Co-funded by
the European Union

Team 06: Week 2

HYDROEUROPE

,tIK

Erasmus+ Programme Cooperation Partnerships
2022-1-FR01-KA220-HED-000089658
HydroEurope

In, g

WP2: Uncertainty in Advanced Hydrological and Hydraulic Modelling
WP3: Climate Change Impacts on Flash Floods
WP4: Accidental Water Pollution

- U.!'I no.
- I
-

Case Study Skawa (Poland)

Team06: Report Week 2:
Modelling and Analysis of the contaminant transport

K.

List of Authors *(to be adapted)*
Version X.Y - 27 February 2025 *(to be adapted)*

Summary

Since this is the third report in a series, it should build on the previous two by focusing on calibration and contaminant transport, while acknowledging the earlier work on conceptual model development and sensitivity analysis. Here's a structured Table of Contents that maintains continuity while keeping the focus on this stage of the study.

1. Introduction

1.1 Background and Context

The Upper Skawa Catchment, located in southern Poland, covers an area of approximately 240.4 km². The Skawa River, a tributary of the Vistula, originates in the Western Carpathians.

The study initially focused on estimating groundwater recharge within the catchment. This recharge was assessed using a formula that incorporates several factors influencing infiltration, including the annual precipitation rate, coefficients related to geological formations, land use, slope, and the depth of the water table. Precipitation data were collected from four stations distributed across the catchment, while the infiltration coefficient was determined based on geological maps. Land use was mapped using CORINE Land Cover data, and the slope coefficient was obtained through the analysis of a Digital Elevation Model (DEM). These elements allowed for the spatialization of recharge rates and laid the foundation for groundwater flow modeling.

A conceptual model was then developed to represent the hydrogeological framework of the catchment. It is based on the assumption of a single unconfined aquifer, delineated by the topography and the aquifer base, with impermeable boundaries corresponding to the catchment limits. Recharge areas were identified based on infiltration analyses, and surface-water/groundwater interactions were accounted for using the River Package (RIV) and Drain Package (DRN) modules of MODFLOW. Numerical modeling was conducted using MODFLOW-2005 with a finite-difference approach and a 100 m × 100 m grid. Key hydrogeological parameters were defined, and their sensitivity within the model was analyzed, with hydraulic conductivity ranging from 5 to 20 m/day, an infiltration coefficient (alpha) between 0.05 and 0.50, and conductance values ranging from 1 m²/day to 1000 m²/day.

To ensure model accuracy, a calibration phase was carried out by comparing observed and simulated groundwater levels. This step included a sensitivity analysis to identify the most influential parameters, as mentioned earlier, along with iterative adjustments to minimize discrepancies between simulated and measured data. These adjustments were made using data from piezometers and groundwater table contours.

Co-funded by the European Union · Universitat Politècnica de Catalunya BarcelonaTech · Vrije Universiteit Brussel · Warsaw University of Technology · Newcastle University · Brandenburgische Technische Universität Cottbus - Senftenberg · Université Côte d'Azur

1.2 Objectives of This Report

The objectives of this report are to ensure an accurate calibration of the numerical model in order to reliably simulate groundwater flow and contaminant transport in the Skawa basin. The first step is to adjust the hydrogeological parameters, including conductance, hydraulic conductivity, and recharge rates, based on piezometer data. A sensitivity analysis is conducted to identify the parameters most influential on the dynamics of subsurface flow and to enhance the robustness of the model.

One of the key objectives is to initiate and parameterize contaminant transport using MT3DMS, incorporating processes of advection, diffusion, and dispersion. Several simulations are carried out to analyze the effects of variations in porosity, longitudinal and transverse dispersivity, as well as spatial and temporal discretization, in order to assess their impact on pollutant migration. The goal is to identify the most vulnerable areas to contamination and to understand the influence of injection on the dispersion of pollutants.

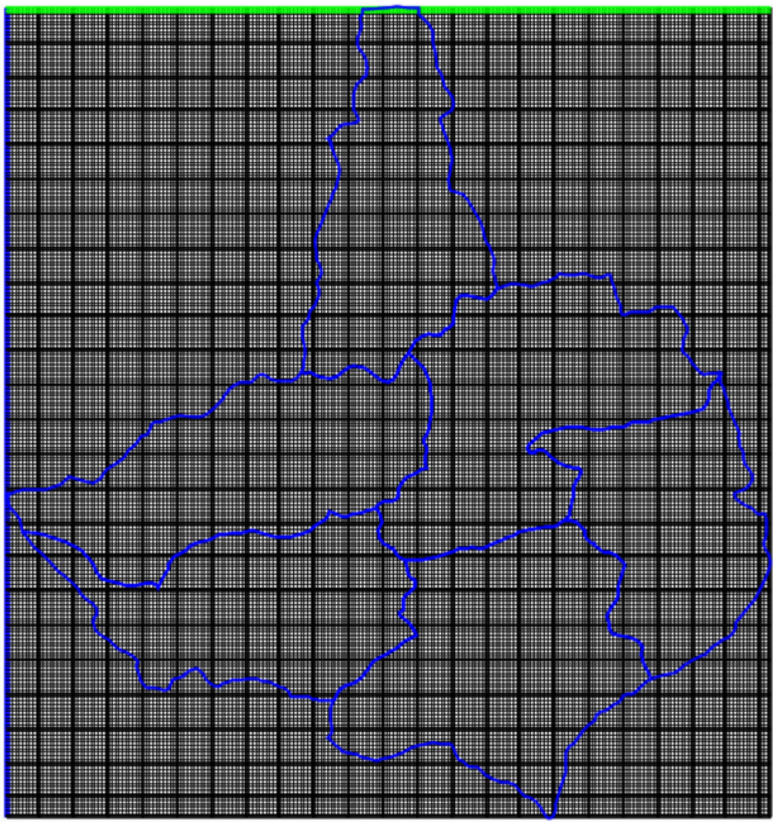
Finally, the report aims to analyze the results by comparing them with the expected behavior from the sensitivity analysis, identifying the main sources of uncertainty, and providing recommendations to improve the accuracy of the simulations.

2. Model Calibration

2.1 Numerical Model

- **Grid Resolution and DEM-Based Representation**

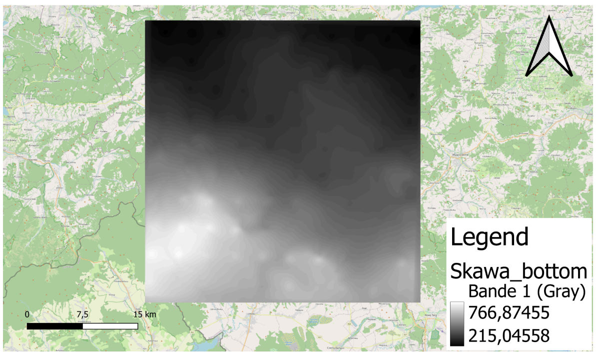
The first step to modelize the Skawa catchment is to create a grid on Modelmuse. The cell size chosen is the same as the one that was used for the processing of the data with GIS, that is to say, a cell size of 100m x 100m. The outline of the grid is defined by the outline of the catchment which was added to Modelmuse as a shapefile.



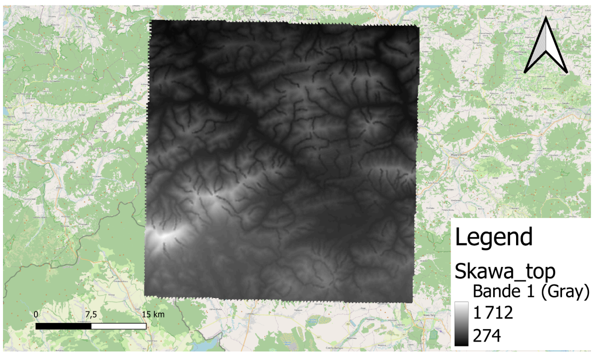
- **Layer Structure and Aquifer Thickness**

After creating the grid, we have to add the bottom and the top of the aquifer. The representation of these layers on QGIS are the following figures :

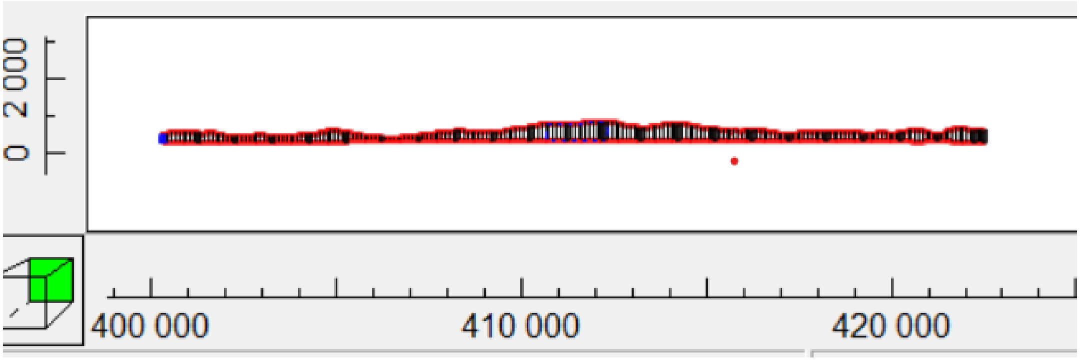
Bottom layer of aquifer

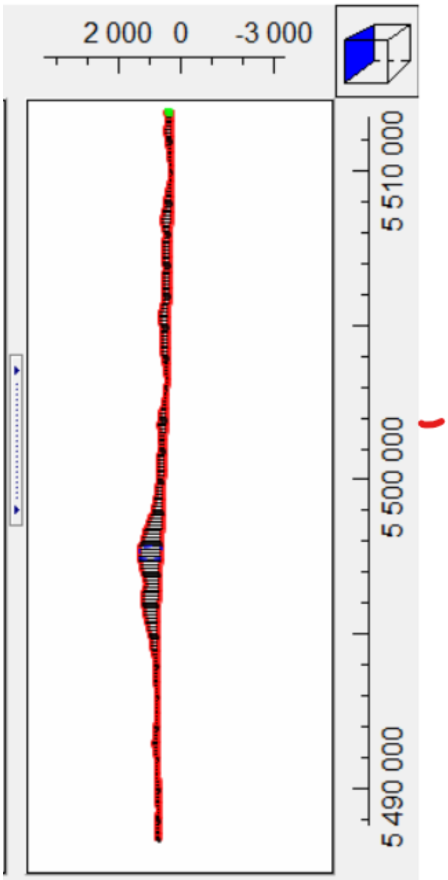


Top layer of the aquifer



After importing these layers, we obtain the thickness of the aquifer at each cell.

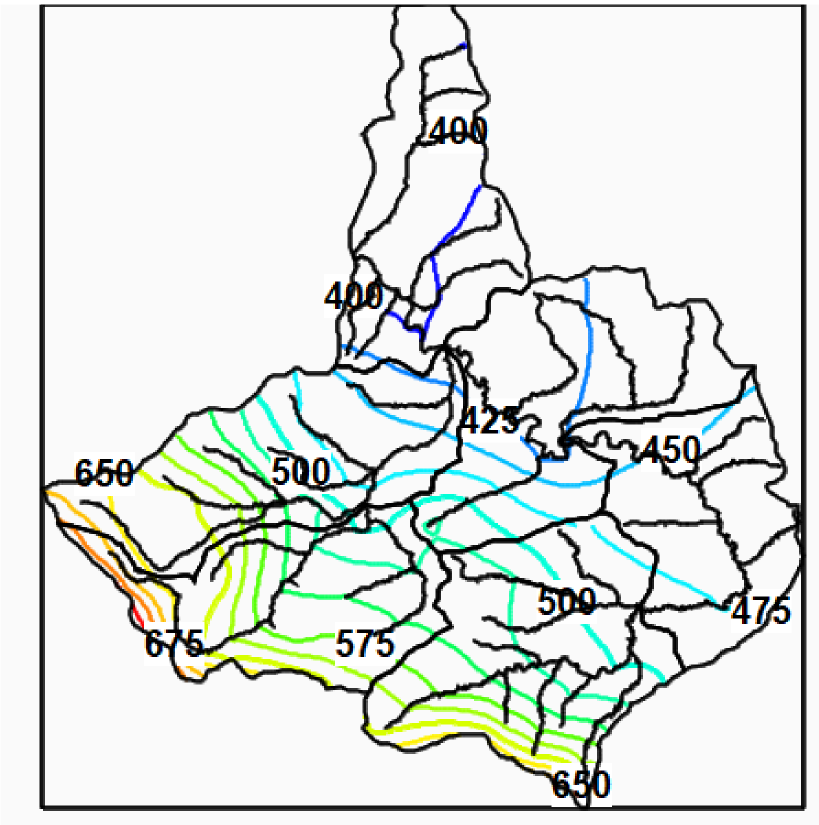




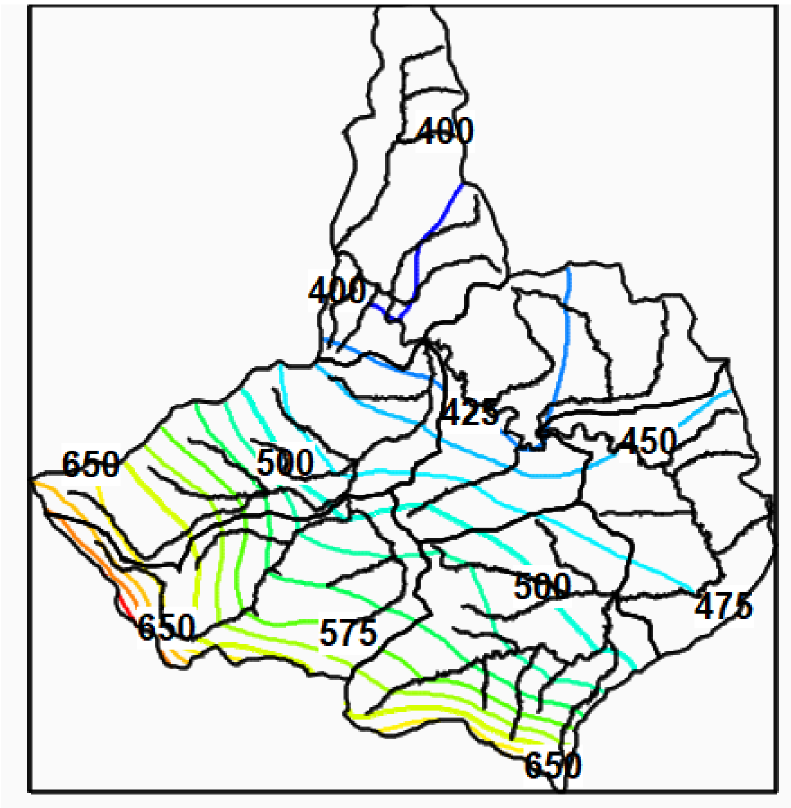
2.2 Overview of Sensitivity Analysis

We change the value of the parameters to estimate the impact of this parameter on the results on the modelisation. That is to say the influence of the parameters on the water table contour.

Hydraulic conductivity :

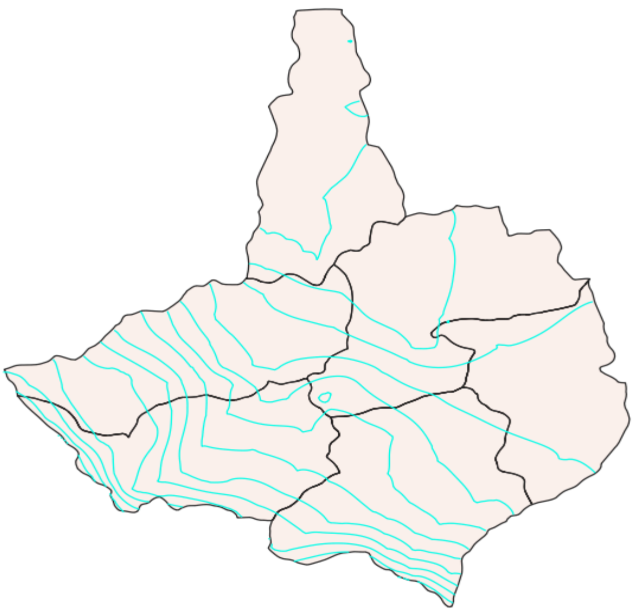


K = 0.5 m/d

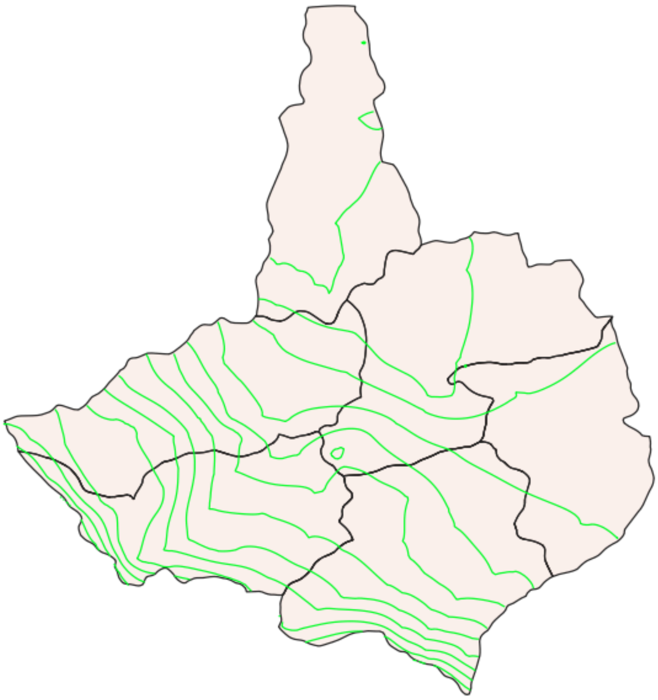


K = 20 m/d

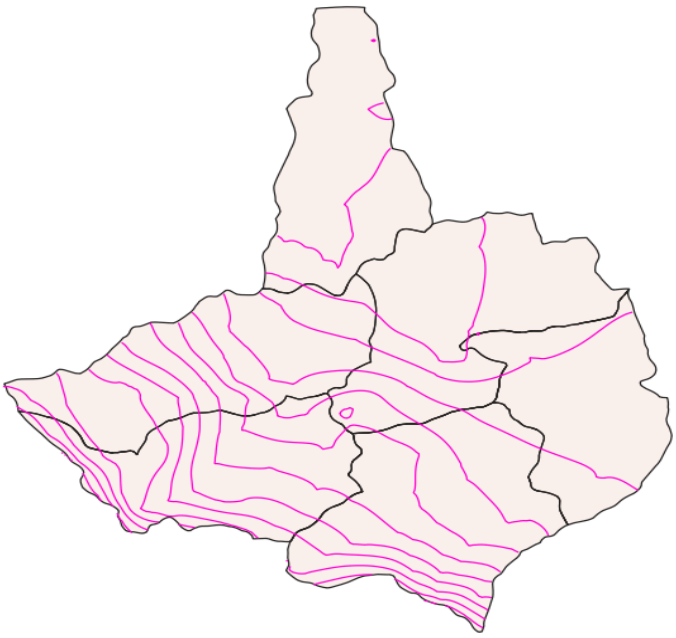
Infiltration coefficient alpha :



α= 0.05

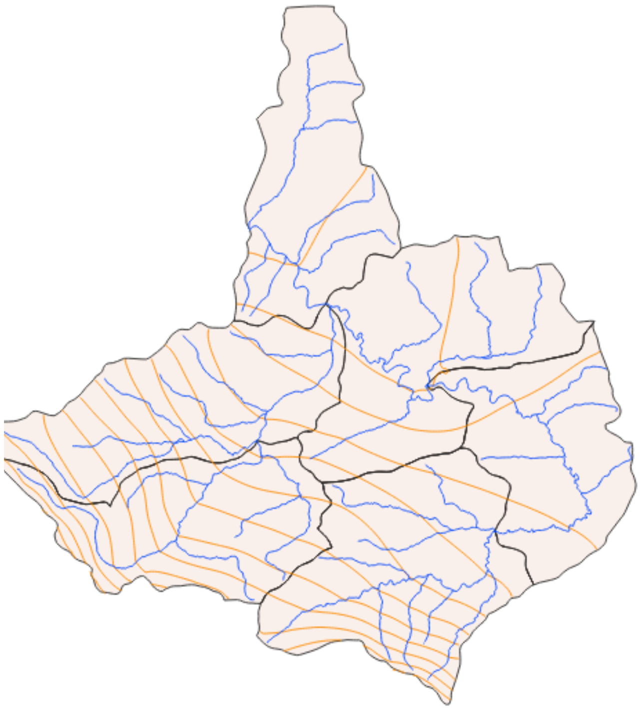


α = 0.15



α = 0.50

Conductance :



C = 1 m²/d

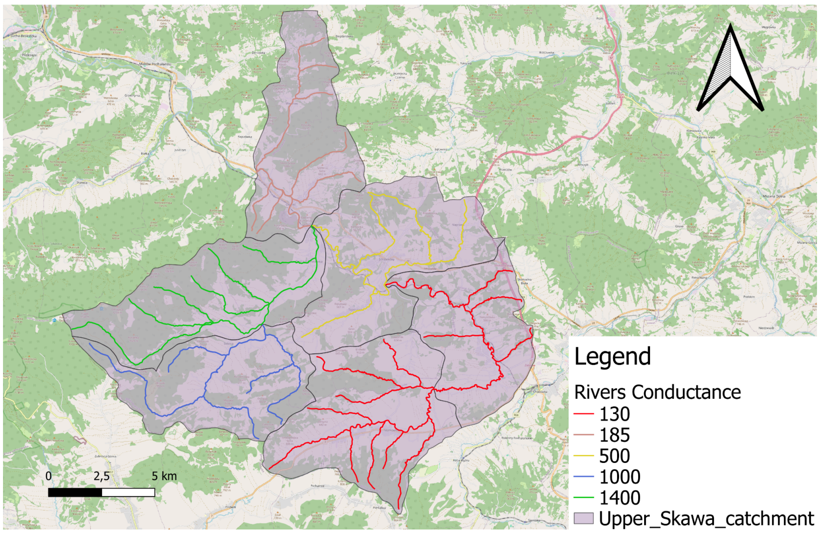
C = 1000 m²/d

Analysis of the result

2.3 Calibration Process in ModelMuse

- Conductance

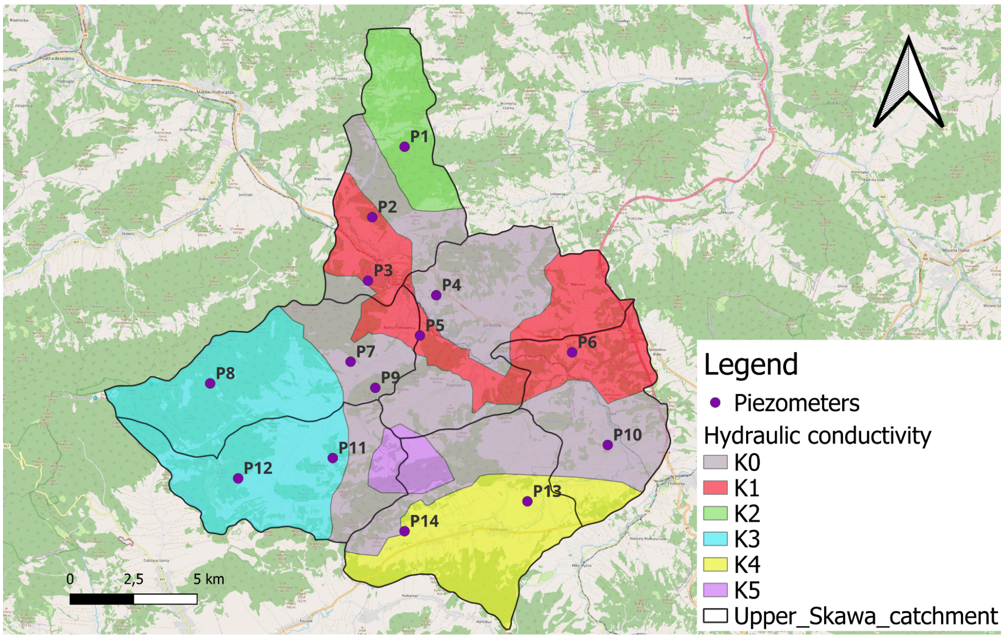
Map of the conductance



	Rivers Conductance BC (m^2/s)	Rivers Conductance AC (m^2/s)
Rivers 1	1000	185
Rivers 2	1000	1400
Rivers 3	1000	1000
Rivers 4	1000	500
Rivers 5	1000	130

- Hydraulic Conductivity

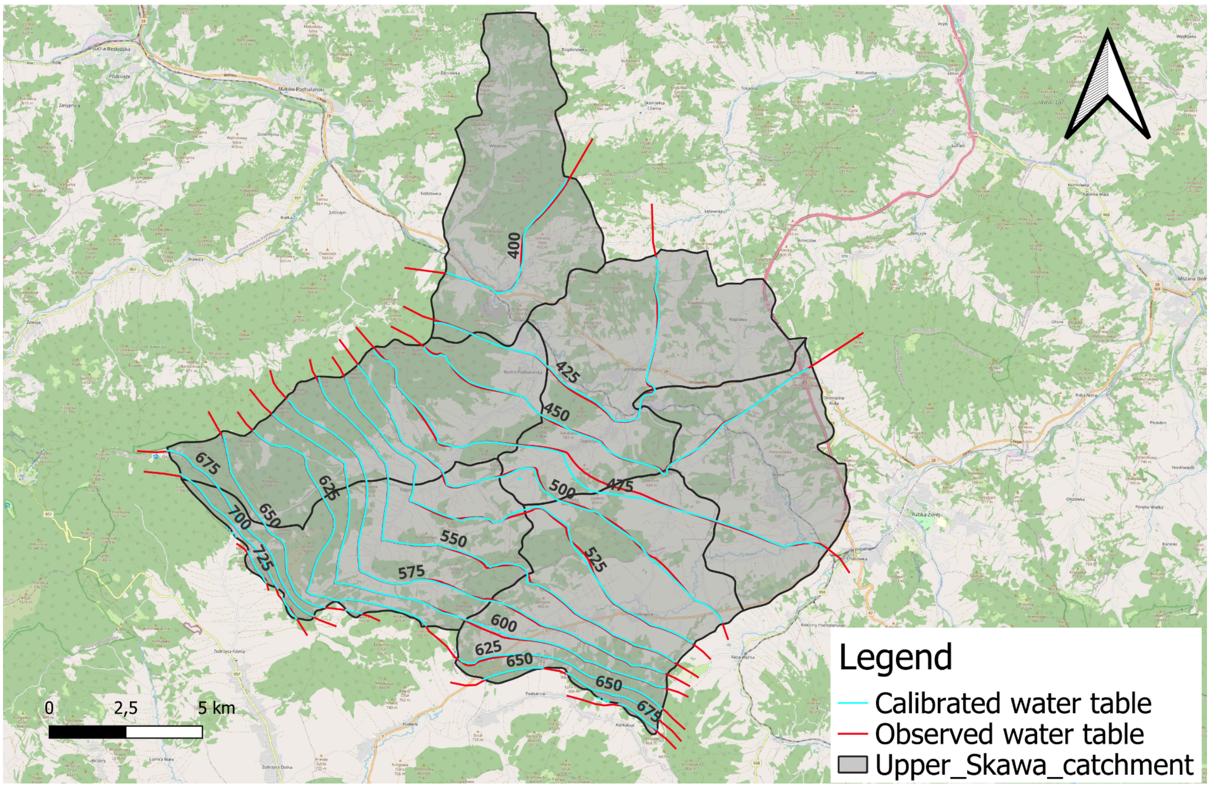
Map of the piezometers and the hydraulic conductivity

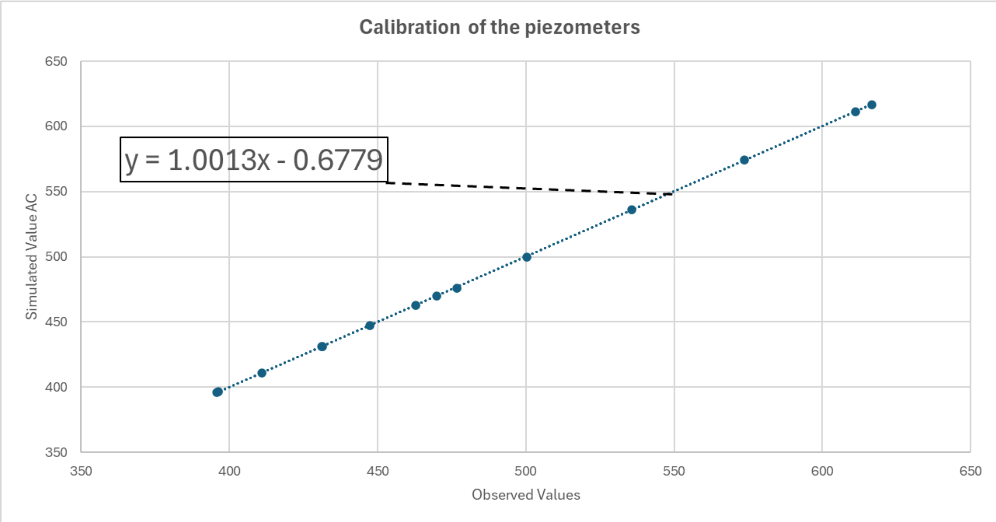


With K0 = 5 m/d, K1 = 10 m/d, K2 = 15 m/d, K3 = 0.5 m/d, K4 = 16 m/d and K5 = 1 m/d

2.4 Analysis and Interpretation of Results

Map of the calibrated model

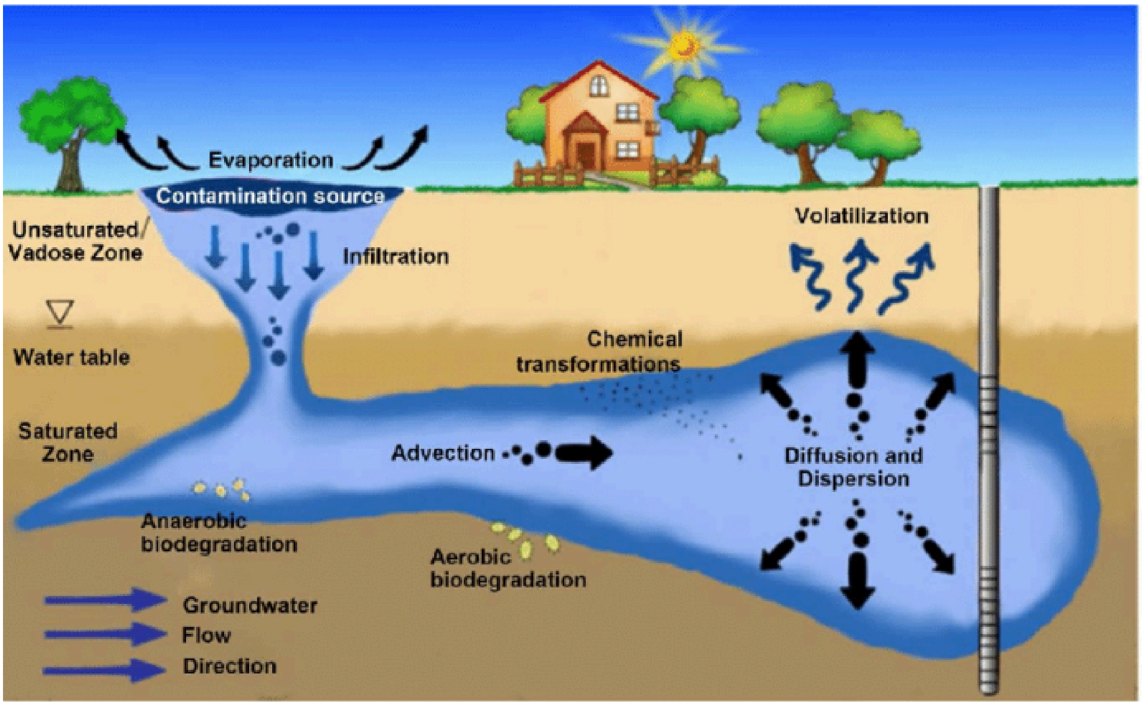




Observation Name	Observed Value	Simulated Value AC	Residual (Observation/simulation)
P1	395.79	396.09	-0.30
P2	396.39	396.35	0.04
P3	411.07	410.90	0.17
P4	431.35	431.08	0.27
P5	431.29	431.08	0.21
P6	447.32	447.28	0.04
P7	462.96	462.82	0.14
P8	611.06	611.05	0.01
P9	476.64	475.97	0.67
P10	469.93	469.99	-0.06
P11	535.72	536.19	-0.47
P12	616.55	616.54	0.01
P13	500.23	499.52	0.71
P14	573.80	574.48	-0.68

3. Contaminant Transport Simulation

3.1 Process Description



Advection: Transport of contaminants with groundwater flow, at a velocity equal to that of the fluid in the pores. (Ex: A pollutant moves with the water flow without spreading.)

$$J^{*}_{adw} = C \cdot \mathrm{v}_{p}$$

Diffusion: Molecular movement of contaminants driven by concentration gradients, even in stagnant water. (Ex: A contaminant slowly spreads in a stagnant zone.)

$$J^{*}_{dyf} = -D^{*}_{d} grad(C)$$

Dispersion: Spreading of contaminants due to local velocity variations, combining mechanical dispersion and diffusion. (Ex: A pollution plume widens as it moves through an aquifer.)

$$J^{*}_{dysp} = -D^{*}_{dysp} grad(C)$$

Total flux of mass in groundwater :

$$J^{*} = J^{*}_{adw} + J^{*}_{dyf} + J^{*}_{dysp}$$

$$J = nC\mathrm{v}_{p} - nD^{*}_{h}grad(C)$$

3.2 Introduction of Contaminant to the Catchment

The introduction of the contaminant into the Upper Skawa catchment occurs when the buried barrels containing chemicals begin to leak, releasing sulphate ions (SO_4^{2-}) into the groundwater. The site of contamination is located approximately 10 meters below the surface in the central part of the catchment. As the sulphate ions are highly soluble in water, they can easily migrate through the groundwater and travel toward the Skawa River.

Upon leakage, the initial concentration of sulphate at the source is 12,000 mg/L, which is significantly higher than the natural background concentration of 10 mg/L. This sharp difference in concentration creates a gradient that drives the movement of the contaminant through the groundwater system. The contaminant will spread through the catchment due to a combination of advection (the movement of water carrying the contaminant) and dispersion (the spreading of the contaminant in different directions).

3.3 Selection of Contaminant and Source Location

For this study, sulphate ions (SO_4^{2-}) have been selected as the contaminant of interest due to their high solubility and ability to easily migrate through groundwater. This makes them ideal for tracking the spread of contamination, especially in a scenario where chemicals may leak from buried barrels into the groundwater. The source of contamination is assumed to be located at the site of the buried barrels, which are approximately 10 meters below the surface. This site is central to the Upper Skawa catchment, and the contamination could potentially reach the Skawa River if the leak occurs.

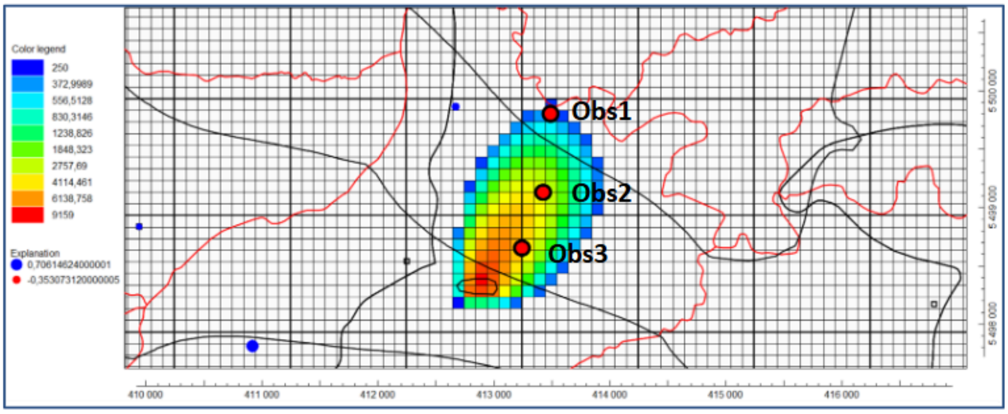
3.4 Parameterisation of Transport Model in MT3DMS

The transport model for this study will be implemented using MT3DMS, a widely used numerical model for simulating the transport of solutes in groundwater. The key parameters to be included in the model are:

- Background concentration of sulphate: 10 mg/L, which represents the natural concentration of sulphate ions in the groundwater before contamination.
- Source concentration of sulphate: 12,000 mg/L, which is the concentration of sulphate ions at the contamination source (buried barrels).
- Longitudinal dispersion coefficient (D_disp): 25 meters, representing the spreading of the contaminant along the flow path.
- Transverse dispersivity coefficients: 10% of D_disp, representing the spreading of the contaminant in the horizontal and vertical directions perpendicular to the flow path.
- Advection: The primary transport mechanism considered in the model, using the standard finite difference method for the advection solution scheme.

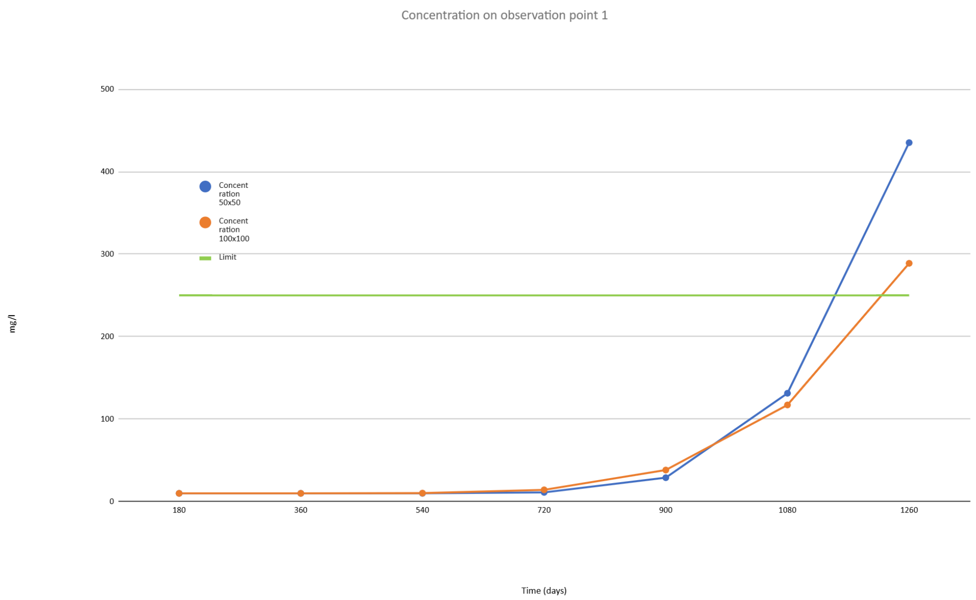
The transport model assumes that diffusion can be neglected, as it is a slower process compared to advection, and is less significant in the context of highly soluble contaminants like sulphate. Additionally, processes such as sorption, retardation, degradation, and chemical reactions are considered negligible and will not be included in the calculations, simplifying the model and focusing solely on the advection and dispersion of the contaminant.

Results and analysis of contaminant transport simulation model

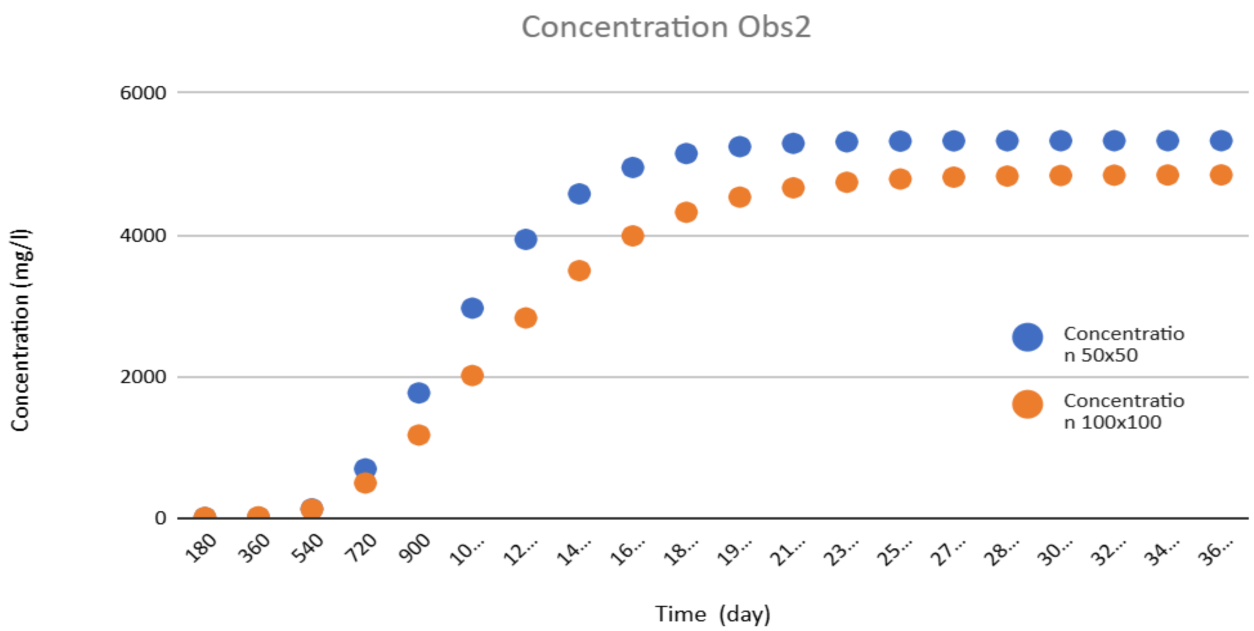


Observation point (difference discretization 50x50 and 100x100)

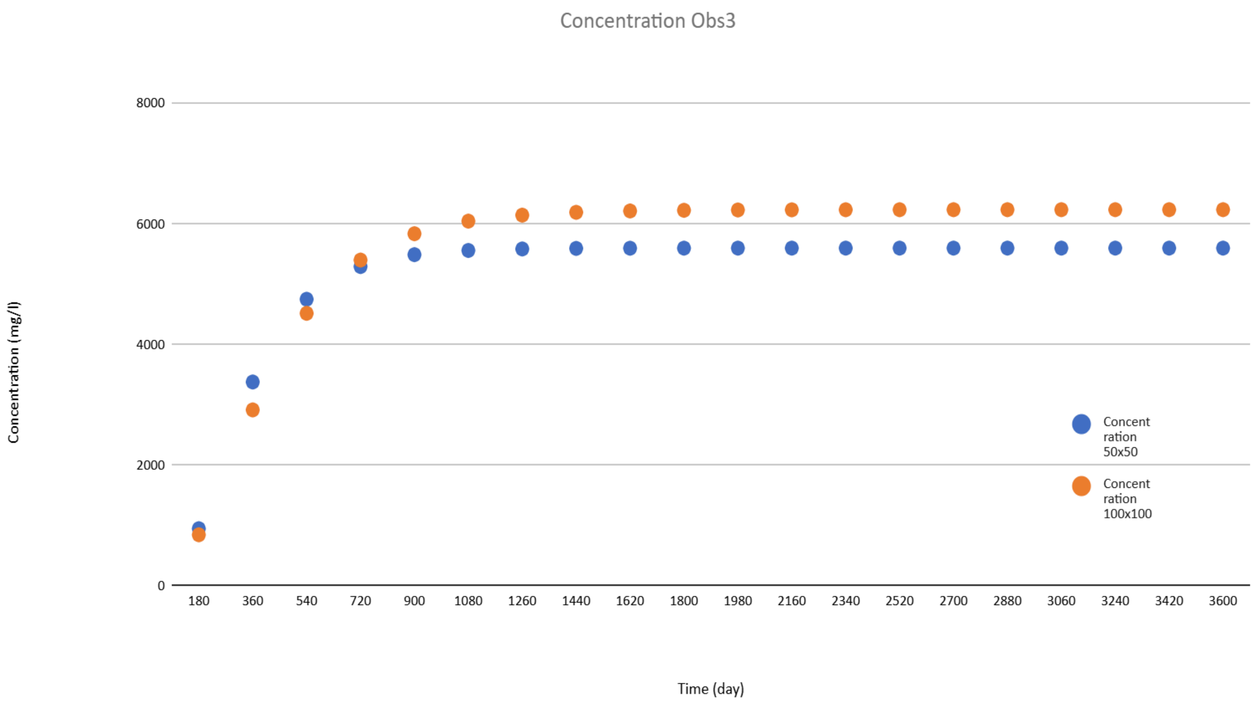
Observation 1



Observation 2



Observation 3



A coarser discretization (100x100) tends to cause a more significant numerical diffusion phenomenon. This means that the contaminant concentration peak is more spread out, and its arrival time at a given observation point is artificially delayed. This phenomenon is due to the numerical method used in the modeling, where large cells lead to an interpolation of concentration gradients.
In contrast, with a finer mesh (50x50), numerical diffusion is reduced, allowing for greater accuracy in capturing contamination fronts. The contaminant's progression is closer to physical reality, with sharper concentration gradients.

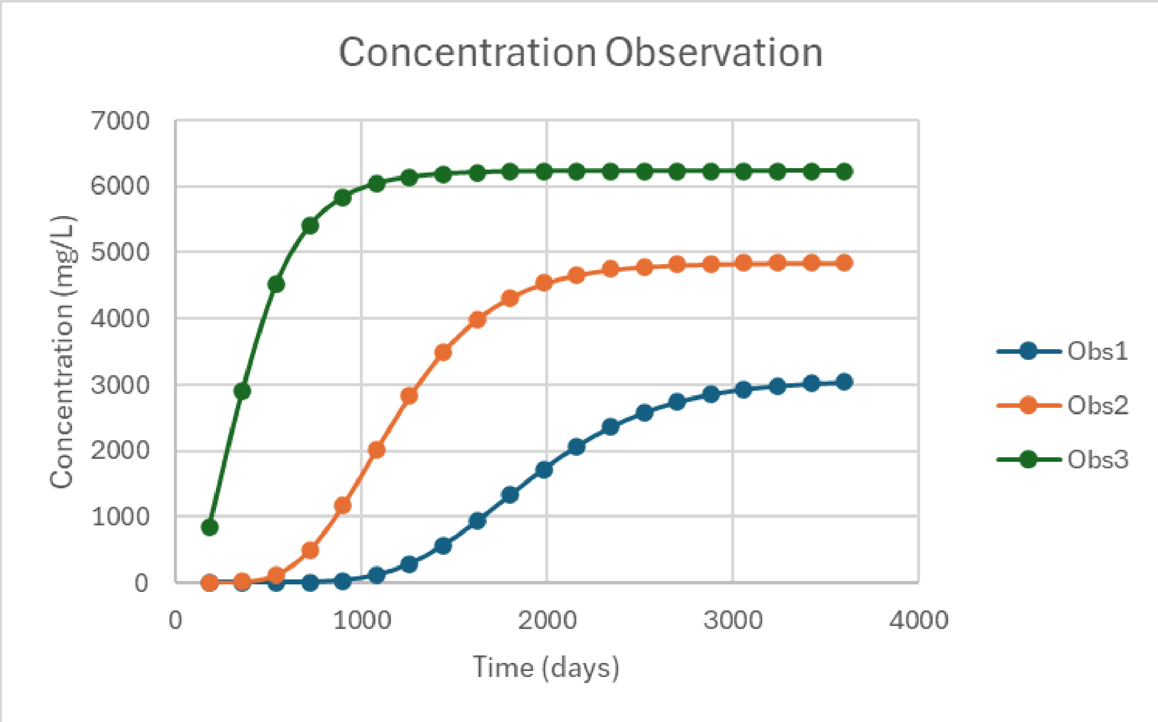
Using a more detailed mesh better represents the dispersion and advection of contaminants in the aquifer. In the case of the 50x50 mesh, the transport follows more realistic pathways, whereas in the 100x100 mesh, there is an overestimation of dilution due to poor spatial resolution. This directly impacts the assessment of groundwater and surface water pollution risks.

A finer discretization leads to a more accurate calculation of contaminant transport time. In the 100x100 mesh, the concentration peak arrives later at observation points compared to the 50x50 mesh. This is due to the inability of the coarser mesh to correctly capture groundwater flow dynamics and local permeability variations.

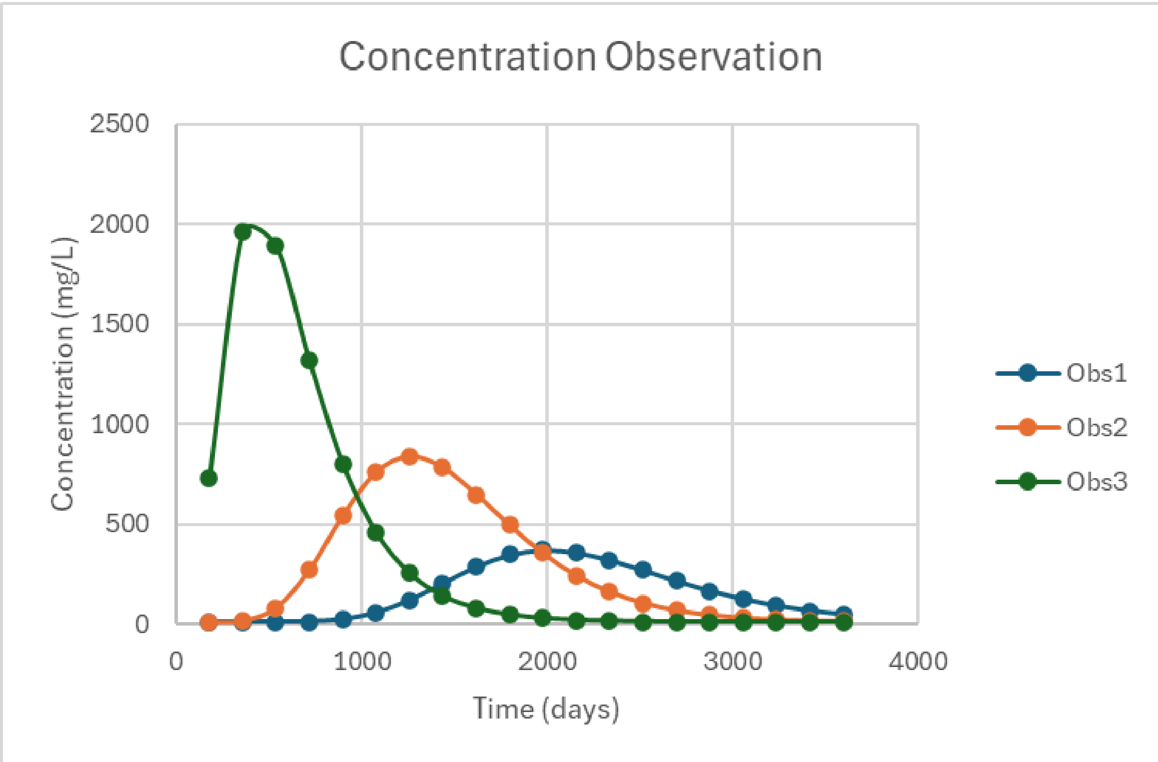
The drawback of a finer mesh is the increased computation time and required computational resources. A coarser mesh allows for faster simulation but at the cost of reduced accuracy, particularly in representing hydrodynamic flows and contaminant transport.

Différence between : excavation, no excavation and P&T

Observation no excavation

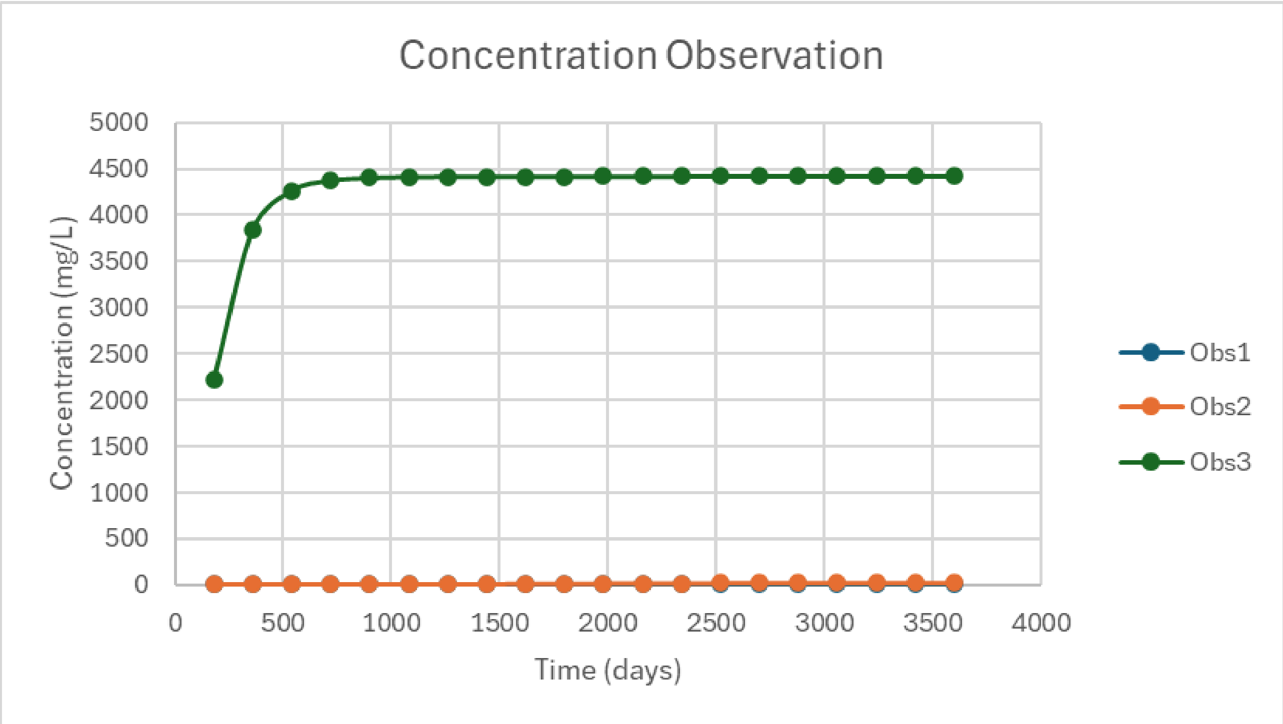


Observation excavation



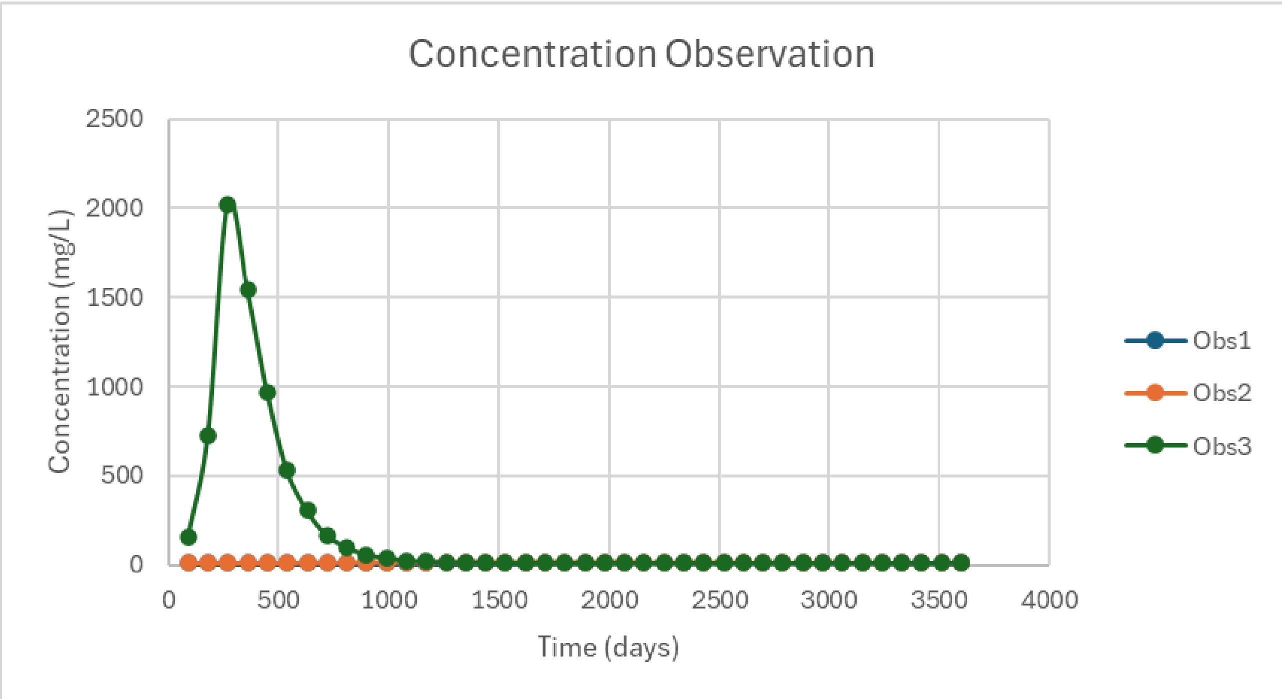
Observation no excavation P&T

x	y	Dist
412995.40	5498896.34	122.15
412995.40	5498774.19	
412998.00	5498774.19	2.60
		124.75
413099.356	5498779.4	103.956644
413099.356	5498675.4	
413101.9549	5498675.4	2.59891611
		106.555561
413195.5159	5498698.8	
413195.5159	5498571.5	**127.346889**
Total distance (m)		**358.65**
Pumping rate (m3/d)		**12552.7648**



Observation excavation P&T

x	y	Dist
412992.8005	5498793.68	110.453935
412992.8005	5498683.23	
412997.9983	5498683.23	5.19783222
		115.651767
413078.5647	5498668.93	105.256103
413078.5647	5498563.68	
413077.2652	5498563.68	1.29945806
		106.555561
413194.2165	5498585.12	111.753393
413194.2165	5498473.37	
413196.8154	5498473.37	2.59891611
		114.352309
Total distance (m)		336.559636
Pumping rate (m3/day)		**10096.7891**



Pumping started on day 180 and can stop on day 720, as the concentration drops below the standard threshold of 250 mg/L by that time.

1. "No Excavation" Scenario

In this case, contaminants from the buried barrels spread freely through the aquifer via advection and dispersion. The results show:

- A persistent high concentration of sulfate around the pollution source.
- The contaminant plume progressing toward the Skawa River over several hundred days.
- A slow decrease in concentrations due to natural dispersion, but without a significant reduction in environmental risk.

This scenario highlights the lack of effective pollution containment and underscores the need for intervention.

2. "Excavation" Scenario

Excavation involves removing the solid contamination sources (the barrels) to stop the continuous release of pollutants into the aquifer. The observed effects include:

- A rapid decrease in sulfate concentrations after the pollution sources are removed.
- A reduction in the contaminant plume, though with persistence of already-diffused pollutants.
- Stabilization of concentrations since there is no longer a continuous sulfate supply.

While this method is effective in stopping contamination at its source, it does not completely eliminate pollutants already dispersed in the aquifer.

3. "Excavation + Pump & Treat (P&T)" Scenario

Pump & Treat (P&T) is an active remediation method where contaminated water is pumped, treated, and either reinjected or discharged. In this scenario, excavation is complemented by strategic pumping, resulting in:

- An accelerated reduction in sulfate concentrations as contaminated water is actively extracted.
- A shorter remediation time, with concentrations dropping below the 250 mg/L threshold within 720 days.
- A decrease in pollutant flux toward the river, minimizing environmental impact.

Conclusion

Scenario	Residual Contaminants	Remediation Time	Technical Complexity	Effectiveness
Without Excavation	High	Very Long	Low	Low
Excavation Only	Medium	Moderate	Medium	Moderate
Excavation + P&T	Low	Short	High	High

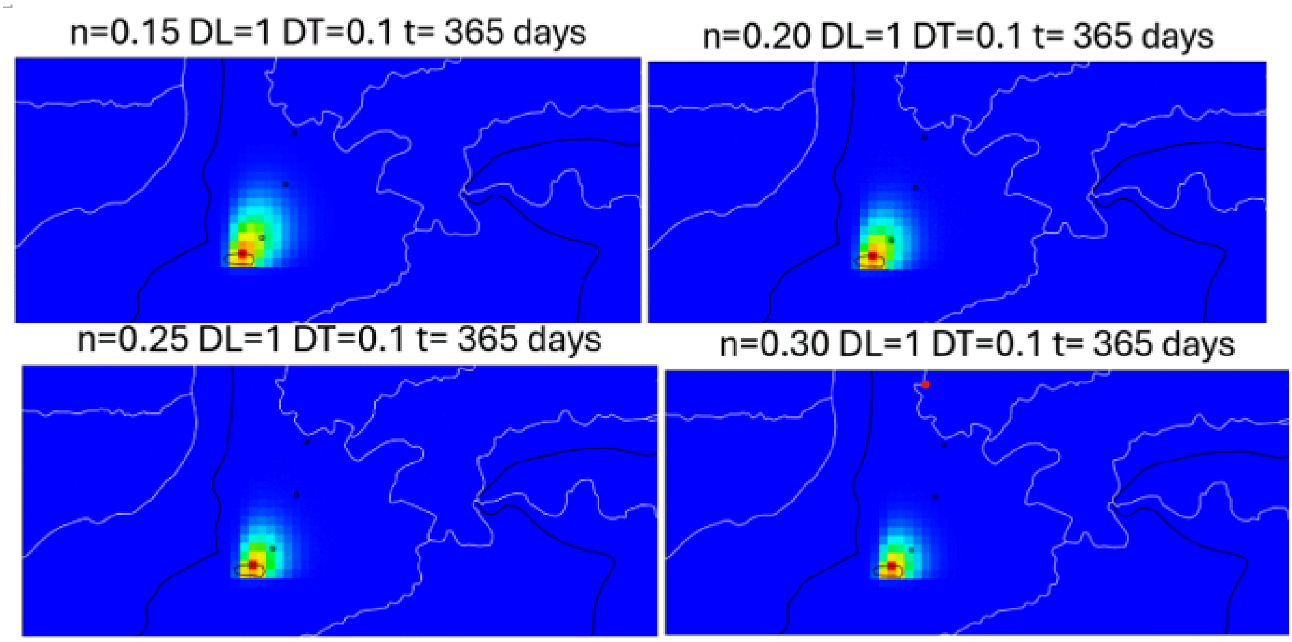
- Excavation alone reduces pollution but does not completely eliminate it.

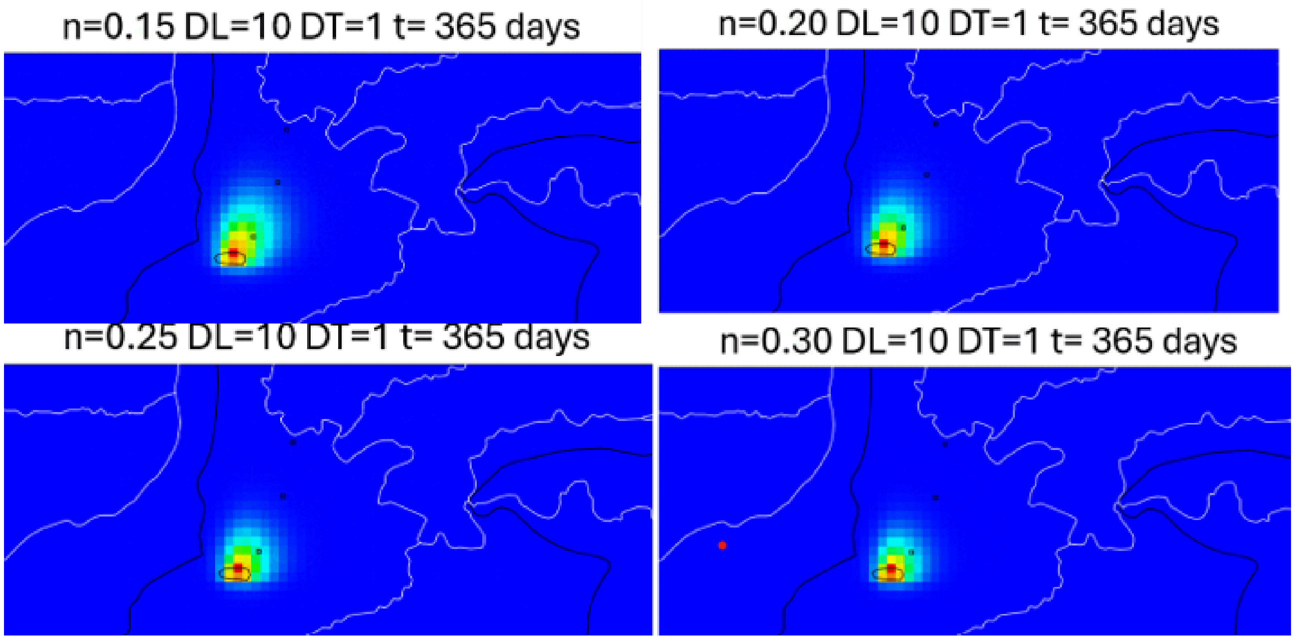
- Adding Pump & Treat is necessary to accelerate decontamination.
- Without intervention, pollution persists in the long term.

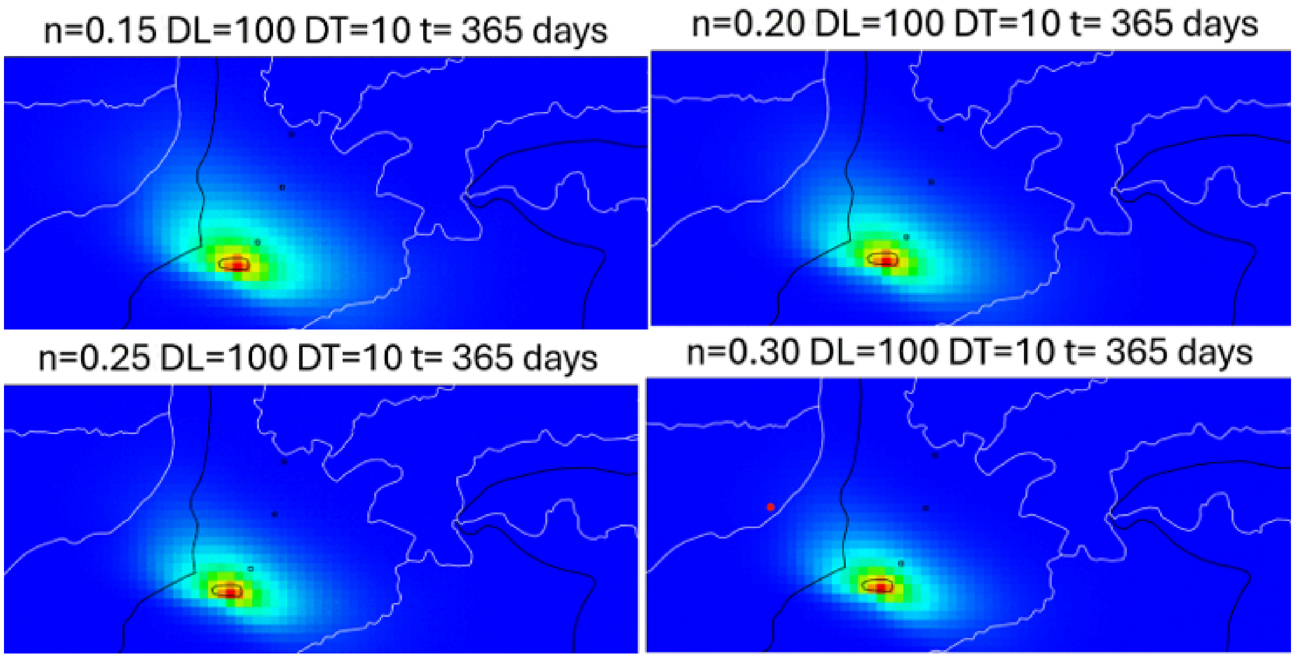
Difference between : Porosity, longitudinal dispersivity, transversal dispersivity

Porosity	*Longitudinal Dispersivity*	*Transversal Dispersivity*
0.05	1	0.1
	10	1
	100	10
0.1	1	0.1
	10	1
	100	10
0.15	1	0.1
	10	1
	100	10
0.2	1	0.1
	10	1
	100	10
0.25	1	0.1
	10	1
	100	10

365 days

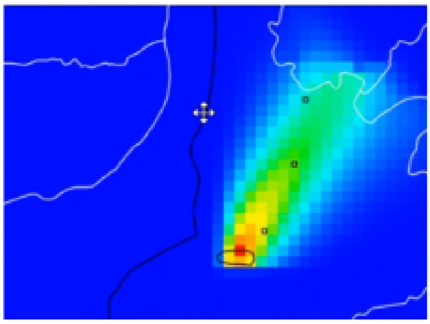



n=0.15 DL=10 DT=1 t= 365 days
n=0.20 DL=10 DT=1 t= 365 days
n=0.25 DL=10 DT=1 t= 365 days
n=0.30 DL=10 DT=1 t= 365 days

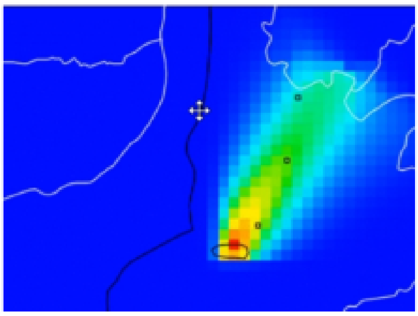

n=0.15 DL=100 DT=10 t= 365 days
n=0.20 DL=100 DT=10 t= 365 days
n=0.25 DL=100 DT=10 t= 365 days
n=0.30 DL=100 DT=10 t= 365 days

3650 Days

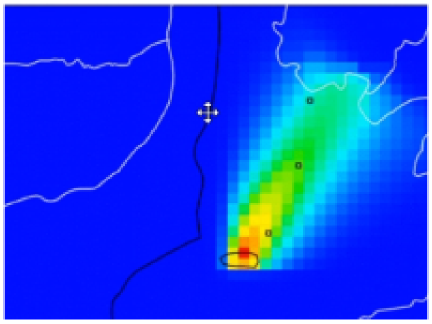
n=0.15 DL=1 DT=0.1



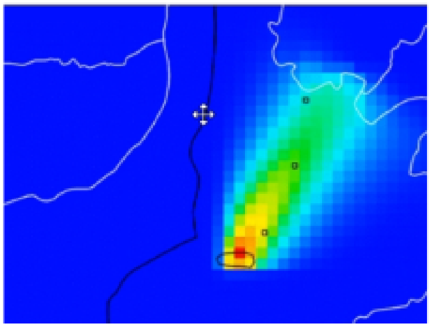
n=0.20 DL=1 DT=0.1



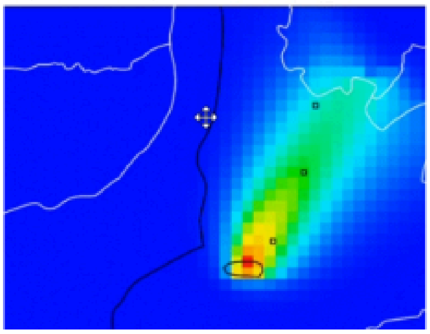
n=0.25 DL=1 DT=0.1



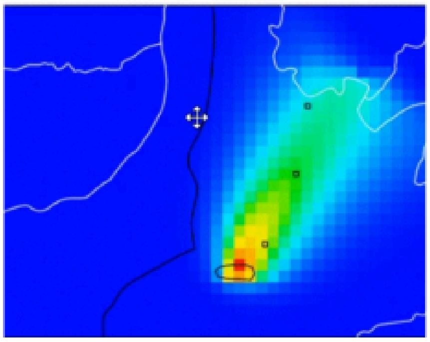
n=0.30 DL=1 DT=0.1



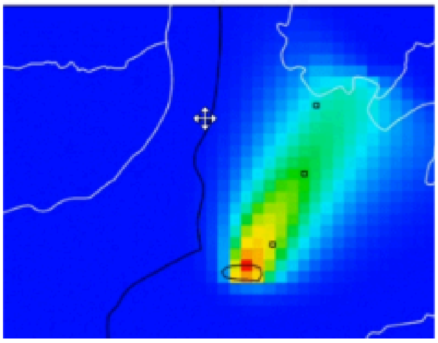
n=0.15 DL=10 DT=1



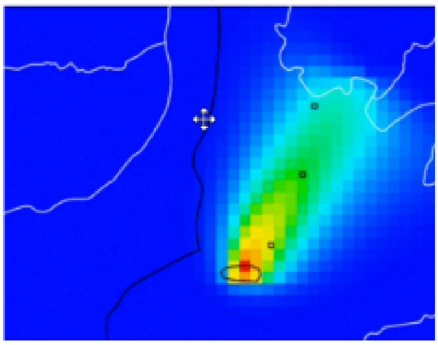
n=0.20 DL=10 DT=1

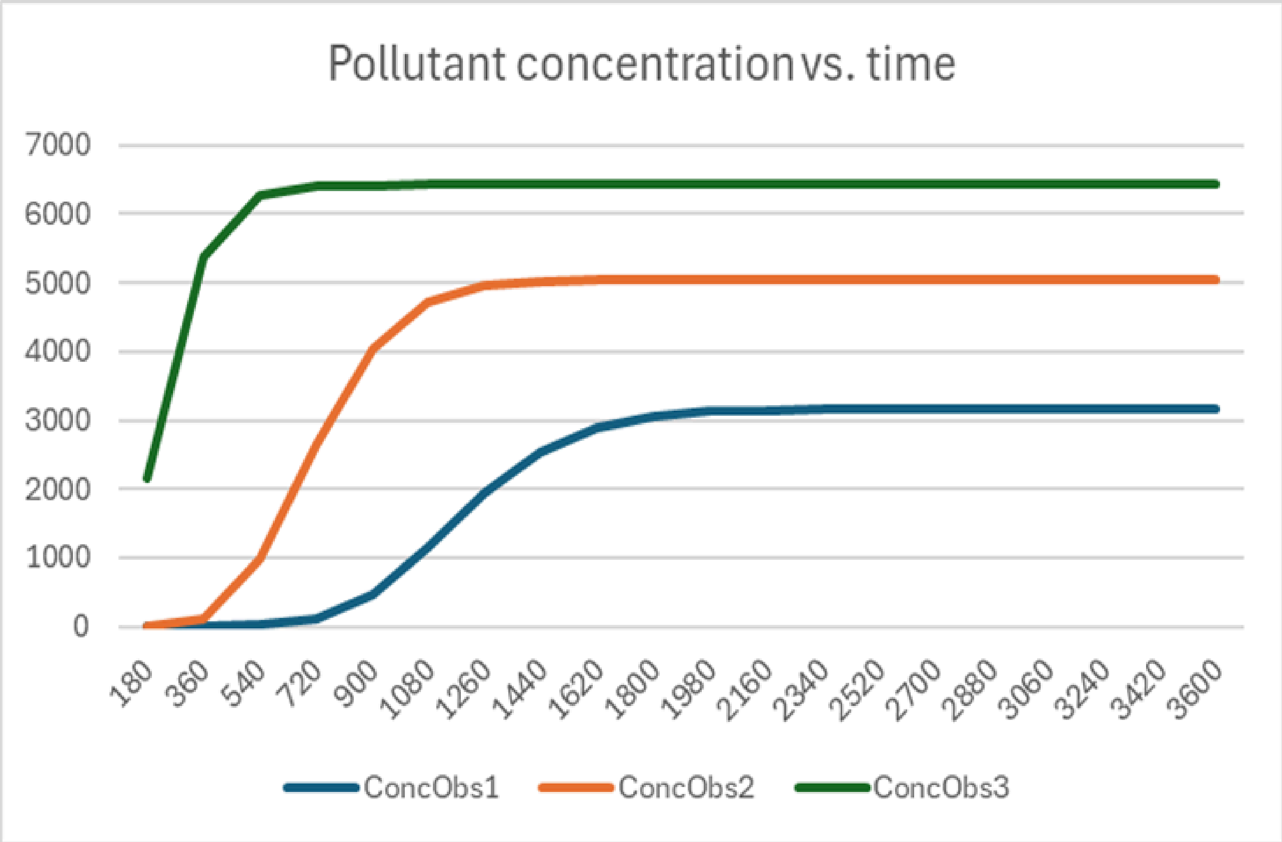


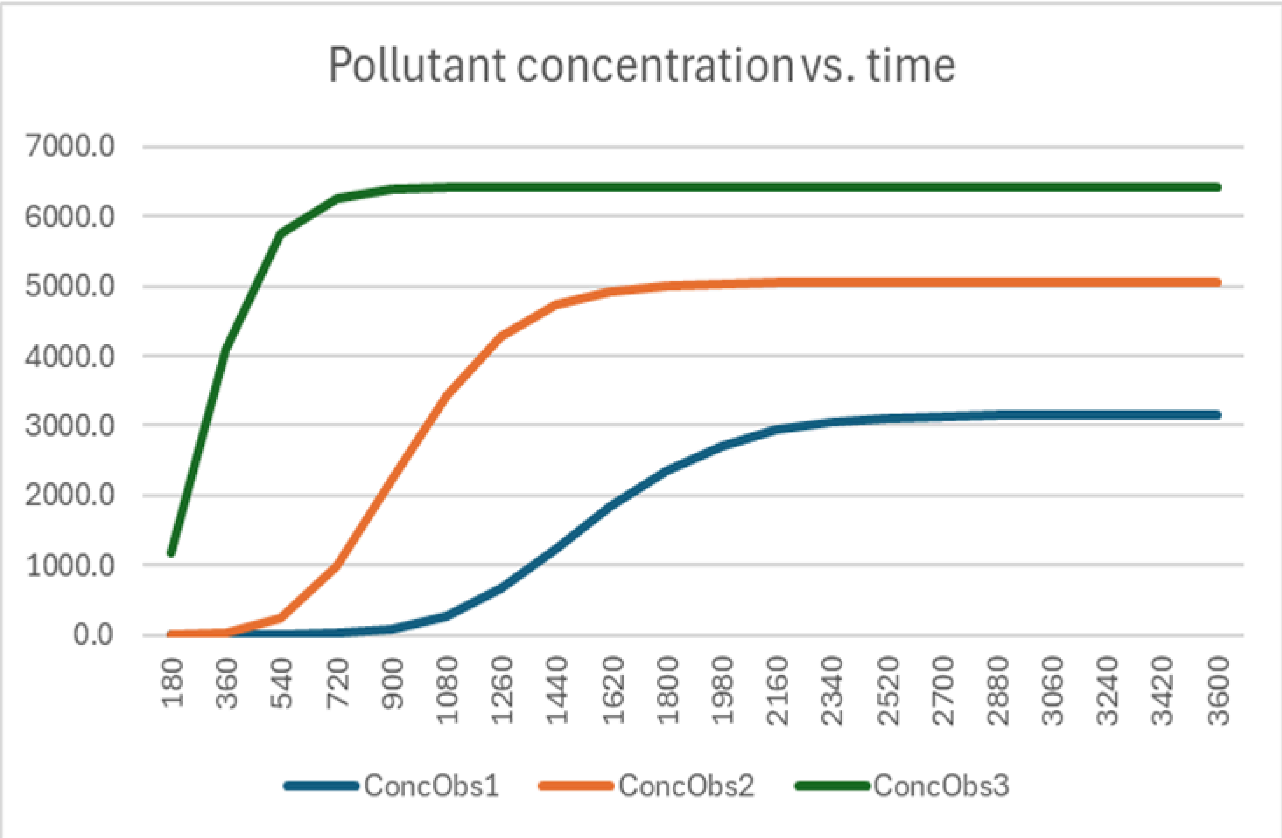
n=0.25 DL=10 DT=1

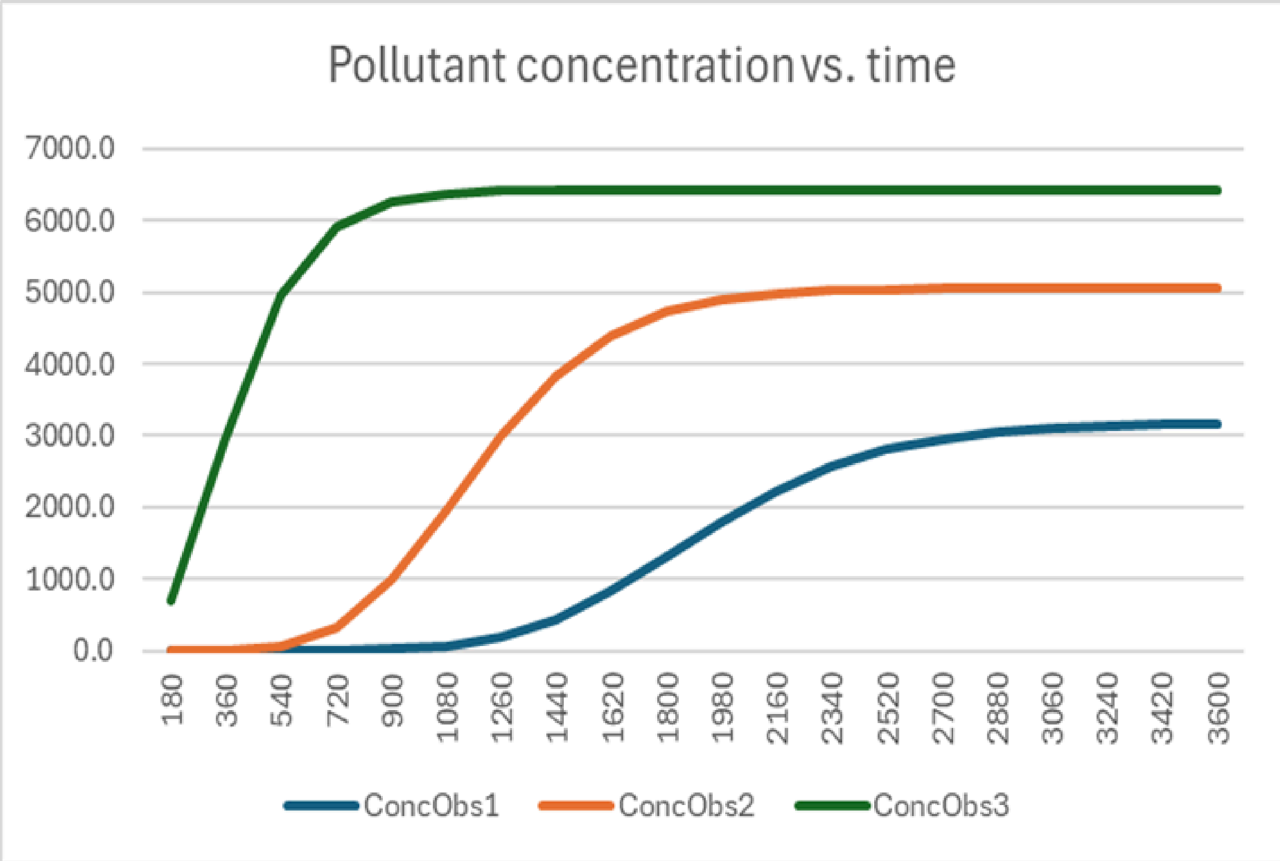


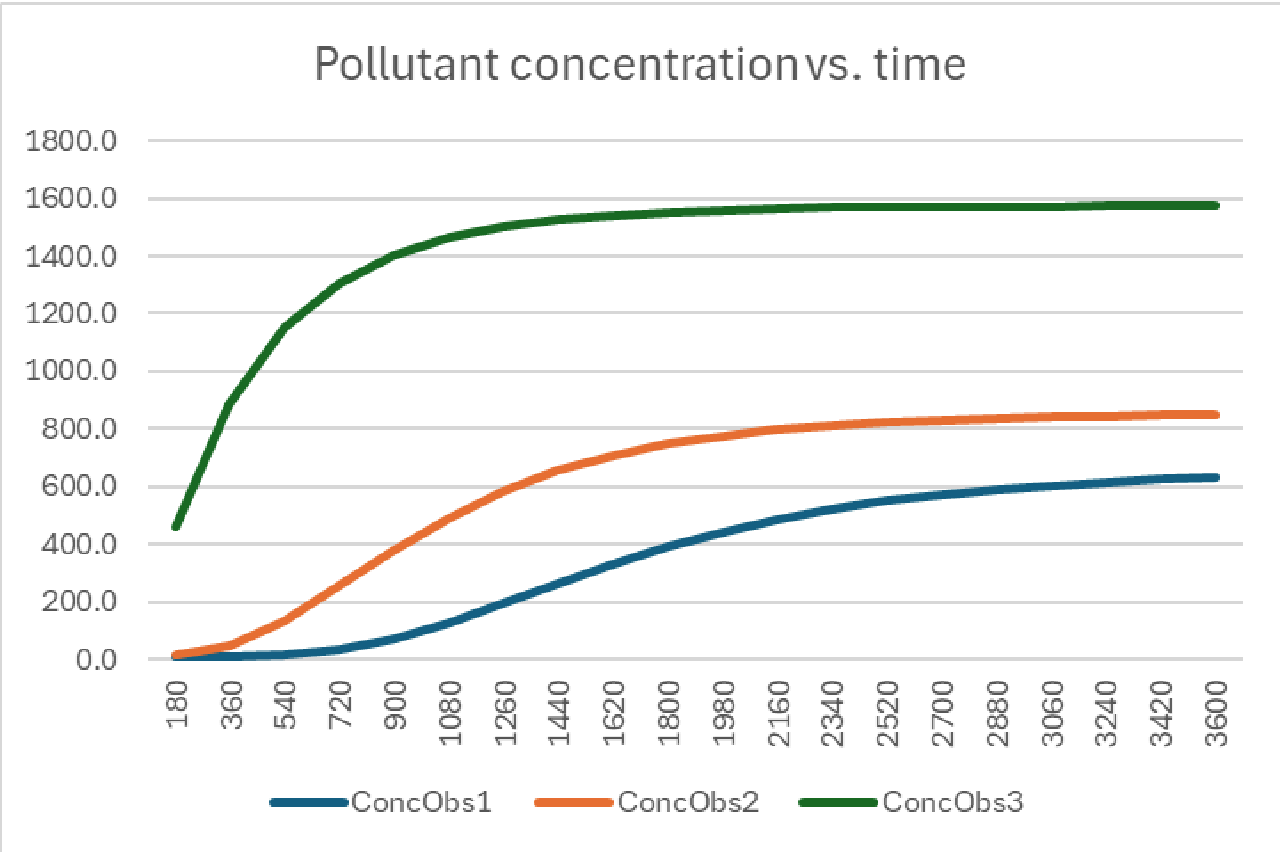
n=0.30 DL=10 DT=1

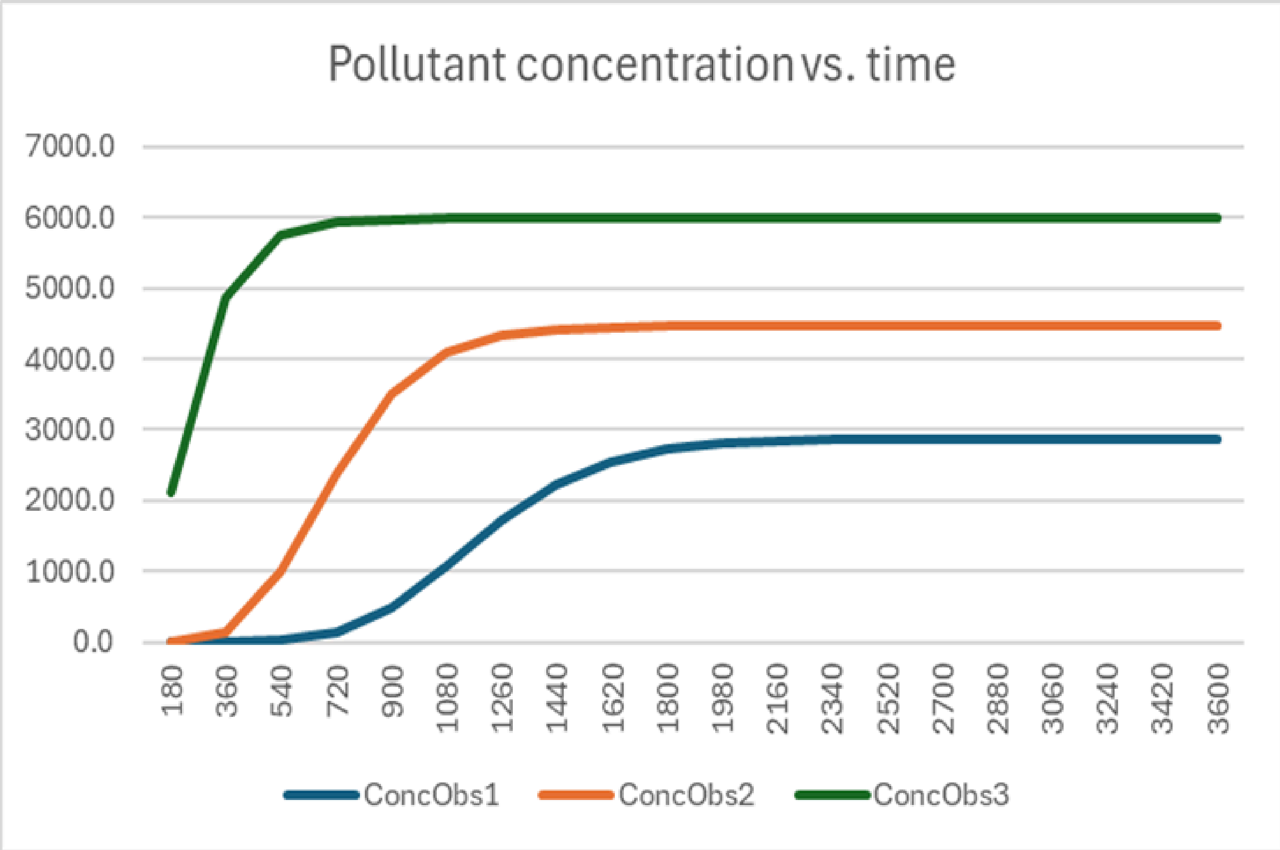


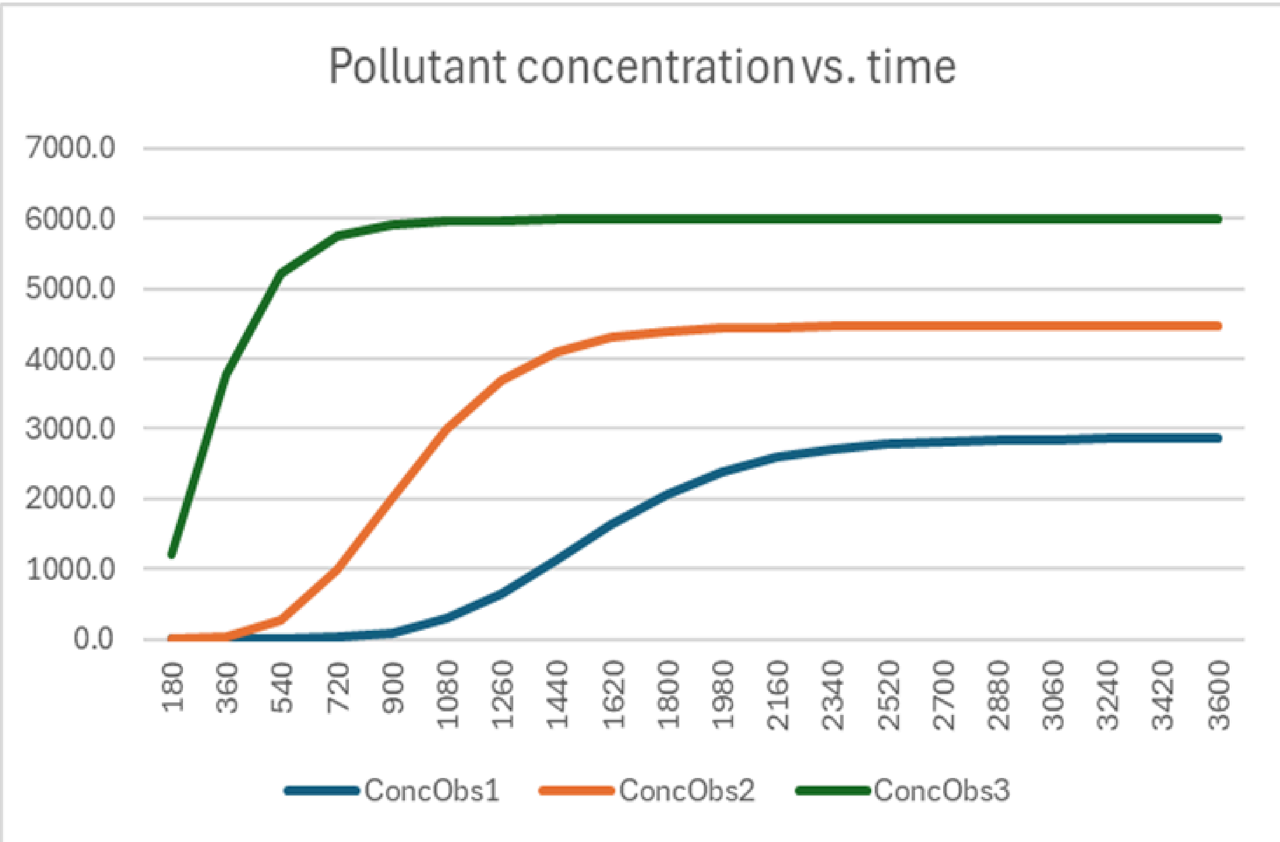

Pollutant concentration vs. time
7000
6000
5000
4000
3000
2000
1000
0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3

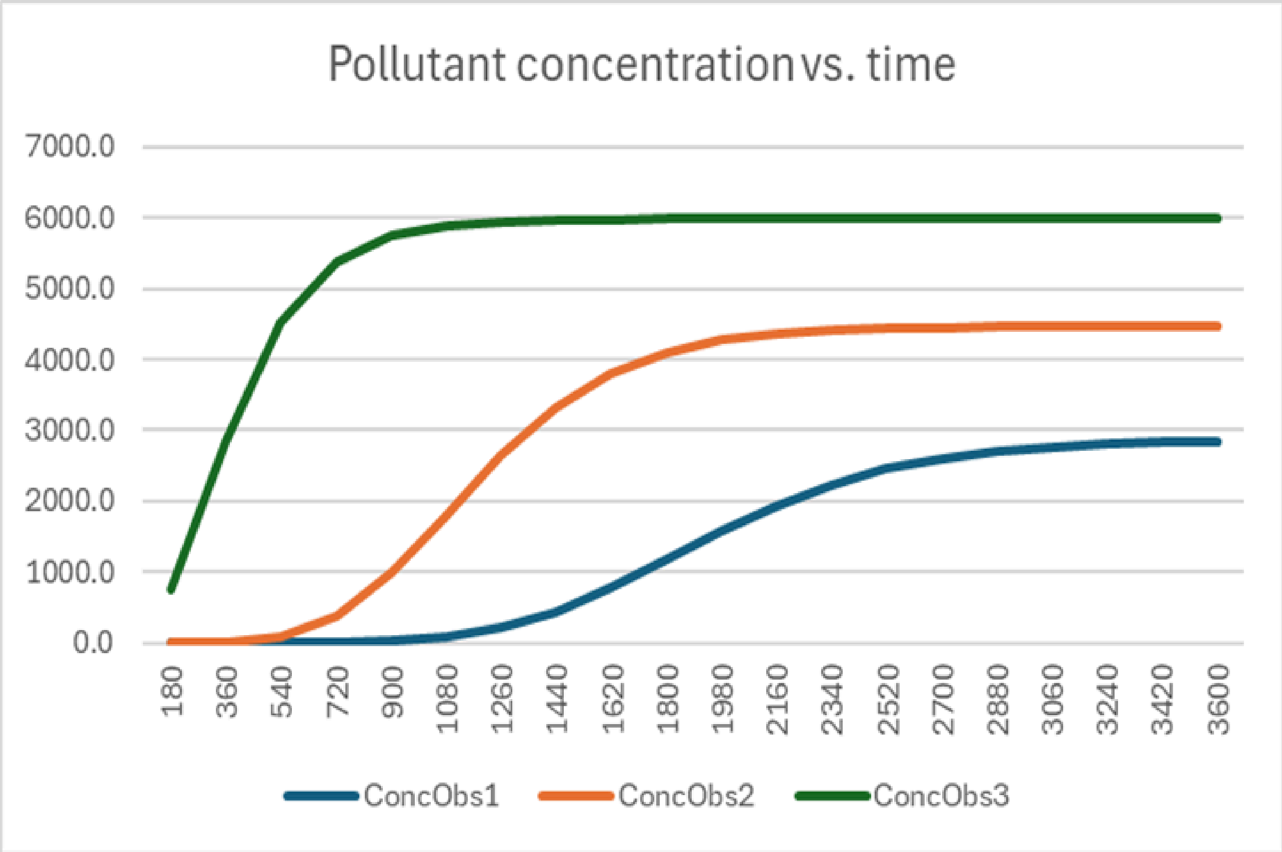

Pollutant concentration vs. time
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3

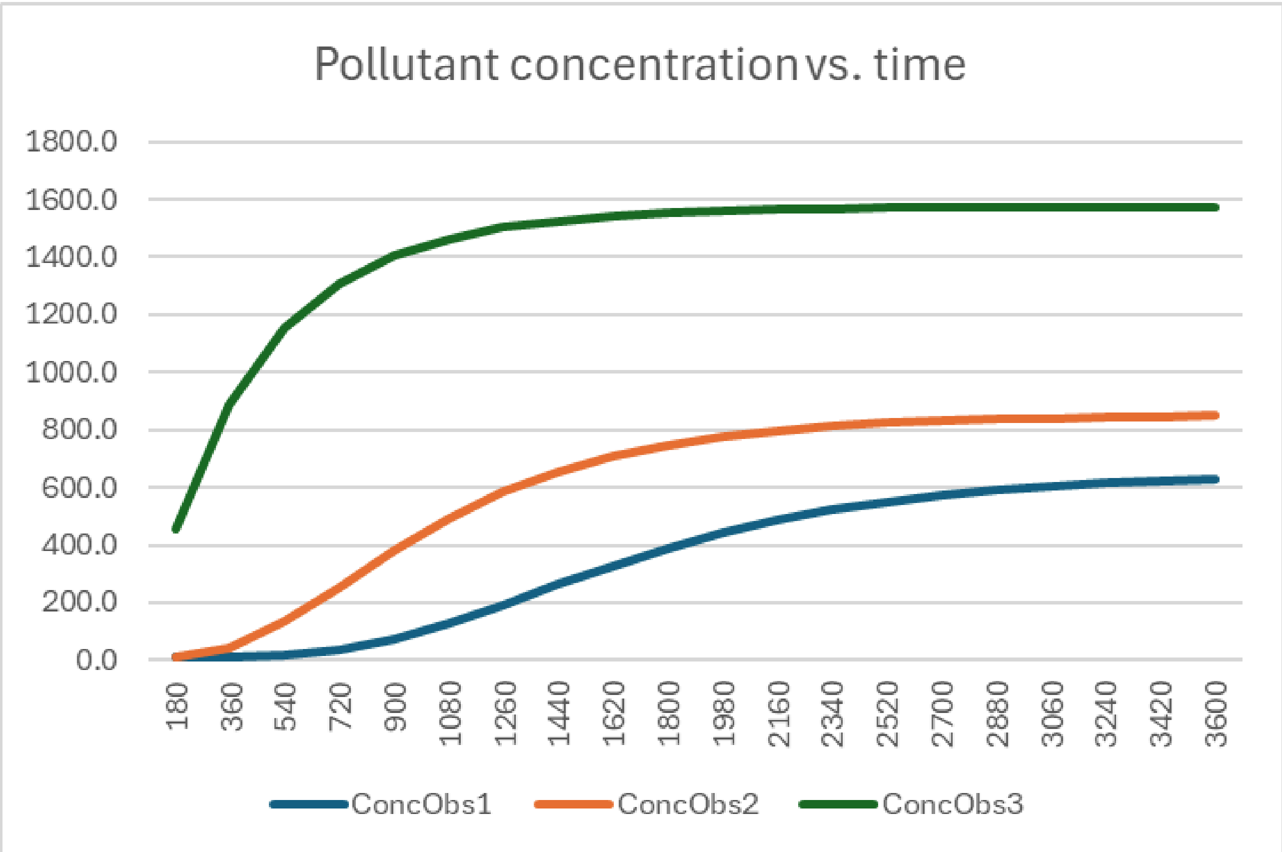

Pollutant concentration vs. time
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3

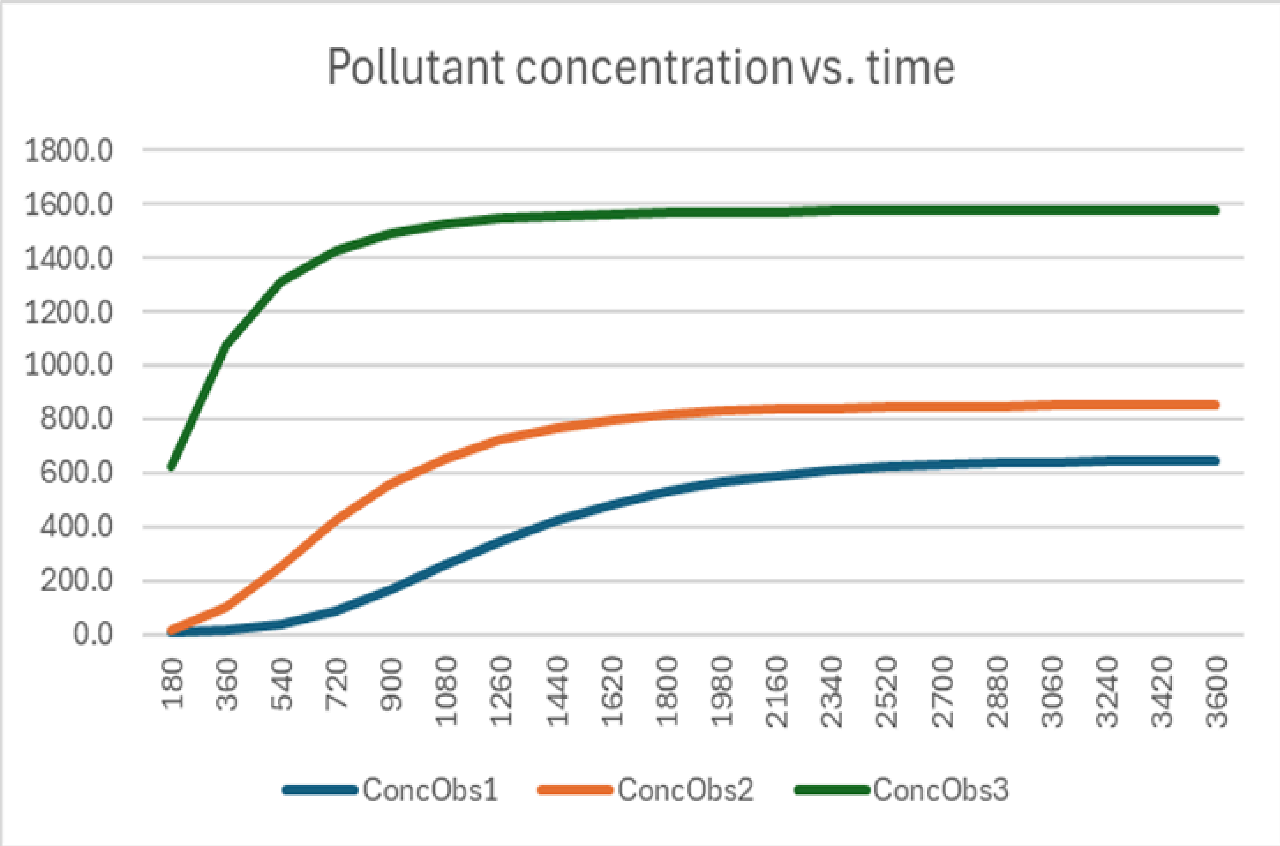

Pollutant concentration vs. time
1800.0
1600.0
1400.0
1200.0
1000.0
800.0
600.0
400.0
200.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3


Pollutant concentration vs. time
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3

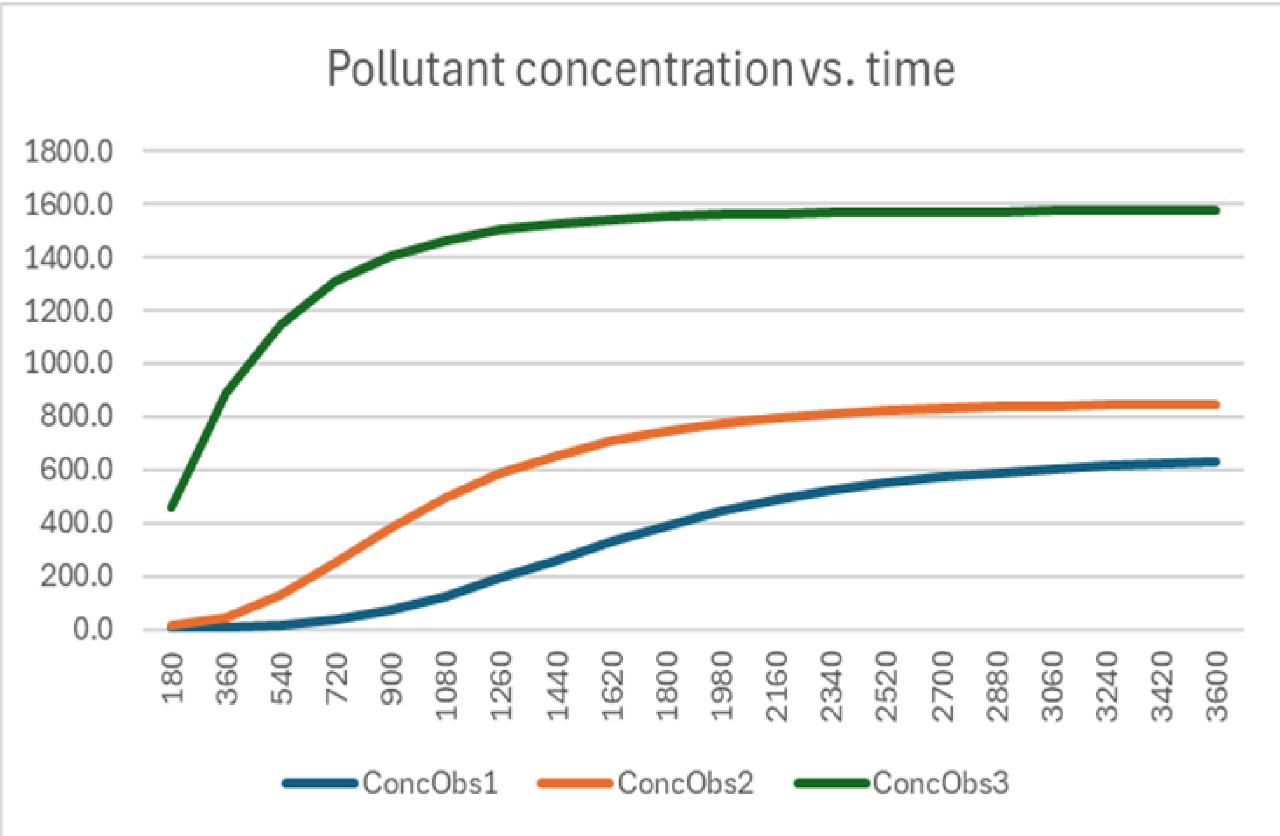

Pollutant concentration vs. time
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3


Pollutant concentration vs. time
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3

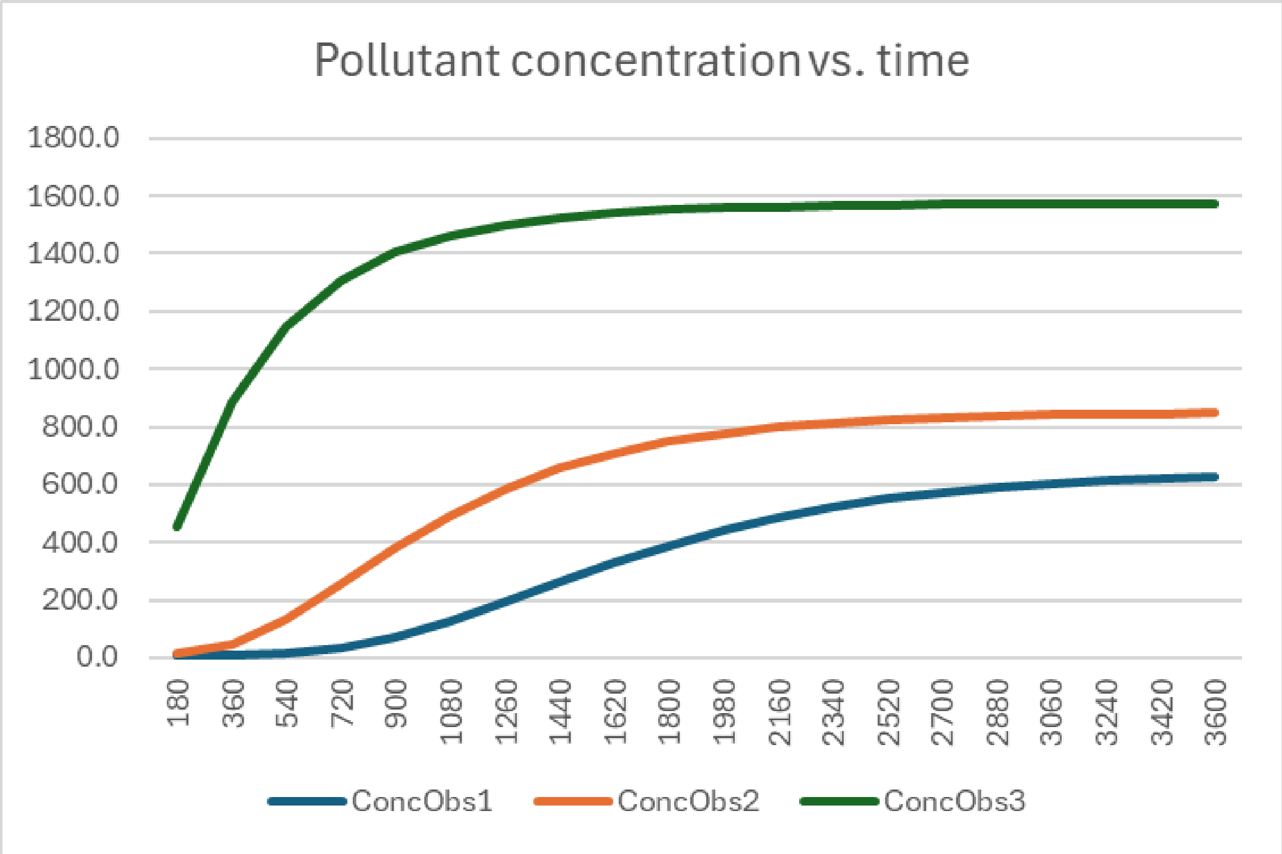

Pollutant concentration vs. time
1800.0
1600.0
1400.0
1200.0
1000.0
800.0
600.0
400.0
200.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3

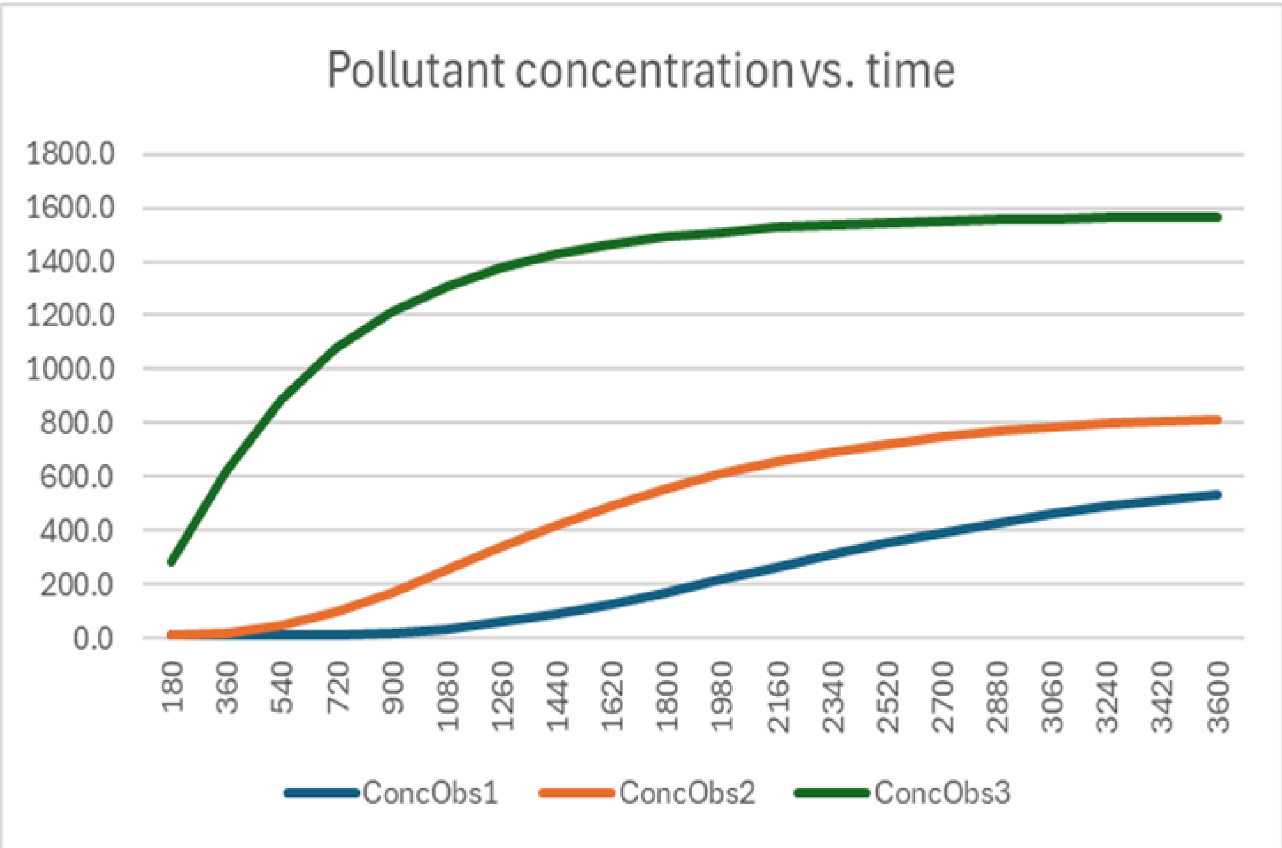


Pollutant concentration vs. time
1800.0
1600.0
1400.0
1200.0
1000.0
800.0
600.0
400.0
200.0
0.0
180
360
540
720
900
1080
1260
1440
1620
1800
1980
2160
2340
2520
2700
2880
3060
3240
3420
3600
ConcObs1
ConcObs2
ConcObs3



Pollutant concentration vs. time
1800.0
1600.0
1400.0
1200.0
1000.0
800.0
600.0
400.0
200.0
0.0
180
360
540
720
900
1080
1260
1440
1620
1800
1980
2160
2340
2520
2700
2880
3060
3240
3420
3600
ConcObs1
ConcObs2
ConcObs3


Pollutant concentration vs. time
1800.0
1600.0
1400.0
1200.0
1000.0
800.0
600.0
400.0
200.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3


Pollutant concentration vs. time
1800.0
1600.0
1400.0
1200.0
1000.0
800.0
600.0
400.0
200.0
0.0
180 360 540 720 900 1080 1260 1440 1620 1800 1980 2160 2340 2520 2700 2880 3060 3240 3420 3600
ConcObs1
ConcObs2
ConcObs3

1. Porosity

Effective porosity directly influences the migration speed of contaminants. Higher porosity implies a greater water storage capacity but a lower flow velocity, as the flow is distributed over a larger water volume. The results show:

- Lower porosity accelerates contaminant migration since water flows more quickly through the reduced interstitial spaces.
- Higher porosity slows down pollutant progression, increasing their residence time in the aquifer.

In the modeling, porosity was adjusted to evaluate its influence on sulfate propagation in the aquifer.

2. Longitudinal Dispersivity

Longitudinal dispersivity represents the dispersion of contaminants in the direction of the main groundwater flow. The higher this value:

- The more the contaminant plume spreads along the flow direction.
- The faster the maximum concentration decreases, as dispersion promotes pollutant dilution.
- Excessive spreading may, however, overestimate dispersion and fail to reflect field observations.

The value used in the simulation is 25 m, which is consistent with large-scale aquifer environments.

3. Transverse Dispersivity

Transverse dispersivity measures the spreading of contaminants perpendicular to the main flow direction. It is generally much lower than longitudinal dispersivity (often a 1:10 ratio). In the model:

- Higher transverse dispersivity broadens the affected pollution zone, increasing the risk of lateral contamination of adjacent aquifers.
- Lower dispersivity keeps the plume more confined, concentrating pollutants in a specific area.

In this study, transverse dispersivity is set at 10% of longitudinal dispersivity, or 2.5 m.

Parameter	Main Effect	Consequences
Porosity	Regulates flow velocity	Low porosity = fast transport, High porosity = increased storage
Longitudinal Dispersivity	Dilution and spreading of the pollutant along the flow direction	Affects dispersion and peak concentration
Transverse Dispersivity	Lateral expansion of the plume	Impacts diffusion into adjacent areas

4. Uncertainty and Model Limitations

ModelMuse is a useful tool for groundwater modelling, but several uncertainties and limitations must be considered when interpreting results.

A primary source of uncertainty is the quality of input data. Hydraulic conductivity, recharge rates, and boundary conditions often vary spatially, yet model inputs are typically based on limited measurements or generalised estimates. Simplifications in the conceptual model, such as assuming uniform geology or treating drains as dry, can also introduce errors by omitting small-scale variations in subsurface conditions.

Numerical discretisation presents another limitation. The model domain is divided into a structured grid, and grid resolution affects accuracy. A coarse grid may fail to capture local flow dynamics, while a fine grid increases computational demands and may lead to numerical instability.

The assumption of steady-state flow further limits the model's applicability. It does not account for seasonal or short-term fluctuations in groundwater levels, which may influence recharge estimates. Additionally, boundary conditions, such as constant head values or river conductance, are often simplified representations that may not fully reflect real-world interactions between groundwater and surface water.

Finally, calibration and validation introduce further uncertainty. Multiple parameter sets can produce similar results, making the process non-unique. If field data for validation are insufficient, model predictions may not be fully reliable for long-term analysis.

Conclusions and Recommendations

Effective porosity directly influences the migration speed of contaminants. A higher porosity means a greater water storage capacity but a lower flow velocity, as the flow is distributed over a larger volume of water. The results indicate that lower porosity accelerates contaminant migration since water moves more quickly through the reduced interstitial spaces. Conversely, higher porosity slows down pollutant progression, increasing their residence time in the aquifer. In the modeling process, porosity was adjusted to assess its impact on sulfate propagation within the aquifer.

Longitudinal dispersivity represents the dispersion of contaminants in the direction of the main groundwater flow. A higher value results in a more extended contaminant plume along the flow path and a faster decrease in maximum concentration, as dispersion facilitates pollutant dilution. However, excessive spreading may overestimate dispersion and fail to accurately reflect field observations. In this study, a longitudinal dispersivity value of 25 meters was used, which aligns with large-scale aquifer environments.

Transverse dispersivity, on the other hand, measures the spreading of contaminants perpendicular to the primary flow direction. It is generally much lower than longitudinal dispersivity, often following a 1:10 ratio. In the model, a higher transverse dispersivity led to a wider affected pollution zone, increasing the risk of lateral contamination in adjacent aquifers. Meanwhile, lower dispersivity helped confine the plume, concentrating pollutants within a more localized area. For this study, transverse dispersivity was set at 10% of the longitudinal dispersivity, equivalent to 2.5 meters.

Recommendations for Future Work and Model Refinements

Improving the model relies on integrating more precise field data, including in situ measurements of sulfate concentrations and piezometric levels. A better characterization of hydraulic conductivity would also help refine calibration and reduce uncertainties.

It would be useful to test additional hypotheses by incorporating processes such as molecular diffusion, biodegradation, and sorption. These mechanisms influence the migration and persistence of contaminants and could improve the accuracy of model predictions.

Optimizing remediation solutions is essential to minimize environmental impact. Adjusting the Pump & Treat pumping network, exploring the use of permeable reactive barriers, or testing in situ treatments could accelerate decontamination while reducing costs and water consumption.

Numerical adjustments, such as refining the mesh and optimizing the time step, would enhance simulation accuracy. Limiting numerical diffusion would provide a better representation of contamination fronts and a more accurate risk assessment.

Finally, a long-term approach is necessary to anticipate pollution evolution. Assessing the impact of climate change, artificial recharge, and long-term simulations over several decades would help ensure sustainable water resource management and prevent potential future contamination.

Results

https://docs.google.com/spreadsheets/d/1e4UAXUeB3KtLQ8tSRZwoto8rhturs553/edit?usp=sharing&ouid=116524212352110548310&rtpof=true&sd=true

https://docs.google.com/spreadsheets/d/1Nt0uUBn4R54ZmaCIrccNpwmbB0bEOrq_/edit?usp=sharing&ouid=116561909395589208677&rtpof=true&sd=true

https://kuleuven-my.sharepoint.com/:x:/r/personal/ferdinan_sunarga_student_kuleuven_be/Documents/Conc_obs.xlsx?d=wf086cdeff3a84386bdefe128747dbd5b&csf=1&web=1&e=v9fRb8