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

Deliverable No.: **TREND2.5**

Title: Input data sets and short report describing the subsoil input data for groundwater and reactive transport modelling at test locations in Dutch part of the Meuse basin, the Brévilles' catchment and the Geer catchment

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

SUMMARY

The establishment of tools for trend-analysis in groundwater is essential for the prediction and evaluation of measures taken within context of the Water Framework Directive and the draft Groundwater Directive. Three-dimensional reactive transport modeling of groundwater and solutes will be the focus of the TREND 2 workpackage in the coming year. Essential to groundwater modeling is the correct and accurate description of inputs to the model: geological features, meteorological data and solute deposition history.

This report describes the subsoil input data for models that will be used in the following three catchments: the Dutch part of the Meuse basin, the Brévilles' catchment and the Geer catchment.

Together with this report, the TREND 2 workpackage partners deliver a set of computer files that describe the input data. These can be found on the accompanying CD or .zip file on the AquaTerra website.

MILESTONES REACHED

T2.5: Subsoil input data prepared for groundwater and reactive transport modelling at test locations in Dutch part of the Meuse basin, the Brévilles' catchment and the Geer catchment

These input data have be collected in close cooperation of the AquaTerra COMPUTE partners, as input data collection and model development are intimately entangled.

These input data may be of interest to other COMPUTE partners for further model development.

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1. Introduction to TREND 2 (TNO)

1.1 Background and objectives

The implementation of the EU Water Framework Directive (2000/60/EU) and the draft Groundwater Directive asks for specific methods to detect the presence of long-term anthropogenically induced upward trends in the concentration of pollutants in groundwater. Specific goals for trend detection have been under discussion during the preparation of the recent draft of the Groundwater Directive. The draft Directive defines criteria for the identification and reversal of significant and sustained upward trends and for the definition of starting points for trend reversal. Figure 1.1 illustrates the trend reversal concept, as communicated by EU Commission Officer Mr. Ph. Quevauviller. The figure shows how the significance of trends is related to threshold concentrations which should be defined by the member states.

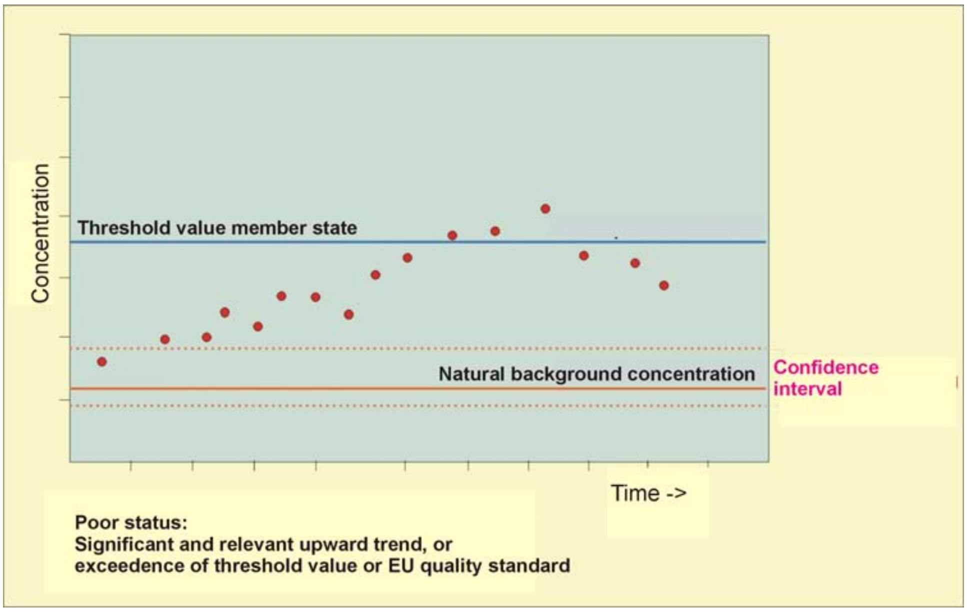

Figure 1.1 Trend reversal concept of the draft EU Groundwater Directive.

Trends should be reversed when concentrations increase up to 75% of the threshold concentration. Member states should reverse trends which present a significant risk of harm to associated aquatic ecosystems, directly dependent terrestrial ecosystems, human health, whether actual or potential, of the water environment, through the program of measures referred to in Article 11 of the Water Framework Directive, in order to progressively reduce pollution of groundwater. Thus, there is a direct link between trends in groundwater and the status and trends in related surface waters. This notion is central to the overall objectives of the AQUATERRA research project.

> Working hypothesis 1:
> Groundwater quality is of utmost importance to the quality of surface waters. Establishment of trends in groundwater is essential for prediction and evaluation of measures taken within the Framework Directive and the draft Groundwater Directive.

Accordingly, the work package TREND-2 of Aquaterra is dedicated to the following overall objectives.

1 Development of operational methods to assess, quantify and extrapolate trends in groundwater systems. The methods will be applied and tested at various scales and in various hydrogeological situations. The methods applied should be related to the trend objectives of the Water Framework Directive and draft Groundwater Directive. In

addition to the Description Of Work DOW, it is our ambition to link changes in groundwater quality to changes in surface water quality.

2 Linking changes in land use, climate and contamination history to changes in groundwater chemistry. We define a temporal trend as '*a change in groundwater quality over a specific period in time, over a given region, which is related to land use or water quality management',* according to Loftis 1991, 1996.

It should be noted that trends in groundwater quality time series are difficult to detect because of (1) the long travel times involved, (2) possible obscuring or attenuating effect of physical and chemical processes, (3) spatial variability of the subsurface, inputs and hydrological conditions and (4) short-term natural variability of groundwater quality time series. The TREND 2 package is dedicated to the development and validation of methods which overcome many of these problems.

Working hypothesis 2:
Detection of trends in groundwater is complicated by spatial variations in pressures, in flow paths and groundwater age, in chemical reactivity of groundwater bodies, and by temporal variations due to climatological factors. Methods for trend detection should be robust in dealing with this inherent variability.

Groundwater pollution is caused by both point and diffuse sources. Large scale groundwater quality, however, is mainly connected to diffuse sources, so that the TREND 2 project will concentrate on trends in groundwater quality connected to diffuse inputs, notably nutrients, metals and pesticides. Although trends in groundwater quality can occur at large scales, linking groundwater quality to land use and contamination history requires analysis at smaller scale, i.e. groundwater subsystems. Thus, the approach zooms in on groundwater system analysis around observation locations. Results will be extended to large scale monitoring.

1.2 General methods used in TREND 2

Research activities within TREND 2 focus on the following issues:

1. *Inventory of monitoring data of different basins and sub-catchments*. The inventory focuses on observation points with existing long time series. The wells should preferably be located in agricultural areas, because pesticides and nutrients are the main concern in trend detection for the Water Framework Directive. Additional information will be collected about historical land use changes and related changes in the input of solutes into the groundwater system.
2. *Development of suitable trend detection concepts.* Trend detection concepts include both statistical approaches (classical parametrical and non-parametrical methods, hybrid techniques) and conceptual approaches (time-depth transformation, age dating)
3. *Methods for trend aggregation for groundwater bodies.* The Water Framework Directive demands that trends for individual points are aggregated on the spatial scale of the groundwater bodies. The project will focus on robust methods for trend aggregation.
4. *Trend extrapolation.* Trend extrapolation will be based on statistical extrapolation methods and on deterministic modelling. Both 1D and 3D models will be applied to predict future changes and to compare these with measured data from time series.
5. *Recommendations for monitoring.* Results from the various case studies will be used to outline recommendations for optimizing monitoring networks for trend analysis

1.3 TREND 2 case studies

The following case studies have been selected for testing the methodologies:

Table 1.1: Case studies in TREND 2

Basin	Contaminants	Institutes
Meuse		
Dommel upper tributaries	Nitrate, sulfate, Ni, Cu, Zn, Cd	TNO/UU
Noord-Brabant region	Nitrate, sulfate, Ni, Cu, Zn, Cd	TNO/UU
Wallonian catchments:	Nitrate	Ulg
• Néblon		
• Pays Herve		
• Hesbaye		
• Floodplain Meuse		
Brévilles		
Brévilles catchment	Pesticides	BRGM
Elbe		IETU
• Czech subbasins	Nitrate	
• Schleswig-Holstein	Nitrate	

These cases have different spatial scales and different hydrogeological situations. Details on the various cases are provided in the subsequent chapters of this report.

1.4 Contents of the current report

Earlier deliverables (T2.3 and T2.4) have concentrated on statistical methods of trend detection and extrapolation. In the coming years the use of modelling approaches will additionally be explored within Aquaterra TREND2. This report focuses on deterministic methods for studying trends in groundwater, using groundwater flow and transport models. Essential to groundwater modeling is the correct and accurate description of inputs to the model: geological features, meteorological data and solute deposition history. This deliverable describes input data used for the groundwater flow and transport models, which are currently being built for the Dutch Dommel basin, the Wallonian Geer basin and the French Brévilles catchment. The report describes the subsoil input data for models that will be used in the following three catchments: the Dutch part of the Meuse basin, the Brévilles' catchment and the Geer catchment. Together with this report, the TREND2 workpackage partners deliver a set of computer files that describe the input data. These can be found on the accompagnying zip-files.

1.5 Structure of the report

This report describes the model input data which have been prepared up to May 2006. Chapters 2 describes the input data for the Dutch Meuse subcatchments of the Dommel river. Chapters 3 describes input data for the Geer basin and Chapter 4 describes the input data for the Brévilles catchment.

2. Subsoil input data prepared for groundwater and reactive transport modelling in Dutch part of the Meuse basin (TNO/UU)

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2.1 Introduction

A three-dimensional reactive transport model will be used for the trend detection and extrapolation of groundwater and surface water quality. The purpose of this document is to shortly describe the input of the three-dimensional reactive transport model. The input of the model has three components: the chemical properties of the subsurface, the groundwater flow system, and the concentrations in recharging groundwater.
Collecting model data, model development and modelling itself are closely entangled. At this moment, we have the input data for cadmium, copper and zinc ready. We are currently working on other solutes.

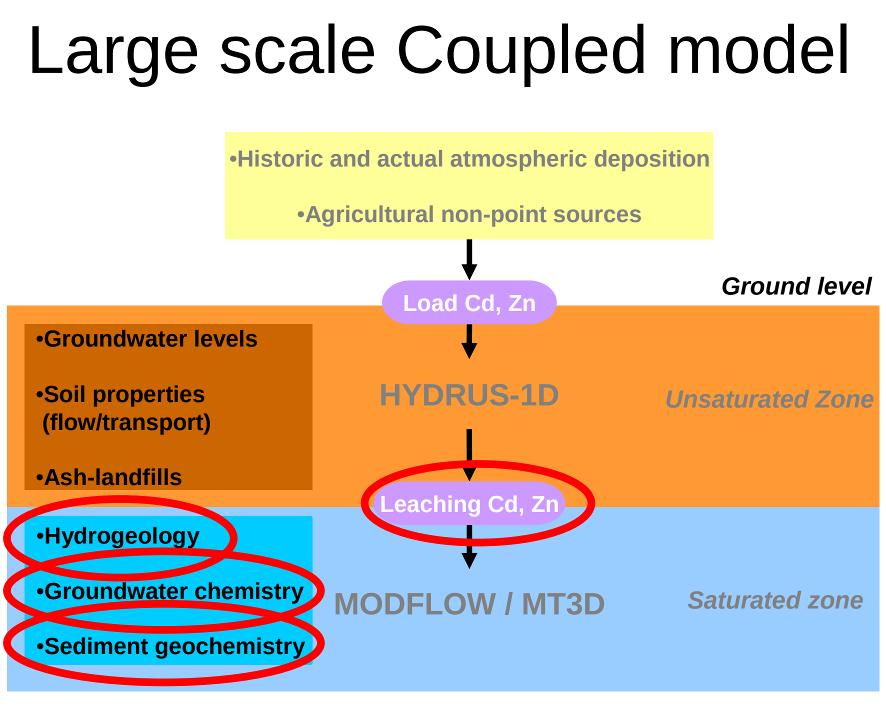


Figure 2.1: Setup of the large scale coupled three-dimensional reactive transport model used in the Dutch part of the Meuse basin.

The three-dimensional reactive transport model which will be used in this project is the Integrated Transport Model, developed by TNO and KIWA. (reference) It combines a stationary groundwater flow model (MODFLOW) with a three-dimensional multi-species transport model (MT3DMS). Figure 1 shows the setup this large scale 3D coupled model, with the input components discussed in this deliverable encircled in red. Further developments of this model are also part of the COMPUTE package.

2.2 Spatial extent of the model and discretization

The model covers a rectangular area of 34.5 km (East-West) by 24 km (North-South). The coordinates of the top-left and bottom-right corners are (51°25’35.6130” N, 5°13’47.1255” E) and (51°12’40.8589” N, 5°43’22.0500” E) respectively (Figure 1). These coordinates correspond to the following coordinates in the Dutch (x, y) reference system: (144000 m, 382000 m) and (178500 m, 358000 m).

Figure 2.2: Spatial extent of the three-dimensional reactive transport model used in the Dutch part of the Meuse basin.

The horizontal size of the grid cells is 100 x 100 meters: the total number of grid cells per layer is 82800 (345x240). Input data is specified for each grid cell. We refer to each grid cell by its coordinates in the Dutch reference system.

The model has 17 horizontal layers. Layer thickness ranges from 0.5 to 10 meters and the total model thickness is 56.5 meters. The vertical discretization is presented in Table 2.1

Layer	Thickness [m]	Bottom below surface [m]
1	0.5	0.5
2	2	2.5
3	2	4.5
4	2	6.5
5	2	8.5
6	2	10.5
7	2	12.5
8	2	14.5
9	2	16.5
10	2	18.5
11	2	20.5
12	3	23.5
13	3	26.5
14	5	31.5
15	5	36.5
16	10	46.5
17	10	56.5

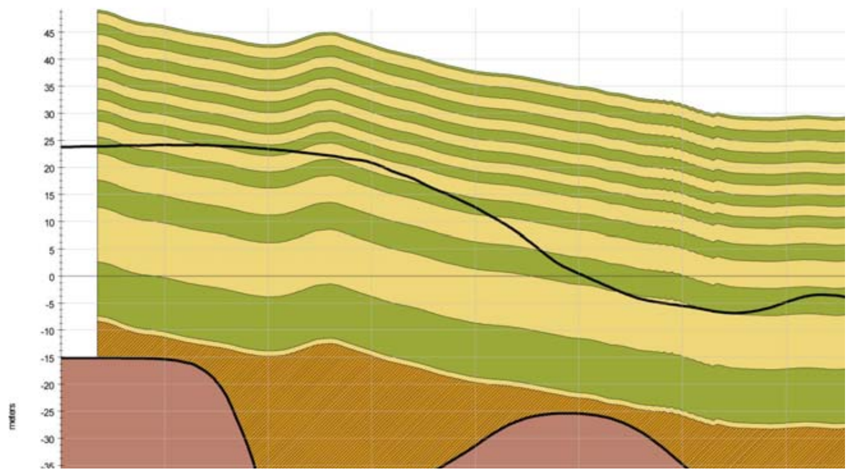


Figure 2.3: Model layers are defined relative to the land surface: each model layer follows the topography of the land surface.

Table 2.1 and: Vertical discretization of the model.

The layers are defined relative to the land surface. Each layer follows the topography of the land surface. (Figure) The altitude of the land surface at the center of each grid cell relative to the Dutch Datum (NAP) is reported in the file *altitude.txt*.

2.3 Hydrological model

The groundwater flow model requires that for each is defined whether the cell is inactive (discarded by the model), has a constant head (at the boundary) or active (part of the groundwater flow system). This information is reported in the file *celltype.txt*. Each row in this file gives the cell type of each layer at a specified x,y location.
The initial heads for the groundwater flow model, as well as the constant heads in for constant head cells, is reported in the file *startheads.txt*. Each row in this file gives the starting head (m above NAP) (and constant head if applicable) for each layer at a specified x,y location.
Vertical conductance for the groundwater flow model are reported in the file *conductance.txt*. Each row in this file gives the vertical conductance (1/day) for each layer at a specified x,y location.
Horizontal transmissivities for the groundwater flow model are reported in the file *transmissivities.txt*. Each row in this file gives the horizontal transmissivity (m/day) for each layer at a specified x,y location.
At this moment we assumed that the precipitation is constant in time and space. However, the net recharge to the groundwater – precipitation minus evapotranspiration - depends on land use and is variable in space. The net recharge reported in the file *recharge.txt*. Each row in this file gives the net recharge (mm/day) at a specified x,y location.

Well abstractions from the 15^{th}, 16^{th} and 17^{th} layer are in the file wells.txt. Each row in this file gives the well abstraction (m^3/day) for model layers 15, 16 and 17 at a specified x,y location.

2.4 Chemical properties of the subsurface

The chemical properties of the subsurface are the initial chemical composition of groundwater (hydrochemical composition), and the reactivity of the subsurface (geochemical properties).

Land use, hydrology and depth strongly influence the chemical composition of groundwater. To predict the *initial chemical composition of groundwater* we classified each grid cell according to land use and hydrology into 5 classes: Nature-recharge, Nature-intermediate, Agriculture-recharge, Agriculture-intermediate, and Discharge. We calculated the median concentration measured by the national and provincial network for each class at three depth intervals: *upper* groundwater (upto 1 meter below the groundwater table), *shallow* groundwater (down to 11 meter below the surface), and *deep* groundwater (below 11 meters below the surface). For example the chloride concentration is printed in table. This yielded 15 groundwater types, based on land use, hydrology and depth. This median concentration represented the the initial chemical composition of groundwater.

Chloride [mg/l]	Nature - recharge	Nature - intermediate	Agriculture - recharge	Agriculture - intermediate	Discharge
upper	8.9	18.1	16.7	22.5	21.0
shallow	14.2	21.4	34.1	33.7	32
deep	13.48	9.42	38.12	42.32	14.39

Table 2.2: Median concentrations (of chloride for example) for 5 classes and 3 depth intervals serve as initial chemical composition of groundwater.

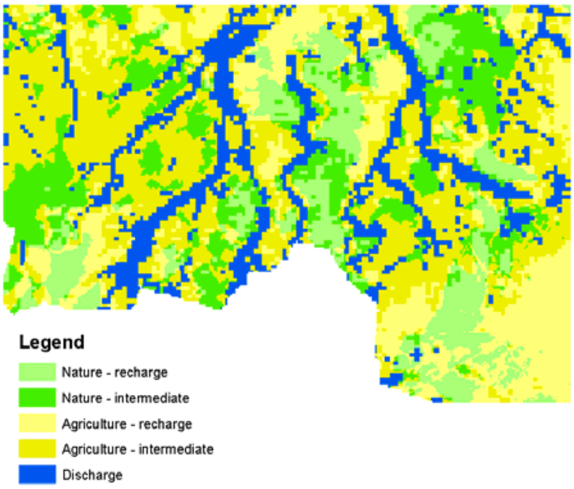


Figure 2.4: The model area was classified into 5 classes according to land use and hydrology to calculate the initial chemical composition of groundwater.

The *geochemical properties of the subsurface* were defined by the sorption constants (Freundlich isotherms) to model the retardation of heavy metals. The sorption constants depend on the macrochemistry of the groundwater and the concentrations of organic matter, clay and ironhydroxides in the subsurface. We used the median concentrations for each groundwater type, mentioned above. We derived the concentrations of organic matter, clay and ironhydroxides in the subsurface from the three-dimensional geological model of the subsurface (REGIS II, reference) and a geochemical analysis of geological formations in the model area by TNO (reference).

We obtained the occurrence of geological formations at 5 depths (10, 20, 30, 40 and 50 meters below surface) from the REGIS II subsurface model (reference). The geological units present in the model area are in table and a cross section is shown in figure.

	origin	N	Clay (%)	S_{total} (%)	FeOX (%)	OM (%)
Boxtel Formation	local and eolian	204	4.24	0.11	0.03	1.92
Beegden Formation	fluvial	5	1.96	0.03	0.00	0.25
Sterksel Formation	fluvial	45	3.33	0.10	0.07	0.68
Stramproy Formation	local and eolian	31	5.15	0.18	0.41	2.55

Table 2.3: Description and chemical characterization of geological units present in the model area.

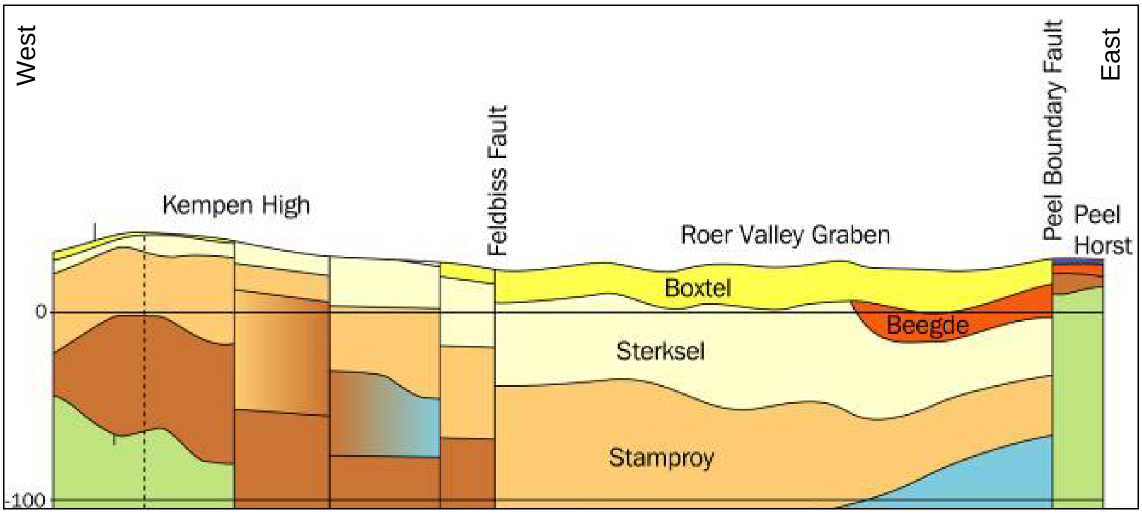


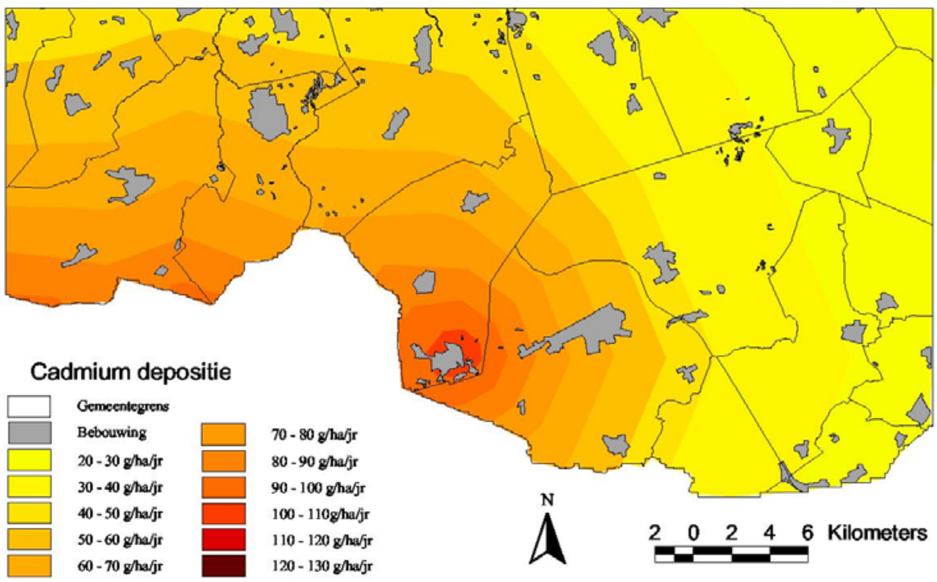
Figure 2.5: Geological West-East profile through the model area.

The combined geological and groundwater type classification is in the file geo.txt. The corresponding parameters of the Freundlich isotherms are in the file *Kfn.xls*.

2.5 Concentrations in recharging groundwater

The concentrations in recharging groundwater are the driving force of trends in groundwater quality. We described the concentrations in recharging groundwater on a provincial scale for agricultural land in deliverable T2.2. We estimated the concentrations under natural land as solely the atmospheric deposition, considering the effect of vegetation. For three-dimensional reactive transport modeling of heavy metals we need to consider the sorption in the unsaturated zone. To do so, we used a one-dimensional unsaturated zone transport model (Hydrus 1D) to calculated the concentrations at the groundwater table. The unsaturated zone transport model was used for 16720 homogeneous areas with similar land use, soil type and hydrology. The sorption of heavy metals was simulated with single-solute-isotherms. The dependence of the sorption isotherms on organic matter content, pH, clay content and metal concentration in the soil was based on partitioning relationships published by Römkes et al. (2002).

The recharging concentrations are in the model input files *concentration_cd.txt*, *concentration_cu.txt* and *concentration_zn.txt*. An example of resulting Cd input concentrations is given in Figure 2.6.



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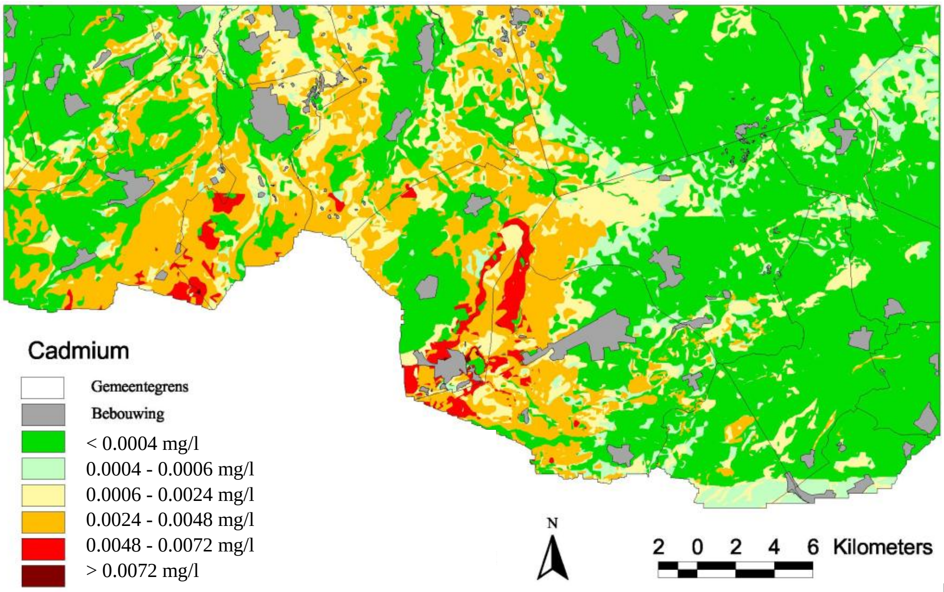

Figure 2.6: A series of 1-dimensional unsaturated zone model converts deposition of cadmium at the surface (a) to the actual concentrations leaching across the groundwater table (b).

2.6 Summary

In summary, the following input data are used.

Input data	unit	file	structure
Altitude top layer	[m above NAP]	altitude.txt	x, y, altitude
Cell type for groundwater flow model	[-]	celltype.txt	x, y, layer_1, layer_2, …
Starting heads for groundwater flow model	[m above NAP]	startheads.txt	x, y, starthead_l1, starthead_l2 …
Vertical conductance for groundwater flow model	[1/day]	conductance.txt	x, y, conductance_l1, conductance _l2, …
Horizontal transmissivity for groundwater flow model	[m^2/day]	transmissivity.txt	x, y, transmissivity_l1, transmissivity_l2, …
Net recharge	[mm/day]	recharge.txt	x, y, recharge
Well extractions	[m^3/day]	wells.txt	x, y, wells_l15, wells_l16, wells_l17
Geo-hydro-chemical units	[-]	geo.txt	x, y, code_l1, code_l2, … (codes refer to data in Kfn.xls)
Geochemical data		Kfn.xls	

3. Input data sets for groundwater and transport modelling in the Geer basin

3.1 Introduction

In the framework of the AquaTerra project, the HGULg team has developed a methodology based on classical statistical tools to infer trends in groundwater quality with an application to nitrate trends in the Geer basin. The subsequent works will focus on the development of modelling tools to predict trends.
The objective of the present deliverable is to summarize information on available hydrogeologic datasets and the methodology that will be used. A detailed description has already been included in other AquaTerra deliverable :

- T2.1 : Documented spatial dataset; subdivision of groundwater systems and subsystems, the selected locations per subsystem for small scale analysis and a description of these sites, available data and projected additional measurements and equipments
- T2.4 : Report on extrapolated time trends at test sites
- R3.16 : Description of hydrogeological conditions in the Geer sub-catchment and synthesis of available data for groundwater modelling
- R3.18 : Groundwater flow and transport delivered for groundwater quality trend forecasting by TREND T2

In the present deliverable, only a brief description is presented.

3.2 The conceptual approach

HGULg has developed a general methodology (Fig 1) for groundwater flow and transport modelling at large scale (Deliverable R3.18). The originality of this approach is to combine, in a single code, different mathematical approaches, ranging from simple linear reservoir and mixing cell models when the hydrogeological system is poorly characterised to more classical flow and advection-dispersion equations when the system is well characterised.
It is proposed to apply this methodology on the Geer basin to predict trends. Water and nitrate fluxes computed by the soil model EPIC Grid (UHAGx) will be used as an input for the groundwater flow and transport model (SUFT3D).
For collaboration with WP T2, estimations of water and nitrates fluxes to groundwater, as computed by UHAGx (Prof. S. Dautrebande) for the PIRENE project, will be used (Deliverable Trend 2.2). These fluxes have been evaluated using the EPICgrid model (UHAGx –FUSAGx) for the last 30 years (1970-2000) for the Walloon part of the Meuse Basin, on the basis of a 1 km² grid. This model simulates hydrological processes such as direct runoff, groundwater recharge, subsurface lateral flows, soil moisture variation, agricultural diffuse nitrates… The model is physically based, without calibration.

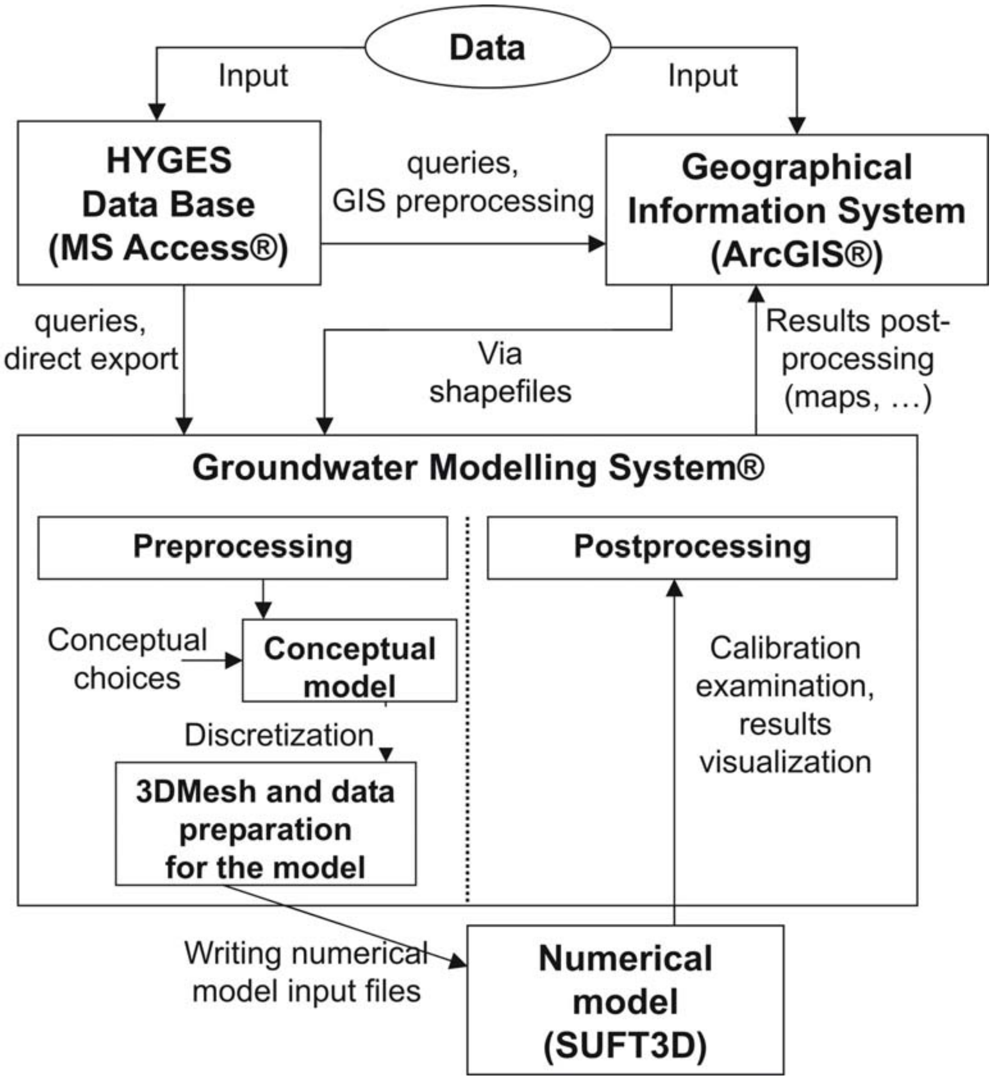

Figure 1 : Scheme of data management

3.3 Available data

To develop a groundwater flow and solute transport model, four kinds of data are required :

- Geometric data to define the spatial extension and the geometry of the aquifer;
- Pumping rates and infiltration rates;
- Values of the parameters used in the equations describing the processes taken into account in the simulation;
- Historical data on groundwater levels and nitrate concentrations in the basin.

As mentioned in Deliverable R3.11 (Batlle et al. 2005), all the hydrogeological data collected in the framework of the AquaTerra project are encoded in the hydrogeological database developed by the HGULg team (Gogu et al. 2001, Wojda et al. 2005). Using requests and GIS, data can be easily prepared and exported for modelling purposes.

All the available data collected are presented in deliverable R3.16. For the available nitrate datasets, readers are referred to deliverable T2.1, T2.2 and T2.4 .