Groundwater flow and contaminant transport in an alluvial aquifer: *in-situ* investigation and modelling of a brownfield with strong groundwater – surface water interactions

PhD thesis

Jordi BATLLE-AGUILAR

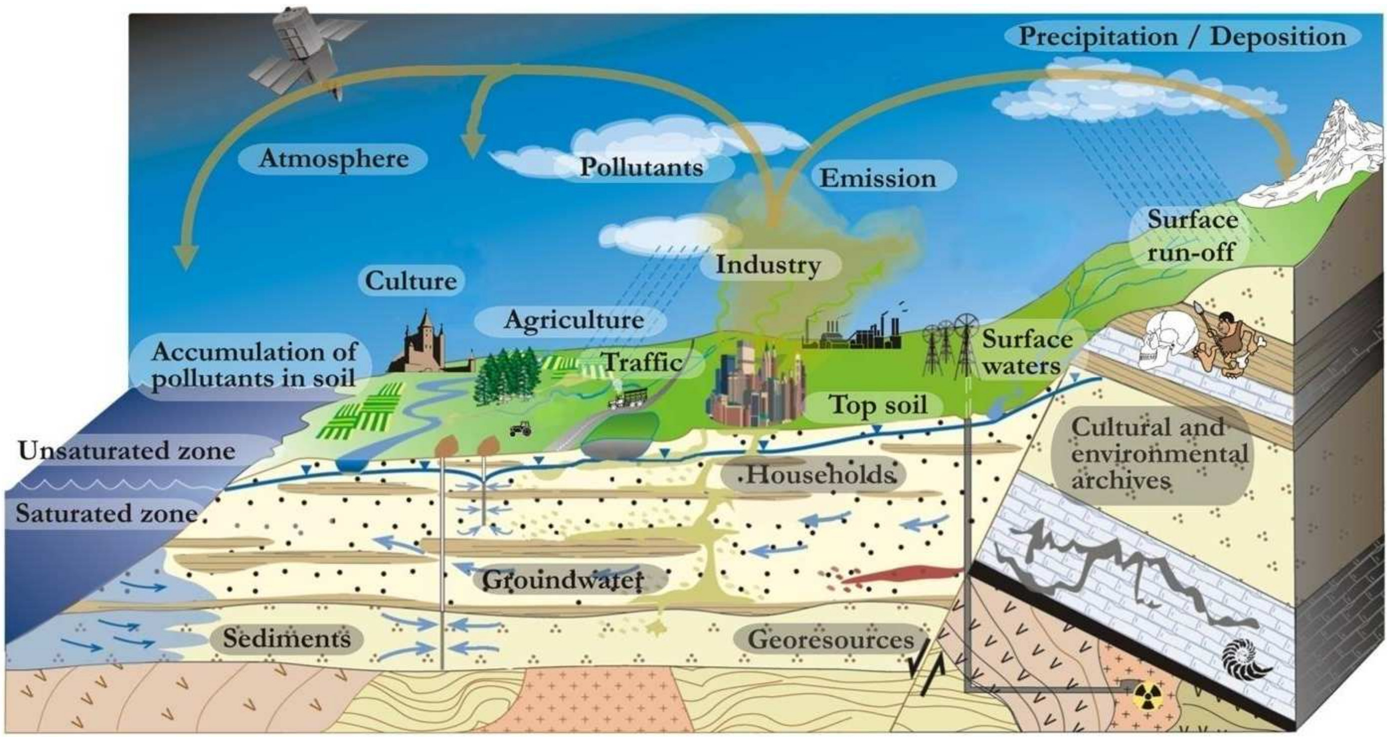
Sart Tilman, 19th September 2008

Overview

1. Context of the research
2. Objectives of the research
3. Hydrogeology of the Flémalle site
4. Summary on data mining and monitoring
5. Summary on field experiments
6. Numerical groundwater flow and transport modelling
7. Benzene transport
8. Conclusions and perspectives

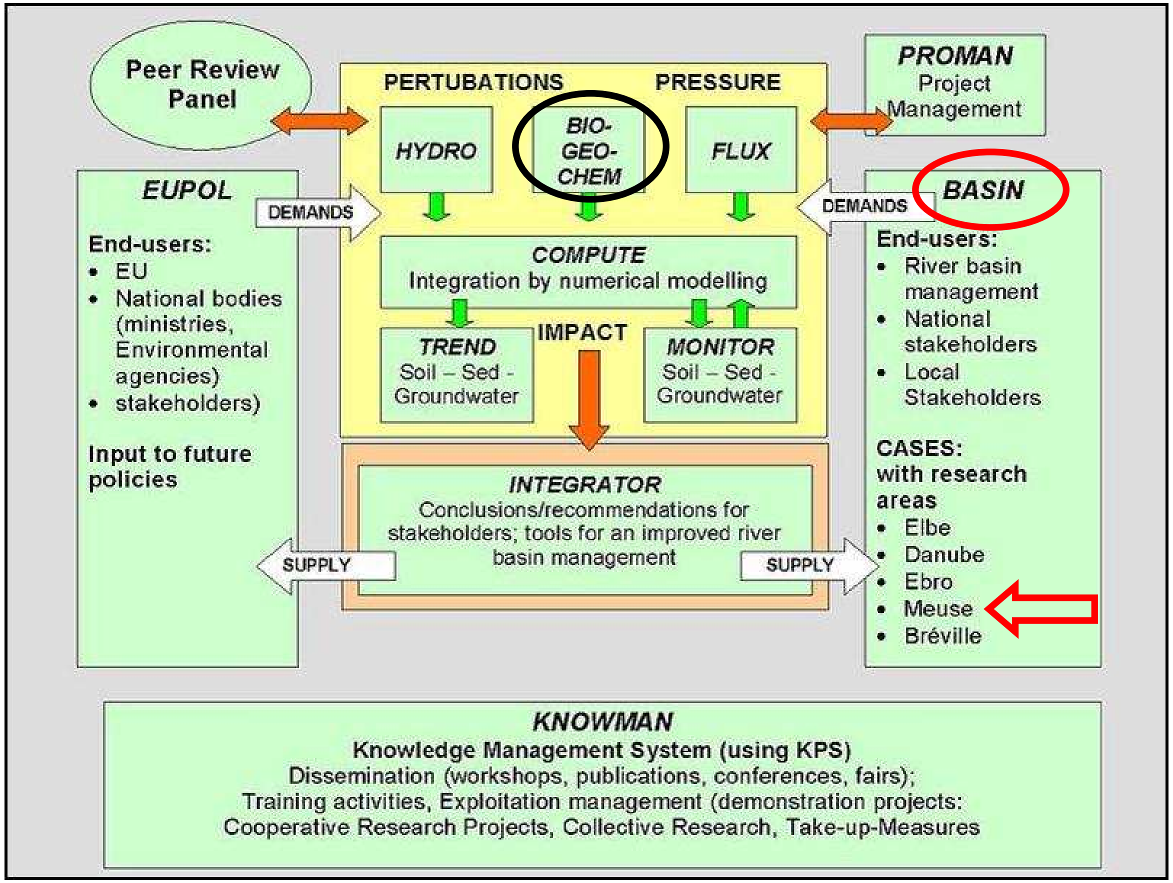
1. Context of the research (Aquaterra project)

• AquaTerra Integrated Project of the 6th EU RTD Framework Programme
• 45 partner organisations (13 EU countries + Switzerland + Serbia)
• Better understanding of the river-sediment-soil-groundwater system as a whole by identifying relevant processes, quantifying the associated parameters and developing numerical models of the groundwater-soil-sediment-river system



1. Context of the research (Aquaterra project)

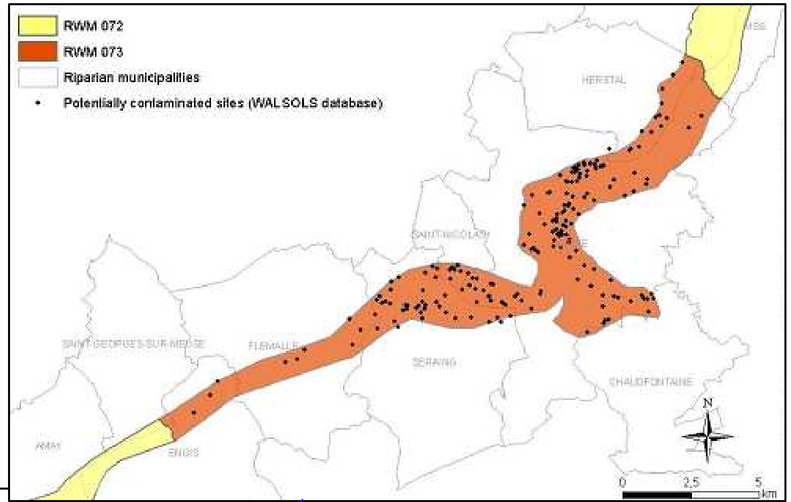
- 11 sub-projects // Basin sub-project // 5 European river basins;
- Meuse work-package (R3);
- Belgian/Walloon catchment & Dutch basin;
- HGULg – CHYN – VITO – LIMOS(UHP).

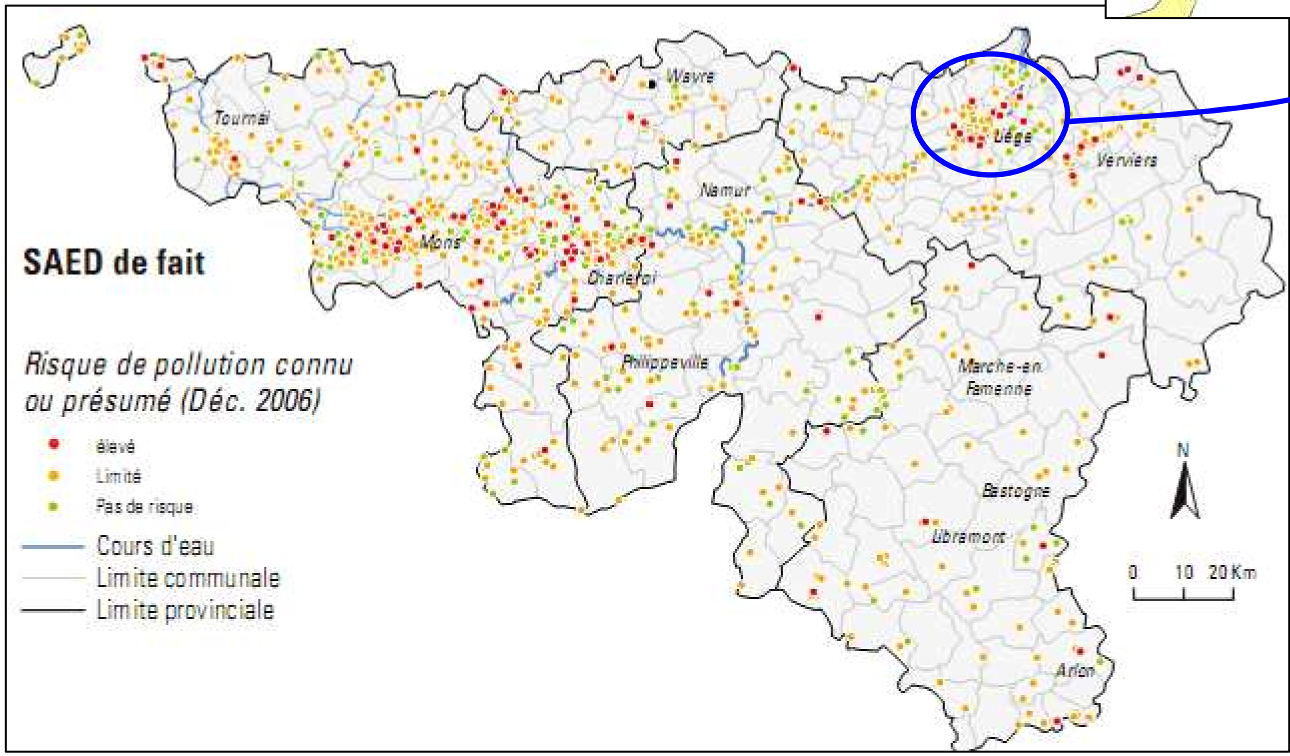


1. Context of the research (Brownfields & Environment)

Former industrial activities (metallurgy) typically located nearby navigable rivers.

Contaminated sites close to rivers and urbanised areas. Risk of contaminant dispersion in the environment.





1. Context of the research (Brownfields & Environment)

What is the environmental risk associated to coke factories?

Air – Soil – Surface water – Groundwater

Iron ore

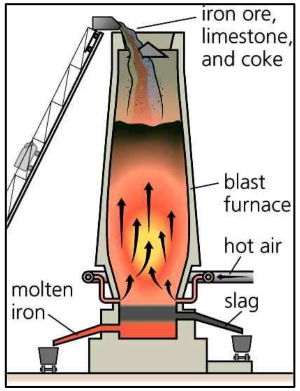
Limestone

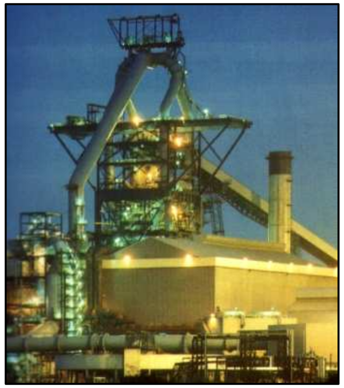
Coke

Coke oven

+

Coal





Blast furnace

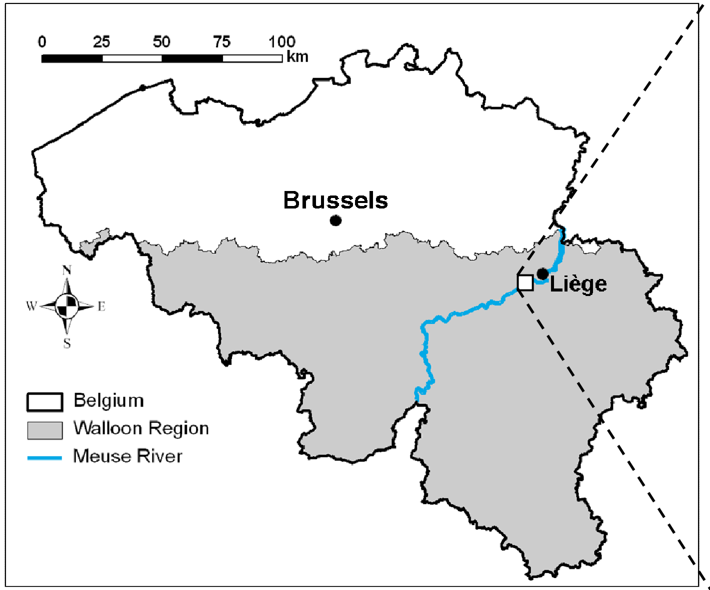
Molten iron

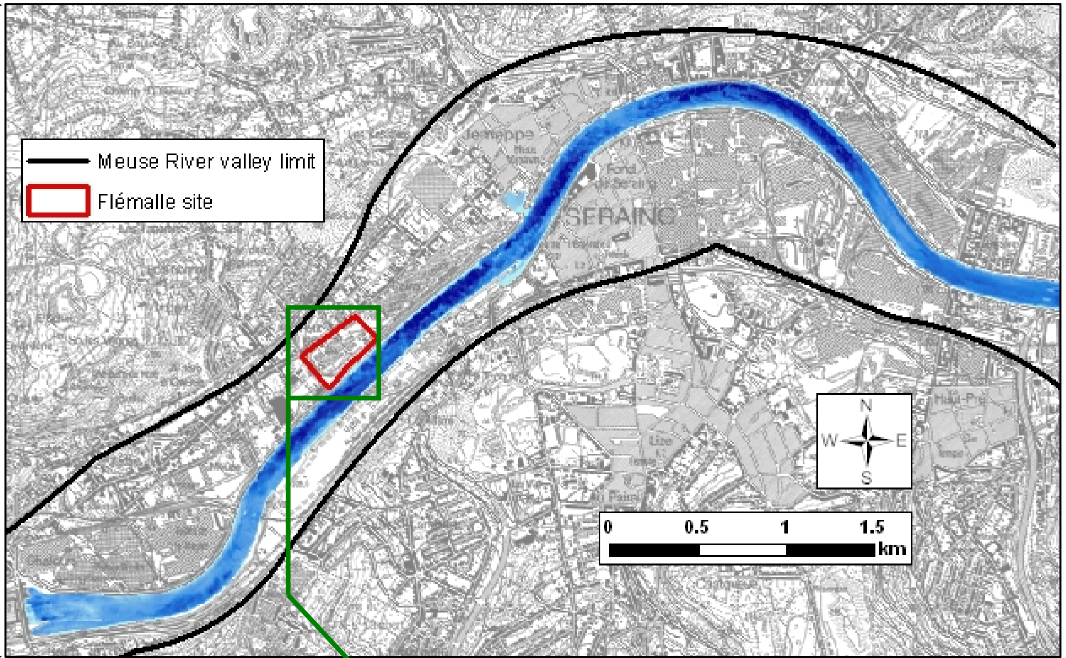
High quantities of wastewater produced:

1. During the quenching of hot coke and;
2. Washing gas produced from ovens.

Ammonia, cyanide, phenols, monoaromatic and polynuclear aromatic hydrocarbons (BTEX and PAHs), sulphate, heavy metals (MTEs),...

1. Context of the research (Brownfields & Environment)





- Proximity to the Meuse River (25 m);
- Pollutant industrial activities (1922 – 1984);
- Soil and groundwater highly polluted by organic (BTEX and PAHs) and inorganic (metals, Fe and sulphate) components.

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2. Objectives of the research

- **Global objective**
  - Investigate risk of contaminant “off-site” dispersion through the groundwater – river system

- **Specific objectives**
  - Evaluate whether a groundwater – surface water interaction exists and contribute to a better understanding / quantification of this interaction
  - Determine factors contributing to (organic & inorganic) pollutant mobility and/or attenuation
  - Estimation and modelling of groundwater and contaminant discharge to the river

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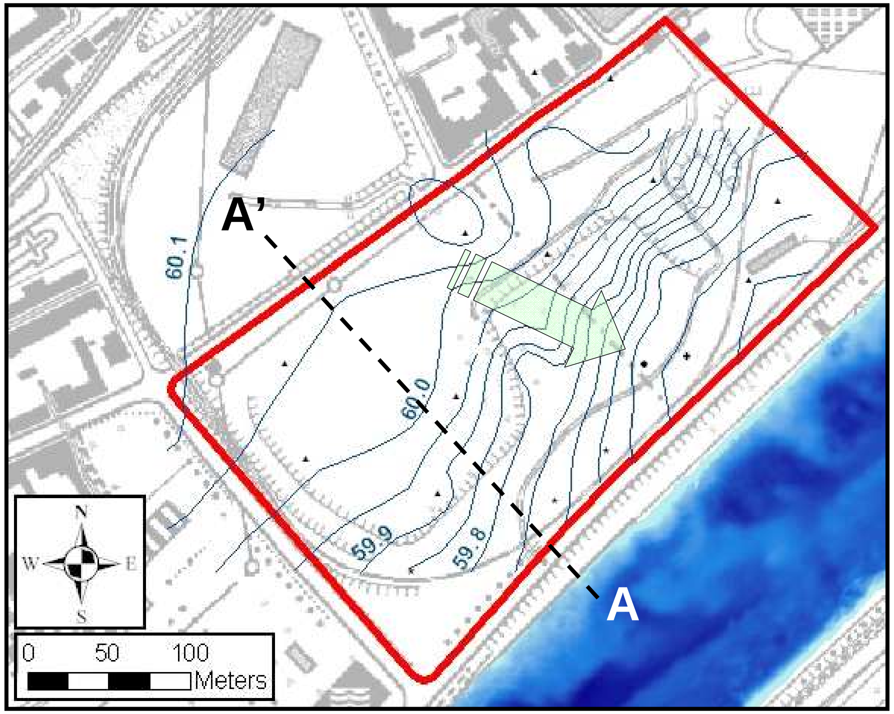
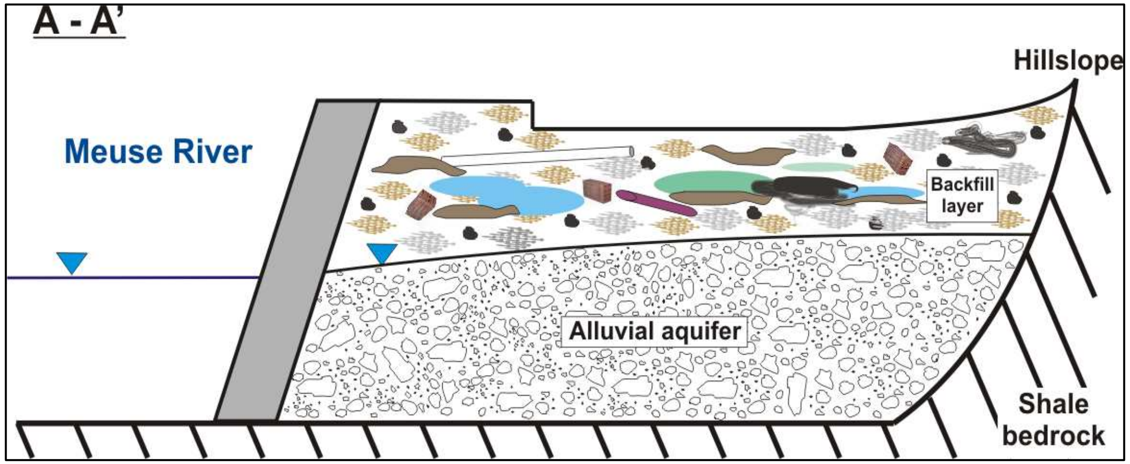
3. Hydrogeology of the Flémalle site

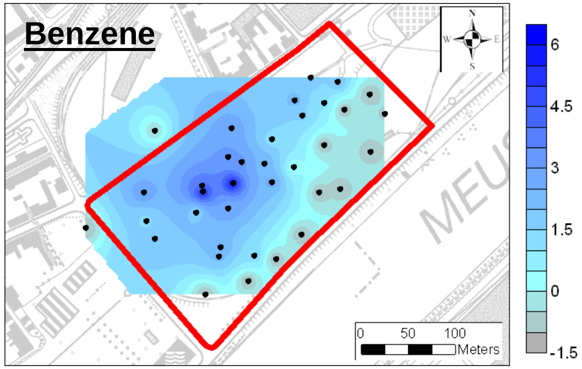


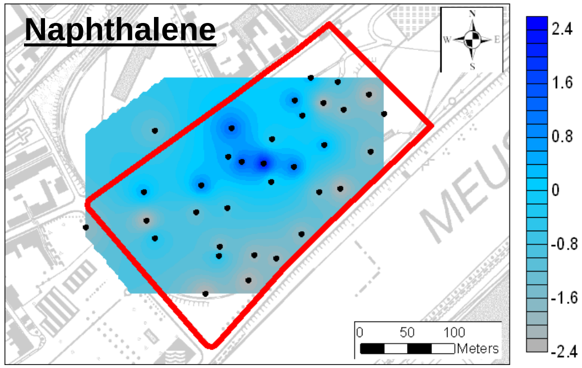
- Hydraulic gradient: 0.15% to 0.45%
- Groundwater flow direction: NW - SE (to the river in regular conditions)

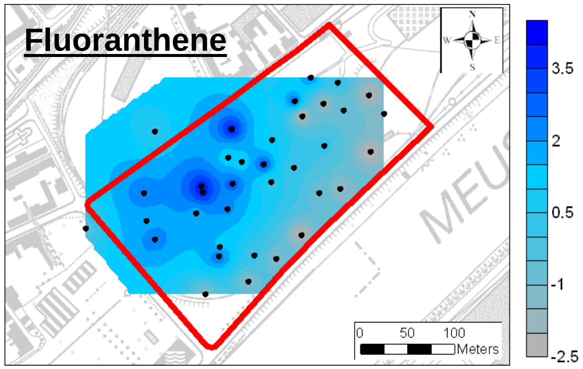


- Backfill layer (5 m th.)
- Alluvial aquifer (8 m. th.)
- Shale bedrock (13 m. depth)

3. Hydrogeology of the Flémalle site







- From 1992 to 2005, 5 characterisation campaigns have been performed,
- 116 piezometers drilled (Φ 5 – 15 cm),
- Depth-averaged conditions,
- Estimation of contamination level and extent in the soil and groundwater.

Contaminant	VI $_{Soil}$ (mg Kg^{-1})*	Soil (mg Kg^{-1})**	VI $_{GW}$ (µg L^{-1})	GW (µg L^{-1})**
Benzene	0.6	**140,000**	40	**750,000**
Toluene	85	**45,000**	5,850	**77,000**
Naphthalene	17	**140,000**	410	**63,000**
Fluoranthene	300	**25,000**	60	**2,000**
Mineral oils	5,000	**130,000**	3000	**38,000**
Zn	1,300	**3,350**	400	**140**
As	300	120	40	**110**

*Industrial use **Maximal concentration

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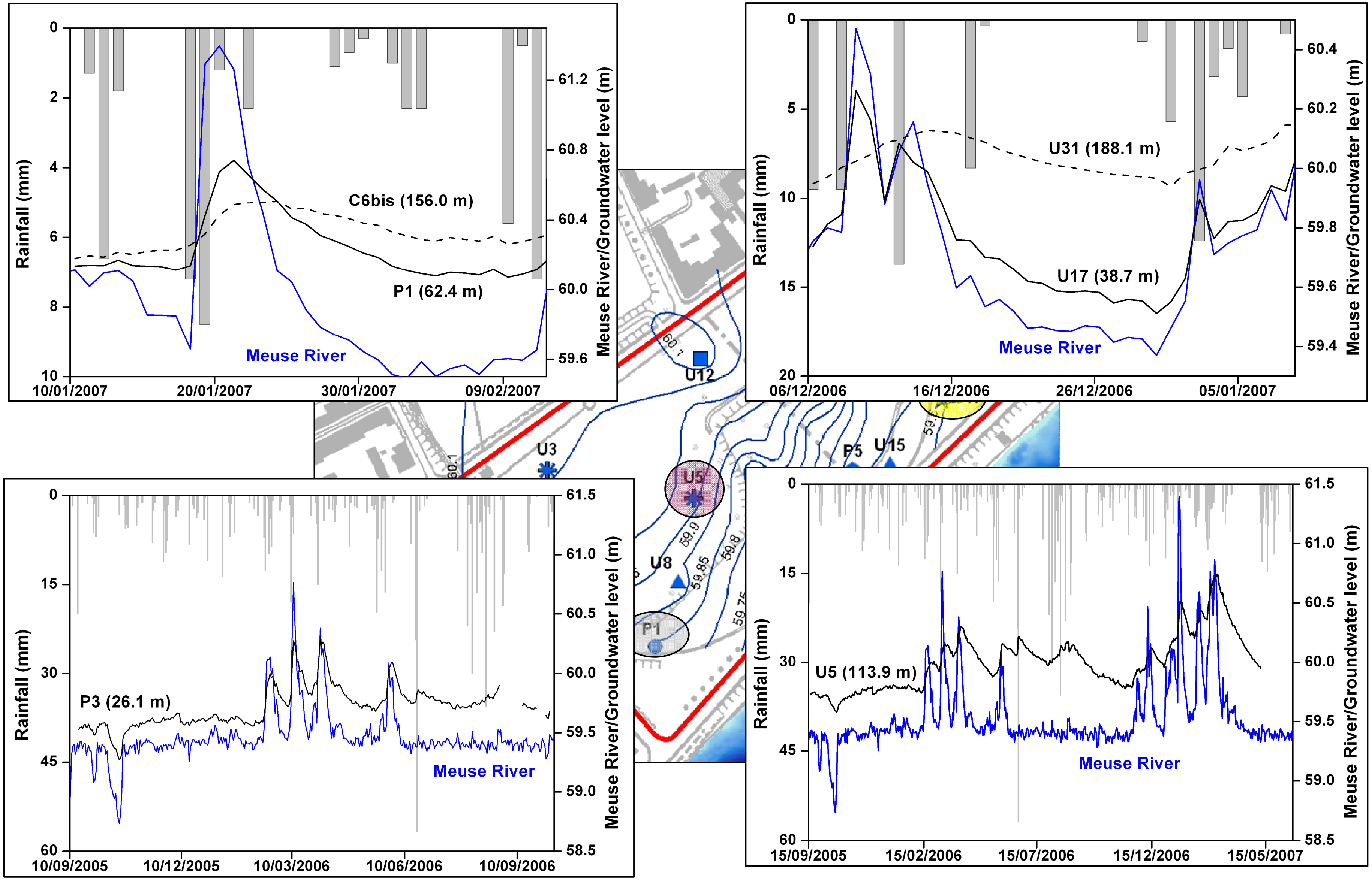
4. Summary on data mining and monitoring

- **Precipitation**
  - Ivoz-Ramet dam (2 kms upstream); daily data.
- **Data on the Meuse River**
  - Water level, discharge and temperature; hourly data.
- **Groundwater head monitoring**
  - 14 monthly monitoring;
  - 16 wells automatically monitored; hourly data.

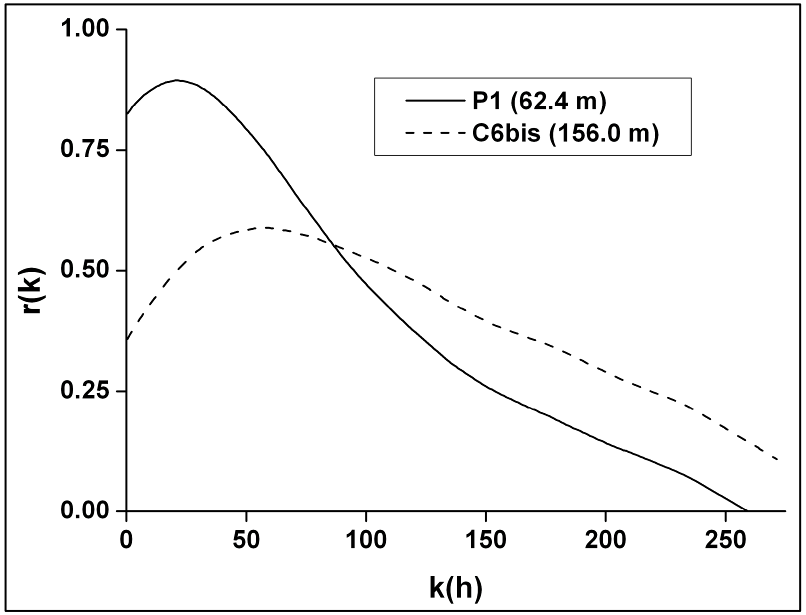
  ⇨ Good spatial cover of the site and at different distances from the Meuse River.
- **Groundwater temperature monitoring**

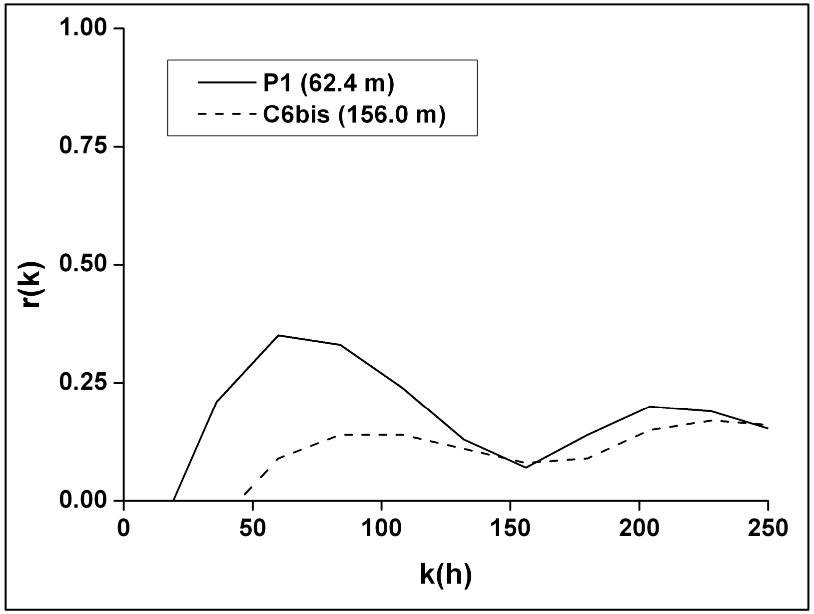
4. Summary on data mining and monitoring



4. Summary on data mining and monitoring

Cross-correlation analysis between surface water level and rainfall (input), and groundwater level (output or response of the system).





Meuse River level and groundwater level:

- up to r(k) = 0.9

Rainfall and groundwater level:

- up to r(k) = 0.3

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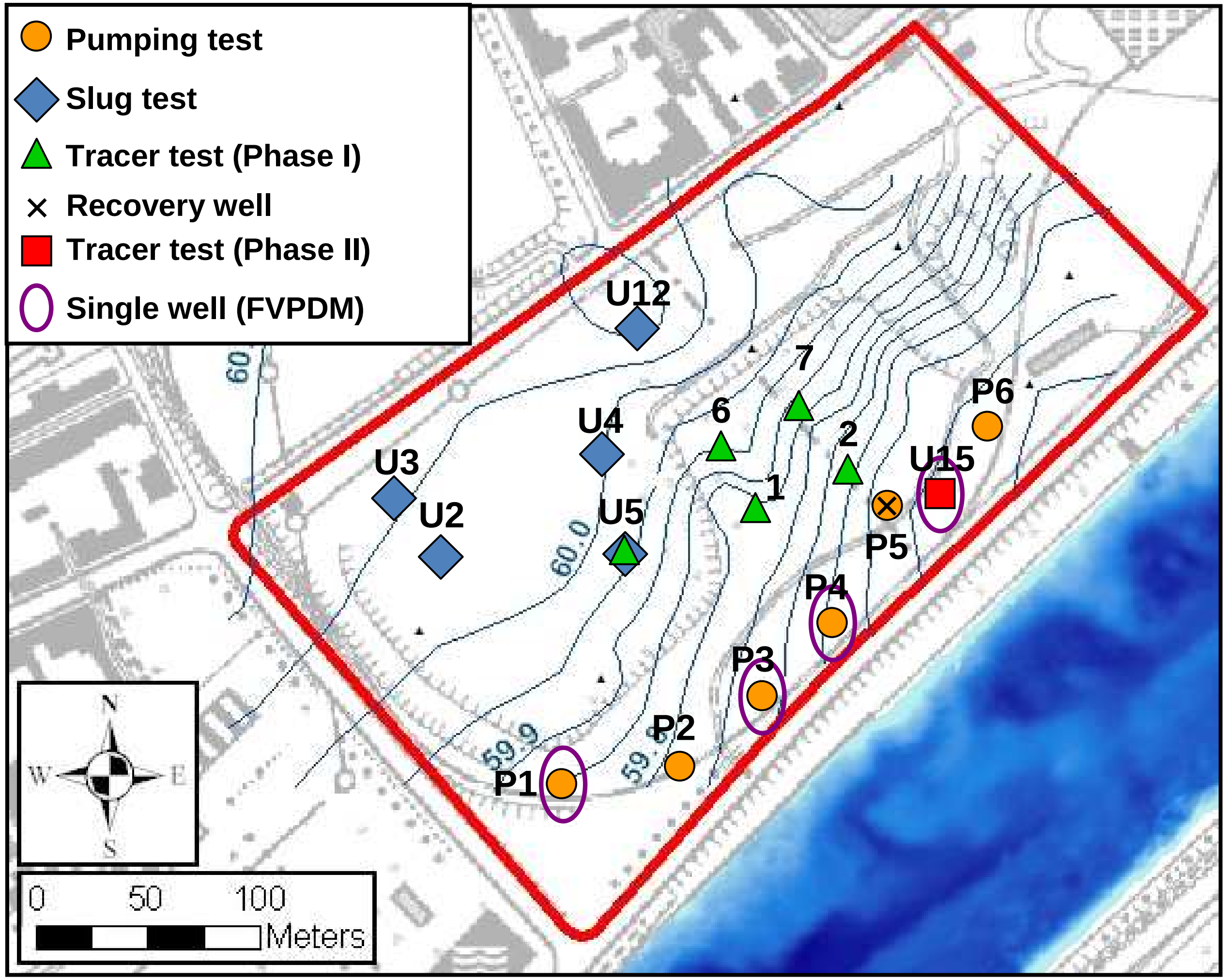
5. Summary on field experiments

- **Pumping tests (6):**
  - 6 to 10 observation wells monitored.
- **Slug tests (5)**
- **Tracer tests:**
  - Radially converging flow (2 phases);
  - Single well (Finite Volume Point Dilution Method).

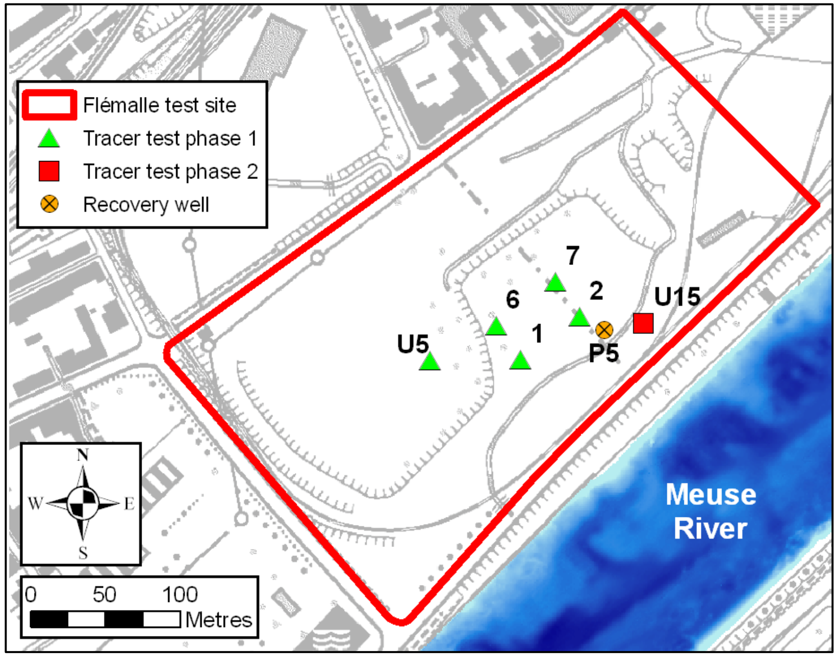
5. Summary on field experiments

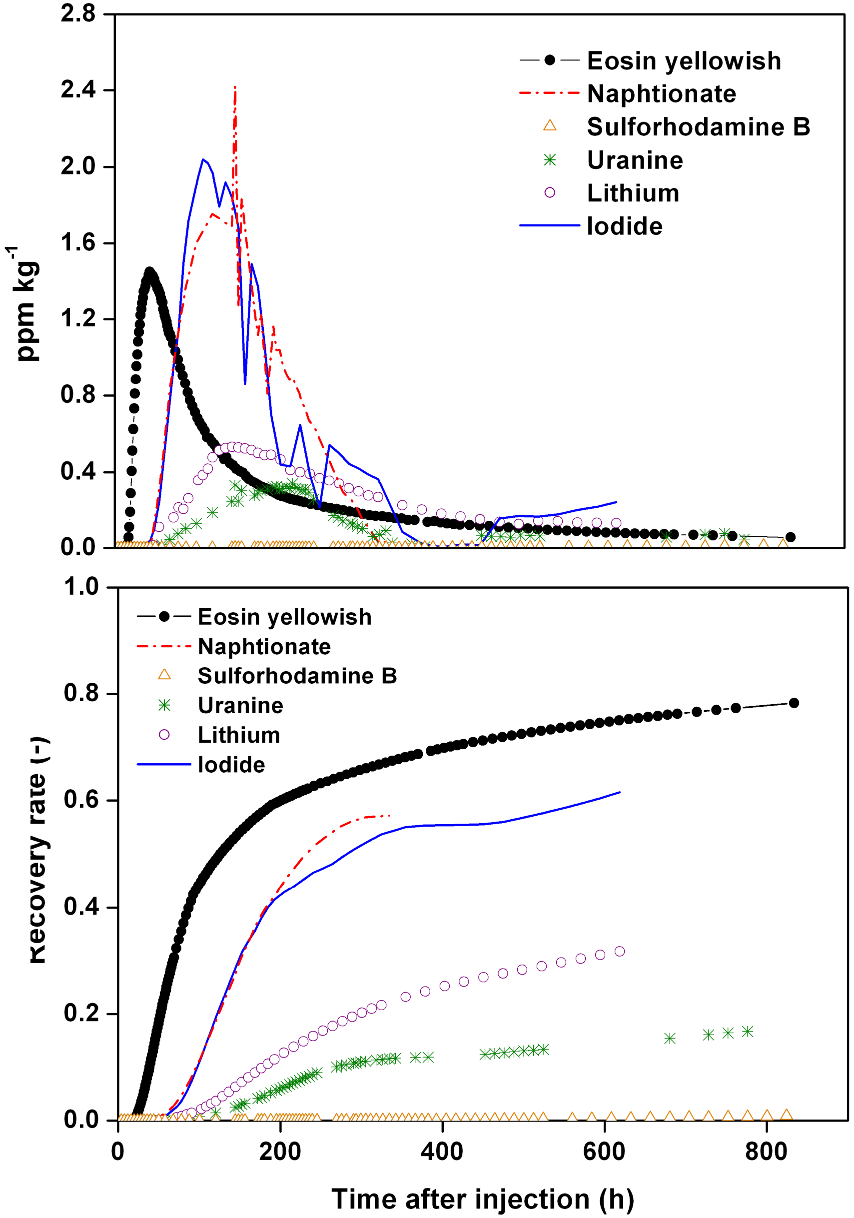


5. Summary on field experiments (Rad. conv. tracer test)

• No arrival of tracers injected during phase I;

• Phase II: different recovery rates, reflecting specific properties of each tracer.





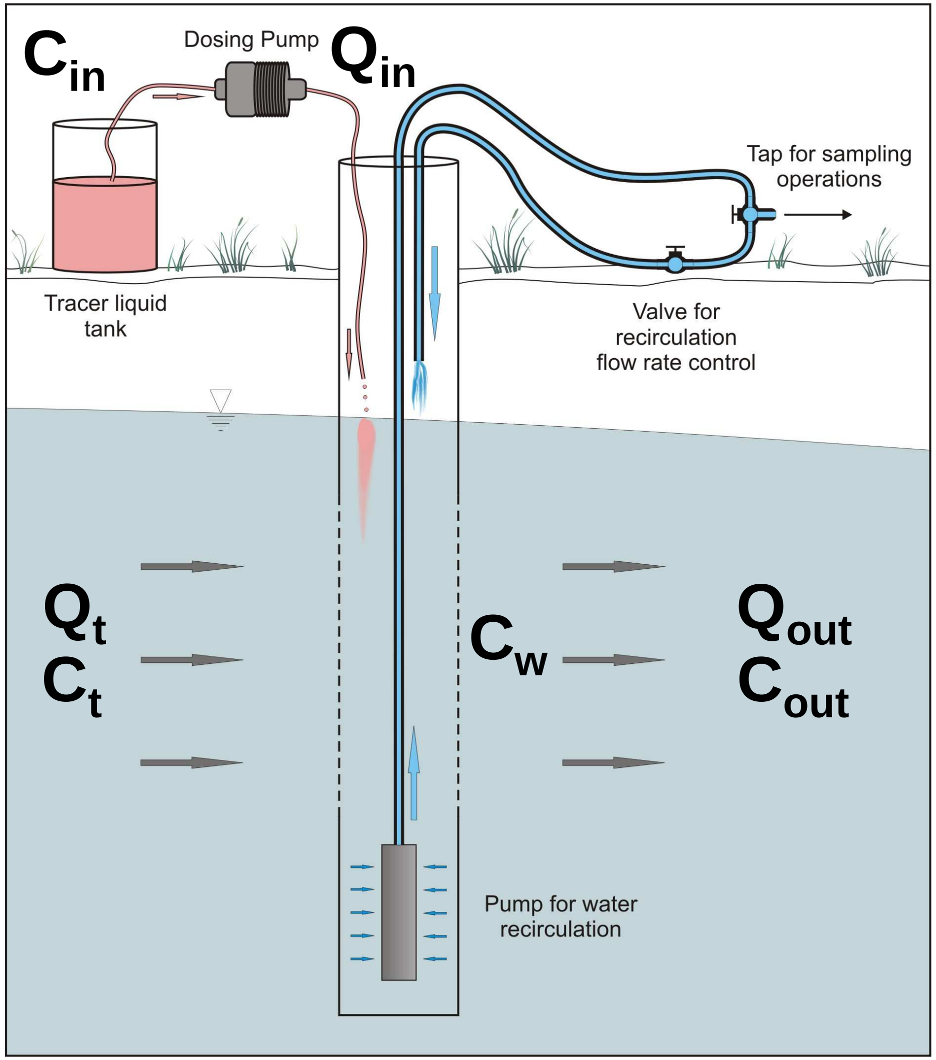
5. Summary on field experiments (Single well tracer test)

Finite Volume Point Dilution Method - FVPDM

(Brouyère *et al.* (2008). J. Contam. Hydrol. **95**: 121-140)

Objectives

- Estimate groundwater Darcy fluxes in the vicinity of the injection well;
- Relate changes in river-stage to changes in groundwater flux.



5. Summary on field experiments (Single well tracer test)

Water conservation

$$\frac{\partial V_w(t)}{\partial t} = \pi . r_w^2 \frac{\partial h_w}{\partial t} = Q_{in}(t) + Q_t(t) - Q_{out}(t)$$

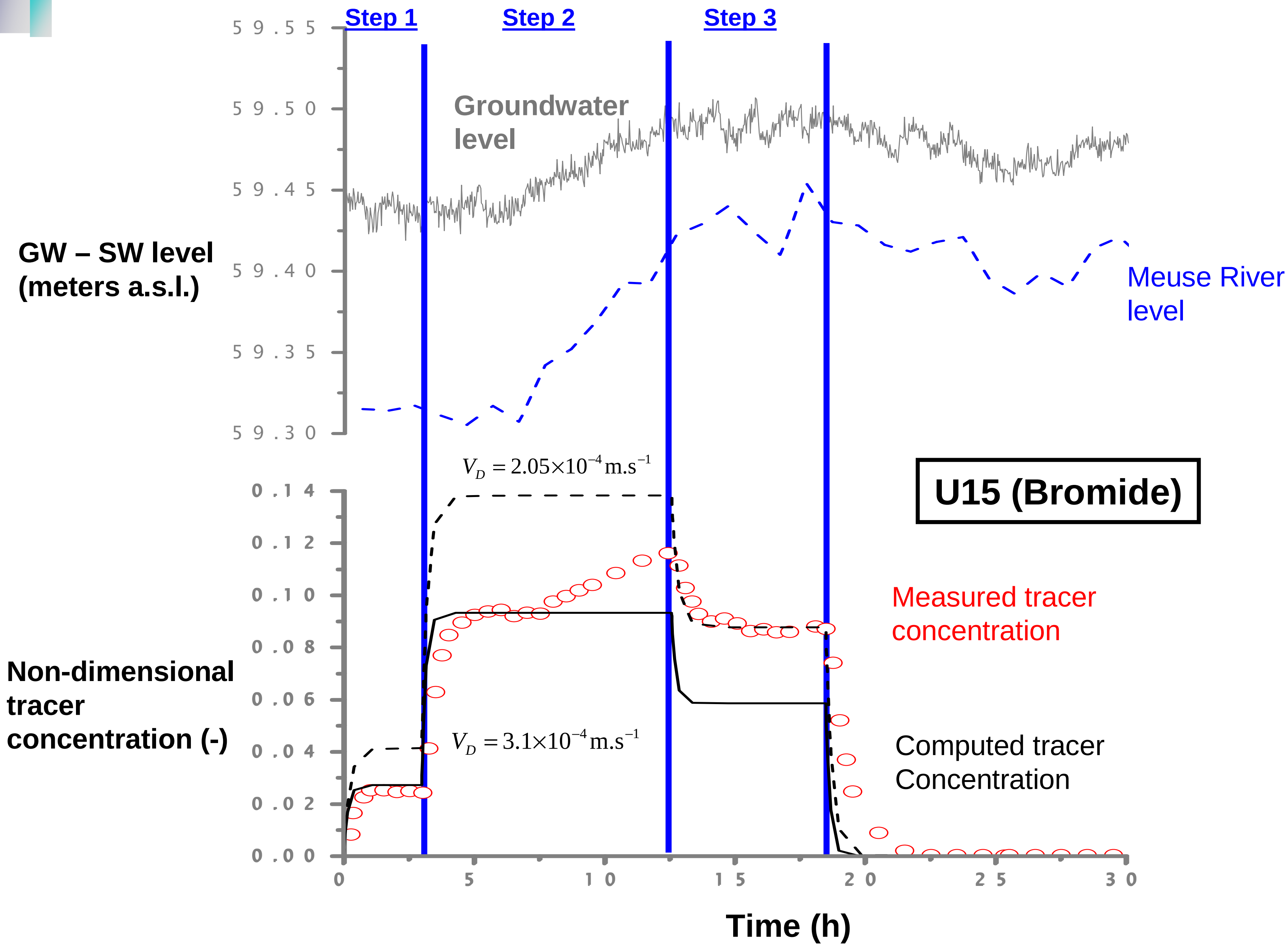
Tracer conservation

$$\frac{\partial M_t}{\partial t} = \frac{\partial}{\partial t}(V_w C_w) = \pi . r_w^2 \left(C_w \frac{\partial h_w}{\partial t} + h_w \frac{\partial C_w}{\partial t} \right) = Q_{in} C_{in} + Q_t C_t - Q_{out} C_{out}$$

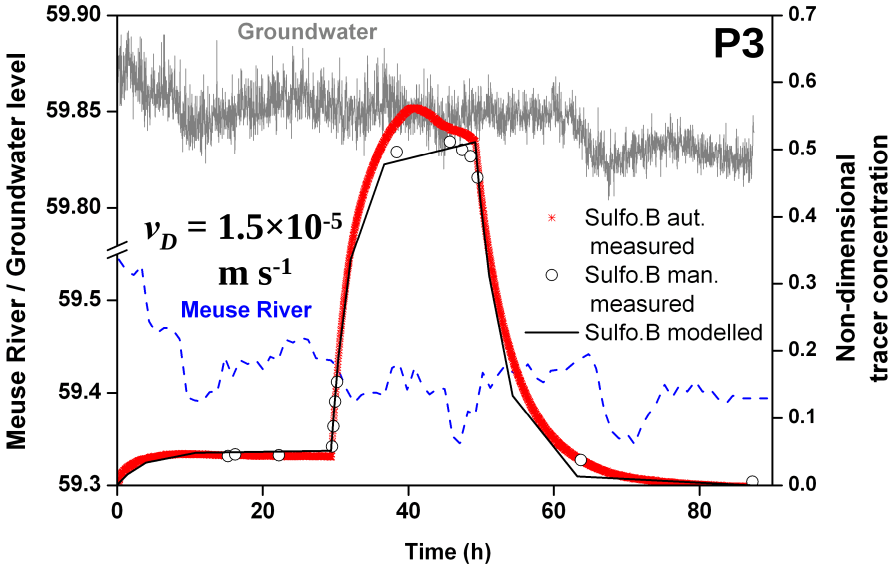
Concentration evolution in the injection well

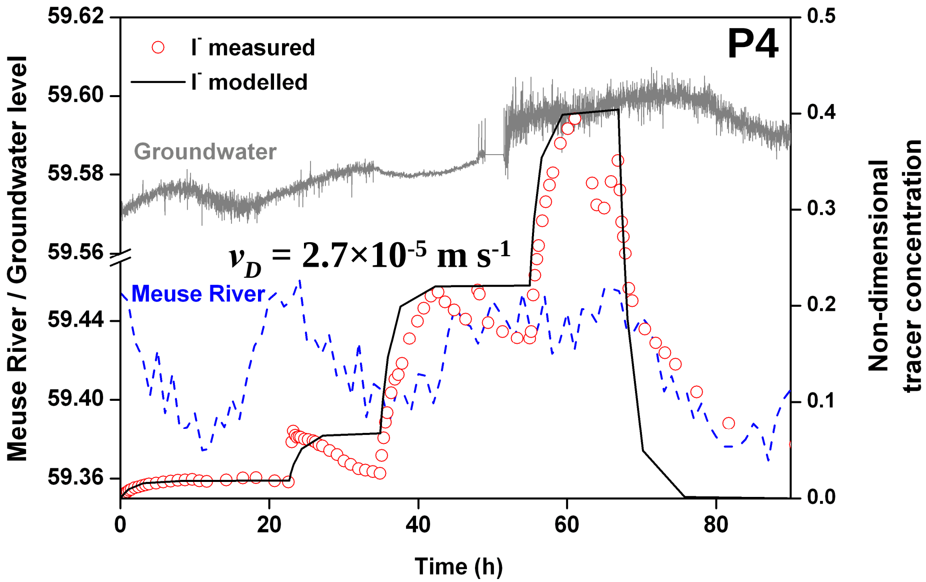
$$C_w(t) = \frac{Q_{in} C_{in} - (Q_{in} C_{in} - Q_{out} C_{w,0}) \exp\left(- \frac{Q_{out}}{V_w} (t - t_0) \right)}{Q_{out}}$$

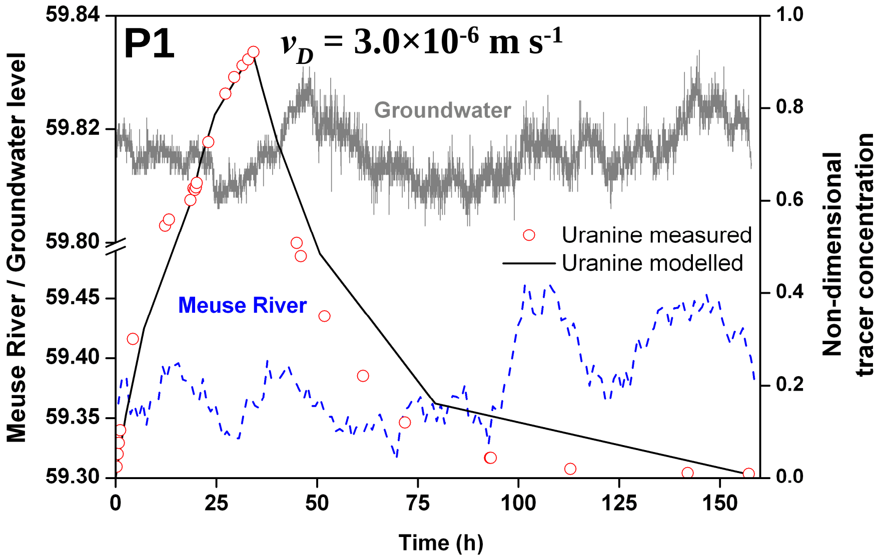
5. Summary on field experiments (Single well tracer test)

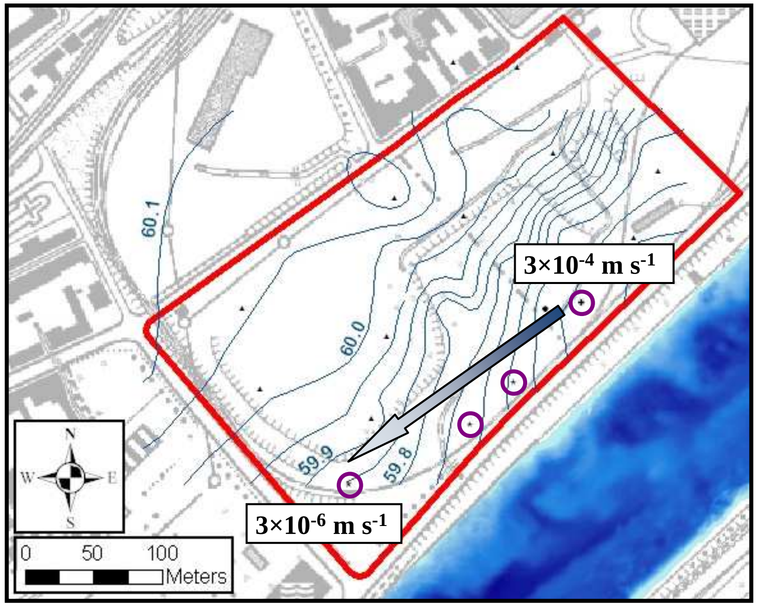


5. Summary on field experiments (Single well tracer test)









5. Summary on field experiments

GROUNDWATER – SURFACE WATER INTERACTION	
Groundwater flux direction	• Groundwater flux direction to the river under regular conditions (H ~ 59.4 m).
Dynamics river – aquifer interface	• Hydraulic gradient inversed when H increases over 60 m; • Changes of water river level induce continuous fluctuations of the Darcy flux; • Surface water flows into the aquifer when important inversions of the hydraulic gradient are produced; • Areas of preferential paths of surface water are highlighted.
HYDRODYNAMIC & HYDRODISPERSIVE PARAMETERS OF THE ALLUVIAL AQUIFER	
Groundwater head	• Groundwater head variations are mainly explained by river fluctuations (80%); • Rainfall has a reduced impact in groundwater levels (20%).
Spatial heterogeneity of the hydraulic conductivity field	• K values ranging between 1×10^{-5} and 1×10^{-3}; • High spatial variability of the hydraulic conductivity field.
Hydrodispersive parameters	• Low values of effective porosity (1.5 – 2.9%); • Low values of longitudinal dispersivity (1.4 – 3.4 m);

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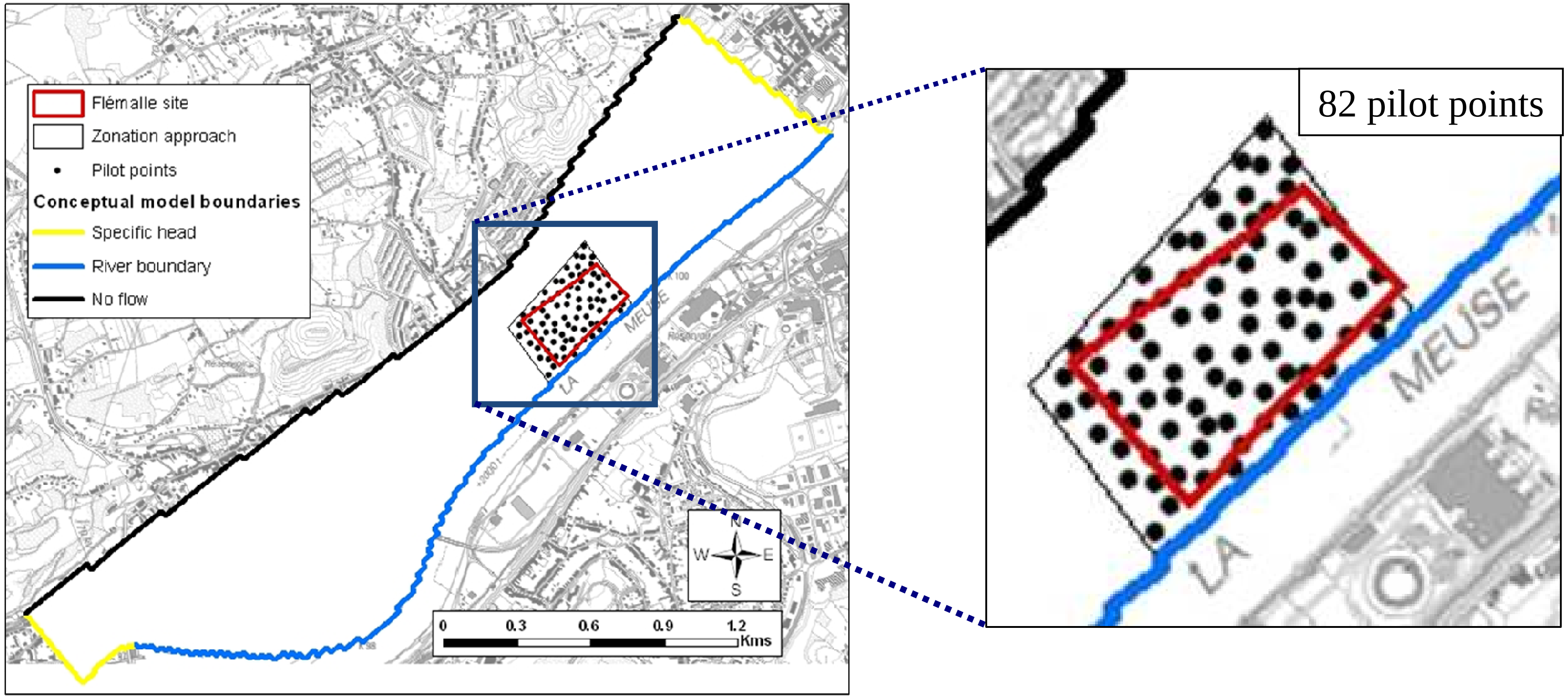
6. Numerical groundwater flow and transport modelling

MODFLOW-2000 (Harbaugh, 2000) with inverse modelling with PEST (Parameter ESTimation), using an innovative combined zonation (**regional**) - pilot points (**local**) parameterisation approach, resulting in a smoothed variation of hydraulic conductivity field of the form:

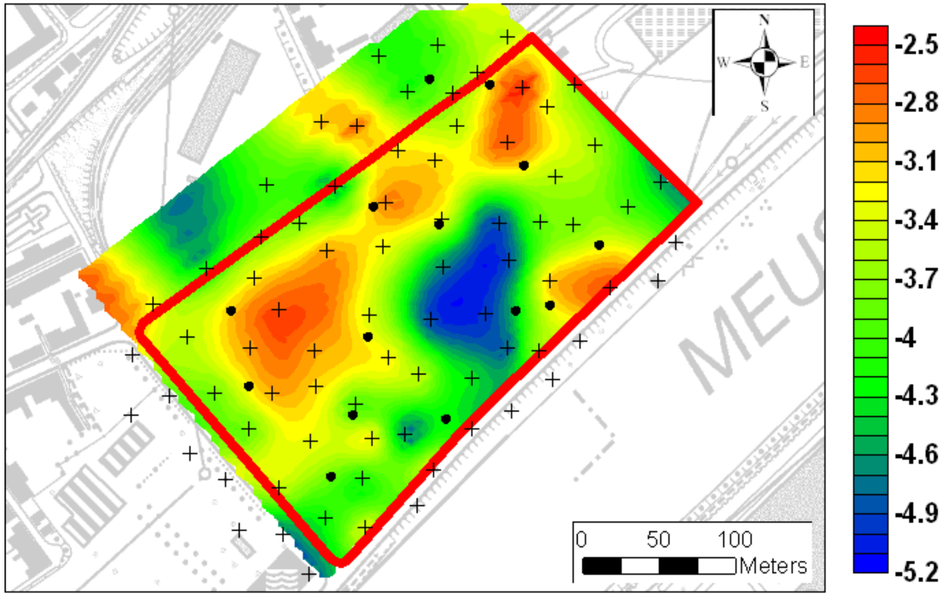
$$K(x) = \Sigma \lambda_j(x) \times k_j$$

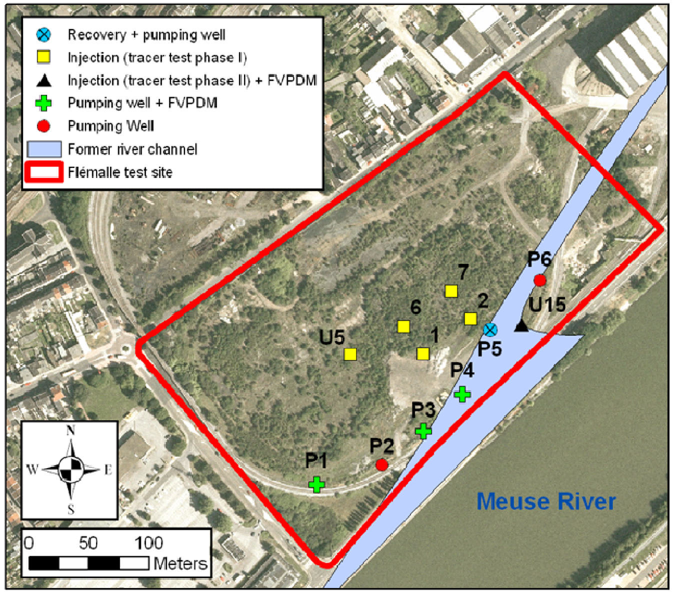
where $\lambda_j(x)$ are interpolation functions multiplying the k_j values defined at the pilot points.

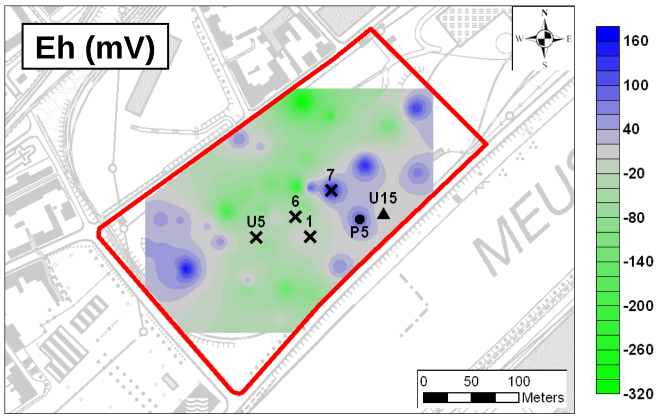


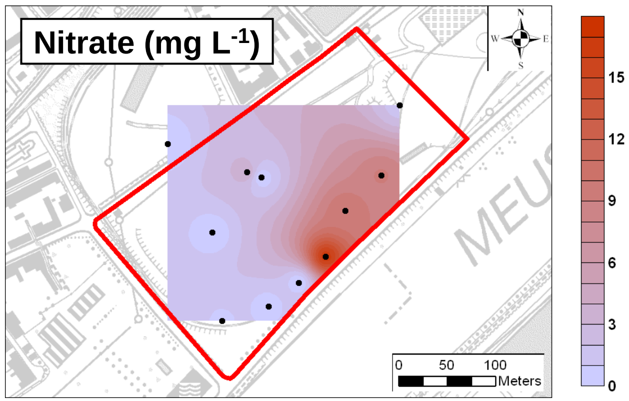
6. Numerical groundwater flow and transport modelling

Spatial heterogeneity (log K m s^{-1})

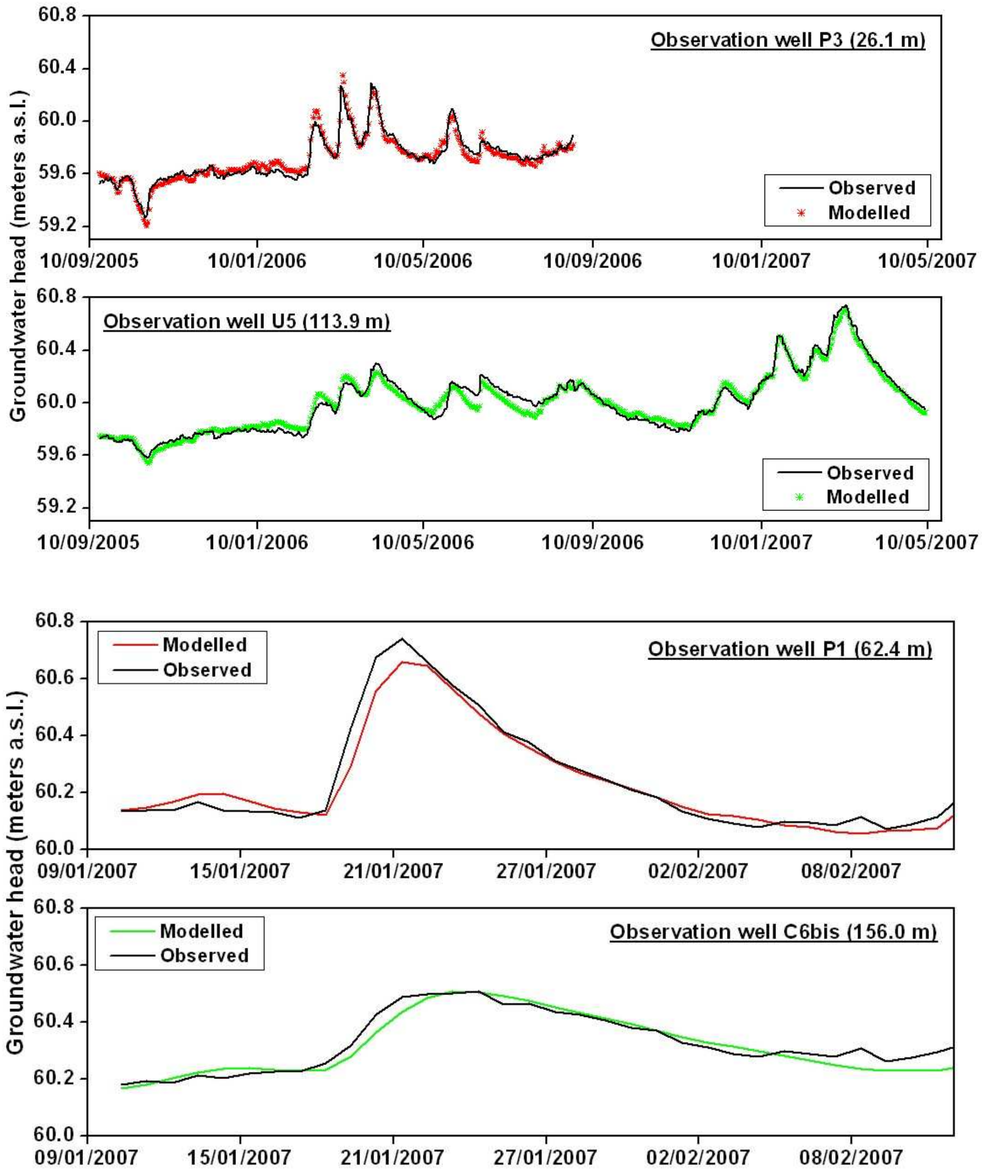


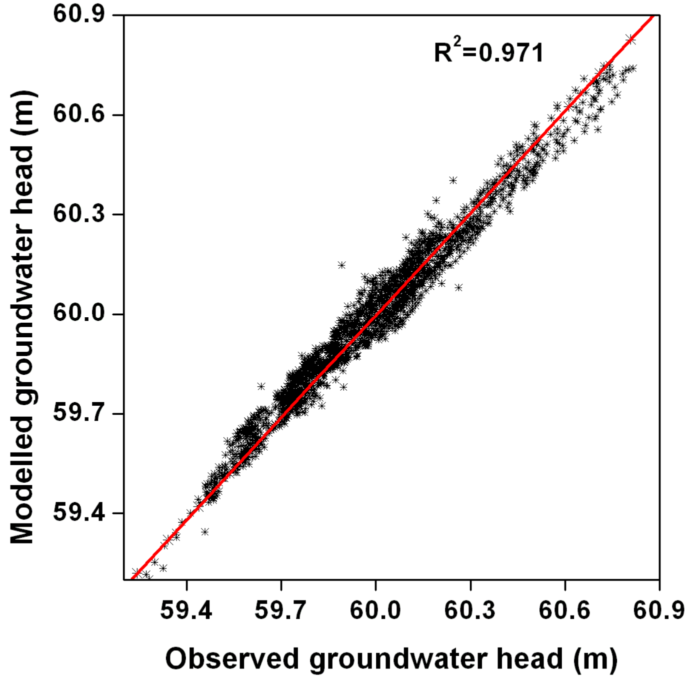






6. Numerical groundwater flow and transport modelling





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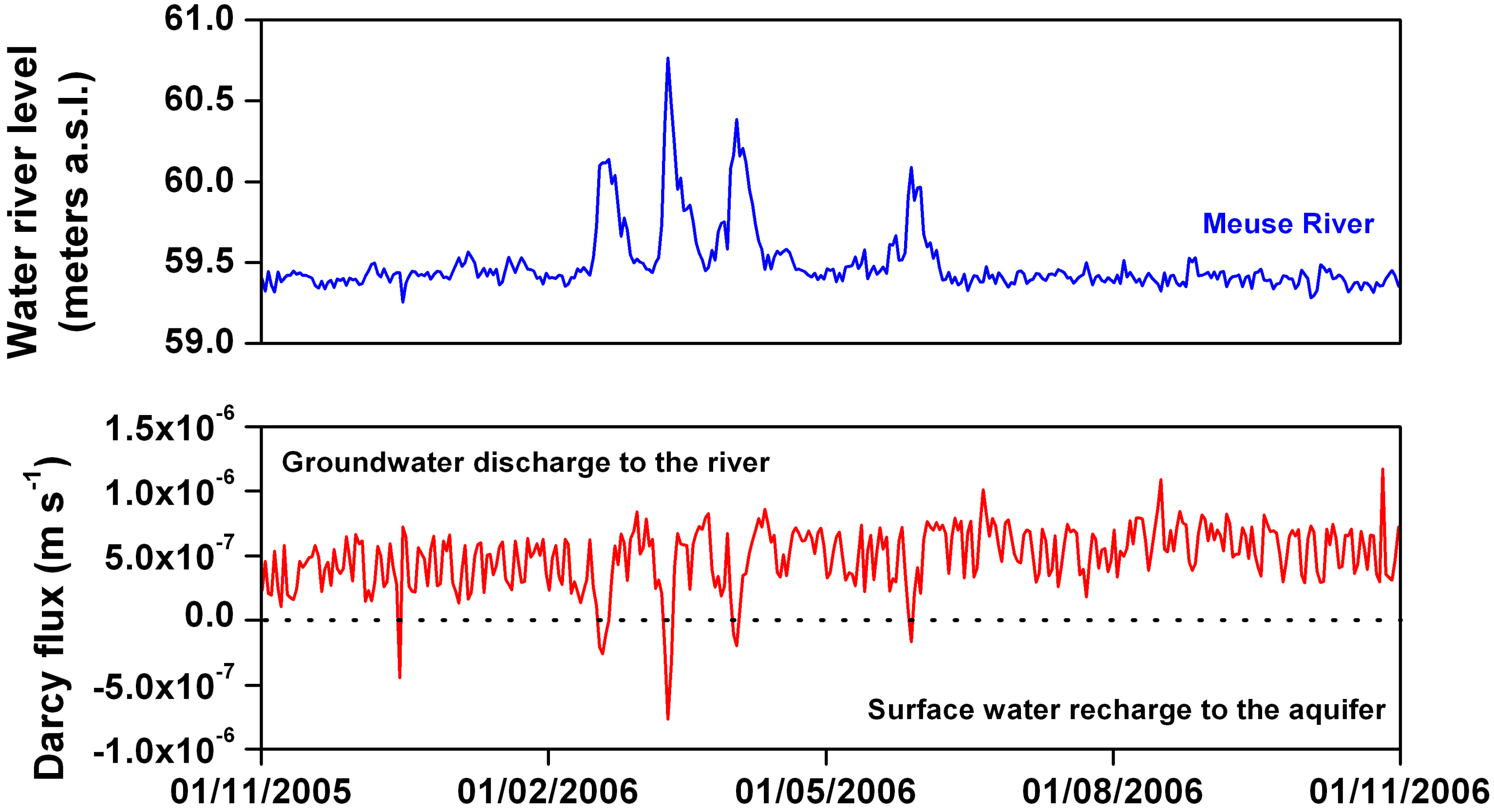
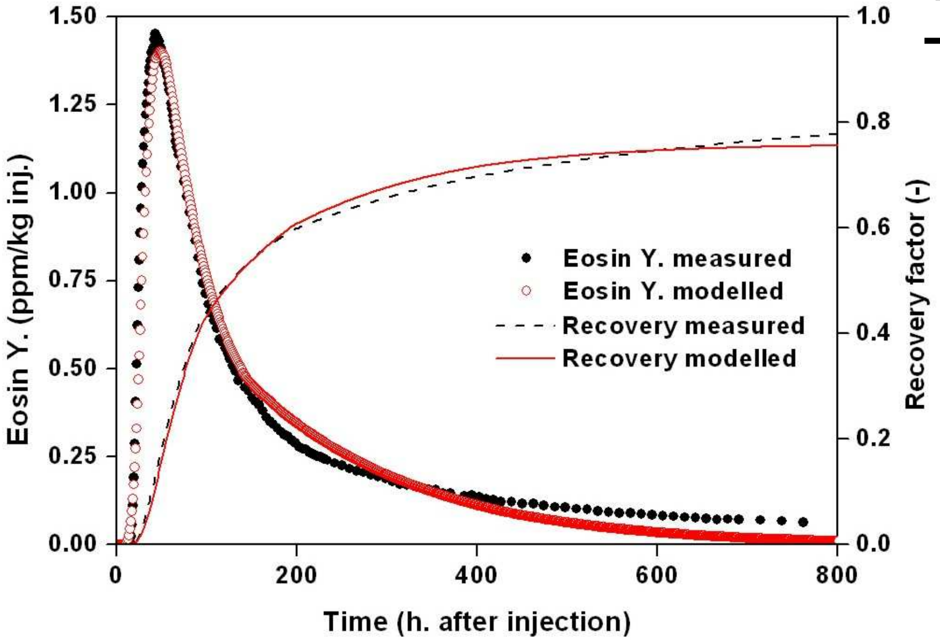


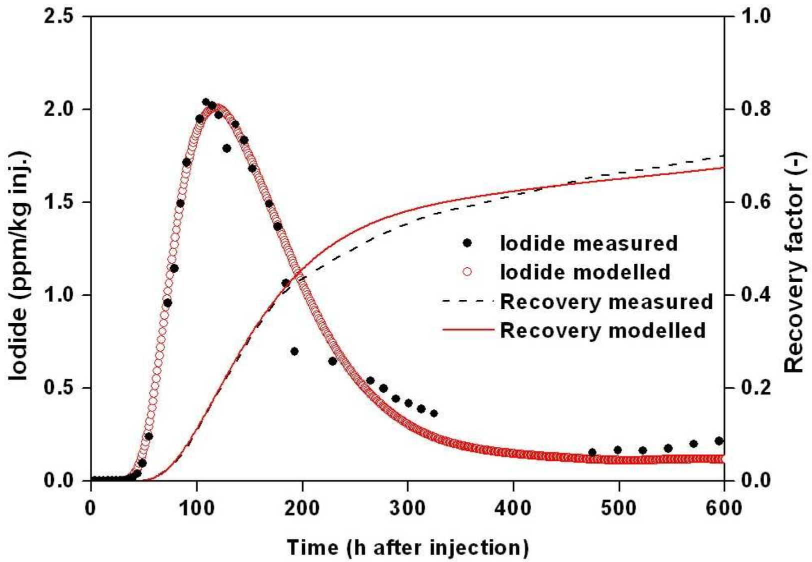
- Darcy flux are continuously changing at the river – aquifer interface.
- Hydraulic gradient inversed when water river level over ~60 m.

6. Numerical groundwater flow and transport modelling

MT3DMS (Zheng and Wang, 1999)

HYDRODISPERSIVE PARAMETERS	
Effective porosity (θ_m) (-)	0.03 – 0.045
Long. dispersivity (α_L) (m)	1.5 – 2.5
Trans. dispersivity (α_T) (m)	0.3 – 0.5
RETARDATION EFFECTS	
Immobile porosity (θ_{im}) (-)	0.05 – 0.1
Exchange coefficient (α) (s^{-1})	2×10^{-7} - 8×10^{-8}





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7. Benzene transport

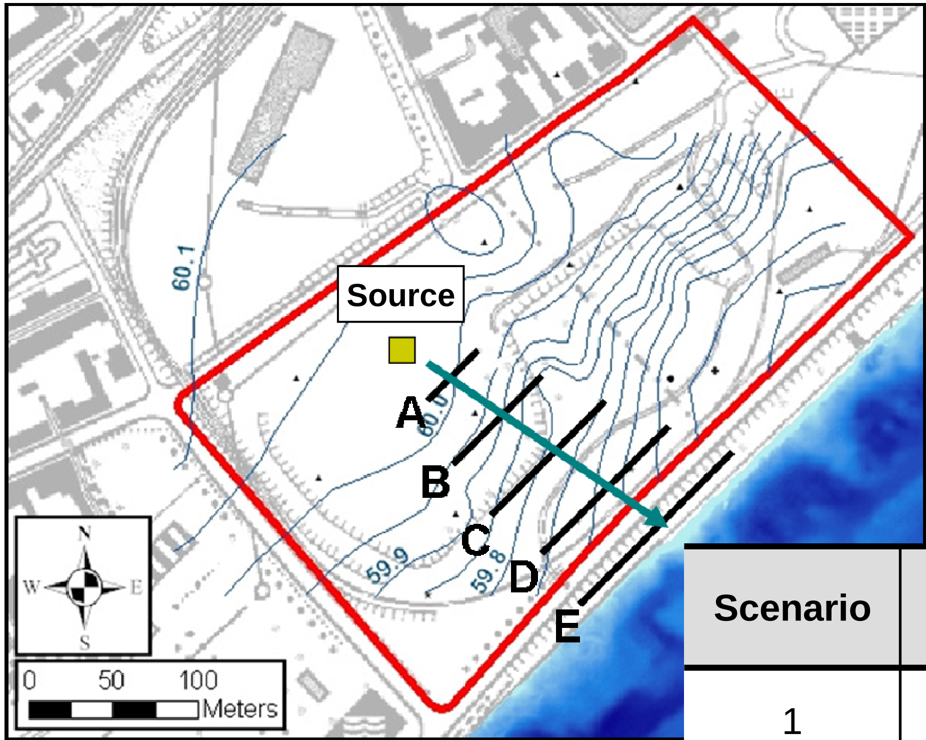
Why benzene?

- One of the main pollutant present in the Flémalle site (2 or 3 sources well identified);
- High concentration in groundwater (up to 750 mg L^{-1});
- High soluble (C_{sol} = 1750 mg L^{-1});
- Mobile in groundwater;
- Highly toxic (VI = 0.04 mg L^{-1});

High risk associated to benzene dispersion

- Useful data on biodegradation from AquaTerra partner CHYN (Centre d'Hydrogéologie de Neuchâtel – Prof. D. Hunkeler, Dr. B.Morasch & P. Höhener).

7. Benzene transport



Benzene concentrations calculated at “control planes” defined downstream from the source

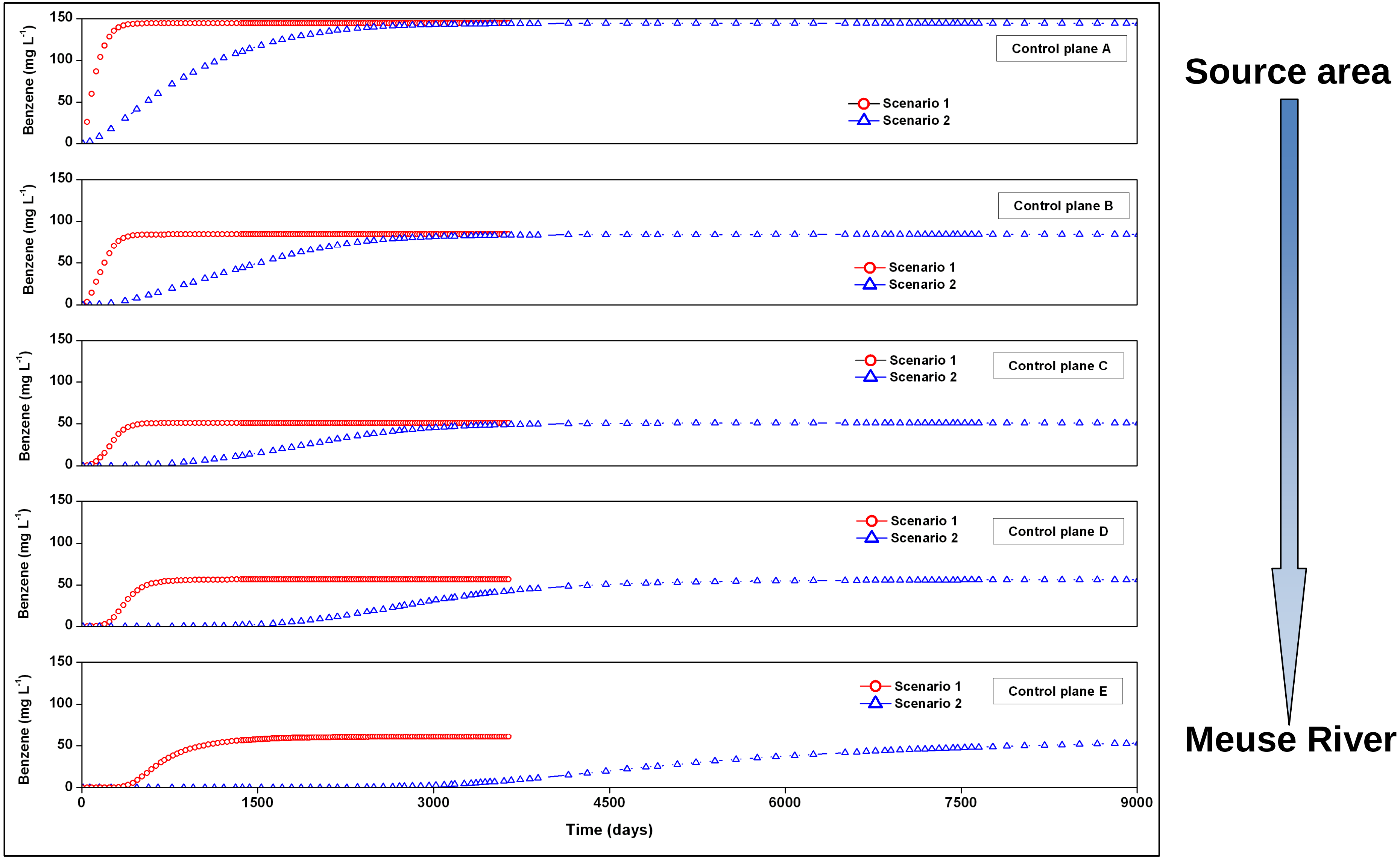
Scenario	Groundwater flow conditions	Transport processes
1	Steady state	Advection – dispersion
2	Steady state	Advection – dispersion – sorption
3	Steady state	Advection – dispersion – sorption – degradation
4	Transient	Advection – dispersion – sorption – degradation

7. Benzene transport

HYDRODISPERSIVE PARAMETERS	
Effective porosity (θ_m) (-)	0.04
Long. dispersivity (α_L) (m)	2.5
Trans. dispersivity (α_T) (m)	0.5
RETARDATION EFFECTS	
Immobile porosity (θ_{im}) (-)	0.1
Exchange coefficient (α) (s^{-1})	1×10^{-7}
Soil sorp. coef. for soil organic carbon (K_{oc}) (m^3 kg^{-1})	0.083
Soil organic carbon (%)	0.05
Distrib. coef. (K_d) (m^3 kg^{-1})	4.15×10^{-5}
Bulk density (ρ_b) (kg m^{-3})	2,000
BENZENE BIODEGRADATION	
Biodegradation ct. rate* (λ) (s^{-1})	3×10^{-7}

*First order rate constant calculated using $^{13}C/^{12}C$ isotope ratios of residual benzene in groundwater.

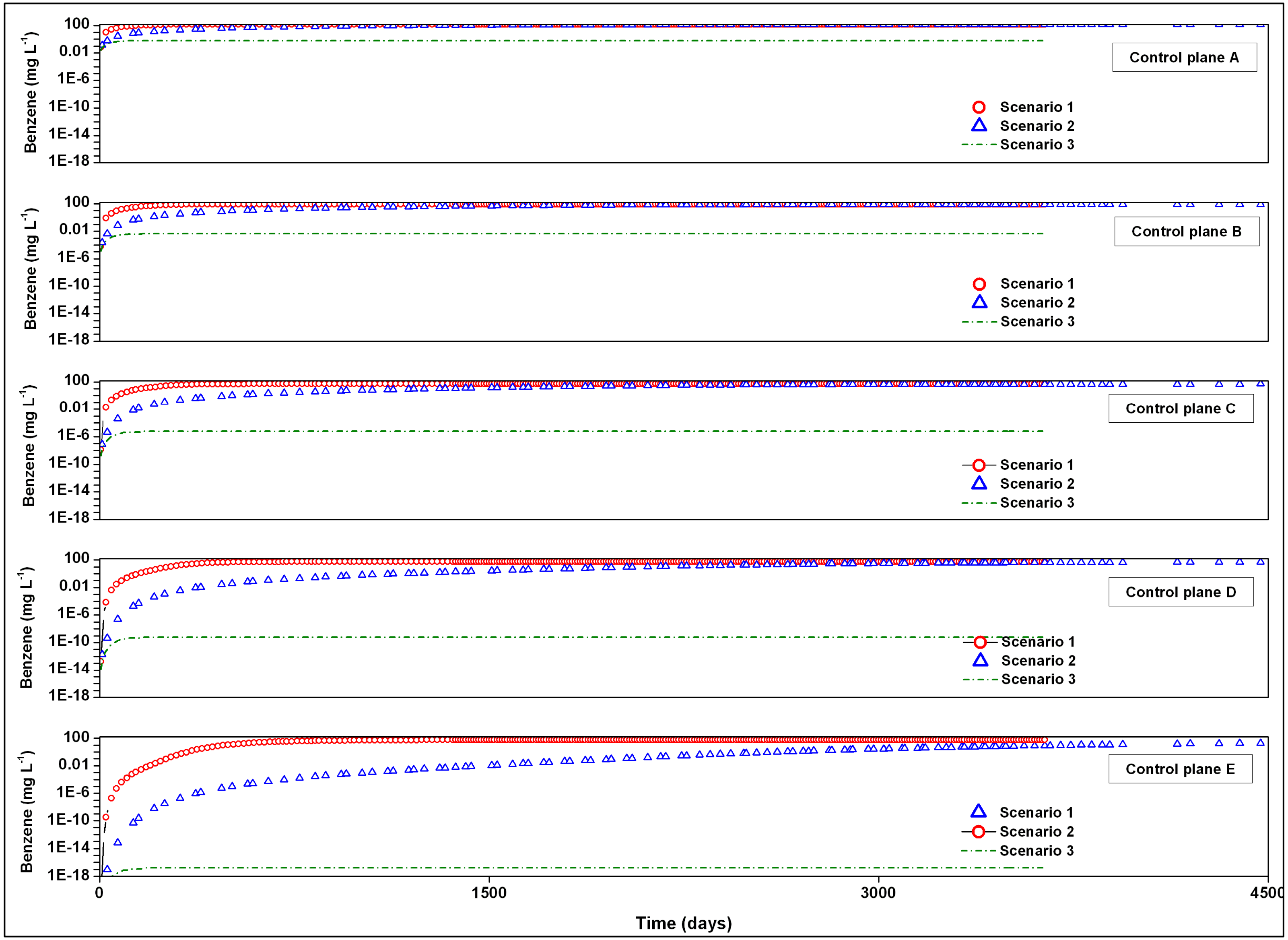
7. Benzene transport



7. Benzene transport

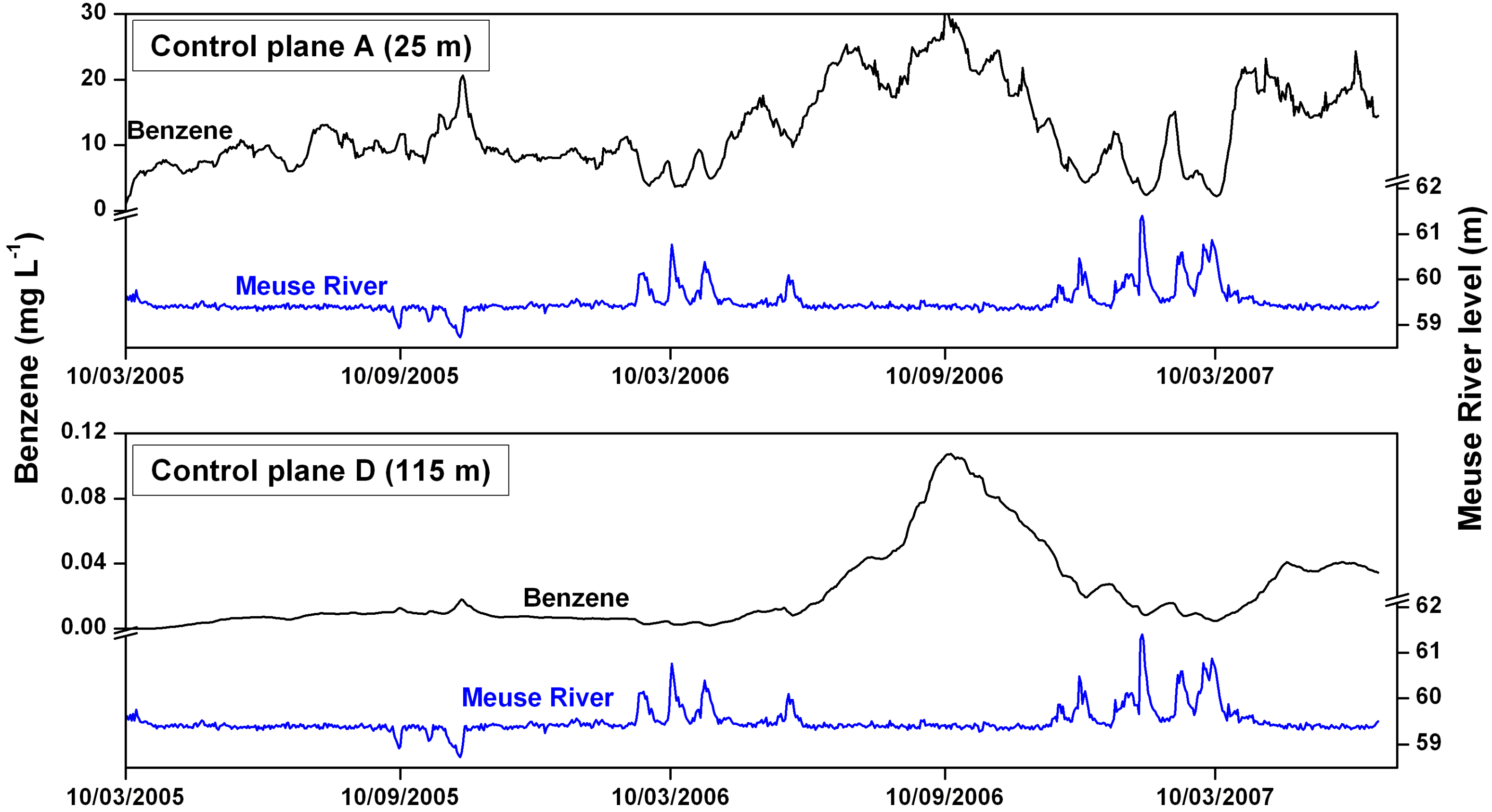
Source area

Meuse River

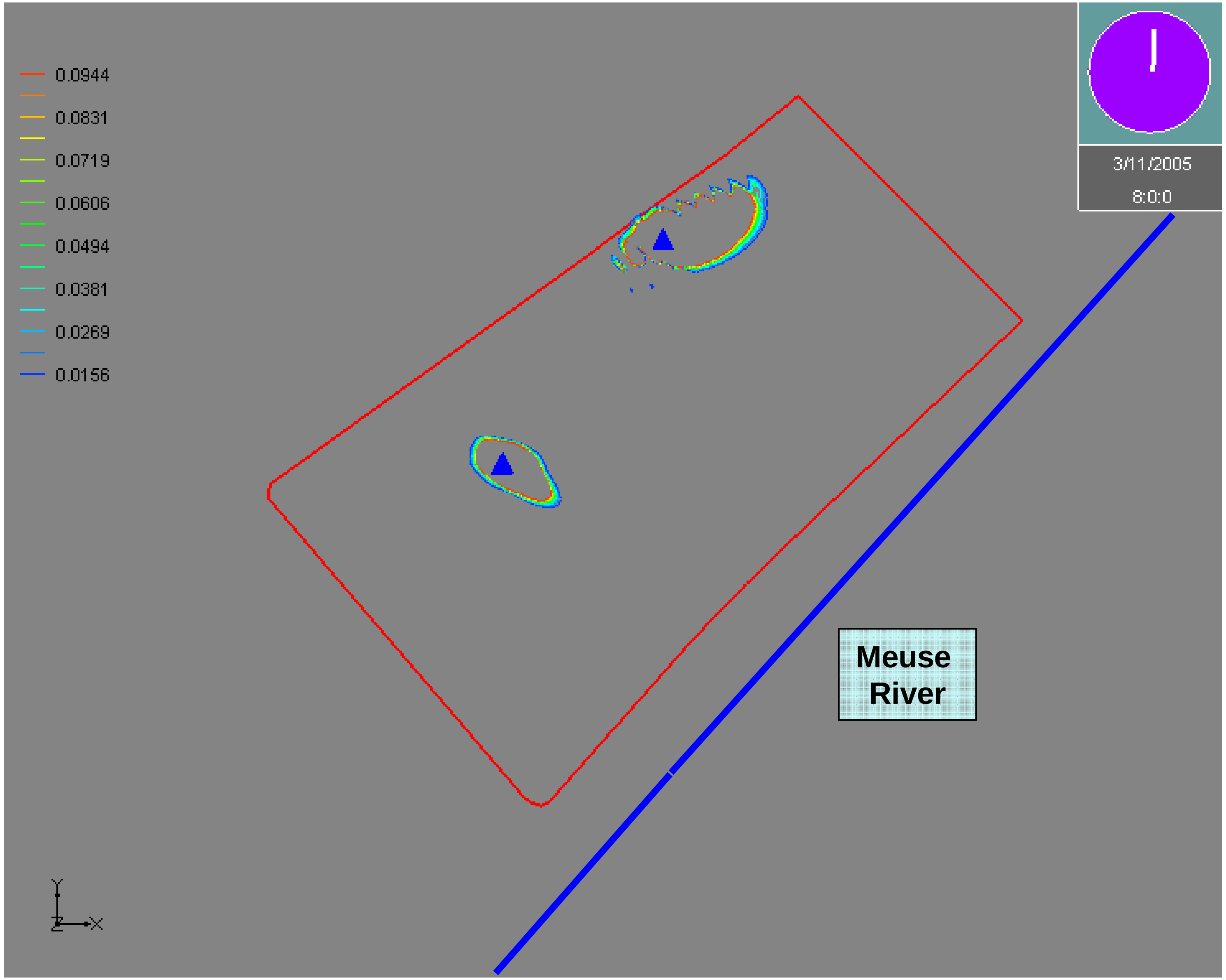


7. Benzene transport

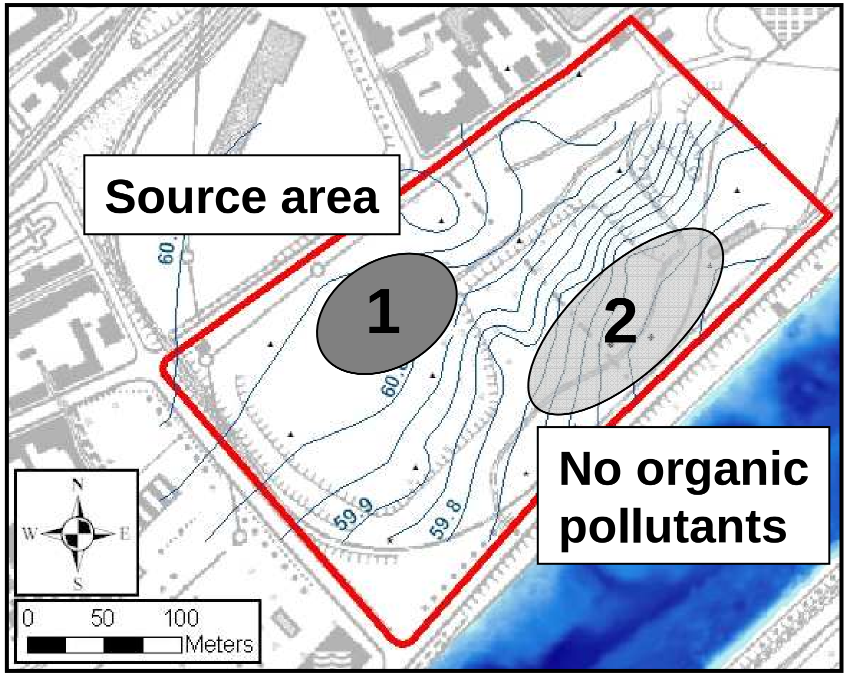
Scenario 4 (transient evolution of benzene plume)



7. Benzene transport



7. Benzene transport



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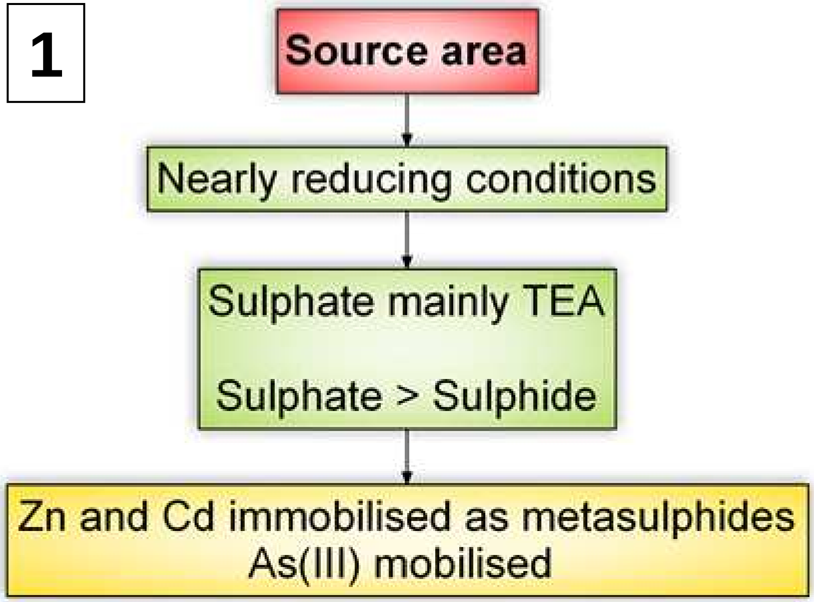

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8. Conclusions & perspectives

• Groundwater dynamics controlled by river fluctuations and heterogeneity of hydraulic conductivity field.

• Benzene dispersion / attenuation controlled by:

  - Biodegradation processes;
  - Aquifer heterogeneity;
  - River stage variations.

• Risk of benzene dispersion low and monitored natural attenuation is a valuable option with:

  - Monitoring benzene at control planes downstream from the sources;
  - Further investigation on risk of sulphate depletion in the alluvial aquifer;
  - Further investigation on mobilisation / immobilisation of heavy metals related to dynamics of organic pollutant.

8. Conclusions & perspectives

- Continuous measurement of DO in wells located nearby the Meuse River;
- Kinetic model of the degradation pattern of benzene under aerobic, nitrate and sulphate reducing conditions, as well as considering reversal of hydraulic gradients and possible inputs of DO from the river to the aquifer (RT3D).

Representativeness of the Flémalle site of a regional problem:

- Industrial activities;
- Proximity to the Meuse River;
- Geological / Hydrogeological context.

Expertise: brownfields located nearby navigable rivers (artificial bank!);

Methodology: cost-effective monitoring scheme, easy to implement in the field, providing important detailed data.

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Applicability to most of the Wallonian brownfields.

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