUNO_PERC/SOIL_ZONE Z=       1V=    405;
/PERCOL_HALF_T/SOIL_ZONE Z=       1V=    4.4;
```

Save this parameters file as "**Didact_Chennetr.mart**"

Defining time steps

The climatic data are available for each month of the 43 years from January 1962 to April 2004, or 508 months. First, create a text file with these climatic data in two columns: one for the monthly rainfall data and the other for the monthly PET data. In practice, we add a third column with the data for easier reading and formatting. It is recommended to put this third column on the right, so as not to disturb the reading of the data columns. Also, add a descriptive text line (starting for safety with a "#" character to indicate that this line is a comment). The file can be very easily created with Excel ® or an equivalent spreadsheet. The data must be in text format. Therefore, do not create an [.xlsx] file but *export* the data by preference with a “text format, separator = tabulation" (Figure 144).

Name this file "**Didact_Chennetr_Meteo_1962_2004.prn**".

```
# Rain and PET_Melun      Date
    82.4   14.3285       15/01/1962
    34.7   15.474        15/02/1962
    79.2   24.9761       15/03/1962
     …        …              …
    43.4   49.5          15/03/2004
    65.6   75.9          15/04/2004
```

Figure 144 – Hydrosystem with GARDENIA hydro-climatic water balance: Time series file of climatic data (extract).

With the “Non-meshed parameters” module, the button 

, creates a new "Time steps" file. Give the starting date of the simulation in calendar format: "**15/12/1961**" as the first time step will be "15/01/1962" (Figure 145).

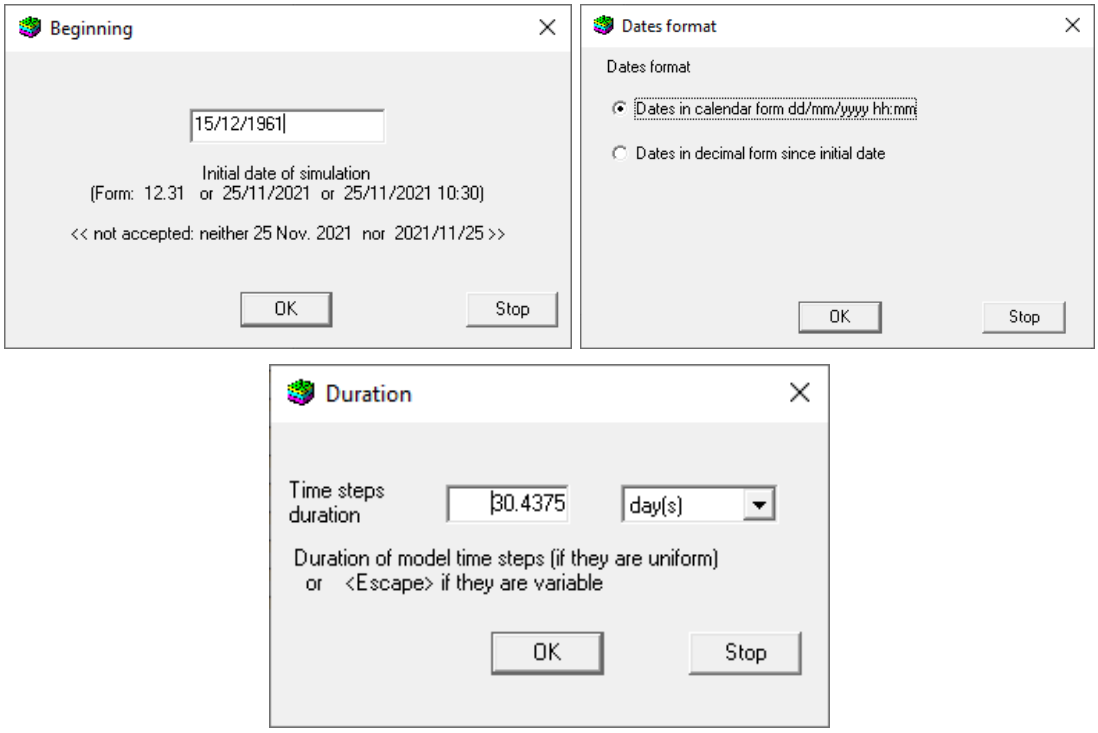


Figure 145 – Hydrosystem with GARDENIA hydro-climatic balance.
Creation of a new time-step file of 1-month duration.

Accept the option to present dates as "**Calendar dd/mm/yyyy hh:mm**" and select Create automatically **508** time steps of duration **30.4375** days, (i.e. 365.25 / 12, the duration of an average month) (Figure 145).

At time step 0, define the rainfall and PET fluxes of all time steps. Select for this: "New Actions" ➔ *Cluster* "Hydro-climatic balance, crops" ➔ *Object* "Precipitations (Rainfall) Flux" (RAIN_FLUX) ➔ *Modified by* "Climatic zones" ZONE_CLIM.

Select soil zone **1** and define an average rainfall flux of **15** mm/month for time step 0. Then define in the window at the bottom the name of the time file containing the 508 values of the monthly time steps from January 1962 to April 2004: "**Didact_Chennetr_Meteo_1962_2004.prn**", and conserve the number **1** proposed for the column of the file to be used for reading these precipitation flux data. Then click on "OK" (Figure 146).

To define the PET flux, click on:

Cluster "Hydro-climatic balance, crops" ➔ *Object* “Potential evapotranspiration (PET) Flux” (PET_FLUX) ➔ *Modification by* "Climatic zone" ZONE_CLIM.

Select soil zone **1** and define a PET flux of **0** mm/month for time step 0; then define in the window at the bottom the name of the time file containing the 508 values of all monthly time steps: "**Didact_Chennetr_Meteo_1962_2004.prn**". Assign number **2** to the column of the file to be used for reading the PET flux data and click "OK" (Figure 147).

Click on "Exit", save the time steps file under the proposed name "**Didact_Chennetr.pastp**" and select as output format for the dates the default one: **"Day: dd/mm/yyyy**" (Figure 148), i.e. in calendar format without hours and minutes, so as to have a more readable file (Figure 149)

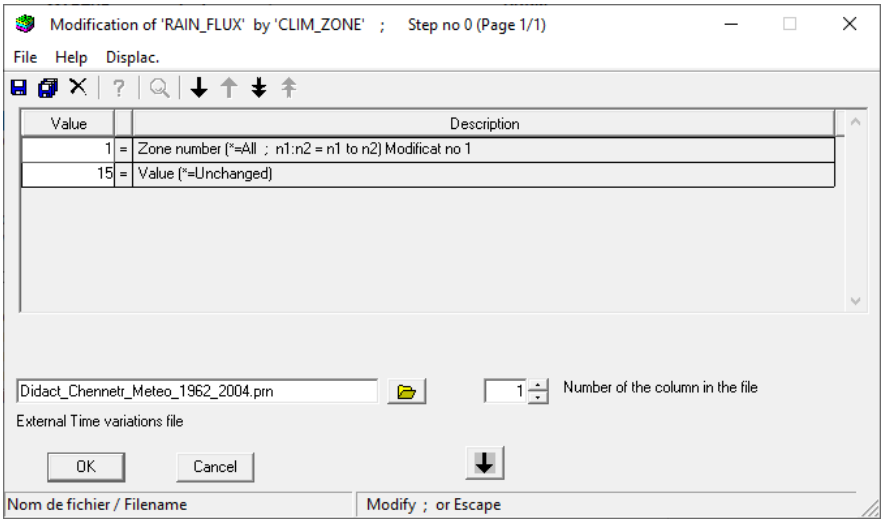


Figure 146 – At time step 0: Definition of rainfall flux with reading of data in column 1 of an external file.

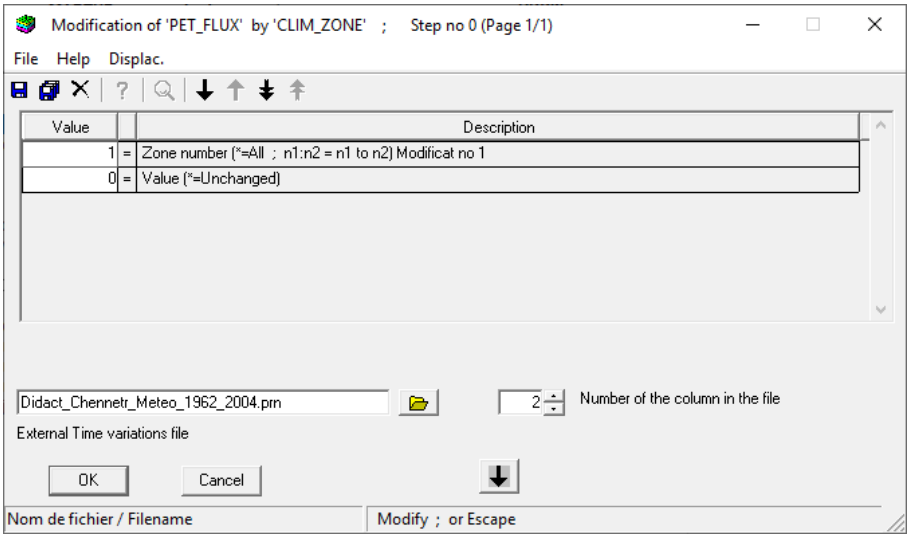


Figure 147 – At time step 0: Definition of the PET flux with reading of data in column 2 of an external file.

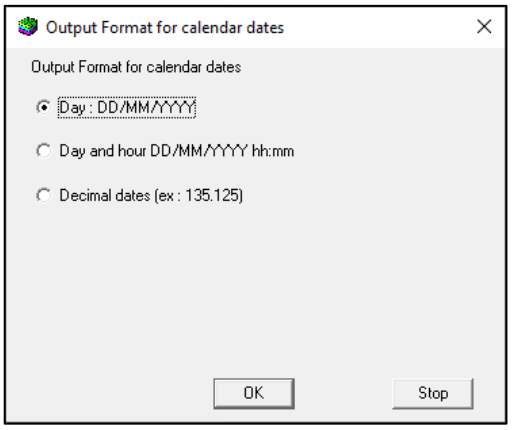


Figure 148 – Definition of the output format for dates in the resulting time steps file.

```
Chennetr 2D : 1962-2004
 #<V7.8># --- End of Header lines --- ; Do not modify/delete this line
 *** Beginning of simulation  at date    : 15/12/1961 ; ***
  /RAIN_FLUX/CLIM_ZONE Z= 1V= 15; File= Didact_Chennetr_Meteo_1962_2004.prn
  /PET_FLUX/CLIM_ZONE  Z= 1V=  0; File= Didact_Chennetr_Meteo_1962_2004.prn; Col=2
  /*****/***** End of this Time Step
 *** Step    :    1:      Ends at date    : 14/01/1962 ; ***
  /*****/***** End of this Time Step
 *** Step    :    2:      Ends at date    : 13/02/1962 ; ***
  /*****/***** End of this Time Step
 *** Step    :    3:      Ends at date    : 16/03/1962 ; ***
  /*****/***** End of this Time Step
    . . .
 *** Step    :  507:      Ends at date    : 15/03/2004 ; ***
  /*****/***** End of this Time Step
 *** Step    :  508:      Ends at date    : 15/04/2004 ; ***
  /*****/***** End of this Time Step
 ***         :     : End of simulation    :            ; ***
```

Figure 149 – Hydrosystem with GARDENIA hydro-climatic balance.
Extract of the resulting time steps file "Didact_Chennetr.pastp".

Defining the "Observations time series" file

This file is created with a spreadsheet from two series of observations. It consists of three columns:

- Column 1: Series of observations of the groundwater level at St Martin Chennetron in monthly time steps from December 1961 to April 2004
- Column 2: Series of observations of flow in the Voulzie at Jutigny in monthly time steps from December 1961 to April 2004
- Column 3: Series of observation dates (*for information; column not used*).

The file has five heading lines, starting with a "#" character, followed by 509 lines, corresponding to time step zero followed by 508 simulation time steps for the period January 1962 to April 2004. The missing values (for instance the levels for the period 1962-1972 and the river flows for the period 1962-1973) are coded by the value 9999.

The file can be very easily created with a spreadsheet, such as Excel ®. The data must be in text format; do ***not*** create an [.xlsx] file, but *export* the data by preference in a "text format, separator = Tabulation". Its recommended file name extension is [.obs_his] and call it "***Didact_Chennetron_Voulzie.obs_his***" (Figure 150).

Click on the button  to bring up the general menu "Marthe non-meshed parameters"; double-click "**Project Files**", at the bottom of the home screen of this module. Go to line "**Observations Time Series**". *To find this line easily, use the search button (magnifying glass) and look for "Observ"*. Once on this line, name it "**Didact_Chennetron_Voulzie.obs_his**". Then click on "Record", confirm, and click on button "Exit".

```
# Observed data: Voulzie River Flow and St Martin Piezom. Level
# Flow           GW_Level      Dates_Mesures
#_Voulzie        St_Martin     Dates_Mesures
#_at_Jutigny     Chennetron    Dates
#_m3/s           m_NGF         For_Info
9999             9999          15/12/1961
9999             9999          14/01/1962
9999             9999          13/02/1962
……               ……            ……
9999             120.6         13/02/1974
1.56             121.35        16/03/1974
1.45             123.55        15/04/1974
……               ……            ……
1.81             131.39        15/03/2004
1.72             131.48        15/04/2004
```

Figure 150 – Extract of the 'Observations Time Series' file "Didact_Chennetron_Voulzie.obs_his".

Defining "Cells with time series"

As in the earlier examples, create a "Cells with time series" [.histo] with the "Non-meshed parameters" pre-processor. Now request:

- A "**H_Head**" (Hydraulic Head) time series in the cell of column 27 and row 8 of the Martin Chennetron observation well in our simplified example.
  - Associate it with **column 2** of the "Observations Time Series" file (Figure 151).
- A "**River_flow**" time series in the cell of column 15 and row 29 that corresponds to the basin outlet.
  - Associate it with **column 1** of the "Observations Time Series" file.
- A time series of "**Runoff flux**", of "**Infiltration flux**" and of the "**Progressive soil reservoir deficit**". Request the time series for a cell located in soil zone 1, i.e. any cell of the domain, for instance in the cell of column 10 and row 10.
  - For these time series, do not associate a column of the "Observations Time Series" file.

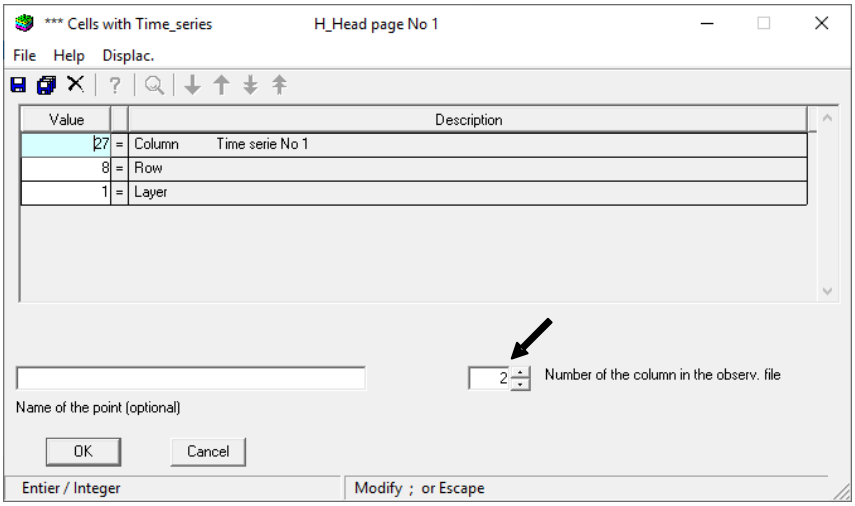


Figure 151 – Cell with time series: Defining the column associated to file "Observations Time Series".

10.4.4 Running the simulation and examining the results

Start the simulation. As there is no cell with a fixed hydraulic head, we get a warning message saying that the initial steady-state simulation might be ill defined. Just ignore this by clicking on the "OK" button and the simulation proceeds in a few seconds.

We specifically obtain the "historiq.prn" file that contains the requested time series, the "histoclim.prn" file with the hydro-climatic balance time series, and the "histobil_riv_dra_lac.prn" file with the time series of river flow. As we also asked for an "Analysis of the simulation discrepancies", we get the following additional files:

- **crit_simul_deviat.prn** containing the comparison criteria between the simulated and observed time series; this text file can be visualized with:
  - A spreadsheet (Excel ® for instance)
  - A text editor.

  It can also be exported as a "shapefile" file for spatialized viewing of the different criteria (for instance with QGIS ® or ArcGIS ®).
- **historiq_sim_obs.prn** containing the observed and simulated time series. This file allows easy visualizing with graphic software, such as Excel ® or Grapher ®).
- **grid_deviat_criter.out** containing the field of each difference criterion.

Figure 152, based on the file "**historiq_sim_obs.prn**" shows that the evolution of river flow at the basin outlet, and the changes in water level as recorded in the observation well, are well simulated by the model.

Figure 153 and Figure 154, based on the "historiq.prn" file, show the changes in calculated runoff and infiltration flux, respectively, as well as the evolution of the percentage of calculated runoff.

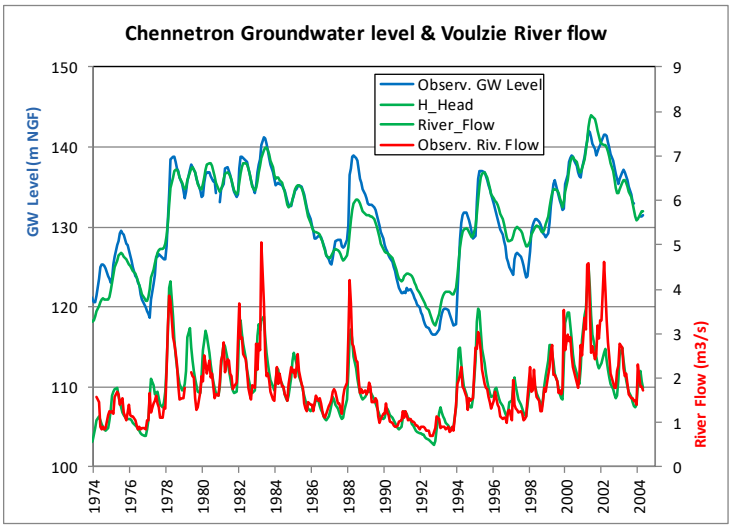


Figure 152 – Simulation with the MARTHE code of the flow of the Voulzie at Jutigny and of the groundwater level in the Saint Martin Chennetron observation well.

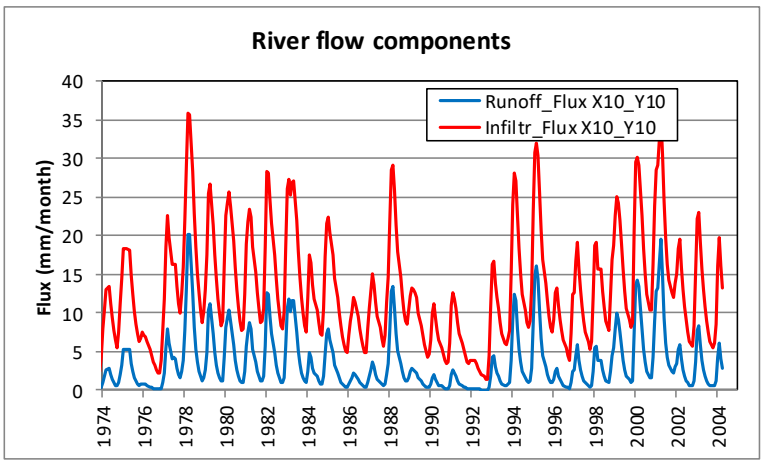


Figure 153 – Runoff and infiltration flux resulting from the coupled GARDENIA hydro-climatic balance.

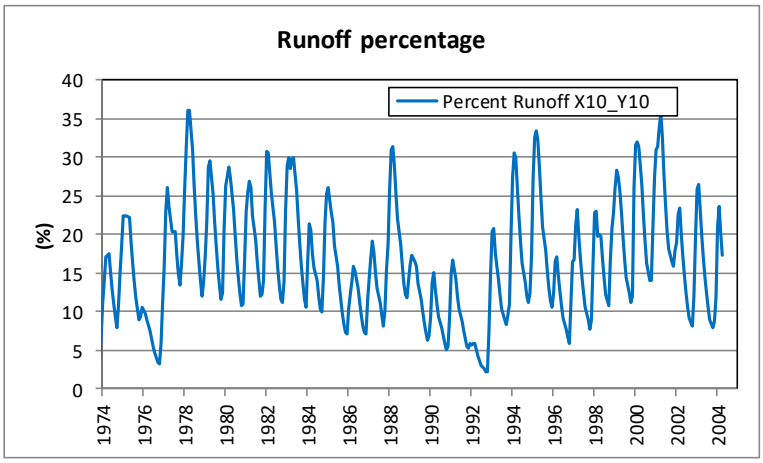


Figure 154 – Percentage of runoff flux
resulting from the coupled GARDENIA hydro-climatic balance.

The "**crit_simul_deviat.prn**" file allows, among the 16 to 18 criteria for each type of time series, the highlighting of the following criteria:

Time series of the groundwater level:

- Number of observations: 372
- Nash coefficient: 0.919
- Maximum simulation error: -7.41 m
- Average quadratic error (Rmse): 1.86 m
- Correlation coefficient: 0.959

Time series of the river flow:

- Number of observations: 359
- Nash coefficient: 0.790
- Nash coefficient over the square root: 0.818
- Maximum simulation error: -2.05 m^3/s
- Average quadratic error (Rmse): 0.34 m^3/s
- Correlation coefficient: 0.893

11 Example 26: Analysis of simulation discrepancies and exporting "shapefile" files

This example is project: ***Rocky_Ecarts.rma***, a simple modelling of mass transport in an aquifer, used for showing the implementation of:

- The feature "**Analysis of simulation discrepancies**", using an "**Observations time series**" [.obs_his] file is compared to simulated time series; and of
- The feature **exporting simulation results to the format "shapefile"** for use with the QGIS software.

Both features are described in report BRGM/RP-69210-FR (Thiéry, 2020c).

The application case as presented is (freely) adapted from the example "Rocky Mountain Arsenal" described by Voss (1984), an alluvial aquifer with the following characteristics:

- General flow direction from north to south;
- Injection of water at a pollutant concentration of 1000 mg/L in the northern zone of the domain;
- Several recovery wells are in the southern part of the domain and a well injecting water at a concentration of 10 mg/L is located in the southwest.

11.1 DEFINITION OF THE MODELLED SYSTEM

The characteristics of the system are:

Geometry

- The domain is modelled by a rectangle of 17,100 m east-west by 21,000 m north-south.
- Regular grid of 300-m-square cells, with 57 columns and 70 rows. The grid origin is at coordinate point (0, 0)
- The topographic elevation is set at 0 m NGF.
- The bottom is set at an elevation of -40 m NGF.

Hydrodynamic parameters

- Permeability = 2.5 10^{-4} m/s;
- Thickness = 40 m;
- Elevation of the top of groundwater (topography) = 0 m;
- Hydraulic head prescribed on the upstream boundary = 250 m;
- Hydraulic head prescribed on the downstream boundary = 38 m;
- Transient groundwater flow simulation

Transport parameters

- Half-degradation time = 20 years;
- Dispersivity: longitudinal = 250 m,
  transverse = 100 m;
- Porosity = 20 %;
- Transient state;
- Transport by the "TVD" method;
- Concentration (outside) of water entering through upstream boundary = 10 mg/L;

Initial transport condition

- Initial concentration = 10 mg/L;

Transportation source terms

- Injected flow = **1** m^3/s at the (outside) concentration = **1000** mg/L: Column **32**; Row **21**;
- Injected flow = **1** m^3/s at the (outside) concentration = **10** mg/L: Column **32**; Row **21**;
- Pumped flow = **0.2** m^3/s (for recovery of the pollution): Columns **12**, **25** and **39**; Row **21**;

Modelling units

Select as user units:

- Hydraulic conductivity = 10^{-4} m/s
- Time = Year (i.e. "Years")
- Porosity = %
- Concentration = mg/L

11.2 CREATION OF THE GRID

- Project title: **Rocky_Ecarts;**
- Southwest corner: X = **0;** Y = **0**;
- Number of columns = **57;**
- Number of rows = **70;**
- Number of layers = **1**;
- Width of columns = **300;**
- Height of rows = **300;**
- Default hydraulic conductivity value = 2.5 (corresponding to 2.5 10^{-4} m/s);
- Topographic elevation = **0** (m);
- Thickness (of each layer) = **40** (m).

11.3 DEFINITION OF THE USER PROFILE

As the simulation will be in transient mode with mass transfer, a "user profile" is defined by assigning the value "1" to the following options:

- 1 = Transient state
- 1 = Standard mass transport

And the profile is saved as "**Rocky_Ecarts.prfu**".

Now return to WinMarthe *sensu stricto*.

11.4 DEFINITION OF THE OTHER FIELDS

As the domain is very simple, all gridded data fields will be defined by "Initialization before simulation" at the end of the parameters [.mart] file.

Defining the General Parameters.

Using the button 

, access the "Non-meshed parameters" menu. Select "General Parameters" and create a new file.

Paragraph: **Control of Aquifer Hydraulic solving process**

```
     0 = Maxi number of iterations for time steps after time step #°0 (transient)
     2 = Maxi number of hydraulic iterat. for time step n°0 (Initial Steady State)
  1e-4 = Average hydraulic head deviation between 2 iterations for convergence
    40 = Maximal number of internal iterations in the solver
Steady = Hydraulic flow Regime [0=Transient state ; 1=Steady state]
```

Paragraph: **Data Units**

```
1e-4 = Aquifer Hydraulic conductivity   unit in m/s (or m2)
Year = Time unit (for model time steps) (second, day, decade, month, year, etc.)
Mg/L = Concentration unit in kg/m3
   % = Porosity = Water Content unit [dimensionless] ['%' when in %]
```

Paragraph: **Transport/Coupling of Concentration, Heat, Salinity**

```
    0 = Maximal number of iterations for Salinity/Heat/Concentr. transport [Def=20]
  TVD = Transport method [3=TVD]
  250 = Longitudinal Dispersivity (m) [ *=Spatialized Field ]
  100 = Transverse   Dispersivity (m) [ *=Spatialized Field ]
```

Paragraph: **Concentration and Pathlines**

```
       1 = Concentration Calculation
    1e-4 = Average concentration variation between 2 iterations for convergence
Transient = Transport scheme for Concentration [0=Transient ; 1=Steady state]
      20 = Degradation half-life time (in time unit) [Def=0]
```

Paragraph: **Optimization / Automatic calibration / Sensitivity analysis**

```
    1 = Analysis of simulation discrepancies [0=No ; 1=Yes]
    1 = Number of time steps to ignore for the analysis simulation discrepancies
```

N.B.: "Ignore" time step zero: As no transport simulation is made at step zero, the simulated concentration at this time step is not significant.

The uniform fields now are simply defined by the pre-processor in paragraph "Initialization before simulation":

- Aquifer Permeability, Porosity, Initial Hydraulic Head, Outside Concentration, Initial Concentration;
- Conditions at the northern (Row 1) and southern (Row 70) boundaries.

The source terms are also defined in this paragraph:

- Pumped and injected flow rates, (Outside) Concentration of the injected flow.

Paragraph: **Initialization before simulation**

```
/PERMEAB/GRID     N: =2.5
/POROSITY/GRID    N: =20
/TOPOGR_ELEV/GRID N: =0
/SUBSTRATUM/GRID  N: =-40
/HYDR_HEAD/GRID   N: =100
/CONCENTR/GRID    N: =10
/EXT_CONCEN/GRID  N: =10
/DISCHARGE/CELL   C=  12R=   54L=    1V=  -0.2;
/DISCHARGE/CELL   C=  25R=   54L=    1V=  -0.2;
/DISCHARGE/CELL   C=  39R=   54L=    1V=  -0.2;
/DISCHARGE/CELL   C=  32R=   21L=    1V=     1;
/DISCHARGE/CELL   C=  15R=   44L=    1V=     1;
/EXT_CONCEN/CELL  C=  32R=   21L=    1V=  1000;
/HYDR_HEAD/CELL   C=   *R=    1L=    1V=   250;
/HYDR_HEAD/CELL   C=   *R=   70L=    1V=    38;
/DISCHARGE/CELL   C=   *R=    1L=    1V=  9999;
/DISCHARGE/CELL   C=   *R=   70L=    1V=  9999;
```

Now save this "General Parameters" file as "**Rocky_Ecarts.mart**"

Defining the time steps

The simulation covers 11 time steps for which concentration values are (hopefully) available in several observation points. The end dates of these time steps, expressed in years, are:

1, 2, 5, 7.5, 10, 15, 20, 30, 40, 60, 80 years

During these time steps, request the following backups:

- At time step zero: Hydraulic head field, Velocity amplitude, Velocity vectors;
- At time step 1: Courant number of the transport;
- At time steps 5, 7, 9, 10 and 11: Field of the calculated concentration.

With the “Non-meshed parameters” pre-processor, button 

, create a "New time steps file" (Figure 155).

Defining the "Observations time series" file

This file is created with a spreadsheet, such as Excel ® or equivalent, from 20 series of (theoretical) concentration observations. It consists of 21 columns: the 20 series and the date in column 21. The date is not used by the simulation, but contributes to the legibility and to verification of the file.

The file has 3 lines of headings starting with the character "#", and then 12 lines corresponding to time step zero followed by 11 simulation time steps. If there is no concentration observation in certain points at certain dates, the corresponding values would have been set at code value "9999", in particular the values of time step zero.

The data must be in text format; do not create an [.xlsx] file, but *export* the data by preference in a "text format, separator = tabulation"; its recommended name is "***Rocky_Ecarts.obs_his***" (Figure 156).

Introduce this file name in the project file with the WinMarthe "Non-meshed parameters" module.

```
Rocky Mountain : *Transient State*
 #<V7.8># --- End of Header lines --- ; Do not modify/delete this line
 *** Beginning of simulation  at date    :          0; ***
  /HYDR_HEAD/OUTPUT         I= 1;
  /VELOCI_AMPLIT/OUTPUT     I= 1;
  /VELOCITY/OUTPUT          I= 1 [C=      0;R=      0;L=      0;Nes=  ]
  /*****/***** End of this Time Step
 *** Step   :    1:       Ends at date    :          1; ***
  /COURANT_NB/OUTPUT        I= 1;
  /*****/***** End of this Time Step
 *** Step   :    2:       Ends at date    :          2; ***
  /*****/***** End of this Time Step
 *** Step   :    3:       Ends at date    :          5; ***
  /*****/***** End of this Time Step
 *** Step   :    4:       Ends at date    :        7.5; ***
  /*****/***** End of this Time Step
 *** Step   :    5:       Ends at date    :         10; ***
  /CONCENTR/OUTPUT          I= 1;V= 0;R= 0;
  /*****/***** End of this Time Step
    . . .
 *** Step   :   11:       Ends at date    :         80; ***
  /CONCENTR/OUTPUT          I= 1;V= 0;R= 0;
  /*****/***** End of this Time Step
 ***        :     : End of simulation    :            ; ***
```

Figure 155 – Mass transport in "Rocky" groundwater: Extract of the time steps file "Rocky_Ecarts.pastp".

Now click on the button 

to bring up the general "Non- meshed parameters" menu and double-click on "**Files of the project**" near the bottom of the screen. Go to the line "**Observations time series**". *Use the search button*  *(magnifying glass) for easily finding this line and search "Observ"*. Once on the line, name the file "***Rocky_Ecarts*.obs_his**" and click “Save”, confirm, and click the "Exit" button.

Defining "Cells with time series"

Create a file "cells with time series" [.histo] with the “Non-meshed parameters” pre-processor. Request the concentration time series in the 20 cells corresponding to the 20 columns of the "Observations time series" file:

- A "Concentration" time series in the cell of column 32 and row 21.
  - Associate with it **column 1** of the "Observations time series" file (Figure 157).
- A "Concentration" time series in the cell of column 32 and row 17.
  - Associate with it **column 2** of the "Observations time series" file.

  etc.
- A "Concentration" time series in the cell of column 45 and row 64.
  - Associate with it **column 20** of the "Observations time series" file.

We could also have asked for the concentration time series in the other cells, without associated observations, or time series of other variables. Such time series would not have an associated column of the "Observations time series" file.

```
# Rocky Mountain : Observed Concentrations
# Conc        Conc          Conc    …      Date
# 32_21       32_17         27_21   …      Date
   10          10            10     …      0
   884         221           173    …      1
   957         429           364    …      2
   984         696           652    …      5
   990         796           766    …      7.5
   992         842           820    …      10
   992         874           856    …      15
   993         886           870    …      20
   993         893           877    …      30
   993         895           879    …      40
   993         896           880    …      60
   993         896           880    …      80
```

Figure 156 – Beginning of the "Rocky_Ecarts.obs_his" observations time series file.

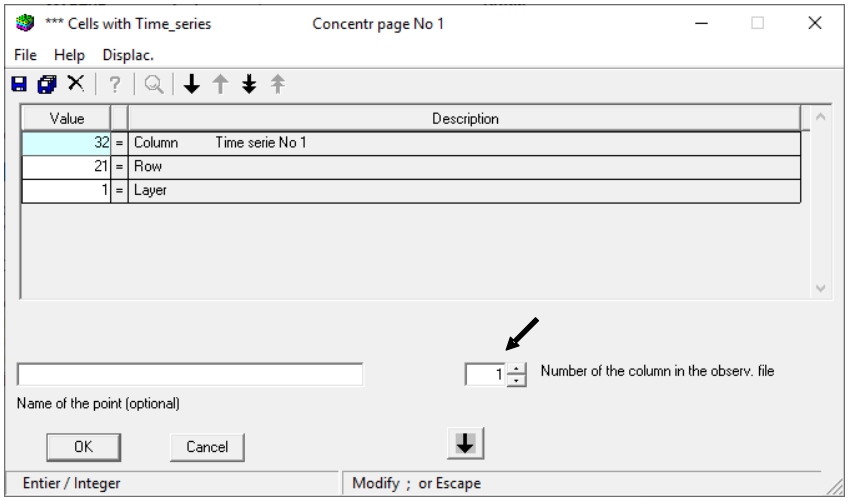


Figure 157 – Cell with time series of the "Rocky" aquifer: Definition of the associated column of the "Observations time series" file.

11.5 RUNNING THE SIMULATION AND EXAMINING THE RESULTS

Run the simulation that takes about one minute. In view of the cell dimensions and the velocities, the TVD transport method imposes a maximum time step of 0.046 years, or 22 transport sub-steps for a model time step of 1 year and 440 sub-time steps for the last time steps of a model duration of 20 years.

We obtain the "**gridsimul.out**" file containing the simulated fields that are saved:

- Hydraulic heads and the velocity magnitude at time step zero,
- Courant number at time step 1,
- Concentration at time steps: 5, 7, 9, 10 and 11.

We also obtain the velocity vectors file "**veloci.out**" and the file of drawn velocity vectors "velocity.bln".

As we ask for an "Analysis of simulation discrepancies", we also obtain the following files:

- **crit_simul_deviat.prn** that contains the criteria for comparison between the simulated and observed time series. This file can be visualized:
  - With a spreadsheet (Excel ® for instance),
  - With a text editor.

  It can also be exported as a "shapefile" file for a spatialized visualization of the different criteria (for instance with QGIS ® or ArcGIS ®);
- **historiq_sim_obs.prn** that contains the observed and simulated time series, and allows easy visualization with a graphic software, such as Excel ® or Grapher ®;
- And a **grid_deviat_criter.out** file that contains the field of each difference criterion.

11.6 EXPORTING THE FILE OF SIMULATED FIELDS "GRIDSIMUL.OUT" AS A "SHAPEFILE" (AND VISUALIZATION WITH QGIS), VISUALIZATION OF VELOCITIES AND PATHLINES

In WinMarthe: use the button  for selecting the file "gridsimul.out".

- In the dialogue that appears accept all default options ("Export all fields", "Export all layers") ➔ OK.
- Then select the default export format: "shapefile".

- As file name [.shp] select (for instance): "Rocky_Ecarts_chasim.shp".

We now instantaneously obtain the following ("shapefile") files:

- Rocky_Ecarts_chasim.shp (containing the coordinates of each cell),
- Rocky_Ecarts_chasim.dbf (containing the attribute table of the eight exported fields),
- Rocky_Ecarts_chasim.shx
- Rocky_Ecarts_chasim_Noms.txt (containing the identification of the fields of the attribute table).

The "Rocky_Ecarts_chasim.shp" file can be directly opened by QGIS (any version), by double-clicking on it if the [.shp] files were associated with QGIS, or by opening QGIS. Hereafter, we show the opening with QGIS v. 3.6.3.

Open QGIS.

Main menu: Layer ➔ Add a layer ➔ Add a vector layer (Ctrl+Maj+V):

- As source of the vector data set, select "**Rocky_Ecarts_chasim.shp**" ➔ Button "**Add**".
- Select the reference coordinate system (RCS): for instance WGS 84 ➔ OK.

This brings up the "Layers" field and a grid drawing of uniform colour. (Figure 158).

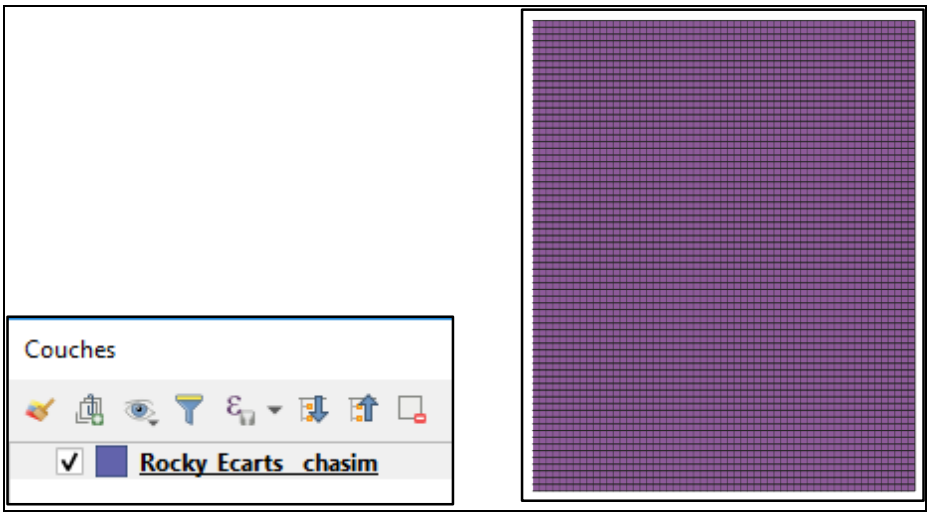


Figure 158 – QGIS: Add the vector layer "Rocky_Ecarts_chasim.shp".

11.6.1 Display of the concentration field after 60 years

In the "Layers" field:

- Select line "Rocky_Ecarts_chasim" and rename it (with right mouse button) "Rocky_Ecarts_concentr". Then double click on it or choose "Properties" with the right mouse button.

In the dialogue box "Properties on display" choose "Symbology":

- At the top, at the place of "Single Symbol" select by default: "**Graduated**".
- Just below one must choose a "Column" (of the attribute table). The "Rocky_Ecarts_chasim_Noms.txt" file indicates that the column named "C_L1_T7" corresponds to the concentration at the date of 60 ans. Select this column.
- Select a "**Colour palette**" among "All colour gradients", by preference a "Rainbow" palette, from blue to red.
- Now select (for instance) "Equal interval", "10" classes.
- **Rank**.
- Apply => A concentration field appears with a legend.

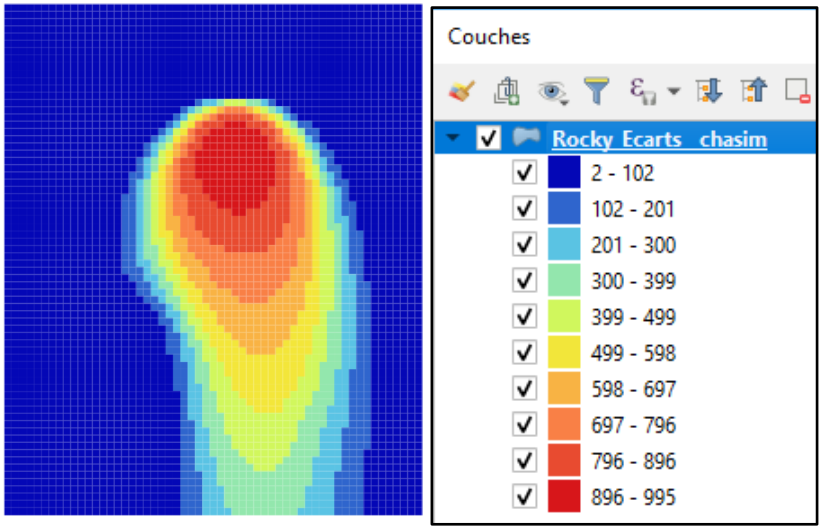


Figure 159 – QGIS: The concentration field after 60 years; Right: Legend in the "Layers" box.

By default, the contour of each cell appears, which can hinder legibility of the drawing in the case of very many cells. The solution is to make the cell contours disappear. In the dialogue box Properties ➔ Symbology that is still displayed, below column, select the line "Symbol – Change":

- Select "Simple infilling" ➔ "Line colour" ➔ "**Transparent contour**".
- OK ➔ OK

Now we see the concentration field after 60 years. The legend appears in the "Layers" box, by "unfolding" the concerned layer. (Figure 159).

11.6.2 Adding the hydraulic head field (calculated at time step 0)

In the "Layers" box menu select the line "Rocky_Ecarts_concentr", and with the right mouse button select "**Duplicate the layer**"

- Choose the same projection => OK

The grid drawing (uniform colour) is superimposed on the concentration field and in the "Layers" box a new line "Rocky_Ecarts_concentr copy" appears below the preceding one. Rename it (right mouse button) "Rocky_Ecarts_head".

- Uncheck the line "Rocky_Ecarts_concentr", check the new line "Rocky_Ecarts_charge" and double click on it, or choose "Properties" with the right mouse button.

The dialogue box "Properties ➔ "Symbology" of the preceding field reappears, with the same palette and the same classes.

- Choose column "C_L1_T1" that corresponds to the hydraulic head (at time step zero).
- Keep the palette and the number of classes, click on "**Rank**" to adapt the classes.
- Then "Apply" to see the result, and on OK if satisfactory.

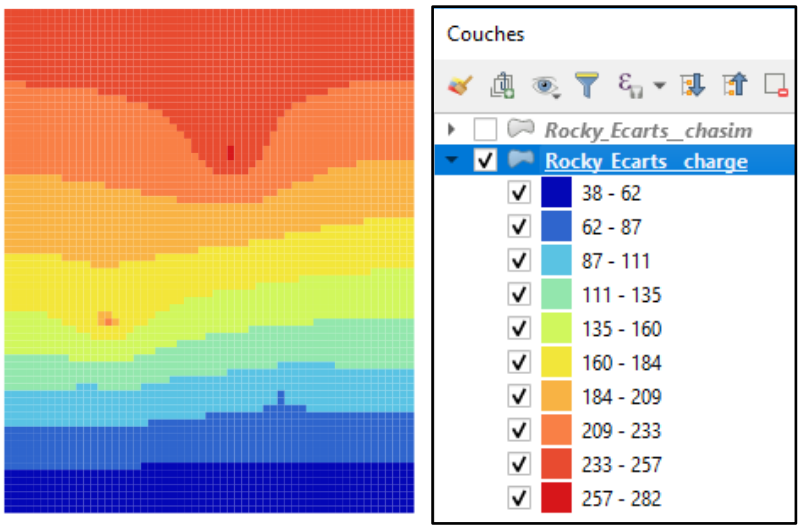


Figure 160 – QGIS: The hydraulic head field; Right: Corresponding legend.

The hydraulic head field now appears (with its legend in the "Layers" box. (Figure 160).

You can show either the concentration field at 60 years, or the hydraulic head field, by checking the required line and unchecking the other in the "Layers" menu.

Save the project file for later use, for instance as "**Rocky_Ecarts_chasim .qgz**".

11.6.3 Adding a drawing of the velocity vectors

We have obtained the velocity vectors file "**veloci.out**" and the file of the velocity vectors drawing "velocity.bln".

When the modelled domain consists of several layers, or if a velocities back-up has been requested at several time steps: "velocity.bln" file is a drawing of the velocity vectors in the first layer during the first back-up, whereas the "veloci.out" file contains all velocity components of all layers, with all velocity back-ups.

Initially, we directly export the velocity vectors drawing file "velocity.bln" as a "shapefile" file. (We will see later that this is not an optimal choice).

Using the WinMarthe's button  , select the file "velocity.bln" and export directly as a "shapefile" file. This gives the shapefile "velocity.shp" and its associated [.dbf] and [.shx] files. To visualize this pathlines "shapefile" with QGIS, proceed as before:

Main menu: Layer ➔ Add a layer ➔ Add a vector layer (Ctrl+Maj+V):

- Source vectoral data set: select "**velocity.shp**" ➔ Button "**Add**".
- Select the reference coordinate system (RCS): choose the same projection WGS 84 ➔ OK

The velocity vectors now appear on the current field, for instance that of the simulated hydraulic head (Figure 161). As there is one velocity vector per cell, and there are many cells, the drawing (right half of the figure) is quite illegible.

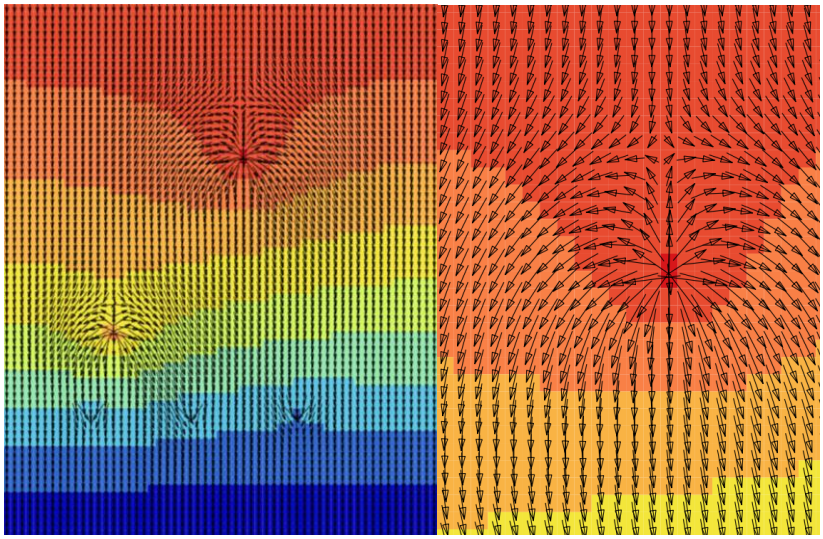


Figure 161 – QGIS: Visualization of the "velocity.bln" vector field, superimposed on the hydraulic head field (on the right, a detail of the surroundings of the injection well).

To obtain a less dense velocity vectors field, we use the WinMarthe menu: "Tools" ➔ "Others" ➔ "Management of Velocity Files". (Figure 162). Select the velocities file "veloci.**out**". If the domain has several layers, or if the velocities were saved at several time steps, we can select:

- The number of time steps, and/or
- The number of the layer.

After these choices (not shown in this example), in the menu that appears we select:
"**3** = Periodicity of the arrows according to the Columns (X)" and,
"**3** = Periodicity of the arrows according to the Rows (Y)".

Record the result in the file called "velocity_bln_Perio_3.bln". This file contains only one arrow every three columns and every three rows (which gives nine times less velocity vectors). Export as before this "velocity_bln_Perio_3.bln" file as a shapefile "velocity_bln_Perio_3.shp" and add to QGIS via "Layer ➔ Add a layer ➔ Add a vector layer".

This gives a more suitable visualization (Figure 163).

Please note that these velocity vectors are real ones calculated in 3D by the MARTHE code, considering any possible heterogeneities in the hydraulic conductivity and porosity fields, as well as any "Impervious connections" etc. This is *not* a simple drawing that might be automatically drawn by a visualization software from the hydraulic head field.

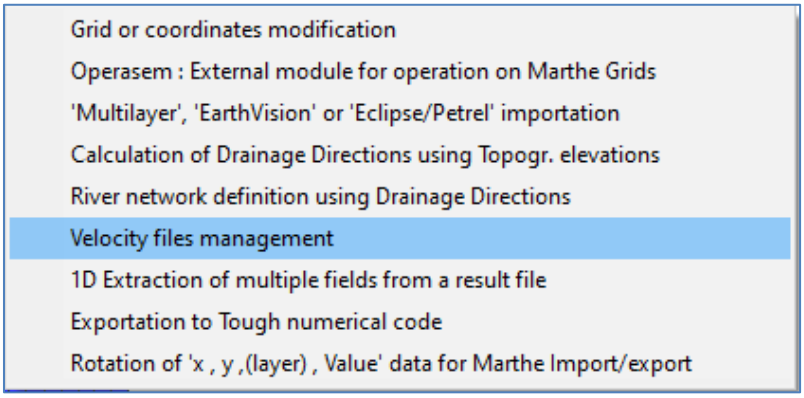


Figure 162 –Velocity files management.

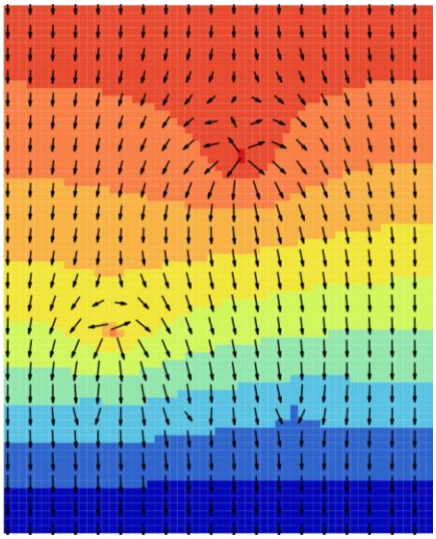


Figure 163 – QGIS: Visualization of the velocity vectors field "velocity_bln_Perio_3.shp", superimposed on the hydraulic head field
(One velocity vector every 3 columns and every 3 rows).

11.6.4 Adding a drawing of the pathlines

Now redo a calculation with a simulation of pathlines. As seen above, we must:

- Select with the pre-processor the simulation of pathlines in the paragraph "Concentration and Pathlines" of the "General Parameters" file [.mart]:
  "**1** = Calculation of Pathlines".
- Define with the pre-processor a file of "Pathline departures" [.deptr]. As "Starting points", select all columns of row 1:
  "Cell; Column = *****; Row = **1**".

Re-run the simulation to get a pathlines file "pathline.out", and a pathline drawing file "pathline.bln" that are renamed “Rocky_Ecarts_trajmar.out" and “Rocky_Ecarts_trajmar.bln”, respectively

In this simple 2D case, the "Rocky_Ecarts_trajmar.bln" file is transformed into a shapefile. For this, use the WinMarthe’s button , select the "Rocky_Ecarts_trajmar.bln" file and export it directly into a "shapefile" file. This gives the shapefile "Rocky_Ecarts_trajmar.shp" file (and the associated [.dbf] and [.shx] files).

To visualize this pathlines "shapefile" file with QGIS, proceed as before:

Main menu: Layer ➔ Add a layer ➔ Add a vector layer (Ctrl+Maj+V):
- Source vector data set: Select "**Rocky_Ecarts_trajmar.shp**" ➔ Button "**Add**".
- Select the reference coordinate system (RCS): Select the same projection: WGS 84 ➔ OK

The pathlines now appear on the current field (for instance, the field of simulated hydraulic heads). (Figure 164).

In a more complex domain, the "Rocky_Ecarts_trajmar.out" file could have been transformed *directly* into a "shapefile" file with the WinMarthe’s button . The attribute table [.dbf] then would have contained complementary information for each pathline segment:
- The elevation of each segment,
- The elapsed time since the start of the pathline,
- The number of the layer concerned.

Such information can be used, for instance, for visualizing the pathlines segments with a colour depending upon ‘time’ or ‘layer’.

It should be noted that these pathlines are real ones calculated in 3D by the MARTHE code, considering any possible heterogeneities in the hydraulic conductivity and porosity fields, any "Impervious connections" etc. This is *not* a simple drawing that might be automatically drawn by a visualization software from the hydraulic head field.

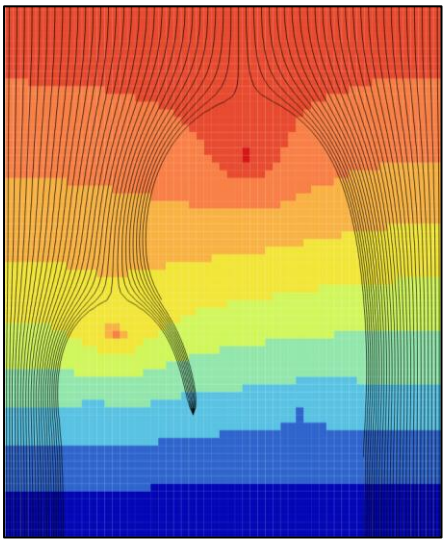


Figure 164 – QGIS: Visualization of the simulated pathlines, superposed on the hydraulic head field.

11.7 ANALYSIS OF SIMULATION DISCREPANCIES BASED ON THE "CRIT_SIMUL_DEVIAT.PRN" FILE

The text file "crit_simul_deviat.prn" that was generated contains 16 comparison criteria between the simulated and observes time series in 20 reference points. Such criteria include:

- The simulation bias,
- The maximum simulation error,
- The root mean square error (Rmse),
- The Nash coefficient,
- The correlation coefficient,
- Etc.

Certain criteria are more pertinent than others, depending on the variable studied.

To visualize the criteria of this "crit_simul_deviat.prn" file, one can:

- Use a text editor;
- Use a **spreadsheet** (Excel ® or similar), for instance to make a statistical analysis of certain criteria;
- Export this "crit_simul_deviat.prn" file as a "shapefile" file to be opened QGIS or ArcGIS ®, for instance, for visualizing the spatial distribution of certain criteria as coloured symbols superimposed on a geographical map or another ‘field’ map. How to export this "crit_simul_deviat.prn" file is described further on.

11.7.1 Spreadsheet analysis of simulation-error criteria of the "crit_simul_deviat.prn" file

As an example, Figure 165 shows, for a concentration of 20 points with time series observations, the comparison of observed and simulated averages and standard deviations (calculated for the 11 dates of the time series).

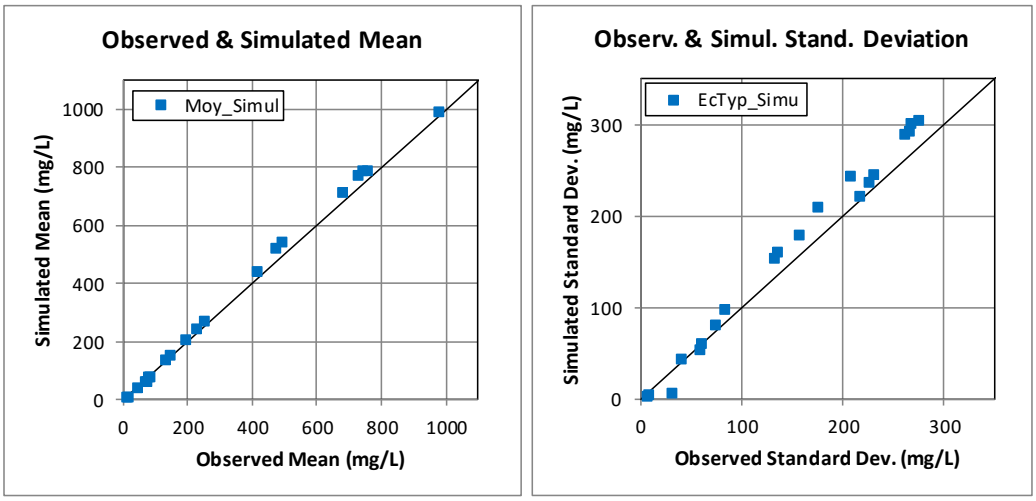


Figure 165 –"Rocky" groundwater: Observed and simulated averages (left) and standard deviations (right) for the 20 time series.

Figure 166 shows that, in each point, both the absolute bias value (Abs_Bias) and the root mean square error (Rmse) increase with a greater variability of the point (large standard deviation in the observation). The correlation coefficient between the Rmse and the standard deviation is 0.96. The bias and the standard deviation therefore are *not* pertinent variables.

Figure 167 shows the statistical distribution of “standardized bias" (standardized by the standard deviation of observations) and of the standardized root mean square error.

Figure 168 shows the statistical distribution of the Nash coefficient and of the correlation coefficient. This figure shows that, in this example at least, the correlation coefficient isn’t a severe criterion as it is over 0.97 for all 20 points, even for the three points where the Nash coefficient is less than or equal to 0.50.

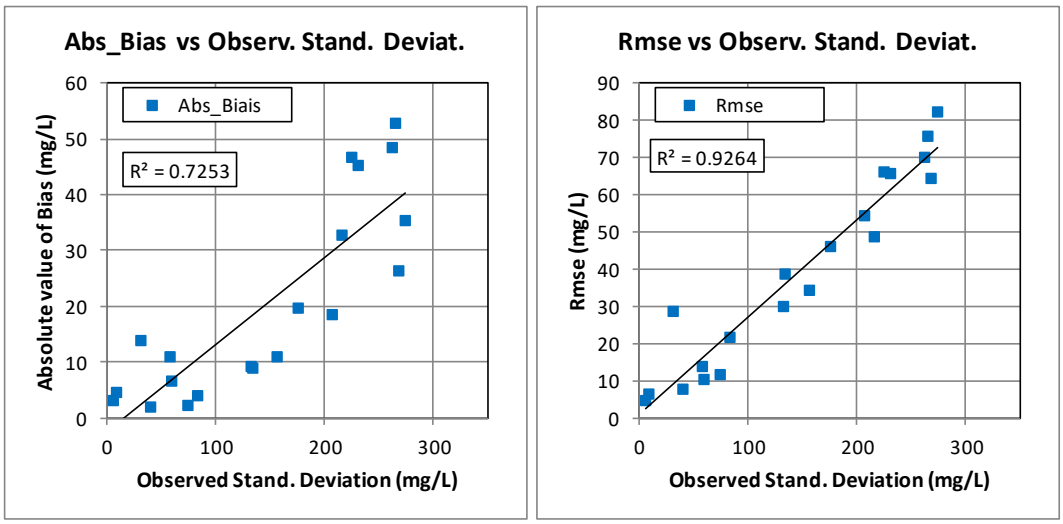


Figure 166 –"Rocky" groundwater. Left: relation between the bias and standard deviation of the observations; Right: relation between the “Rmse” and the standard deviation. Each point represents a time series.

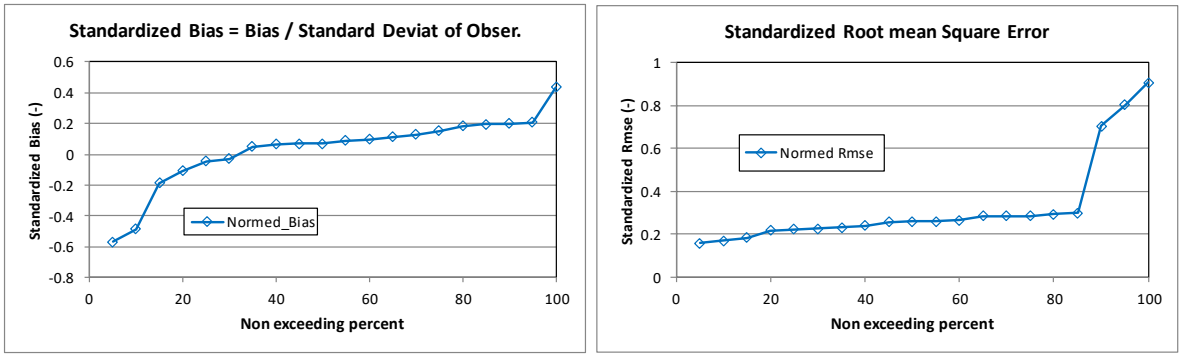


Figure 167 –"Rocky" groundwater. Statistical distribution of the standardized bias (left) and the standardized root mean square error (right).

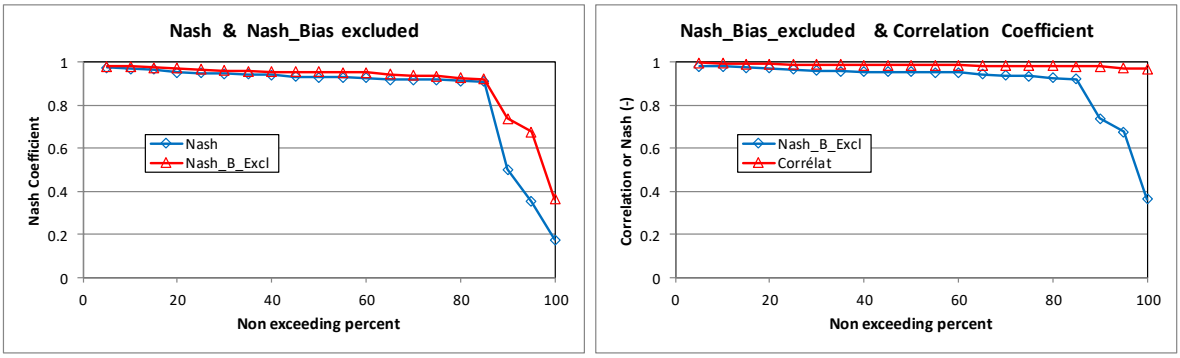


Figure 168 –"Rocky" groundwater. Statistical distribution of Nash coefficients (left) and of the correlation coefficient compared to the Nash coefficient (right).

11.7.2 Exporting the criteria file "crit_simul_deviat.prn" into a "shapefile" file (and visualization with QGIS)

In WinMarthe use the button  and select the "crit_simul_deviat.prn" file.

- In the dialogue box "Advanced options - Change of coordinate system", validate ➔ OK.
- Then select the default export format: "shapefile".
- As [.shp] file name, give (for instance): "Rocky_Ecarts_crit_ecart_simul_Concentr.shp".

We now immediately obtain the following ("shapefile") files:

- Rocky_Ecarts_crit_ecart_simul_Concentr.shp (contains the coordinates of each time series point with criterion);
- Rocky_Ecarts_crit_ecart_simul_Concentr.dbf (contains the attribute table of the 16 exported criteria);
- Rocky_Ecarts_crit_ecart_simul_Concentr.shx.

The "**Rocky_Ecarts_crit_ecart_simul_Concentr.shp**" file can be directly opened with QGIS (any version), by double-clicking on it (if the [.shp] files have been associated with QGIS), or by first opening QGIS. Hereafter, we show with QGIS v. 3.6.3 how to superimpose the criteria on a map of the concentration field.

Open QGIS for visualization of the hydraulic head field and of the preceding concentration field (by opening the earlier saved QGIS project file "**Rocky_Ecarts_chasim .qgz**").

- In the "Layers box, deselect the hydraulic heads field (Rocky_Ecarts_charge).
- Still in the "Layers box, check the concentration field at 60 years (Rocky_Ecarts_concentr). Then, to modify its "**Opacity**" (i.e., to render it clearer, double click on it or choose "Properties" with the right mouse button).

- In the dialogue box "Symbology" that appears at the bottom, click on "Rendu de couche and set the "Opacity" at 30 % (instead of 100 %) ➔ OK.

Then load the "shapefile" file with the criteria:

Main menu: Layer ➔ Add a layer ➔ Add a vector layer (Ctrl+Maj+V):

- Source vectoral data set: Select "**Rocky_Ecarts_crit_ecart_simul_Concentr.shp**" ➔ Button "**Add**".
- Coordinate system selector (RCS): Choose the same projection: WGS 84 ➔ OK

In the concentration field, 20 circles of a uniform colour appear, that correspond to the 20 points with different criteria. In the "Layers" box a new "Rocky_Ecarts_crit_ecart_simul_Concentr" line appears.

- Double-click on this new line (or choose "Properties" with the right mouse button).

As before, in the dialogue box "Properties" choose "Symbology":

- At the top, at the default place "Single symbol", select "**Graduated**".
- Just below, choose a "Column" (in the attribute table). Select for instance the column "**Bias**".
- Now select a "**Colour palette**" (colour scheme), for instance the same as before.
- Choose (for instance) "Equal interval", "9" classes.
- **Rank**.
- Apply => Now appear circles coloured by the bias value, with a legend (in the "Layers" box).

In this "Symbology" menu, the size of the coloured circles can be increased by the line "Symbol – Change":

- In the dialogue box that appears, on the line "Size" increase the value from "2" to "3" for instance => OK

In the "Layers" box, rename the layer line as "Rocky_Ecarts_crit_ecart_simul_Concentr_Bias".

Figure 169 shows the result.

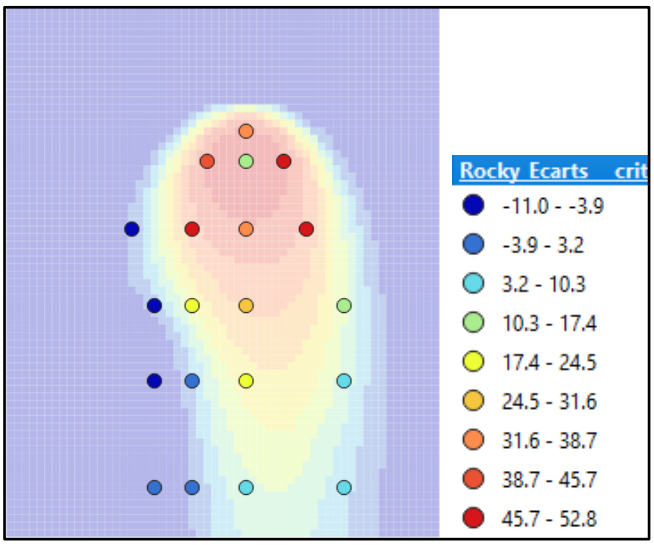


Figure 169 – QGIS: Bias (mg/L) of the simulated concentration time series in 20 points.

One can easily visualize the other criteria with the same procedure as above:

In the "Layers" box: right button "Duplicate the layer", then select another column, for instance the standardized root mean square error and visualize it. (Figure 170).

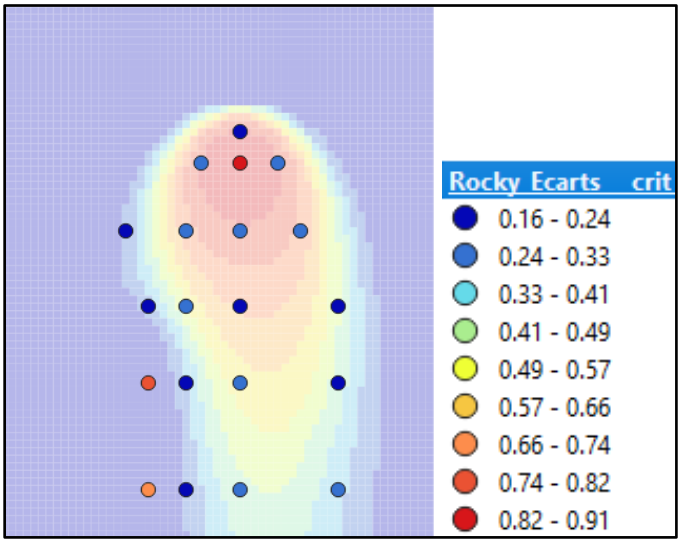


Figure 170 – QGIS: Standardized root mean square error (Rmse_Stand) (no dimension) of the simulated concentration time series de in 20 locations.

11.8 SIMPLE COMPARISON OF SIMULATED AND OBSERVED TIME SERIES BASED ON THE "HISTORIQ_SIM_OBS.PRN" FILE

The generated "historiq_sim_obs.prn" file allows a simple and rapid comparison of the simulated and observed time series at each time step. In this text file for each point with an observed time series, a column gives the simulated time series and the next column gives observed time series. This file can thus be immediately visualized with a spreadsheet, for instance Excel ®.

Figure 171 compares the simulated and observed time series in the cells:

- Left: Column 32, row 17: Nash coefficient = 0.95, correlation coefficient = 0.986
- Right: Column 20, row 50: Nash Coefficient = 0.55, Nash_Bias_Exclu = 0.67. But, notwithstanding a very poor simulation, the correlation coefficient = 0.985.

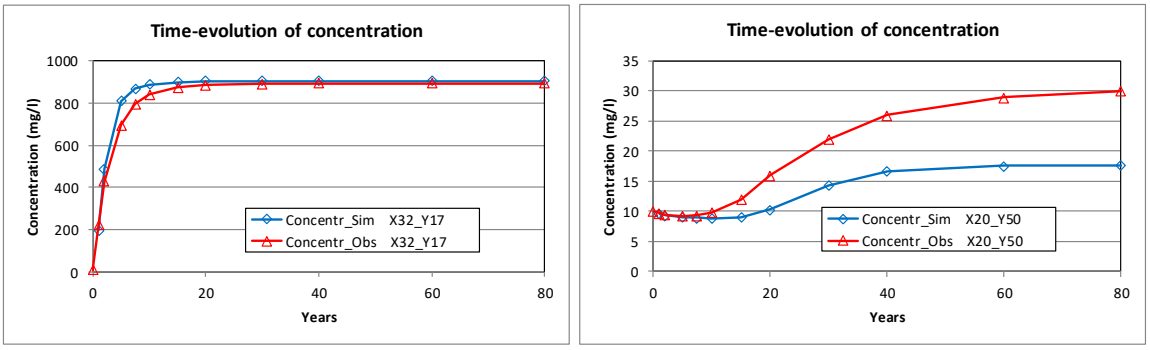


Figure 171 – Comparison of simulated and observed concentration time series in two points based on the "historiq_sim_obs.prn" file.

11.9 COMPARISON OF TWO SIMULATIONS CARRIED OUT WITH DIFFERENT HYPOTHESES

With the same "Discrepancies analysis" approach, it is possible to compare two simulations made with different hypotheses, for instance two mass-transfer simulations with different dispersivities.

Create a file of "observations time series" in which, instead of time series of "observed" data, and introduce values of simulated time series with the first hypothesis in certain cells in sensitive or strategical zones.

Then run a simulation with the second hypothesis. Analysis of the differences and the calculated criteria then refers to the differences in simulated time series in these cells between the two hypotheses.

The "historiq_sim_obs.prn" file now allows comparing the simulations with these two hypotheses, which is a sort of simple "sensitivity analysis".

11.10 SIMULATION WITH "MODEL SUB-TIME STEPS"

When carrying out a simulation with model sub-time steps, the calculated time series files ("historiq.prn", "histobil_debit.prn", "histomas.prn", etc.) generally contain the values calculated at all sub-time steps.

- For reasons of compatibility, the [.obs_his] file must contain the values observed (or absent) at all sub-time steps.

Thus, if the simulation is run with, for instance, 10 model sub-time steps, the file [.obs_his] will have ten times more lines than the number of "model time steps", or 10 times the number of time steps in the “Time steps” [.pastp] file.

An example with 10 model sub-time steps is in the "**Rocky_Ecarts_10_ss_Pas.rma**" project.

Specific case: If a "**Periodicity for time series output**" of "**-1**" is selected in the paragraph "Outputs and controls" of the "General Parameters" [.mart] file:

```
-1 = Periodicity for time series output [Def=0 => Every time step]]
```

- The files of a simulated time series ("historiq.prn", etc.) only contain the values calculated for the dates of the "Model time steps".
- The file of the observed time series must contain observed (or absent) values only on the dates of the "Model time steps".

Such an example, with 10 model sub-time steps, and a “time series output periodicity” of "**-1**" is given in the "**Rocky_Ecarts_10_ss_Pas_Perio.rma**".

12 How to …

In this chapter we show how to back-up projects, how to modify grids, how to format data, and how to import geometric models or export result files.

The operations that can be carried out include:

- Back-up all files of a MARTHE project.
- Modify a grid.
- Recover data of all fields after modification of a grid.
- Import a 3D geological model into the "Multilayer" ® (BRGM), Eclipse-Petrel ® or "EarthVision" ® formats, for the direct generation of a MARTHE model.
- Calculate automatically drainage directions from a topographical grid.
- Calculate automatically a drainage network from drainage directions and from a minimum value of catchment area drained by a reach of the network.
- Manage velocities from a "veloci.out" file: generate a “drawing” file for a given layer or a given date. Conserve the velocities only every "*C*" columns and every "*R"* rows.
- Extract multiple 1D fields from a *"gridsimul.out*" results file: Extract multiple 1D series along a given row, column or layer, for different fields and/or multiple dates.
- Visualize a grid directly in 3D.
- Generate a "Vrml" file from a grid (for instance a hydraulic head field) for 2.5 D visualization.
- Export a 3D grid for a visualization by "Paraview" ®, "3Dview" ® or "Tecplot" ®.
- Use a "*gridsimul.out*" file for exporting to QGIS, ArcGIS ® or Mapinfo ® of fields calculated for various layers and at different dates.

12.1 BACK-UP ALL FILES OF A MARTHE PROJECT

This feature allows saving all files of a project, for instance for transmission to another user, or for safety reasons before a major modification. To use the functionality:

WinMarthe: "File" ➔ "Make a Backup copy of the Project".

12.2 MODIFY A GRID

The possible modifications are the following:

- Subdivide layers,
- Suppress layers,
- Add layers under the deepest layer,
- Add or suppress nested grids,
- Extract a nested grid, conserving only this nested grid,
- Extract a sub-model (a parallelepiped),
- Extend a grid: add rows up- and/or down-ward, add columns to the right and/or the left,
- Change coordinates (offset and/or change of units).

To use this feature (Figure 172): WinMarthe: "Tools" ➔ "Others" ➔ "Grid or coordinates modification".

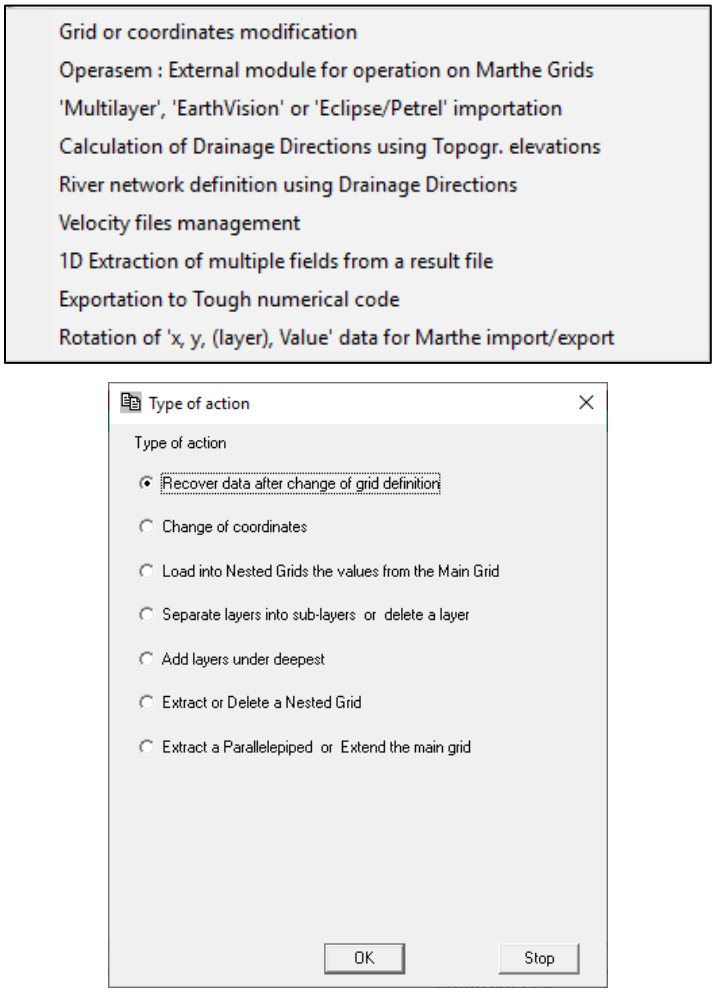


Figure 172 – Grid or coordinates modification.

12.3 RECOVER DATA OF ALL FIELDS AFTER MODIFICATION OF A GRID

In case of a project with many gridded fields, it is not always possible to load all fields in WinMarthe before modifying the grid, such as changing the heights of rows or widths of columns. Such grid modifications can also be made by creating a new, empty, project with irregular column and row widths. Only the “Hydraulic conductivity” (Permeability) file that defines the grid structure, will correspond to the new grid, and there will be for instance no "Concentrations" file, nor a "Temperature" file.

It is thus recommended, **before modifying the grid**, to "Make a Backup copy of the project" (for instance called "Project_Before_Modif.rma").

Now modify the grid or create a new one. The modified project will be called for instance "Proj_Maill_Modif.rma" and contains the modified Hydraulic conductivity file called "Proj_Maill_Modif.permh".

It is now possible to **load into the new grid** ("Proj_Maill_Modif"), through optimal interpolation, adapted to each field, the data of all fields of the saved project ("Project_Before_Modif.rma").

Proceed as follows:

- Load the saved project ("Project_Before_Modif.rma"),
- Use the WinMarthe menu (Figure 172): "Tools" ➔ "Others" ➔ "Grid or coordinates modification" ➔ "Recover data after change of grid definition".
- Give the name of the "Permeability" file of the modified grid ("Project_Before_Modif.rma") that contains the definition of the new grid, with the new rows and columns dimensions,
- Assign a name to the resulting project (for instance "Project_Final.rma").

At the end of the operation close the project "Project_Before_Modif.rma" and open the new project "Project_Final.rma" to make any adjustments, if necessary.

12.4 IMPORT A 3D GEOLOGICAL MODEL

We can import the geometry resulting from 3D geometric models or geo-modellers, such as GDM ®, Multilayer ®, EarthVision ® or Eclipse/Petrel ® for the direct generation of a MARTHE model.

To use this feature (Figure 173): WinMarthe: "Tools" ➔ "Others" ➔ "'Multilayer' or 'EarthVision' or 'Eclipse/Petrel' data importation".

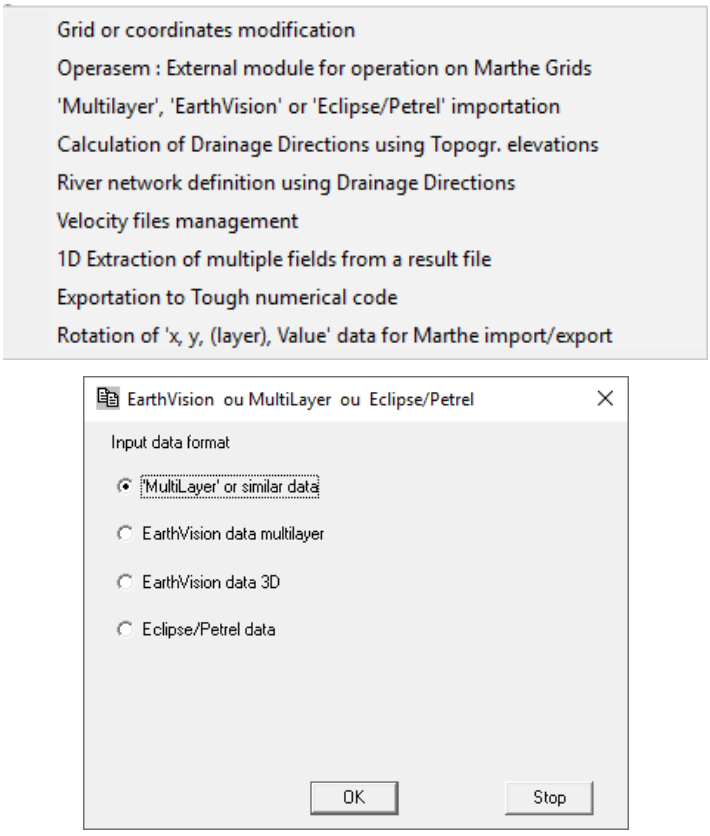


Figure 173 – Importing data from a geo-modeller (Multilayer, EarthVision, Eclipse/Petrel).

12.5 AUTOMATIC CALCULATION OF DRAINAGE DIRECTIONS

Automatically calculates drainage directions from a topographical grid.

To use this feature: WinMarthe: "Tools" ➔ "Others" ➔ "Calculation of Drainage Directions using topographic elevations".

12.6 AUTOMATIC DETERMINATION OF THE RIVER NETWORK.

Automatically defines the river network from drainage directions, and a minimum catchment area value drained by a reach of the network.

To use this feature: WinMarthe: "Tools" ➔ "Others" ➔ "River network definition using Drainage Directions".

12.7 MANAGING VELOCITIES FROM A "VELOCI.OUT" FILE

This feature allows managing velocities from a "veloci.out" file:

- Generation of a drawing file for a given layer, at a given date.
- Conservation of velocity vectors only every "*C*" columns and every "*R"* rows.
- Definition of the reference length of velocity vectors.

To use this feature: WinMarthe: "Tools" ➔ "Others" ➔ "Velocity files management".

12.8 1D EXTRACTION OF MULTIPLE FIELDS FROM A "GRIDSIMUL.OUT" RESULTS FILE

This feature allows the one-dimensional extraction of multiple fields from a "gridsimul.out" results file.

Data can be extracted for:

- A given row,
- A given column,
- A given vertical.

The data of a given field, or of all fields, can be extracted for a given date, or for all dates of the de "gridsimul.out" results file.

To use this feature: WinMarthe: "Tools"➔"Others"➔"1D extraction of multiple fields from a results file".

12.9 DIRECT 3D VISUALIZATION OF A GRID

It is possible directly to visualize in 2.5 D (basic visualization) a 2D data field (for instance a temperature field or a hydraulic head field).

To use this feature: press WinMarthe button 

12.10 GENERATION OF A "VRML" FILE

It is possible to generate a "Vrml" file from a grid (e.g. a hydraulic head field) for 2.5 D viewing.

To use this feature: press WinMarthe button 

12.11 3D EXPORTING TO "PARAVIEW" ®, "3DVIEW" ®, "TECPLOT" ®.

It is possible to export a 3D grid for visualization by "Paraview" ®, "3Dview" ®, "Tecplot" ®.

To use this feature: press WinMarthe: button 

12.12 "SHAPEFILE" EXPORT FOR VISUALIZATION WITH QGIS, ARCGIS ® OR MAPINFO ®

From a "gridsimul.out" file: export as a "shapefile" file useable by QGIS, ArcGIS ® (or as mif/mid files useable by MapInfo ®) of 2D calculated in various layers of the model and at diverse dates.

To use this feature: press WinMarthe's button  .

A model file, whose name appears in the [.rma] project file, can also be exported directly in "shapefile" format.

To use this feature: Menu "File ➔ Export values from the current field ➔ current field => Shapefile".

12.13 EXTRACTING THE COORDINATES OF A "SHAPEFILE" FILE TOWARD A [.BLN] FILE

From a "shapefile" [.shp] file, export the coordinates of the shapes as a file in [.bln] format. This [.bln] file can be visualized immediately by WinMarthe.

To use this feature: WinMarthe: press the button  .

13 Conclusions

We present some concepts of groundwater flow and transport processes available in the MARTHE software of BRGM. We also discuss guidelines for using the general 3D applications for calculating hydraulic head, flow rates and mass transport, related to Managed Aquifer Recharge (MAR) / artificial recharge and active aquifer management.

Among the features of the MARTHE code are:

- Multilayer aquifer, groundwater, unsaturated zone with or without density effects;
- River networks;
- Groundwater recharge and runoff.

Other features of the MARTHE code, available in this version v.7.8 (or v.7.5), are described in more detail in specific documents, such as:

- Mass transport in a saturated or unsaturated porous medium, in steady-state or transient modes (report BRGM/RP-64765-FR);
- Salinity transport with coupled interaction of the fluid density on calculation of the hydraulic head (report BRGM/RP-64765-FR);
- Heat or thermal-energy transfer with coupled calculation of density and viscosity (report BRGM/RP-64765-FR);
- Unsaturated Zone (UZ) flow (report BRGM/RP-64495-FR);
- The effect of vegetation and crops on evaporation and transpiration (report BRGM/RP-65918-FR)
- Automatic calibration of parameters with sensitivity analysis;
- Flow of gaseous fluids;
- Flow with consideration of density-dependent salinity (report BRGM/RP-64765-FR);
- Geochemical coupling (in certain versions) (report BRGM/RP-65010-FR).

The following features are available as well:

- Two-phase flow of Water/Gas;
- Two-phase flow of Water/Hydrocarbons.

To make use of all features of the BRGM MARTHE code, one should refer to the associated descriptive reports, the "Tutorial for the MARTHE software v7.8", report BRGM/RP-69542-FR (Thiéry, 2020b, *in French*). One should also refer to the report "Tutorial for the WinMarthe v4.0 pre-processor", BRGM/RP-54652-EN (Thiéry 2007) (or the report BRGM/RP-54652-FR, Thiéry, 2006 *in French*) that describes the WinMarthe pre-processor in more detail.

14 Bibliographic references

Brooks, R.H., Corey, A.T. (1964) - Hydraulic properties of porous media. Hydrology Paper n°3. Colorado State University, Fort Collins, Colorado, 27 p.

Brutsaert, W. (1966) - Probability laws for pore-size distributions. *Soil Science* 101, p. 85-92.

Burdine, N.T. (1953) - Relative hydraulic conductivity calculations from pore-size distribution data. *Petrol. Trans., Am. Inst. Min. Eng.* 198, p. 71-77.

Cooley, R.L. (1983) - Some new procedures for numerical solution of variably saturated flow problems. *Water Resour. Res.* 19, p. 1271-1285.

Douez, O., Bichot, F., Petit, V. (2011) - Contribution à la gestion quantitative des ressources en eau à l'aide du modèle Jurassique de Poitou-Charentes. Rapport BRGM/RP-59288-FR. 411 p., 286 fig.

Gardner, W.R. (1958) - Some steady state solutions of unsaturated moisture flow equations with application to evaporation from a water table. *Soil Sci.* 85, p. 228-232.

Haverkamp, R., Zammit, C., Bouraoui, F., Rajkai, K., Arrue, J.L., Heckmann, N. (1998) - GRIZZLY, Grenoble Catalogue of Soils: Survey of soil field data and description of particle-size, soil water retention and hydraulic conductivity functions. Laboratoire d'Etude des Transferts en Hydrologie et Environnement (LTHE), Grenoble, France.

Leonard, B.P. (1988) - Universal Limiter for transient interpolation modeling of the advective transport equations: the ULTIMATE conservative difference scheme, *NASA Technical Memorandum 100916 ICOMP-88-11*.

Mualem, Y. (1976) - A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water Resour. Res*. 12, p. 513-522.

Parkhurst, D.L., Appelo C.A.J. (2013) - Description of Input and Examples for PHREEQC Version 3 - A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations. *U.S. Department of the Interior, U.S. Geological Survey Techniques and Methods 6–A43*.

Parkhurst, D.L., Wissmeier, L. (2015) – PhreeqcRM: A reaction module for transport simulators based on the geochemical model PHREEQC. Advances in Water Resources 83(2015) 176-189. http://dx.doi.org/10.1016/j.advwatres.2015.06.001

Richards L.A. (1931) - Capillary conduction of liquids through porous mediums. *Physics,* 1, p. 318-333.

Saltel M., Pédron N. (2012) – Contribution à la révision du SAGE Nappes Profondes de Gironde : Utilisation du Modèle Nord-Aquitain dans le cadre du module « Tendances et Scénarios ». Rapport BRGM/RP-60416-FR, 56 p., 24 fig., 5 ann.

Schaap M.G., Leij F.J. (1998) - Database related accuracy and uncertainty of pedotransfer functions, *Soil Science*, 163, p. 765-779.

Schaap, M.G., Leij, F.J., van Genuchten, M.T. (2001) - ROSETTA: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions, *J. of Hydrol.* 251, p. 163-176.

Šimůnek, J., Šejna, M., van Genuchten, M.T. (2006) - The HYDRUS software package for simulating the two- and three-dimensional movement of water, heat, and multiple solutes in variably-saturated media - User Manual - Version 1.0. http://ars.usda.gov/sp2UserFiles/

Place/53102000/pdf_pubs/P2164.pdf (*Access August 2020*)

Thiéry, D. (1990) – Software MARTHE. Modelling of Aquifers with a Rectangular Grid in Transient state for Hydrodynamic Calculations of Heads and Flows. Release 4.3. Rap. BRGM 4S/EAU R 32548.

Thiéry, D. (1991) - Modelling contaminant transport through the unsaturated zone in transient date with a random walk particles scheme. Proceeding of the Internat. Conf. on Groundwater, Flow and Pollution, Nanjing Univ. Press, China, p. 311-316.

Thiéry, D., (1993) – Modélisation des aquifères complexes - Prise en compte de la zone non saturée et de la salinité. Calcul des intervalles de confiance. *Revue Hydrogéologie*, 1993, n°4 pp. 325-336. https://hal-brgm.archives-ouvertes.fr/hal-01062466 (*Accès August 2020*).

Thiéry, D. 2005 – Saltwater intrusion modelling with an efficient multiphase approach: Theory and several field applications. *In: Groundwater and saline intrusion. Selected papers from the 18th Salt Water Intrusion Meeting 18 SWIM Carthagena 2004. Eds. L. Araguas, E. Custodio and M. Manzano, ISBN 84-7840-588-7, pp. 97-110*. www.swim-site.nl/pdf/swim18/swim18_009.pdf (*Access August 2020*).

Thiéry, D. (2006) – Didacticiel du pré-processeur WinMarthe v4.0. Rapport final. BRGM/RP-54652-FR, 86 p., 54 fig. http://infoterre.brgm.fr/rapports/RP-54652-FR.pdf. (*Access August 2020*).

Thiéry, D. (2007) – Tutorial for the WinMarthe v4.0 pre-processor. BRGM/RP-54652-EN, 89 p.,48 fig.

Thiéry, D. (2009a) – Modèles d'hydrogéologie. *in Traité d'hydraulique environnementale – Volume 3 - Modèles mathématiques en hydrologie et en hydraulique fluviale*. Tanguy J.M. (Ed.) - Éditions Hermès - Lavoisier. Chapitre 4 pp. 95-117. ISBN 978-2-7462-1838-3.

Thiéry, D. (2009b) – Modèles à Réservoirs en Hydrogéologie. *in Traité d'hydraulique environnementale – Volume 4 - Modèles mathématiques en hydraulique maritime et modèles de transport*. Tanguy J.M. (Ed.) - Éditions Hermès - Lavoisier. Chapitre 7 pp. 239-249. ISBN 978-2-7462-2006-5.

Thiéry, D. (2010a) – Modélisation des Ecoulements Souterrains en Milieu Poreux avec MARTHE. *in Traité d'hydraulique environnementale – Volume 9 – Logiciels d'ingénierie du cycle de l'eau*. Tanguy J.M. (Ed.) - Éditions Hermès - Lavoisier. Chapitre 4 pp. 77-94. ISBN 978-2-7462-2339-4.

Thiéry, D. (2010b) – Hydrogeologic Models. *in "Mathematical Models Volume 2, chapter 4, pp. 71-92 • Environmental Hydraulics Series"*. Tanguy J.M. (Ed.) –Wiley/ISTE London. ISBN: 978-1-84821-154-4.

Thiéry, D. (2010c) – Reservoir Models in Hydrogeology. *in "Mathematical Models Volume 2, chapter 13, pp. 409-418 • Environmental Hydraulics Series". Tanguy J.M. (Ed.) – Wiley/ISTE London. ISBN: 978-1-84821-154-4*.

Thiéry, D. (2010d) – Groundwater Flow Modeling in Porous Media Using MARTHE. *in "Modeling Software Volume 5, Chapter 4, pp. 45-60 • Environmental Hydraulics Series"*. Tanguy J.M. (Ed.) –Wiley/ISTE London. ISBN: 978-1-84821-157-5.

Thiéry, D. (2013) - Didacticiel du code de calcul Gardénia v8.1. Vos premières modélisations. Rapport BRGM/RP-61720-FR, 136 p., 101 fig. http://infoterre.brgm.fr/rapports/RP-61720-FR.pdf . (*Access August 2020*).

Thiéry, D. (2014b) – Logiciel GARDÉNIA, version 8.2. Guide d'utilisation. Rapport BRGM/RP-62797-FR, 140 p., 74 fig., 2 ann. http://infoterre.brgm.fr/rapports/RP-62797-FR.pdf.

(*Access August 2020*).

Thiéry, D. (2015b) – Modélisation 3D du transport de masse et du transfert thermique avec le code de calcul MARTHE – version 7.5. Rapport BRGM/RP-64765-FR, 338 p., 159 fig. http://infoterre.brgm.fr/rapports/RP-64765-FR.pdf (*Access August 2020*).

Thiéry, D. (2015c) – Modélisation 3D des écoulements en Zone Non Saturée avec le code de calcul MARTHE - version 7.5. Rapport BRGM/RP-64495-FR. 87 p., 36 fig. http://infoterre.brgm.fr/rapports/RP-64495-FR.pdf (*Access August 2020*).

Thiéry, D. (2015d) – Modélisation 3D du Transport Réactif avec le code de calcul MARTHE v7.5 couplé aux modules géochimiques de PHREEQC. Rapport BRGM/RP-65010-FR, 172 p., 89 fig. http://infoterre.brgm.fr/rapports/RP-65010-FR.pdf (*Access August 2020*).

Thiéry, D. (2015e) – Validation du code de calcul GARDÉNIA par modélisations physiques comparatives. Rapport BRGM/RP-64500-FR, 48 p., 28 fig. http://infoterre.brgm.fr/rapports/RP-64500-FR.pdf. (*Access August 2020*).

Thiéry, D. (2016) – Prise en compte de la végétation pour le calcul de l'Évaporation et de la Transpiration dans le code de calcul MARTHE v7.6. Rapport BRGM/RP-65918-FR, 78 p., 47 fig. http://infoterre.brgm.fr/rapports/RP-65918-FR.pdf (*Accès August 2020*).

Thiéry, D. (2018) – Logiciel ÉROS version 7.1. Guide d'utilisation. Rapport BRGM/RP-67704-FR, 177 p., 82 fig. http://infoterre.brgm.fr/rapports/RP-65918-FR.pdf. (*Access August 2020*)

Thiéry D. (2020a) – Code de calcul MARTHE v7.8 - Modélisation 3D des écoulements et des transferts dans les hydrosystèmes - Notice d'utilisation. Rapport BRGM/RP-69541-FR, 353 p., 161 fig.

Thiéry, D. (2020b) – Didacticiel du code de calcul MARTHE v7.8 - Exploration des fonctionnalités de modélisation des écoulements et des transferts dans les hydrosystèmes. Rapport BRGM/RP-69542-FR. 381 p., 256 fig.

Thiéry, D. (2020c) – MARTHE v7.8 - Analyse des écarts de simulation ; Exportations de fichiers de résultats en « shapefiles ». Rapport BRGM/RP-69210-FR. 38 p., 27 fig.

Vandenbeusch, M. (1976) - Essai et mise en production des aquifères profonds. Rapport n°2. Correction de salinité, pression et température sur les mesures piézométriques. *Rapport BRGM* 76 SGN 482 AME.

van Genuchten, M.T. (1980) - A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Amer. J.* 44, p. 892-898.

van Genuchten, M.T. (1982) - A comparison of numerical solutions of the one-dimensional unsaturated-saturated flow and mass transport equations. *Advances in Water Resour*. 5, p. 47-55. doi : 10.1016/0309-1708(82)90028-8. http://www.sciencedirect.com/science/article/pii/0309170882900288 (*Access August 2020*).

van Genuchten, M.T. (1985) – Convective-dispersive transport of solutes involved in sequential first-order decay reactions, Computers & Geosciences, 11(2), 129-147.

Vinsome, P.K.W., Westerveld, J. (1980) – A Simple Method for Predicting Cap and Base Rock Heat Losses in Thermal Reservoir Simulators, J. Canadian Petr. Techn. 19, 87-90, July-September 1980.

Voss, C. (1984) - SUTRA, a finite element simulation model for saturated unsaturated fluid density dependent groundwater flow with energy transport or chemically reactive single species solute transport. USGS National Center. Reston, Virginia.

Warrick, A.W., Biggar, J.W., Nielsen, D.R. (1971) - Simultaneous solute and water transfer for an unsaturated soil. *Water Resour. Res*. 7, p. 1216-1225.

Xu, T., Sonnenthal E., Spycher N., Pruess K. (2004) - TOUGHREACT User's Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media, *Lawrence Berkeley National Laboratory Report LBNL-55460*.

Zheng, Chunmiao, and P. Patrick Wang, (1999) - MT3DMS, A modular three-dimensional multi-species transport model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater systems; documentation and user¡¯s guide, U.S. Army Engineer Research and Development Center Contract Report SERDP-99-1, Vicksburg, MS, 202 p.

Annexe 1

Exchange coefficients between cells

Lateral exchanges

The exchange coefficient "T" between two adjacent cells with a hydraulic head difference "dH" allows calculating the exchange flow "Q":

$$Q = T \cdot dH$$

In the standard case of a harmonic average, the lateral exchange coefficients (T_N, T_S, T_E, T_O), in the north, south, east and west directions, respectively, are given by the following equation, here written for exchanges with the north:

$$T_N = 1/\left(\frac{1}{\frac{K \cdot dZ \cdot dX}{dY/2} / \sqrt{A_{Kx/Ky}}} + \frac{1}{\frac{K_N \cdot dZ_N \cdot dX}{dY_N/2} / \sqrt{A_{Kx/Ky}}} \right)$$

or, after development:

$$T_N = \frac{2 \cdot dX \cdot K \cdot dZ \cdot K_N \cdot dZ_N}{K \cdot dZ \cdot dY_N + K_N \cdot dZ_N \cdot dY} / \sqrt{A_{Kx/Ky}}$$

with:

K, K_N = horizontal hydraulic conductivities

DX = cell lengths (direction ox)

DY, DY_N = cell widths (direction oy)

DZ, DZ_N = water height in the cells (direction oz)

$A_{Kx/Ky}$ = plan anisotropy coefficient of the hydraulic conductivity

= K_{West_East} / K_{North_South}

N, S, E, W, H, B = North, South, East, West, Higher, Lower.

For exchanges with the south, the equation is identical by replacing the letter "N" (North) by "S" (South).

For exchanges with the east, we obtain:

$$T_E = \frac{2 \cdot dY \cdot K \cdot dZ \cdot K_E \cdot dZ_E}{K \cdot dZ \cdot dX_E + K_E \cdot dZ_E \cdot dX} \cdot \sqrt{A_{Kx/Ky}}$$

For exchanges with the west, the equation is the same, replacing the letter "E" (east) by "W" (west).

Exchanges with higher and lower cells:

The exchange coefficients with ‘Higher’ (H) and ‘Lower’ (L) cells are given by the equations:

$$T_H = 1/\left(\frac{1}{\frac{K_V \cdot dX \cdot dY}{dZ/2}} + \frac{1}{\frac{K_{VH} \cdot dX \cdot dY}{dZ_H/2}} \right)$$

or, after development:

$$T_H = \frac{2 \cdot dX \cdot dY \cdot K_V \cdot K_{VH}}{K_V \cdot dZ_H + K_{VH} \cdot dZ}$$

For the exchanges with lower layers, we obtain, after replacing the index "H" by "L":

$$T_B = \frac{2 \cdot dX \cdot dY \cdot K_V \cdot K_{VB}}{K_V \cdot dZ_B + K_{VB} \cdot dZ}$$

with:

K_V, K_{VH} and K_{VB} = vertical hydraulic conductivities of the centre, and of the upper and lower cells.

Annexe 2

Description of the "MARTHE Grids"

What is a "MARTHE grid"?

The MARTHE grid is an auto-documented file that describes a field of values at the centres of cells of a rectangular regular or irregular grid.

The rectangles are defined by rows and columns of variable width. The files are self-documented; the absolute abscissae of the columns and the absolute ordinates of row centres appear in clear in the file. The coordinates can be (generalized) Lambert coordinates in France, or for instance UTM coordinates, or any other orthonormal non-terrestrial system. The files are in “text format" and are easily used.

The system is compact as only the abscissae of the columns and the ordinates of the rows appear. For instance, a grid of 200 rows x 300 columns contains only 200 ordinates and 300 abscissae, or 500 values (instead of 60,000 abscissae and 60,000 ordinates: 120,000 values if the data were listed in a sequential format, or 240 times less).

The interest of a "MARTHE grid"

The values of a field are self-documented (geo-referenced) and can be re-used without any localization problems.

"MARTHE grids" can be created:

- Directly by WinMarthe;
- With Surfer ®, QGIS ®, or ArcGIS ® software;
- By importing files from Multilayer® (BRGM), GDM® (BRGM), EarthVision®, or Petrel® software.

"MARTHE grids" are accepted as input, and generated as output, by the following BRGM software packages: WinMarthe, MARTHE and Operasem.

Description of a "MARTHE grid"

Figure 174 shows an example of a MARTHE grid, version 9.0., with the following characteristics:

- Point of origin, lower left: x0 = 50; y0 = 110 (*x_Left_Corner=**50**; y_Lower_Corner=**110***)
- Number of columns = 5; Number of rows = 4 (*Ncolumn=**5**; Nrows=**4***)
- Abscissae of the centres of the 5 columns = **55 62.5 66.5 69 75**
- Ordinates of the 4 rows (top to bottom) = **165 155 140 120**
- Width (dx) of the 5 columns = **10 5 3 2 10**
- Width (dy) of the 4 rows (top to bottom) = **10 10 20 20**

- values in the grid:

4	**4.5**	**7.2**	**8.1**	**9.6**
3.3	**3.2**	**3.6**	**6**	**5**
1.5	**2.2**	**4.3**	**5.5**	**6.6**
-7	**-6.5**	**-5.5**	**-4.5**	**-3.5**

```
MARTHE_Grid Version=9.0
Title=Example of Marthe Grid                                    PERMEAB  1
[Infos]
Field=
Type=
Elem_Number=0
Name=
Time_Step=-9999
Time=0
Layer=0
Max_Layer=0
Nest_grid=0
Max_NestG=0
[Structure]
X_Left_Corner=50
Y_Lower_Corner=110
Ncolumn=5
Nrows=4
[Data_Descript]
! Row 1        :  0   ,    0        , <   1 , 2 , 3 , Ncolumn   >
! Row 2        :  0   ,    0        , < X_Centre_of_all_Columns >
! Row 2+1     :  1   , Y_of_Row_1     , < Field_values_of_all_Columns > , Dy_of_Row_1
! Row 2+2     :  2   , Y_of_Row_2     , < Field_values_of_all_Columns > , Dy_of_Row_2
! Row 2+Nrows : Nrows , Y_of_Row_Nrows , < Field_values_of_all_Columns > , Dy_of_Row_2
! Row 3+Nrows :  0   ,    0        , <     Dx_of_all_Columns   >
[Data]
0       0       1       2       3       4       5
0       0       55      62.5    66.5    69      75
1       165     4       4.5     7.2     8.1     9.6     10
2       155     3.3     3.2     3.6     6       5       10
3       140     1.5     2.2     4.3     5.5     6.6     20
4       120     -7      -6.5    -5.5    -4.5    -3.5    20
0       0       10      5       3       2       10
[End_Grid]
```

Figure 174 – Example of a MARTHE grid of 5 columns with 4 rows.

Tabs separate the numbers of the different columns, allowing easy import under Excel ® or any other spreadsheet. This helps extracting a row or column for graphic representation. The numbers can also be separated by one or several spaces instead of a (single) tabulation.

In the case of the grid of a uniform field (all field values are the same), the form is simplified. (Figure 175).

At the end of the simulation, supplementary parameters are indicated (field code, number of chemical elements, number of time steps, date of the time steps, etc.). These data are used by the WinMarthe preprocessor for sorting the simulation results by data type and according to the different time steps. This allows exporting the values of certain fields, at certain time steps, or for creating animations. On Figure 175, the field values are filled (Concentration in Mineral 2, Calcite, at time step 15, at date 120, in layer 1, of a unit of 1 layer).

```
MARTHE_Grid Version=9.0
Title=Example of Uniform Marthe Grid                    CONCENTR  1
[Infos]
Field=CONCENTR
Type=Miner
Elem_Number=2
Name=Calcite
Time_Step=15
Time=120
Layer=1
Max_Layer=1
Nest_grid=0
Max_NestG=0
[Structure]
X_Left_Corner=50
Y_Lower_Corner=110
Ncolumn=5
Nrows=4
[Constant_Data]
Uniform_value=7
[Num_Columns_/_x_/_dx]
1       2       3       4       5       Number of the 5 columns
55      62.5    66.5    69      75      Abscissae of the 5 column centres
10      5       3       2       10      Width of the 5 columns
[Num_Rows_/_y_/_dy]
1       2       3       4       Number of the 4 rows
165     155     140     120     Ordinates of the centres of the 4 rows (top to bottom)
10      10      20      20      Width of the 4 rows (top to bottom)
[End_Grid]
```

Figure 175 – Example of a MARTHE grid relative to a uniform field.

Annexe 3

Structure of a “bln” file

The structure of a "bln" file is very simple, as it is a text file that combines several polygons. An example is shown as Figure 176.

Each polygon is described by:

- A descriptive line,
- X and Y coordinates of each point of the polygon, one point per line. The X and Y coordinates can be separated by a space or by a tabulation.

The descriptive line gives:

- The number of points of the polygon (9 for the first polygon of the example, 7 for the second);
- The number "0" after the number of points, not used here;
- A descriptive name of the polygon ("Traj_0004" for the first polygon). This name can be a number, for instance the value of an isovalue, or a date);
- The letters "xy" (indicating a view in the x, y plane), or "xz" for a view in the x, z plane.

```
 9 0 Traj_0004 xy
550.000   2350.000
540.627   2300.000
535.084   2200.000
535.530   2100.000
565.387   2000.000
600.000   1932.299
620.743   1900.000
700.000   1821.899
798.049   1828.933
 7 0 Traj_0048 xy
1150.000   550.0000
1100.000   528.3288
1000.000   513.7328
913.7367   600.0000
900.0000   602.6250
800.0000   601.7477
700.0000   600.0000
```

Figure 176 – Example of a [.bln] file containing two polygons (the 1st of 7 points, the 2nd of 9 points).

Annexe 4

Description of application examples

Application examples are presented in the following sections:

- **Application example 1: Flow and mass transport in a three-layer aquifer system.**
- *Vertical anisotropy of the hydraulic conductivity*.
- *Pathlines.*
- *Recharge from rainfall.*
- *Transient state hydraulic simulation.*
- *Mass transport: TVD and MOC methods.*
- *Definition of a contaminated zone.*
- *Partition coefficient kd.*
- *Insertion of a nested grid.*
- *Automatic calibration of the parameters.*

- **Application example 4: Fine Radial Simulation of a rise of the free surface resulting from local recharge through the unsaturated zone.**
- *Radial grid.*
- *Vertical cross-section.*
- *Free surface.*
- *Dewatering or re-watering in transient state.*
- *Under-relaxation coefficient.*
- **Application example 5: Flow with density effects near the sea. Henry saltwater wedge.**
- *Simulation with density effects (salinity variations)*.
- *Diffusion*.
- **Application example 7: Flow below a River, through the unsaturated zone.**
- *Flow simulation with an "Unsaturated zone" scheme in transient state*.
- *Pseudo*-vertical cross-section.
- *Under-relaxation.*
- *Radial grid.*
- *Mass transport in the unsaturated zone.*
- *Infiltration in a pseudo-vertical cross-section.*
- **Application example 10: Multi-layer hydrosystem with Rivers.**
- *Multilayer system with wedging layers*.
- *River network*.
- *Stage-Discharge relation with the de Manning-Strickler formula.*
- *River flood in transient state.*
- *Mass transport in aquifer and in* rivers.

- **Application example 11: Simple hydrosystem with GARDENIA hydro-climatic scheme, Analysis of simulation variance.**
- *Coupled hydro-climatic GARDENIA balance*.
- *Coupling rain, evapotranspiration, runoff, recharge, groundwater-river exchanges.*
- *Analysis of simulation variance by using "observations time series" files.*

<< Others applications examples are described in report BRGM/RP-69542-FR (Thiéry, 2020b, *in French*). **>>**:

- **Application example 20: Effect of viscosity in thermal transfers: Flow in a horizontal column.**
  - *Effect of viscosity in heat transfer.*
  - *Hydraulic / heat-transport coupling.*
- **Application example 21: Unsaturated zone flow and transport in a column containing macropore**
  - *Flow and mass transport in a vertical column in the unsaturated zone containing a vertical drain.*
  - *"Unsaturated Zone" simulation scheme.*
  - *Van Genuchten retention law and relative permeability law*
  - *Preferential flow.*
- **Application example 22: Multiphase flow. Infiltration of tetrachlorethylene in a layered sandy soil initially saturated in water.**
  - *Multiphase "water-oil" flow in a heterogeneous environment.*
  - *Vertical cross-section.*
- **Application example 26: Analysis of simulation discrepancies and export in "shapefiles"**
  - *Transient state mass transfer simulation in a monolayer aquifer.*
  - *Direct export of simulated fields in a "shapefile" file and immediate visualization with QGIS or ArcGIS ®.*
  - *Analysis of simulation variance when using an "observations time series" file*.
  - *Automatic calculation of 15 criteria on the variance between observed and simulated time series.*
  - *Direct export of the variance criteria on the simulated time series as "shapefile" files and immediate visualization with QGIS or ArcGIS ®.*
  - *Analysis of the difference between two simulations made with different hypotheses.*

Table 9 lists the application examples that are used by each feature.

Functionality	Examples
Analysis of simulation deviation	26, 11
Automatic calibration of parameters	1
Crops and vegetation	
Dewatering	1, 4
Drainage network	10
Drain-conduit	
Export as "shapefile" GIS file	26
Free surface	4
Fresh water – saltwater interface	
GARDENIA balance: Rainfall – PET	11
Gas flow, venting	
Geothermal doublet well	
Hydraulics- Heat-transport coupling	
Lakes	
Langmuir or Freundlich isotherm	
Manning-Strickler relationship	10
Mass transport	1, 5, 7, 10
Mass transport in river	10
Mass transport in UZ	7
Mass transport method MOC	1
Multilayer with wedging layers	10
Multiphase flow	
Nested grid	1
Partition coefficient k_d	1
Pathlines	1
Preferential flow	
Radial grid	4, 7
Reactive transport (PHREEQC)	
Recharge by rainfall	1, 11
Production temperature coupling	
Salinity, density effects	5
Seepage surface	
Simulation of well	
Successive degradation	
Thermal transfer	
Impervious connections	
Transient state hydraulics	1, 4, 7, 10
Under-relaxation coefficient	1, 4, 7 10
Unsaturated zone (UZ) flow	4, 7
Velocities	5, 26
Vertical anisotropy	1
Vertical cross-section, Pseudo-vertical cross-section	4
Viscosity	

Table 9 - List of application examples used by each functionality.

Annexe 5

Icons and buttons of the WinMarthe preprocessor

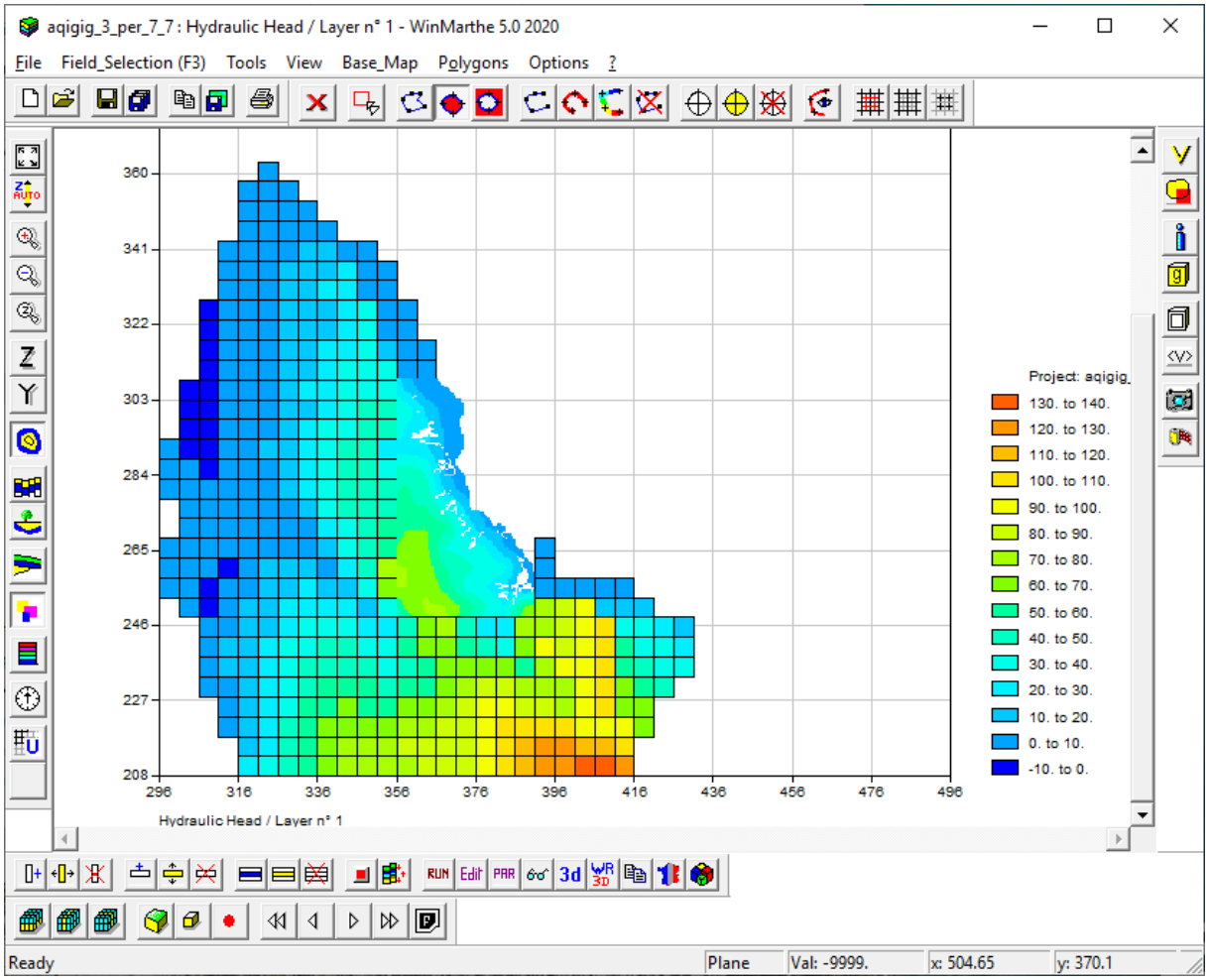


Figure 177 – Main window of the WinMarthe graphic pre-processor.

Buttons of the upper toolbar


Create a new project.


Open an existing project, [.rma] file.


Save the current project (save the edited files).


Save the current project under a new name (save the edited files).


Copy view to clipboard.


Save the view as a bitmap file [*.bmp].


Print screen image, for working documents.


Unselect all cells of the model (in all layers).


Select the cells within a rectangular domain defined by a scalable rectangle.

Ctrl + Scalable_Rectangle = Alt Gr + Scalable_Rectangle = Unselect.

Shift + Scalable_Rectangle = Invert the selection.


Digitize a closed boundary (double-click to finish and close the boundary).


Select the cells within the selected (or to be selected) boundary.


Select the cells outside the selected (or to be selected) boundary.


Create a line (double-click to finish).


Select the cells located on the selected line or boundary.


Interpolate or number the values along a(n) (open) line.


Delete the selected line or closed boundary.


Create points for "dressing" the drawing.


Modify the selected point.


Delete the selected point.


Display the polygons management dialogue box.


Create a new nested grid.


For a nested grid: hide the selected nested-grid cells (and show the main grid) => Create a "partial" nested grid.


For a "partial" nested grid: show the nested-grid cells hidden below the selected cells.

Buttons of the left toolbar

These buttons concern the visualization in plan or cross-section:


"Fit to page": the view fills the whole WinMarthe screen.

Determine an automatic vertical scale (for vertical cross-sections).


Zoom in: increase the image size. Also possible to define a zone for zooming by holding down the right-hand mouse button and defining a scalable rectangle.


Zoom out: reduce the image size.


Define a zoom factor. One centimetre on the screen will represent (100/zoom factor) coordinate units. For example, with a zoom factor of 5, 1 cm on the screen will represent (100/5) = 20 coordinate units.

Modify the Z amplitude coefficient for visualizing in vertical cross-section.

 Distort the Y ordinate with respect to the X abscissa (for plan views).

 Visualize a plan view.

 Visualize a "model"-style vertical cross-section along a preselected column or row.

 Visualize a "real"-style (interpolated) vertical cross-section along a preselected column or row.

 Colour cells according to layer number.

 Colour cells according to fieldvalue.

 Define customized colour classes.

 Shift from an East-West cross-section (along ox) to a North-South cross-section (along oy) or vice versa.

 Refresh the drawing: refresh colours.

Buttons of the right toolbar

Buttons mainly for actions concerning parameter values: selection by value, assignment and/or modification.

 Assign a value to a preselected cell or cell area.

 Provides access to cells outside the domain.

 Display the values of the different fields loaded in a cell and its neighbouring cells. After clicking on  , double-click on a cell to select it. If any values are modified, do not forget to click on **"Apply modifications"** in the Dialog box.

 Provides information on the model geometry: elevation of the top and bottom of the different layers. After clicking on  , double-click on a cell to select it. The values can be modified.

 Allows defining "watertight connections". After clicking on  , double-click on a cell. A Dialog box appears that allows selecting the sides of the cell where a tight connection is to be imposed.

 Select the cells whose parameter value is between given mini and maxi values. Or, select the cells whose values differ from a given value. Select either in the displayed layer or in all layers.

 Memorize the values of the current field in the selected cells. First, select cells in the current field. Then press this button => The values of these cells are memorized. It will be then possible, using button  to paste these values in another field.

 Paste the memorized selection => Into the current field. After having used button  , and then memorized the values of a field in a selected zone, choose another field: Use the button  to paste these values into the current field.

Buttons on the lower toolbars

First bottom row: buttons for constructing and refining the grid and for running external modules

 Add a column; divide the selected column into two columns of the same width. One must first be in "Column selection" mode and have selected a column.

 Modify the width of the selected column.

 Delete the selected column; group with the following column.

 Add a row; divide the selected row into two rows of the same width.

 Modify the width of the selected row.

 Delete the selected row; group with the following row.

 Add a layer: insert a layer above the current layer. **Use of this button is discouraged**. Instead, use the menu "Tools➔ Others ➔ Grid or coordinates modification".

 Modify the thickness of a layer. **Use of this button is discouraged**. Instead, use the menu "Tools➔ Others ➔ Grid or coordinates modification".

 Delete current layer. **Use of this button is discouraged**. Instead, use the menu "Tools➔ Others ➔ Grid or coordinates modification".

Attention: All grid-definition operations must be done before introduction of field values. WinMarthe does not allow to manage the transfer of fields from one mesh to another different mesh. However, one can use the grid modification tool ("Tools➔ Others ➔ Grid or coordinates modification"). **If one wants to construct an irregular grid, it is much easier directly to use the option "Create an irregular grid", rather than modify a regular grid**.

 Check the geometric consistency (compares the top and bottom [substratum] elevations); offers the possibility of correcting inconsistencies.

 Update the cell elevations from the topography and the substratum. This operation may be necessary after certain imports or transformations that modify the topography or substratum.

Run the "MARTHE" computer computational engine.

Edit the numerical values of the selected field and layer.

Run the "**Paramart**" module for introducing the computation parameters and options of the MARTHE computational engine.

 Examine [.txt] , [.out] , [.avi] , [.pdf] , [.hlp] , [.htm], etc., files. Particularly suitable for examining the convergence and balance results at the end of a computation ("flowbalance.txt", "mart_ver.txt" files) or any other text file.

3D visualization.

3D VRML visualization.

File management: Copy / Delete / Rename / Edit.

Export of files in "shapefile" format that can be used by QGIS ® or ArcGIS ® software, or in the mif/mid format that can be used by MapInfo®. The files that can be exported are "Marthe-Grid" files, [.bln] files (lines, boundaries, velocities, etc.), pathline files (pathline.out) and particles files. Also for transforming MapInfo line or boundary files [.mif] into WinMarthe [.bln] format with a coordinate system change.

Also transformation of lines or contours [.mif] files into the [.bln] format with change of coordinate system for use in WinMarthe.

Also transformation of "shapefile" [.shp] files into line [.bln] files.

3D visualization:

- Visualization with 3D View (Winteracter ®)
- Export in VTK format for visualization with Paraview ®
- Export to Tecplot ®

Second bottom row: buttons for different layer-, row-, column- or cell selection modes

Shift to "Layer selection" mode. To select all cells of the layer, double-click on a cell of the layer that then turns red.

Shift to "Column selection" mode. To select a column, double-click on the column that then turns red.

Shift to "Row selection" mode. To select a row, double-click on the row that then turns red.

Select the whole domain (select all cells in all layers).

Shift to "Cell selection" mode. Double-click on a cell to invert its mode (select the cell if it had not been selected; unselect it if it had been selected). The selected cells turn red (or purple if they are outside the grid).

When visualizing in vertical cross-section, during a change of row or column, allows to move the selected row or column (*not very useful*).

Return to the first row / column / layer of the grid, depending on whether the view is a North-South vertical cross-section, an East-West vertical cross-section, or a plan view.

Visualization in vertical cross-section: Move back a row / column / layer of the grid.

Visualization in vertical cross-section: Move forward a row / column / layer of the grid.

Move to the last row / column / layer of the grid.

Keyboard shortcuts

- **F3** : Select a field
- Control_**A** : Select **A**ll
- Control_**B** : Open a "Work" page (Draft = "**B**rouillon" in French)
- Control_**C** : **C**opy the view (or part of it) in the clipboard
- Control_**D** : **D**ouble contour lines Isovalues
- Contrl_**E** : Grid **E**ditor
- Control_**F** : **F**it to Page
- Control_**G** : **G**o to column, row, layer
- Control_**H** : Visualization of cells with time series ("**H**istorique" in French)
- Control_**I** : Single Field contour lines (**I**sovalues)
- Control_**L** : Classes with **L**inear spacing
- Control_**P** : **P**rint the window
- Control_**Q** : Classes with e**Q**ual distribution spacing
- Control_**R** : Open a **R**esults file (simulated fields)
- Control_**S** : **S**ave the project
- Control_**T** : Classes with logari**T**hmic spacing
- Control_**U** : Classes with **U**ser-defined spacing
- Shift+Control_**S** : **S**ave the project as
- Shift **F5** : Run the simulation

- Alt_**C** : Visualization of cell boundaries (**C**ontours in French)
- Alt_**F** : Display the base map ("**F**ond de carte" in French)
- Alt_**M** : Display the grid ("**M**esh")
- Alt_**O** : **O**peration among parameters
- Alt_**P** : **P**olygons management
- Alt_**S** : **S**tatistics
- Alt_**T** : Numerical **T**ransformation

- Contr+Alt_**T** : Colour classes for the whole (**T**otal) domain

Géosciences pour une Terre durable
brgm

Centre scientifique et technique
Direction de l'Eau, de l'Environnement, des Procédés & Analyses (DEPA)
3, avenue Claude-Guillemin
BP 36009 – 45060 Orléans Cedex 2 – France – Tél. : 02 38 64 34 34
www.brgm.fr