



Project no. 505428 (GOCE)

## AquaTerra

**Integrated Modelling of the river-sediment-soil-groundwater system; advanced tools for the management of catchment areas and river basins in the context of global change**

### Integrated Project

**Thematic Priority: Sustainable development, global change and ecosystems**

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<b>Dissemination Level</b>		
<b>PU</b>	<b>Public</b>	<b>X</b>
<b>PP</b>	Restricted to other programme participants (including the Commission Services)	
<b>RE</b>	Restricted to a group specified by the consortium (including the Commission Services)	
<b>CO</b>	Confidential, only for members of the consortium (including the Commission Services)	

## SUMMARY

In the framework of Workpackage R3 Meuse, the Hydrogeology Group of the University of Liège (HGULg) develops a groundwater flow and transport model for the Geer sub-catchment (tributary of the Meuse) (Figure 1, Deliverable R3.16 (Orban et al 2006)). In the scope of TREND T2, the model will be used to develop trend forecasting tools.

The objective of the deliverable is to describe new concepts for large-scale transport modelling, more particularly a modelling approach, the Hybrid Finite Element Mixing Cell (HFEMC) developed by HGULg and implemented in the 3D simulator SUFT3D. First steps for the application to the Geer basin are also presented.

## MILESTONES REACHED (from DOW II p. 81 to 86)

**ONLY LIST MILESTONES RELEVANT TO THIS DELIVERABLE AND  
QUICKLY OUTLINE WHICH OTHER GROUPS AND  
WORKPACKAGES CAN BENEFIT FROM IT**

**No milestones are associated to this deliverable**

**The groundwater flow and transport model developed for the Geer basin has been delivered to T2 to model nitrate trends in the Geer basin.**

## Glossary

Eulerian approach	Numerical approach to solve the advection – dispersion equation in a fixed mesh.
Lagrangian approaches	Numerical approach to solve the advection – dispersion equation in a mobile mesh.
Mixed eulerian-lagrangian approach	Numerical approach to solve the advective part of the advection – dispersion equation in a mobile mesh and the dispersive part in a immobile mesh.
TVD shemes	TVD = Time variation diminishing. High order upstream scheme
Dirichlet boundary condition	Main variable (pressure or concentration) is prescribed
Neumann boundary condition	Flux is prescribed
Cauchy boundary conditions	The exchanged water flux is a function of the difference of water level
The SUFT3D	Saturated Unsaturated Flow Transport 3D
CVFE	Control volume finite element
HFEMC	Hybrid Finite Element Mixing Cell
EMS-I company	Environmental Modeling System, Inc. Head distributor the GMS (Groundwater Modeling System)
EPIC-GriD soil model	Semi-distributed physically based soil model developed by UHAGx

## Introduction

In the framework of Workpackage R3 Meuse, the Hydrogeology Group of the University of Liège (HGULg) develops a groundwater flow and transport model for the Geer sub-catchment (tributary of the Meuse) (Figure 1, Deliverable R3.16 (Orban et al 2006)). In the scope of TREND T2, the model will be used to develop trend forecasting tools.

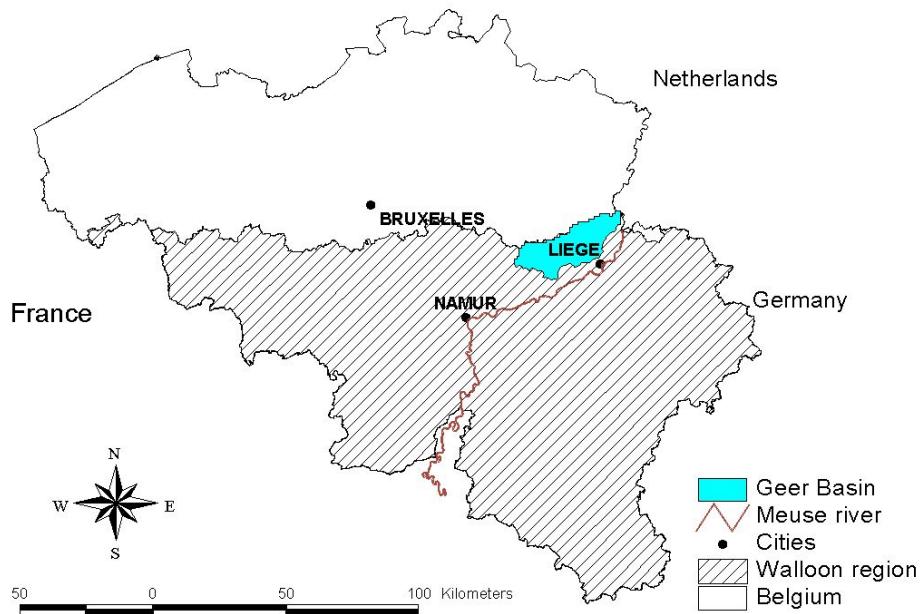


Figure 1: Location of the Geer basin

The objective of the deliverable is to describe new concepts for large-scale transport modelling, more particularly a modelling approach, the Hybrid Finite Element Mixing Cell (HFEMC) developed by HGULg and implemented in the 3D simulator SUFT3D. First steps for the application to the Geer basin are also presented.

## Concepts of large-scale transport modelling

Efficient and sustainable management of water resources should be considered from an integrated way, at the basin scale. For understanding physical mechanisms, interactions between different components of the water cycle and for defining optimal ways of water management, physically-based, spatially distributed modelling tools has turned to be very useful. Regional groundwater models have been developed for years now (e.g. BRGM 1998, Besbes et al. 2003, Brouyère et al. 2004, Drobot 2004), however, models dealing with large scale contaminant transport models and methods for assessing transport processes and calibrating models at such scales are still almost nonexistent.

The first problem that arises when modelling large scale transport relates to the difficulty in quantifying and/or scaling transport processes (mostly advection and hydrodynamic dispersion) at such scales. Classical techniques used to quantify transport processes in the field, such as tracer experiments (eg. Käss 1998, Brouyère et al. 2005) do apply at local to medium scales (from a few meters to a few hundred meters). Because of these limitations, important research efforts have been devoted to upscaling techniques from local to large scale (e.g. Gelhar & Axness 1983, Desbarats 1990, Dagan 1994). Such researches have however always been limited to relatively theoretical aspects. For diffuse pollution, due to the dispersion of the source, local dispersivities have little effects on the concentration measured at discharge points (Eldor and Dagan 1972, Duffy and Lee 1992)

The second problem relates to the numerical solution of mathematical equations classically used for modelling transport processes in the underground (advection-dispersion equation). Classical techniques require long computation times and large computer memory because refined meshes are required in order to avoid problems such as numerical dispersion or instabilities. An alternative is to use simplified approaches for modelling transport at large scale, such as transfer functions (linear reservoir, piston-flow...) but with the drawback that modelling results are not spatially distributed anymore and they loose precision.

The challenge consist thus in finding a good compromise between a good physical description of the phenomena governing the groundwater flow and solute transport and the numerical approach. HGULg proposes a mixed approach made of a compilation of existing solutions.

## **Existing approaches for modelling large scale contaminant transport in groundwater at the basin scale**

Generally speaking, existing mathematical approaches used to model contaminant transport at large scale can be grouped into three main categories: transfer function approaches, compartment models and models relying on advanced solution of the advection-dispersion equation.

Transfer function models, sometimes referred to as “black box” models, are usually used for the interpretation and correlation of datasets at the entry and outlet of the underground system (e.g. recharge and discharge zones). The transfer function can be obtained through deconvolution of available time series. It can also be expressed as a more or less elaborated parametric mathematical equation (e.g. Jury 1982, Skaggs et al 1998, Amin & Campana 1996, Stewart & Loague 1999). Such approaches are relatively simple and they require a limited number of parameters to be assessed. However they provide a relatively low accuracy and because these models rely on integral mass balance formulations relating mass flux and concentrations at the system entry and output, the spatial distribution and time evolution of concentrations within the underground system remain unknown. Such approaches have been mostly applied to isotopic and environmental tracer data (e.g. Duffy & Gelhar 1986, Ritzi et al 1991, Maloszewski & Zuber 1996).

Even if they are still based on simplified mathematical concepts such as transfer functions, compartment modelling approaches have the advantage of being spatially distributed. They are usually made of black-box models connected in series or spatially distributed (e.g. Campana & Simpson 1984, Harrington et al. 1999). Such models have also been predominantly applied to studying isotopic and environmental tracer distributions in groundwater systems.

Modelling large scale transport models based on the advection-dispersion equation need that a compromise be found between the degree of spatial refinement and computational costs (memory and time). Various advanced numerical techniques have been developed based on eulerian, mixed eulerian-lagrangian or purely lagrangian approaches. Recently, new promising numerical schemes have been proposed (TVD schemes) that are able to control numerical dispersion inherent to using less refined groundwater meshes (Harten 1983).

Because all approaches, from simple transfer function models to spatially distributed models based on the advection dispersion equation, might be adapted to specific situations (available data, complexity of the hydrogeological context or details expected in the results), a methodology and modelling tool that allows choosing different kinds of modelling concepts and changing from one approach to another (e.g. from a simplified approach to a more advanced approach) has been developed recently (Orban et al. 2005) and applied to large scale groundwater modelling (Brouyère et al. 2004b).

## **General approach for groundwater flow and transport modelling**

In 2001, the Government of the Walloon Region (Belgium) initiated the PIRENE project to develop tools for integrated water quantity/quality modelling in the Walloon region. As a partner of this project, HGULg has developed a physically based, transient groundwater flow and transport model for the Walloon part of the Meuse Basin (approximately 18.000 km<sup>2</sup>). The methodology (Figure 2) and the numerical code group together different approaches (non distributed or distributed mixing cells, advection-dispersion equation...). It allows the transition from a simplified approach to a deterministic model (Orban et al 2004). This new methodology was tested on the Walloon part of the Meuse basin (Brouyère et al. 2004c).

This methodology is now used and improved to develop a groundwater flow and transport model for the Geer basin for nitrate trend forecasting. The model will integrate the results of the nitrate trend analysis developed for the Geer basin in the framework of the Aquaterra project (Deliverable T2.4).

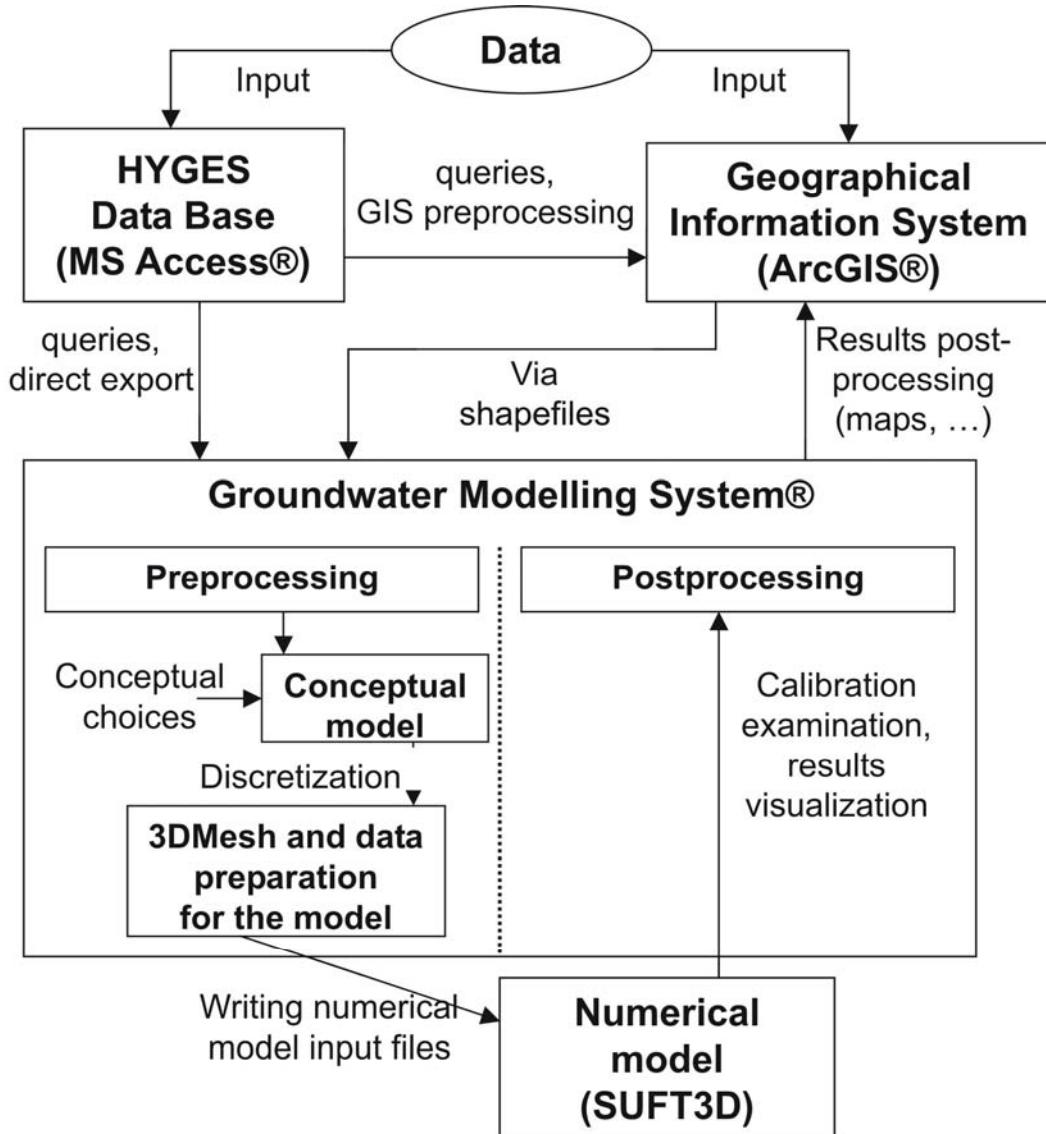


Figure 2: Scheme of data management

### ***Data management and model preprocessing***

Large amounts of data are required for large-scale groundwater flow and transport modelling when adopting a spatially distributed and physically consistent approach. Geological data such as maps, borehole data and logs, data from geophysical surveys have to be used in an optimal way to create the spatial discretization. Parameters such as values of hydraulic conductivity, specific yield and porosity of the different distinguished hydrological units are needed to constrain the calibration of the model. Historical values of piezometric levels and concentrations are needed for calibration and validation procedures. These data have been collected and introduced in a hydrogeological database (HYGES) coupled with a GIS system (ArcGIS®) (Gogu et al. 2001, Wojda 2005). Based on queries and GIS preprocessing, data are transferred into the pre- and post-processor package Groundwater Modelling System (GMS®). A conceptual model is developed that consists in different layers of information built independently of any numerical and discretization choices. This information is transferred in a further step to the mesh used for the computation. This procedure allows new data being easily introduced

and processed. After computation, visualization of results can be performed using GMS, ArcGIS, or any other visualization tools for calibration, output production...

## ***Numerical development***

### **Conceptual model**

In large scale models, one has to play with spatial heterogeneities:

- many hydrogeological basins can be covered;
- the knowledge or hydrogeological characterisation can vary strongly from one part of the modelled area to another one;
- various geological contexts generate drastically different hydrogeological conditions (eg less permeable formations, porous, fissured and karstic media...).

To face this reality, two basics assumptions have been adopted for cutting the global area. First, hydrogeologically independent sub-basins can be modelled independently. Secondly, different ways of modelling are considered in function of the investigation degree and the data availability. The global model is therefore divided in subdomains in function of the local hydrogeological characteristics and the degree of hydrogeological characterisation.

Exchange of water fluxes is made possible and eventually simulated between these subdomains and with the others compartments of the water cycle (recharge computed by a soil model, exchanges of water with the rivers). These interactions are conceptualised by classical boundary conditions (ie Dirichlet, Neumann, Cauchy boundary conditions).

### **Adapted version of the SUFT3D code: Hybrid Finite Element Mixing Cell (HFEMC) method**

The SUFT3D (Saturated Unsaturated Flow Transport 3D) is a control volume finite element (CVFE) code developed by the HGULg (Carabin et al 1999, Brouyère 2001). For the purpose of the PIRENE project, the code has been translated in Fortran 90, using dynamic allocation and progressive object-oriented coding (new Fortran derived-types such as subdomains, elements,...). In its original version, the code solves the classical flow and advection-dispersion equations. However such equations require a large amount of parameters and thus are not always adapted for large scale modelling. A new flexible and modular method, called the Hybrid Finite Element Mixing Cell (HFEMC) approach has thus been coded and implemented in the SUFT3D code. In each subdomain, different mathematical and numerical solutions of the groundwater flow and transport equation can be selected in function of the actual degree of knowledge of the hydrogeological conditions. Basic approaches such as linear reservoir, distributed reservoir or mixing cells can be used where the hydrogeological knowledge is limited. In subdomains where the hydrogeological characterisation is sufficiently detailed, more detailed, physically consistent solutions based on Darcy's law and the advection-dispersion equation can be applied. The choice of a simplified solution for simulating groundwater flow conditions implies to choose also a simplified method for solving the transport

problem (Table 1). Actually, for example, to solve the advection-dispersion equation, Darcy's fluxes exchanged between nodes are needed so it's necessary to solve the classical flow equation.

		TRANSPORT		
		<i>Simple Linear Reservoir</i>	<i>Distributed Mixing Model</i>	<i>Advection-dispersion</i>
FLOW	<i>Simple Linear Reservoir</i>	OK	impossible	impossible
	<i>Distributed Linear Reservoir</i>	OK	OK	impossible
	<i>Flow in porous media</i>	OK	OK	OK

Table 1: Solutions implemented in the SUFT3D code and restrictions of use.

Linear reservoir models imply that the characteristics at the outlet of the aquifer are linearly linked to the mean behaviour of the reservoir which is made of a single entity. In continuity between the linear reservoir model and the classical flow model, distributed linear reservoir models have also been implemented in the SUFT3D. This continuity allows, if further data are acquired, to move from a simplified approach to a more complex one.

Classical spatial discretisation used for distributed linear reservoir models are based on simple geometric form like parallelepiped mesh. If such a kind of mesh simplifies the discretisation work and the computation of the fluxes exchanged between the cells, it is not possible to represent complex geometries such as the ones met in hydrogeology. In the HFEMC method, a complex spatial discretisation based on the finite element with control volume is used to define the geometry of the problem and the mixing volumes associated to each node. In order to apply the simple linear reservoir in a given subdomain, all the elements of the subdomain are grouped together, a single unknown (ie : mean groundwater level, mean concentration) being applied for the whole subdomain. The finite element discretisation is then only used to define the external boundary of the subdomain, its interactions with the other subdomains or the other compartments of the water cycle and to compute the global volume of the reservoir as the sum of the effective volumes associated to each element.

### ***Groundwater flow modelling with the code SUFT3D***

#### Single linear reservoir model

The single linear reservoir model is conceptually very simple. Mathematically, this model means that the flux at the outlet of the reservoir varies linearly in function of the water level in the reservoir:

$$Q_{res} = V_{res} \frac{\partial \theta}{\partial t} = S A_{res} \frac{\partial \bar{H}}{\partial t} = -\alpha_{res} \bar{H} \quad (1)$$

where,

- $V_{res}$  is the total geometric volume of the reservoir ( $L^3$ ) ;
- $\theta$  is the volumic proportion of water in the reservoir (-) ;
- $S$  is the storage coefficient of the reservoir (-) ;
- $A_{res}$  is the area of the reservoir ( $L^2$ ) ;
- $\bar{H}$  is the mean water level in the linear reservoir. It is the unknown of the problem ( $L$ ) ;
- $\alpha_{res}$  is the recession coefficient at the reservoir outlet ( $L^2 T^{-1}$ )

This model is often used by hydrologists to evaluate the groundwater recession in the river to model the contribution of groundwater to the base flow.

This model can be easily improve by the addition of base drainage level of the reservoir ( $H_b$ ) and a sink/source term  $Q$  ( $L^3 T^{-1}$ ),

$$S A_{res} \frac{\partial \bar{H}}{\partial t} = -\alpha_{res} (\bar{H} - H_b) + Q \quad (2)$$

### Distributed linear reservoir model

It is possible to connect different linear reservoirs all together, in which case the term  $H_b$  of Equation 2 is replaced by the mean water level  $H_j$  in reservoir  $J$  connected to reservoir  $I$ . Equation 2 becomes:

$$\frac{\partial V_{w,I}}{\partial t} = V_{res,I} \frac{\partial \theta_I}{\partial t} = S A_{res,I} \frac{\partial H_I}{\partial t} = \sum_{J \in \eta_I} \alpha_{IJ} (H_J - H_I) + Q_I \quad (3)$$

where  $V_I$  ( $L^3$ ) is the volume of reservoir  $I$ ,  $V_{w,I}$  is the volume of water contained in reservoir  $I$ ,  $\theta_I$  (-) is the volumic proportion of water in reservoir  $I$ ,  $H_I$  ( $L$ ) is the water level in reservoir  $I$ , the terms  $H_J$  ( $L$ ) are the water levels in cells  $J$  hydraulically connected with cell  $I$ , the terms  $\alpha_{IJ}$  ( $L^2 T^{-1}$ ) are the exchange coefficients between cell  $I$  and the cells  $J$  located in its neighbourhood  $\eta_I$ .

### 3D flow equation in porous media

The 3D flow equation in porous media can be written as :

$$F \frac{\partial h}{\partial t} = \nabla \cdot (\underline{\underline{K}} \cdot \nabla (h + z)) + q \quad (4)$$

where,  $F$  is a generalised specific storage coefficient ( $L^{-1}$ ),  $\underline{K}$  is the tensor of hydraulic conductivity,  $h$  is the pressure potential ( $L$ ),  $z$  is the gravity potential ( $L$ ) and  $q$  ( $T^{-1}$ ) is the possible volumic sink/source term.

In the SUFT3D simulator, this equation is solved by the application of the classical finite element method or by the control volume finite element method (Brouyère, 2001).

### **Solute transport modelling with the code SUFT3D**

#### Simple linear reservoir transport model or simple mixing

Solutes migrating in the subsoil are subject to hydrodynamical dispersion and diffusion leading to a progressive mixing with groundwater. The assumption of perfect mixing consists in assuming that water entering is instantly and perfectly mixed with the water in a cell. The solute concentration within this volume is thus assumed uniform. The same model allows easily considering partial mixing by reduction of the mixing volume.

Mathematically, this model is defined as:

$$\frac{\partial(V_{\text{eff},\text{res}} \bar{C})}{\partial t} = Q_{\text{in}} C_{\text{in}} - Q_{\text{out}} C_{\text{out}} \quad (5)$$

where  $V_{\text{eff},\text{res}}$  ( $L^3$ ) is the effective mixing volume of the reservoir,  $\bar{C}$  ( $ML^{-3}$ ) is the mean concentration in the reservoir (unknown of the problem),  $Q_{\text{in}}$  et  $Q_{\text{out}}$  are ( $L^3T^{-1}$ ) the flow rates coming in and out the reservoirs at concentrations  $C_{\text{in}}$  et  $C_{\text{out}}$  ( $ML^{-3}$ ) respectively.

The assumption of linearity is reflected mathematically by the fact that the concentration in the flow rate coming out of the reservoir is set equal to the mean concentration in the reservoir:

$$C_{\text{out}} = \bar{C} \quad (6)$$

The linear reservoir transport model can then be written :

$$\frac{\partial(V_{\text{eff},\text{res}} \bar{C})}{\partial t} = Q_{\text{in}} C_{\text{in}} - Q_{\text{out}} \bar{C} \quad (7)$$

This model can be generalised to multiple flow rates coming in and out :

$$\frac{\partial(V_{\text{eff},\text{res}} \bar{C})}{\partial t} = \sum_k Q_{\text{in},k} C_{\text{in},k} - \sum_l Q_{\text{out},l} \bar{C} \quad (8)$$

Under the assumption of perfect mixing, the effective mixing volume  $V_{\text{eff},\text{res}}$  is equal to the volume of water ( $V_{\text{eff},\text{res}} = V_{\text{res}} = SA_{\text{res}} \bar{H}$ ). Under the assumption of partial mixing it

is limited to a part of the volume of water ( $V_{eff,res} = \mu V_{res}$ ). The  $\mu$  ( $0 \leq \mu \leq 1$ ) coefficient is called mixing coefficient or coefficient of mixing efficiency.

### Distributed mixing model

To apply the simple mixing model, the volume of the mixing cell and the fluxes exchanged with its neighbourhood have to be defined. If the mixing cell exchanges with other mixing cells, we have a compartment mixing cell or a distributed mixing model.

Mathematically, a transport equation of linear reservoir has to be written for each mixing volume  $V_{eff,I}$  defined in the subdomain. In a general way, this equation can be written as :

$$\frac{\partial(V_{eff,I} C_I)}{\partial t} = \sum_{J \in \eta_I} Q_{IJ} C_{IJ} + Q_I C' \quad (9)$$

where  $V_{eff,I}$  ( $L^3$ ) is the mixing volume associated to the cell  $I$ , the terms  $Q_{IJ}$  ( $L^3 T^{-1}$ ) are the flow rates between the volume  $I$  and the volumes  $J$  connected to  $I$ , the  $C_{IJ}$  ( $ML^{-3}$ ) are the concentrations associated to the exchanged flow rates  $Q_{IJ}$ ,  $C'$  ( $ML^{-3}$ ) is the concentration associated to the sink/source term  $Q_I$  ( $L^3 T^{-1}$ ).

### Advection – dispersion equation in porous media

The numerical schemes (method of Galerkin and SUPG scheme) at the moment implemented in the code do not allow solving the advection-dispersion equation for large scale problems without numerical difficulties. Moreover, it is difficult to obtain transport parameters (mainly dispersion coefficient) representative of this scale.

Some particular hydrodispersive processes such as immobile water effect, linear degradation, or equilibrium sorption laws, usually used with the advection-dispersion equation, remain available with the distributed mixing model.

### **Development of an interface for the SUFT3D**

Previously, the interface of the SUFT3D code was limited to a few pre-processing (building of the mesh, definition of boundary conditions) and post-processing operations with the GMS software (Groundwater Modelling System) developed by the Brigham Young University and the EMS-I company. In practice, to develop a groundwater flow or transport model with the SUFT3D code, the user had to write some input file with text editors. For large scale modelling, it was essential to develop new tools to simplify the pre-processing operations and to allow direct interactions between database – SIG and the numerical code. Different modules were developed with MatLab tools to manage the cutting of the global mesh into subdomains and the interactions between these subdomains, to introduce the boundary conditions (more particularly interactions with the river network and recharge) and to create the input file.

## Mesh module

A 3D finite element based spatial discretization is adopted for each subdomain. The possible exchange of water between the subdomains is modelled by internal boundary conditions of three types. If the piezometric level can be considered as continuous between two subsequent subdomains, a Dirichlet boundary condition (1<sup>st</sup> type) is prescribed. If, the piezometric level cannot be considered as continuous, the two subdomains exchange water based on the difference in piezometric levels between the two adjacent nodes and a Cauchy boundary condition (3<sup>rd</sup> type) is prescribed. If there is no exchange of water, a no flow boundary is prescribed. Numerically, the second and the third internal boundary condition require the unknowns on the boundary be duplicated. So, in practice, the nodes of the arc representing the limit between these subdomains have to be doubled (Fig. 3). For this operation, a mesh division module has been developed. Using polygons for representing the subdomains, it is allowed (a) to define the type of internal boundary conditions between subdomains, (b) to divide the original mesh into submeshes by duplicating the boundary nodes, (c) to renumber the elements and the nodes for obtaining a continuous numbering in each submesh. Subdomains and internal boundary conditions can also be useful to represent two aquifers separated by a thin less permeable layer (aquitard). Each aquifer becomes a subdomain and the exchange of water through the thin less permeable layer is represented by a Cauchy internal boundary condition.

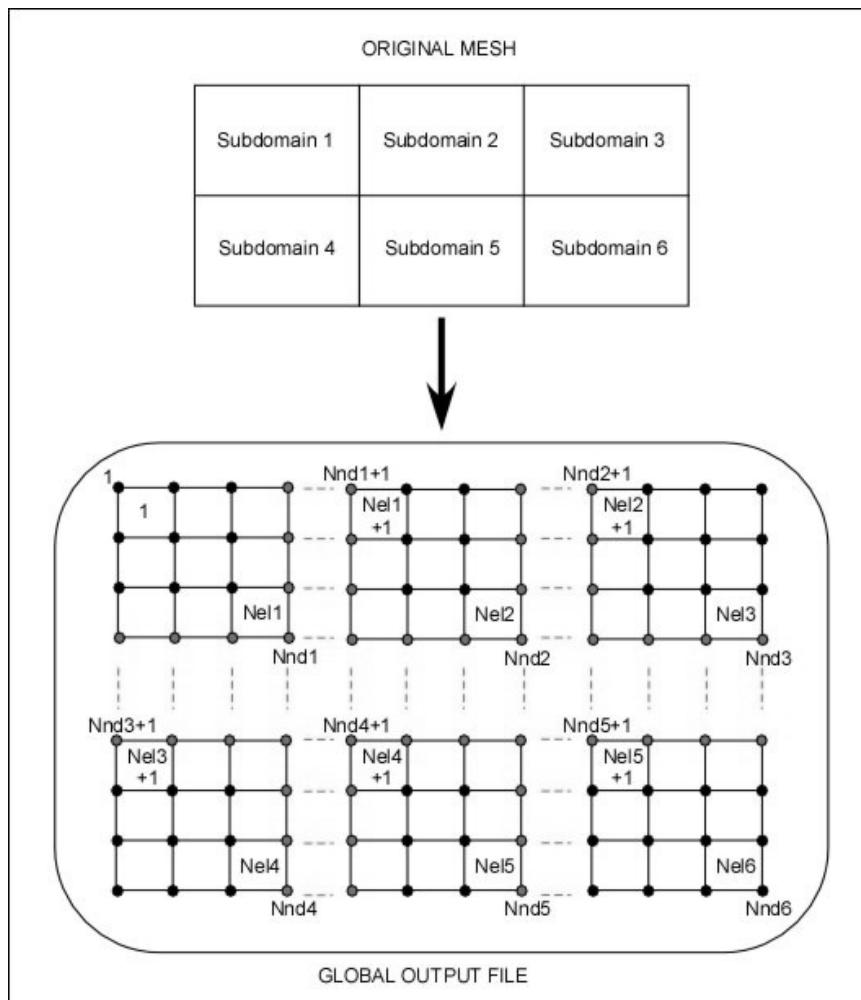


Figure 3: Scheme of renumbering of the mesh

## River module

In hydrogeological models, rivers are often introduced through the use of Cauchy boundary conditions (i.e. the exchanged water flux is a function of the difference of water level in the river and the aquifer). At large scale, it is often difficult and inefficient to take the river network into account explicitly in the 3D discretization process. To perform the mapping between the river network and the 3D mesh, a module has been developed to compute the length of the river segment crossing the upper face of each element  $e_i$  (Fig. 4) and a conductance coefficient  $\alpha_i$  allowing computing the water flux between the aquifer and the river:

$$Q_i = \alpha_i (h_{riv,i} - h_{aq,i}) = \frac{K_i L_i l_i}{E_i} (h_{riv,i} - h_{aq,i}) \quad (10)$$

where  $Q_i$  is the water flux exchanged between the river and the aquifer through element  $e_i$  ( $m^3/s$ ),  $K_i$  the hydraulic conductivity of the river sediments ( $m/s$ ),  $L_i$  the length of the river segment in element  $e_i$  (m),  $l_i$  the width of the river (m),  $E_i$  the thickness of the river sediment (m),  $h_{riv,i}$  the mean water level in the river in the element  $e_i$  (m),  $h_{aq,i}$  the groundwater level in the element  $e_i$  (m).

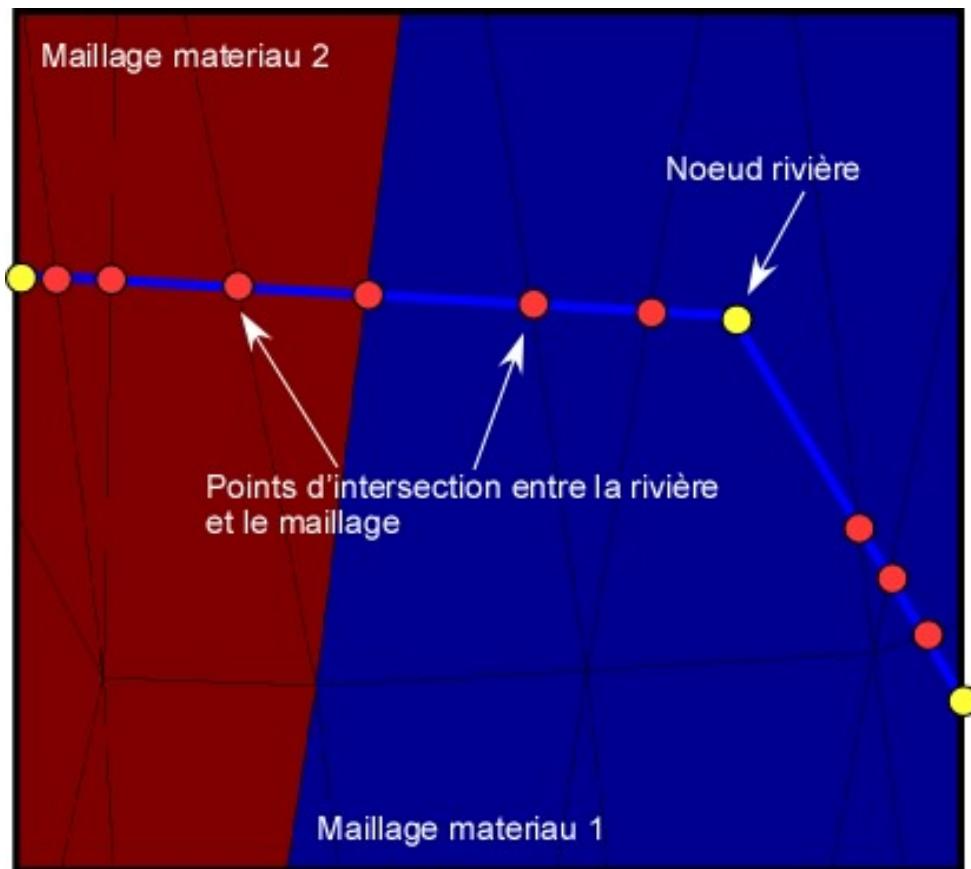


Figure 4: Intersection (red points) between the mesh and the river network (yellow points)

## Recharge module

Recharge to the aquifer can be simply computed based on hydrological budgeting and then defined as a prescribed flux at the top of the mesh. UHAGx team develops the EPIC-GriD soil model (Dautrebande et al. 2005; Deliverable T2.2). With this

model, water and nitrates fluxes to groundwater are computed for the whole Walloon region on the basis of a 1 km<sup>2</sup> squared-grid for the period 1960-2000 with a daily time step. A module has been developed to assure the spatial and temporal mapping between the two models and to input these results into the groundwater model.

## ***The model developed for the Geer basin***

### **Introduction**

This section describes the first steps that were performed in order to develop a groundwater flow and transport model for the Geer basin. These first developments consist in the establishment of a 3D finite element discretization of the geology in the basin, the definition of appropriate boundary conditions (recharge, exchanges with rivers, flowing boundaries,...) and the transposition of stress factors (galleries, pumping wells,...).

A first calibration of groundwater flows has been obtained in steady state condition, using two contrasted groundwater level scenarios (high and low groundwater levels).

This model will still be improved (transient calibration of groundwater flows etc) but it can be already used for running first solute transport (nitrate) scenarios in the basin.

A complete description of the Geer basin and of the available datasets was proposed in Deliverable R3.16. As mentioned in the same deliverable, for collaboration with T2 and trend predictions, water and nitrate fluxes introduced as an input for the groundwater model are computed by the soil model EPIC-Grid (UHAGx).

### **Conceptual model for the Geer basin**

Horizontally, the limits of the modelled area have been defined as corresponding to the Geer hydrological basin. In the South, the hydrogeological basin limit varies slightly because of fluctuations of groundwater levels. However, these variations can be neglected and this boundary considered as impervious (groundwater divide). The Geer river is the main outflow of the chalk aquifer. However, on an annual basis, water balance in the Geer basin shows a water loss estimated to range between 15 mm (Monjoie 1967) and 62 mm (Hallet 1999). The lost groundwater flows under the Geer river to the groundwater basin located northwards, due to sloping and deepening of chalk layers towards the North. Such losses will be considered through the definition of a Cauchy boundary condition on the lateral northern boundary of the model. All the other lateral boundaries are considered as impervious.

The basis of the chalk aquifer is made of smectite clay of very low hydraulic conductivity. This is used as the bottom of the model with a no-flow boundary condition.

For defining the vertical discretisation, different aspects have to be taken into account:

- The main aquifer is located in the chalk:

The aquifer is made up of two main layers of chalk separated by a thin layer (approximatively 1m) of indurate chalk called “the Hardground”. This layer has a lower hydraulic conductivity than the surrounding chalk. It does not have any aquifer

capacity and it rather acts as a confining unit with an impact on vertical groundwater exchanges between the upper and lower chalk aquifer layers.

- o The influence of the unsaturated zone:

Many datasets coming from the Geer basin exhibit clear periodic variations in nitrate concentrations. As discussed by Brouyère et al., (2004), such periodic variations are explained by groundwater table fluctuations in the variably saturated dual-porosity chalk. In principle, nitrates spread over the land surface progressively infiltrate across the unsaturated zone and they migrate slowly, downward through the unsaturated chalk matrix. Under low groundwater level conditions, the nitrate contamination front is disconnected from the aquifer and nitrate concentrations in the aquifer tend to diminish because of dispersion and mixing processes. When groundwater levels rise, the contamination front is quickly reached and washed: the contamination source is re-activated and nitrate concentrations are likely to increase rapidly in the saturated zone. It is, therefore, important to represent adequately the unsaturated zone.

The groundwater recharge and the nitrate fluxes are computed by the EPIC-Grid soil model (UHAGx team). In the present version of the EPIC-Grid, the fluxes transmitted by UHAGx are computed at the mean groundwater table. Because the aquifer is unconfined, these fluxes computed at the top of the chalk layers would be more adequate to represent the time variations in groundwater levels and in nitrate concentrations in the unsaturated zone.

Vertically, the model has thus been divided into three layers of finite elements (Figure 5): one layer for the bottom chalk aquifer and two for the upper chalk aquifer in order to better represent the variations in groundwater levels in the unsaturated zone. The Hardground being very thin, it is not represented explicitly. In order to take into account its influence on groundwater flows, it is taken advantage of the possibility to define, in the SUFT3D code, the upper and lower chalk aquifer layers as separated subdomains, the Hardground being assimilated to the separating interface, using a leakage coefficient. The loess layer is not represented in the model as the fluxes in this layer are simulated by the EPIC-Grid soil model.

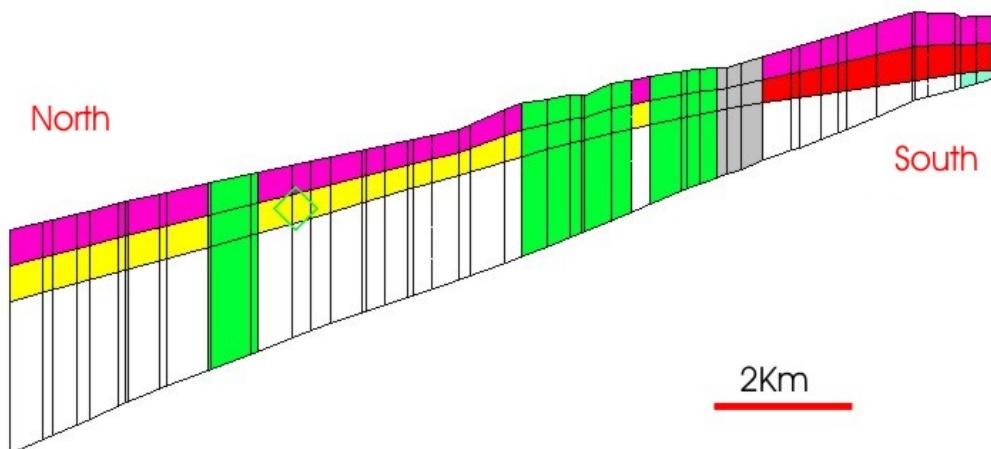


Figure 5: Vertical cross-section in the 3D-Mesh  
(The different colours symbolise different geological units)

## Discretisation

A two dimensional finite element mesh was first created considering explicitly the boundaries of the hydrological basin and the location of the pumping galleries. The mesh is based on triangular elements with a mean side of 700m. The resulting mesh is made up 1370 nodes and 2551 2D elements.

This two-dimensional mesh was then used to elevate four levels of nodes delimiting three layers of elements: one for the bottom layer of chalk, two for the top layer, as explained before. The bottom and the top of the layers were linearly interpolated based on available information from different boreholes and wells drilled in the basin. The three dimensional mesh is made up 5480 nodes and 7653 elements (Figure 6). Laterally, the layers may represent different geological units (symbolised by the different colours in Figure 5 and Figure 6).

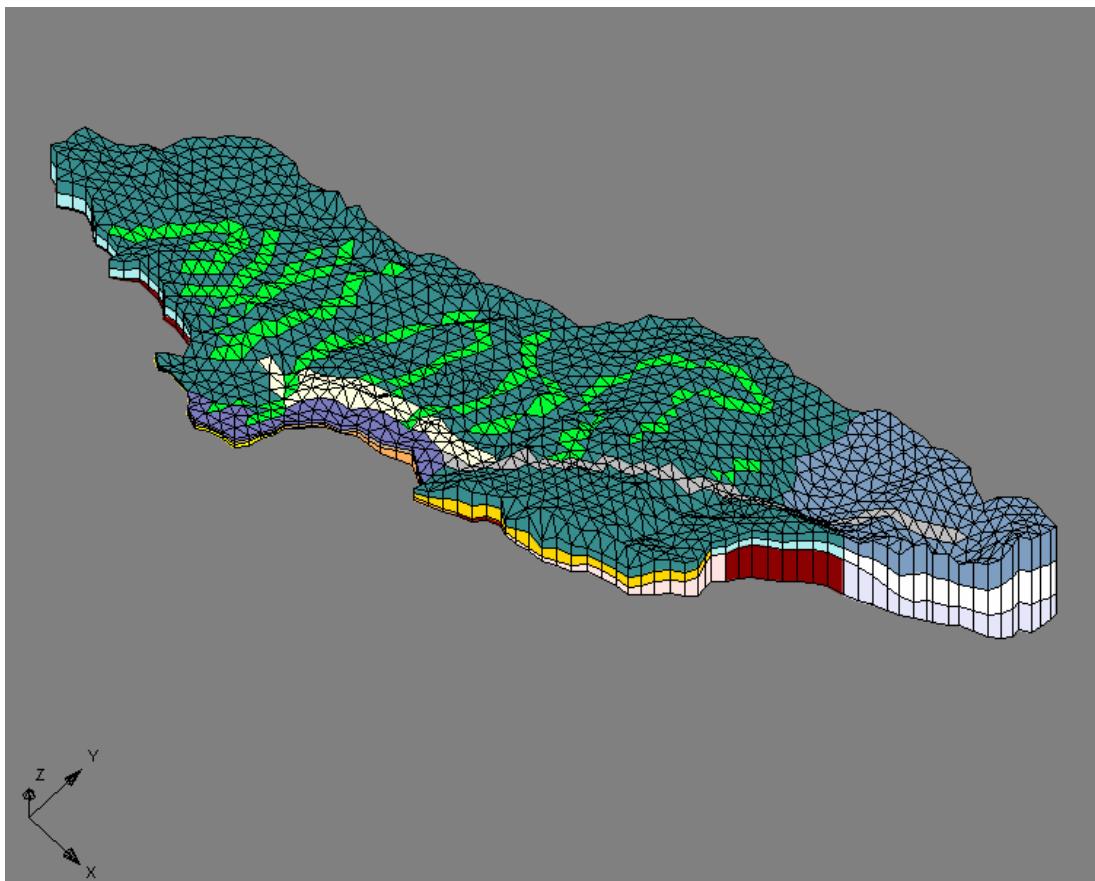


Figure 6: 3D – Mesh (vertical scale multiplied by 100)

## Boundary conditions

On the Eastern, Western and Southern lateral boundaries, no-flow boundary conditions are prescribed. On the Northern boundary, a Cauchy boundary condition is prescribed, the fluxes through this boundary depending on groundwater levels computed in the aquifer at the given locations.

At the top of the aquifer, water fluxes are prescribed using Neumann boundary conditions based on values computed by the EPIC-Grid soil model.

Interactions between the rivers and the aquifer are modelled using face-based Cauchy boundary conditions, the exchanged fluxes being a function of the difference of water level between the river and the aquifer.

### **Stresses**

The pumping galleries are represented explicitly in the horizontal discretisation. However, it turned out very difficult to consider exactly and explicitly the complex vertical locations of the galleries. As a first approximation, the Southern gallery, catching groundwater at a mean depth of 30 meters, has been defined at the top of the bottom chalk aquifer. The northern gallery, catching groundwater at a mean depth of 60 m, has been defined at nodes of the bottom of the bottom chalk layer.

Other groundwater fluxes pumped from wells have been taken into account by sink terms defined in the elements in which the well screens are located.

### **Calibration**

A first calibration of groundwater flows has been obtained in steady state conditions, using two contrasting piezometric situations : one corresponding to high groundwater levels (during the period 1983-1984), the second to low groundwater levels (during the period 1991-1992). For this calibration step, the groundwater model has been runned in stand-alone mode (without using EPIC-Grid) using a constant and uniformly distributed recharge calculated based on water budget for the corresponding years (Deliverable R3.16). For the period 1983-1984 and 1991-1992, respectively 43 and 54 piezometric measurements were used (Figure 7). Computed piezometric levels were compared to annually averaged groundwater levels.

In Figure 8 and 9, a general quality of the calibration is presented in the form of a scatter plot diagram of observed versus computed groundwater levels for the period respectively 1983-1984 and 1991-1992.

This model will still be improved in particular by a calibration step in transient conditions (transient recharge computed by the soil model, transient pumping rates...), using transient water fluxes computed using the EPIC-Grid model.

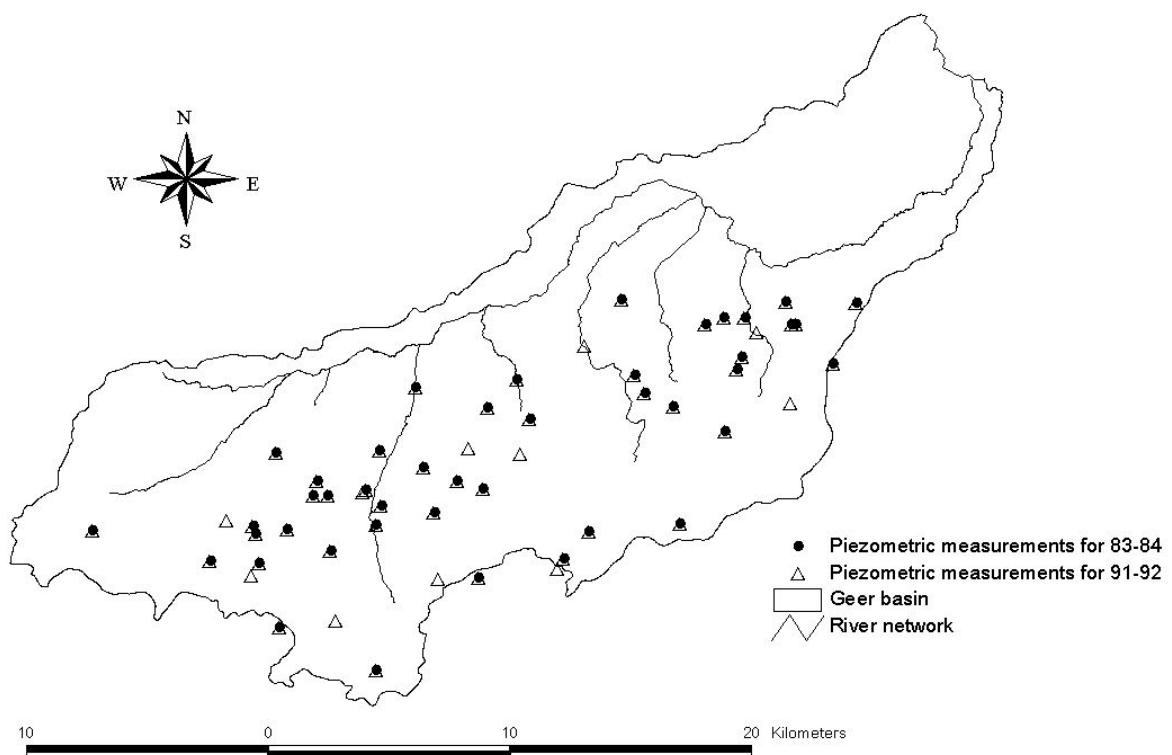


Figure 7: Location of the piezometric measurement points used for the steady state calibration

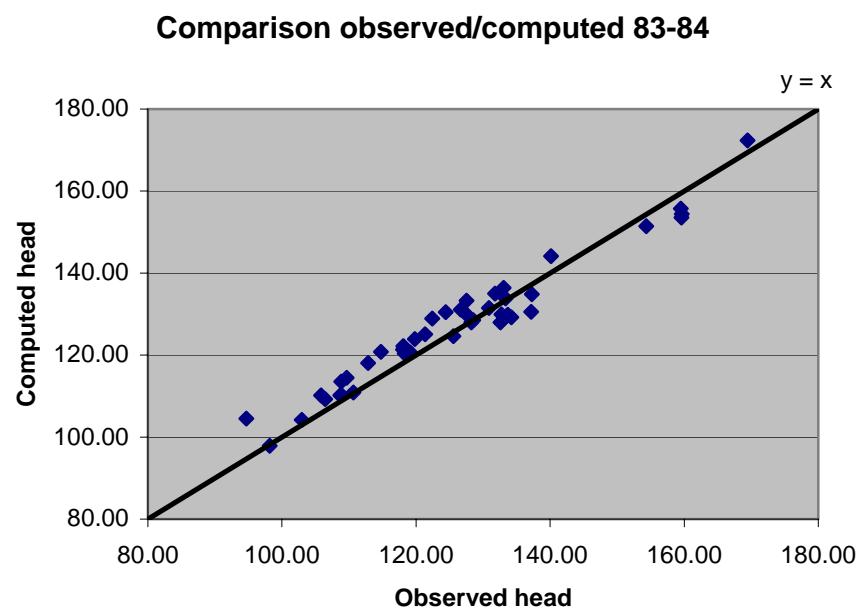


Figure 8: Comparison between observed and computed head for the period 83-84

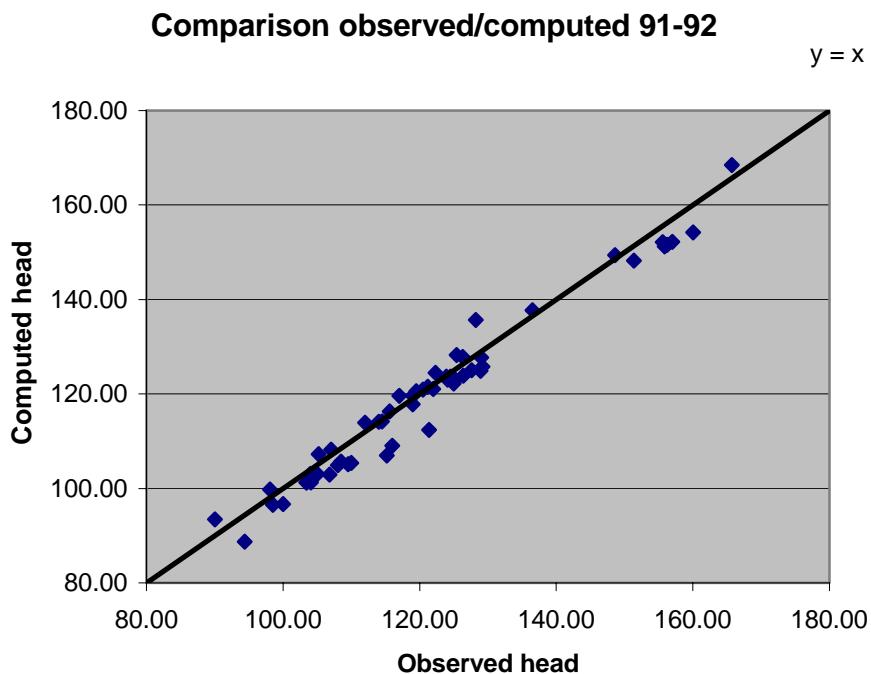


Figure 9: Comparison between observed and computed head for the period 91-92

### Further works and delivery to TREND T2

As mentioned in the previous section, the model still has to be calibrated in transient conditions. However, it can already be used for running first nitrate transport scenarios in the framework of the TREND T2 sub-project. For example, it could be an interesting exercise to model transient nitrate fluxes recharge under mean steady state groundwater flow conditions.

Trend analysis results presented in deliverable T2.4 will be used as calibration and validation datasets for the groundwater flow and transport model. Then the model will be used to perform trend forecasting.

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