PHISHES

PHysically-based Integrated Soil HEalth Simulation platform

Predicting soil health to protect ecosystems

WP 4 report from the test sites

Authors: Zeman, E., Devau, N., Earon, R., Brandyk, A., Kok, E.

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Table of Content

List of Figures 6
List of Tables 8
Executive Summary 9
Keywords 9
List of acronyms and abbreviations 9
1. General summary – concept of the test sites for PHISHES project 11
2. Experimental fields 11
2.1. Zelivka basin (CZE) 12
2.1.1. Purpose of the sites within the PHISHES project 12
2.1.2. Description of the basin/site 13
2.1.3. Existing data available 23
2.1.4. Additional – optional – monitoring within the project frame 25
2.1.5. Tools, model trains, scenarios expected to be employed or utilized 26
2.1.6. Activities executed on site up to date 31
2.1.7. Planned activities for the upcoming period 33
2.2. River Koprzywianka (PL) 34
2.2.1. Purpose of the sites within the PHISHES project 34
2.2.2. Description of the basin/site 34
2.2.3. Existing data available 37
2.2.4. Additional – optional – monitoring within the project frame 38
2.2.5. Tools, model trains, scenarios expected to be employed or utilized 39
2.2.6. Activities executed on site up to date 40
2.2.7. Planned activities for the upcoming period 41
2.3. BRGM Test Facility - Soil Laboratory (FRA) 41
2.3.1. Purpose of the sites within the PHISHES project 42
2.3.2. Description of the basin/site 43
2.3.3. Existing data available 47
2.3.4. Additional – optional – monitoring within the project frame 51
2.3.5. Tools, model trains, scenarios expected to be employed or utilized 53
2.3.6. Activities executed on site up to date 55
2.3.7. Planned activities for the upcoming period 56
2.4. Airport in Örnsköldsvik (SWE) 56
2.4.1. Purpose of the sites within the PHISHES project 56
2.4.2. Description of the basin/site 56
2.4.3. Existing data available 62
2.4.4. Additional – optional – monitoring within the project frame 64
2.4.5. Tools, model trains, scenarios expected to be employed or utilized 64
2.4.6. Activities executed on site up to date 65
2.4.7. Planned activities for the upcoming period 65

2.5. The Rotterdam Urban Area (NL) 66
2.5.1. Purpose of the site within the PHISHES project 66
2.5.2. Description of the basin/site 67
2.5.3. Existing data available 68
2.5.4. Additional – optional – monitoring within the project frame 74
2.5.5. Tools, model trains, scenarios expected to be employed or utilized 75
2.5.6. Activities executed on site up to date 77
2.5.7. Planned activities for the upcoming period 77

List of Figures

Figure 1 Delineation of Martinicky creek basin and location of Zelivka basin within Czech Republic 15
Figure 2 Landuse of Martinicky creek 17
Figure 3 Leaf area index – main parameter describing vegetation in MIKE SHE 17
Figure 4 Extent of Cambisol, main soil type of Martinicky creek 18
Figure 5 Soil and shallow saturated zone hydraulic properties 19
Figure 6 Outflow rate of saturated zone conceptual drainage 19
Figure 7 Martinicky creek – orthophoto map with existing and new monitoring profiles used for project execution 20
Figure 8 Cascade of sub-basins in the Martinicky basin. White fields are drainage systems built in the last century 20
Figure 9 PVL s.p. has data available for the period 2019-2023 from reports on the application of treatment substances on plots within the B4 program. Data is not commonly available on other plots. This information is a key input for all analyses and models – calibration and verification. 21
Figure 10 Cernici Basin A included specific drainage and permanent monitoring sites 22
Figure 11 An Example of the results of sampling in Martinicky creek and concentration of some metabolites in the basin, year 2024 - left Y axis shows discharge, right concencration and X axis time. Blue line represents discharge at Senozaty station and colored points represent Dimethachlor (as an example) concentration at various sampling places along Martinicky creek. 26
Figure 12 Location of Koprzywianka catchment within Poland territory 35
Figure 13 Soil types in the Koprzywianka catchment 36
Figure 14 Land use classes of Koprzywianka catchment. 37
Figure 15 Water sampling and gauging points. 39
Figure 16 Illustrative examples of 1D column set up to assess transport properties of the porous medium and fate and transport of inorganic contaminants 45
Figure 17 Illustrative example of an experiment on Light non aqueous phase fluid filtration in a sandy material in the 2D tank set up 45
Figure 18 Schematic sketch of the lysimeters used in the metric platform 46
Figure 19 Schematic sketch of the plurimetric pilot. 47
Figure 20 Implementation of the monitoring tools of the PMP 49

Figure 21 Conceptual design of the PMP experiment (modified from Zessner et al., 2025)..... 50

Figure 22: Sketch of the model train developed to simulate fate and transport of PFAS in soil-groundwater continuum..... 54

Figure 23 Soil types according to the Geological Survey of Sweden's 1:25 000 – 1:100 000 Soil types map. 57

Figure 24 Summary of sedimentation analyses (left, n=16) and 28 sieve analyses (right, n=22). Sedimentation analyses were performed using the hydrometer method (blue, n=6) and pipette method (red, n=10). 58

Figure 25 Piper plot of proportional chemistry data prior to the installation of the CAC barrier. Points represent the relative ion composition of groundwater samples collected in the vicinity of the AFFF site at Örnsköldsvik Airport during 2022. 59

Figure 26 Minimum, average and maximum daily temperature 2000-2024 (left), Örnsköldsvik's airport (SMHI station 138240) and snow depth observations 1947-2024, Örnsköldsvik (SMHI station 138180). Average length of the vegetation period (158 days) shown with green line. 59

Figure 27 Relative groundwater level to April 2023 measured at selected wells at the AFFF site, 2023-2024. Dashed lines indicate extrapolated groundwater decline (assuming no recharge) during groundwater recharge events..... 60

Figure 28 Example of return period for accumulated daily precipitation, SMHI station 138180 Ornsköldsvik. Period 1945-1994 (left) and 1995-2024 (right). 60

Figure 29 Groundwater level September 2023 (m.a.s.l.). Interpolation of the groundwater surface using kriging (cm a.s.l., Ordinary, Spherical) is shown. 61

Figure 30 Relative frequency of Log(K) data (a) and cumulative frequency of Log(K) data from different hydrogeological units measured using the HPT..... 62

Figure 31 Hydraulic gradient calculated from groundwater level time-series measurements from selected wells. 62

Figure 32 Location of Rotterdam in the Netherlands (bottom left) and cross section of harbour and urban area. 67

Figure 33: Locations of the available groundwater level monitoring wells..... 68

Figure 34: Timeseries of groundwater levels for a specific location in Rotterdam at a depth of NAP – 2.59 m. NAP stands for 'Normaal Amsterdams Peil', the national reference level for the Netherlands. This approximately corresponds to the geoid. 69

Figure 35: Soil quality classification of up to 1 m below ground level for the city of Rotterdam. Within the urban area, the classifications residential (orange), industrial (red), agriculture (yellow) and nature (green) are present. The black lines represent the boundaries between various neighbourhoods. 70

Figure 36: In red the locations of available (historical) soil investigations 72

Figure 37: Location of borehole profiles (light brown) and CPT profiles (dark brown). 72

Figure 38: Borehole profile for a specific location. 73

Figure 39: A north–south cross-section of GeoTOP (TNO) showing the most probable lithological classes. In grey: anthropogenic fill; in yellow: sandy deposits; in brown: peat; and in green: clay. 74

Figure 40. Pilot field soil health experiments. 75

Figure 41: coupling scheme for MF6 – UZF - Reservoir-model. 76

List of Tables

Table 1 The list of the most important streams/creeks/rivers in the River Zelivka Basin 14

Table 2 Hydrological characteristics of Martinicky creek at Senozaty profile (catchment area 113.28 km²) 16

Table 3 Data overview in Martinicky creek basin 25

Table 4 Scenarios on the River Zelivka Basin – cascades of experimental sites – broad overview and preliminary scenarios set-up, where “x” indicates the scenario is considered relevant and is planned to be addressed within the given test case, and “o” indicates the scenario is not planned for that test case or is lower priority, for example because it is not relevant to the site, the required data are not available, or the respective modelling approach is not applicable. 31

Table 5 Table summarizing the data issued from the PMP experiment 51

Table 6 Median chemical concentrations from groundwater samples collected during 2018 (NIRAS) 58

Table 7 Overview of the data collected at Örnsköldsvik within the Swedish Geotechnical Institute’s governmental assignment regarding PFAS. 63

Table 8: Reference values for metal parameters, for the soil quality classifications ‘soil quality map’. In the Rotterdam Urban area the class ‘(L)MW Wonen’ is dominant (residential areas in orange). 71

Executive Summary

Work Package 4 (WP4) of the PHISHES project aims to validate innovative tools and simulation models through five diverse test sites, each representing different soil types, land uses, and environmental conditions. These sites serve as real-world environments to test methods developed in other work packages, ensuring their effectiveness across various data quality and spatial scales. WP4 supports the creation of a digital soil and water platform for data sharing and scenario analysis, contributing directly to sustainable land management strategies and informed policymaking. This report provides a summary of each test site, detailing the available data and the application of simulation tools within the project.

Keywords

PHISHES, WP4, test sites, Zelivka, Koprzywianka, Örnsköldsvik, Soil Laboratory, Rotterdam Urban Area

List of acronyms and abbreviations

1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
AD	Advection-dispersion
ADE	Advection-dispersion equation
AFFF	Aqueous filming-forming foam
AOM	Added organic matter
API	Application programming interface
AWI	Air-water interface
BMP	Best management practice
BRGM	French geological survey, FRA
CAC	Colloidal activated carbon
CF	Channel flow
CG	CzechGlobe (Global Change Research Institute CAS), CZE
cm	Centimeter
CMIP6	Coupled Model Intercomparison Project Phase 6
CPT	Cone penetration test
CZE	Czech Republic
ET	Evapotranspiration
FRA	France
g	Gram
GC	General Circulation Model
ha	Hectare
HPT	Hydraulic profiling tool
Kh	Hydraulic conductivity
km	Kilometer
KNMI	Royal Netherlands Meteorological Institute
KU	Copenhagen University, Denmark
L	Liter
LAI	Leaf area index

LNAPLs	Light non-aqueous phase liquids
m	Meter
MF6	MODFLOW 6 software program
mg	Milligram
mm	Millimeter
MoA	Ministry of Agriculture
ng	Nanogram
NL	The Netherlands
NNF	Non-Newtonian fluids
NTM	Numerical Terrain Model
OL	Overland Flow
PFAS	Polyfluoroalkyl substances
PL	Poland
PMP	Plurimetric Platform
PV	Pore volumes
PVDF	Polyvinylidene difluoride
RCP	Representative Concentration Pathway
s	Second
SDBS	Sodium Dodecyl Benzene Sulfonate
SGGW	Warsaw University of Life Sciences, PL
SGI	Swedish Geotechnical Institute, SWE
SGW	Soil–groundwater
SMB	Soil microbial biomass
SMHI	Swedish Meteorological and Hydrological Institute
SOM	Soil organic matter
SSP	Shared socioeconomic pathway
SWE	Sweden
SWI	Soil-water interface
SY	Specific yield
SZ	Saturated Zone
TMDL	Total maximum daily load
TNO	Geological Survey of the Netherlands
UZ or UNZ	Unsaturated Zone
UZF	Unsaturated Zone Flow
VN	Reservoir
VUMOP	Research Institute for Soil and Water Conservation, CZE
W	Watt
WP	Work Package
WQ	Water quality
WWTP	Wastewater treatment plant

WP 4 report from the test sites

1. General summary – concept of the test sites for PHISHES project

Work Package 4 (WP4) focuses on validating innovative tools, methods, and simulation models through carefully selected test cases across five diverse sites. These test sites represent various soil types, land uses, and environmental conditions, offering a robust platform to demonstrate how simulation-based approaches can support sustainable land and soil management. The primary goal of WP4 is to serve as a testing ground for methods developed in other work packages, assessing their effectiveness across different data levels, quality, and spatial scales—from laboratory to basin level.

The outcomes from WP4 will provide concrete evidence to guide policy and decision makers in implementing best practices for soil conservation and ecosystem sustainability, especially in the context of future challenges such as climate change. The test sites will serve as real-world demonstrations showcasing how innovative approaches can work under practical conditions, including data limitations and the complexities of current agricultural practices.

Additionally, WP4 will support the development of a digital soil and water platform, facilitating data sharing, scenario analysis, and dissemination among project partners, stakeholders, and the broader community. Through its integrative role, WP4 connects and supports the objectives of the broader project, ensuring that all proposed tools and approaches are tested, validated, and effectively aligned to deliver meaningful, evidence-based results.

This report provides a detailed overview of each test site, including the specific data available and utilized, as well as the development and application of the simulation tools used within the PHISHES project at individual test sites.

2. Experimental fields

The five selected test cases represent distinctly different conditions, ensuring comprehensive coverage and minimizing gaps or limitations in validation activities within the PHISHES project.

- Zelivka River Basin (Czech Republic)
  Lead: CzechGlobe; support: DHI, KU
- Koprzywianka River Basin (Poland)
  Lead: SGGW; support: DHI, CzechGlobe
- BRGM Test Facility - Soil Laboratory (France)
  Lead: BRGM; support: SGI
- Airport in Örnsköldsvik (Sweden)
  Lead: SGI; support: BRGM
- The Rotterdam Urban Area (Netherlands)
  Lead: DELTARES; support: BRGM, DHI

2.1. Zelivka basin (CZE)

The river Zelivka (Želivka in Czech) basin is situated in Central Bohemia and Highlands Region in the Czech Republic. The Zelivka stream basin covers an area of 1188 km^2, of which the area of the Svihov (Švihov in Czech) water reservoir's own catchment area is 1178 km^2. The primary purpose of the Svihov water reservoir on the Zelivka River (hereafter referred to as VN, which means water reservoir in Czech language) Svihov is to supply drinking water to the capital city of Prague, the Central Bohemian Region, and parts of the South Bohemian and Vysocina Regions. In terms of both storage volume and extracted quantity, this water management structure represents the largest water supply reservoir in the Czech Republic and the Central Europe. The water management complex also includes the pre-reservoirs Trnavka on the Trnavka River, Nemcice on the Sedlicky Stream, and Sedlice on the Zelivka River, which serve to trap sediment and a portion of the pollution carried by the watercourses.

VN Svihov has been subject to long-term pollution from diffuse agricultural sources (primarily nitrates and pesticides). For instance, this load accounts for approximately 75–85% of the total nitrate pollution. Due to the limited percentage of grassland areas and the creation of large land blocks during the period of agricultural collectivization, the VN Svihov catchment experiences significant problems with soil erosion. This erosion results in the siltation of local ponds, pre-reservoirs, water bodies, and water supply infrastructure with sediments. These sediments, along with nutrients (nitrogen and phosphorus) and pesticides, subsequently compromise the water quality in the main reservoir, which is crucial for its uninterrupted abstraction and subsequent treatment into potable water.

The basin area of the VN Svihov is densely populated and intensely utilized for agriculture, with approximately 58% of the area comprising arable land. Extensive areas are dedicated to cultivating crops with combined uses, partly as a source of substrates for biogas plants. This primarily involves wide-row and industrial crops, especially maize, rapeseed, and potatoes. Plant protection products are used on a large scale. From a long-term perspective, the shift to cultivating industrial crops within the reservoir catchment poses a significant risk with potentially serious implications for water quality. Potential issues with nitrate levels have been signaled for a long time.

New wastewater treatment plants (WWTPs) were extensively constructed, and older ones were intensified to mitigate the impact of pollutant loads, initially organic substances, and later phosphorus. Erosion problems and agricultural practices in general have also been addressed.

In recent decades, partly due to the availability of modern analytical techniques, the problem of plant protection products has come to the forefront, particularly where maize and rapeseed are cultivated over larger areas. The consequence of extensive agricultural activity is primarily elevated concentrations of nitrates and pesticide substances in groundwater, in drainage outlets and surface waters. Along with nutrients from wastewater (mainly phosphorus), other chemical substances, such as pharmaceuticals, hormonal preparations, cosmetic products, anti-corrosives, bisphenol A, and more, also enter the watercourses. The local sewage treatment plants are a probable source of these pollutants. Both pesticide substances and pharmaceuticals transform into various metabolic products that persist in the water in different forms.

To reduce the negative impact of the aforementioned factors, Program B4 was adopted within the Svihov reservoir catchment, and procedures based on the approved methodology (Methodology for Management in the OPVZ VN Svihov 2020) have been implemented in selected localities.

2.1.1. Purpose of the sites within the PHISHES project

The work for the test case site Zelivka, within PHISHES project, is on 3 scale levels:

- whole basin
- selected experimental area of the Martinicky creek;
- sub-catchments within Martinicky creek, and related potable water reservoir Svihov with volume 309 Mil m^3

The cascade of catchments was carefully selected. All selected catchments are explained in section 2.1.2.

Relevant Users: Regional Water Authority, regional decision makers, Vltava River Basin Authority (supervisor of ecosystem - Soil-vegetation-water-groundwater-surface-reservoir to protect groundwater for drinking water purposes). The VN Svihov represents the strategic - key water sources in the Czech Republic and that is why is important to understand the development of the water quantity and quality parameters in the basin under the climate change.

The main purpose of using the basin, which is very rich in monitoring data, within the framework of the PHISHES is as follows. The Martinicky creek (basin E - 116 km^2) has its own confluence with the reservoir and has only a few ponds scattered throughout the basin, so it is a good candidate for an experimental site. Furthermore some of the tributaries of the sub-catchment of the Martinicky creek have unique information about the fertilizer load and protective chemicals at least during a certain period of knowledge thanks the reduction program of the MoA (Ministry of Agricultural, Methodology for Management in the OPVZ VN Svihov 2020). The Water Authority and the project partner CzechGlobe have adopted a program for extraordinary monitoring focused on pesticide and fertilizers and their forms in surface waters. These data from the soil – groundwater – surface water system provide a solid foundation for applying modeling techniques to simulate the transport processes of fertilizer and pesticide substances within the defined system. The goal is to identify best practices or adaptation measures that can improve these transport processes under changing climate conditions.

Special objectives:

1. Assessment of the overall impact of point and non-point source pollution in the Zelivka River Basin or its sub-catchments (primarily the Martinicky Creek, where most of the current data is available). The analysis is based on baseline time series (approximately 30 years) and includes projections of boundary conditions influenced by expected climate change over the next 100 years, focusing mainly on hydrological variables and water balance;
2. Impact of adaptation measures in soil management and resulting in soil health improvements and the impacts on soil ecosystem services – baseline scenario and climate change impact scenarios;
3. Define special treatment of selected kinds of pollution and contaminants, which are monitored in the streams by the Water Authority in their monitoring stations and also reported by farmers and landowners on the production side;
4. Using the cascade of models in the experimental basin to track the pollution in the system soil -water body- potable water reservoir by using modeling train tools.

2.1.2. Description of the basin/site

The Zelivka River basin covers an area of 1188.4 km^2, of which the catchment area of the Svihov Reservoir (VN Svihov) itself is 1178.5 km2. The Zelivka basin is part of the Lower Vltava sub-basin, as defined by Ministry of Agriculture Decree No. 393/2010 Coll., concerning river basin areas.

The Zelivka River, also known as Hejlovka in its upper reaches, is a third-order stream and a left side tributary of the Sazava River, into which it flows below Zruc nad Sazavou. It originates in the Kremesnicka Highlands on the northern slope of Trojak, approximately 10 km from Pelhrimov, at an elevation of 677 m above sea level. The average discharge at its confluence with the Sazava River is 7 m^3/s. The river's length is 103.89 km, and its basin area is 1188.4 km^2.

Within the basin, there are 136 water bodies larger than 1 ha, with a total area of 1935.8 ha. The largest of these is the Svihov water reservoir, covering 1396.6 ha. In its southern part, the Zelivka has major right side tributaries, the Bela and Jankovsky creek. In its central part, it has the left side tributary Trnava. In its northern part, the Sedlicky creek, Blazejovicky creek, and Martinicky creek directly enter the VN Svihov from the left. Parameters of the more significant watercourses within the Svihov water supply reservoir catchment are provided in Table 1.

Table 1 The list of the most important streams/creeks/rivers in the River Zelivka Basin

Hydrologic parameters of main tributaries of the River Zelivka	*Basin area (km^2)*	*Length of the creek - river (km)*	*Tributary of the River Zelivka*
Zelivka	1 188.4	103.9	-
Cerekvicky creek	54.5	16.9	left side
Bela	130.6	25.1	right side
Jankovsky creek	130.0	22.8	right side
Trnava	340.2	56.3	left side
Martinicky creek	116.0	38.7	left side
Blazejovicky creek	33.41	14.1	left side
Sedlicky creek	95.8	23.6	left side

Martinicky creek in detail

The Martinicky creek is a left side tributary of the River Zelivka (Figure 1). The creek drains an area of 116 km^2, nearly 10% of Zelivka river basin. It is a significant tributary to the Zelivka Reservoir, the primary drinking water source for Prague. Situated within the Ceskomoravska vrchovina (Bohemian-Moravian Highlands), its hydrological regime, water quality, and overall ecological health are intricately linked to the region's meteorology, geology, soil composition, and intensive agricultural land use.

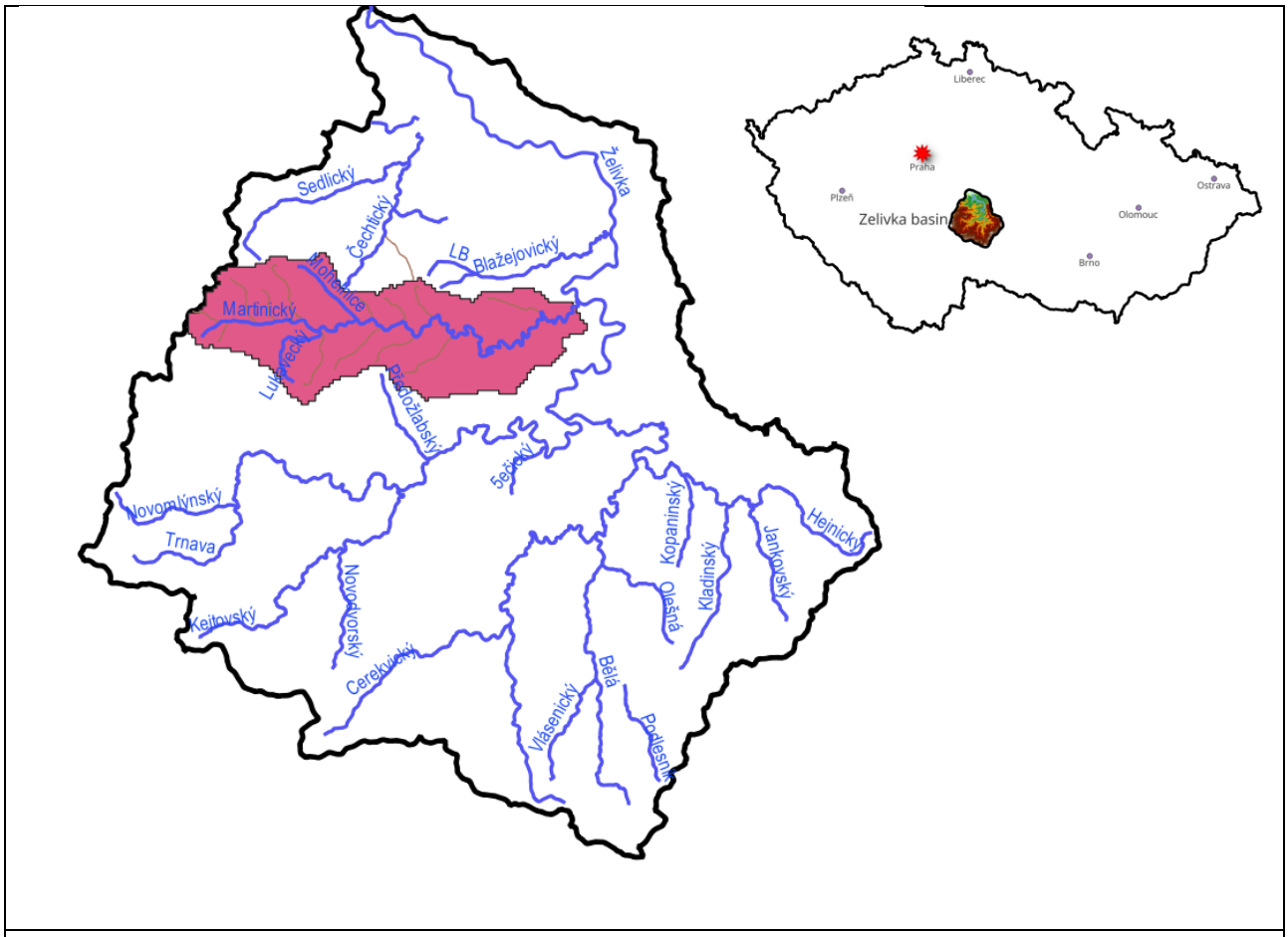


Figure 1 Delineation of Martinicky creek basin and location of Zelivka basin within Czech Republic

The MIKE SHE model of Martinicky creek includes a detailed description of the main river and tributaries Mohelnice and Lukavecky creek with channel parameters described by data from a geodetical survey. Smaller creeks are simplified but still represented in the hydrodynamic part of the MIKE SHE model.

Meteorological and Hydrological Characteristics

The Martinicky creek catchment lies in a temperate climate zone, characterized by warm summers and cold, cloudy, and humid winters. Regional climate data for the broader Vltava basin, of which the Zelivka is a part, indicates a trend of increasing average annual temperatures. This trend, coupled with potential shifts in precipitation patterns and an increased frequency of extreme weather events such as intense rainfall and droughts, is likely to impact the hydrological regime of the creek.

The hydrological characteristics of the Martinicky creek are well-documented, with a key gauging station located at Senozaty. The creek has a length of 35.9 km and a catchment area of 116.1 km². The hydrological regime is pluvio-nival, with the highest flows typically occurring in spring due to snowmelt and precipitation, and lower flows in the late summer and autumn.

Table 2 Hydrological characteristics of Martinicky creek at Senozaty profile (catchment area 113.28 km²)

Hydrological characteristics of Senozaty profile	Value (m^3/s)
Average discharge (Qa)	0.52
1-year flood flow (Q1)	11.20
5-year flood flow (Q5)	25.50
10-year flood flow (Q10)	34.00
100-year flood flow (Q100)	64.00

Geology and Soil Composition

The Zelivka River basin is located in the western part of the Crystalline Hydrogeological Region within the Sazava River basin, encompassing the Zelivka catchment and the Sazava catchment downstream to Zruc. Crystalline rocks in this region exhibit reduced fracture permeability, which, within the reach of weathering processes, primarily depends on the character of the weathering material. Granitoids of the Moldanubian Pluton, found in the southern part, possess relatively better fracture permeability.

Among Quaternary sediments, fluvial accumulations of floodplain sediments and some thicker eluvium deposits hold greater hydrogeological significance. Quaternary permeability varies depending on the specific deposits. The area is characterized by shallow aquifers linked to the surface zone of Quaternary deposits, the weathering zone, or near-surface rock disintegration. Water circulation is localized. Infiltration occurs across the entire collector area, contingent on the permeability of the regolith. Drainage takes place at or above the local erosion base.

The geological underpinning of the Martinicky potok catchment is dominated by the Moldanubian Zone of the Bohemian Massif. The primary rock type is metamorphosed paragneiss, specifically biotite and sillimanite-biotite paragneiss. These crystalline rocks are relatively resistant to weathering, influencing the topography and soil development in the region. The landscape is characterized by rolling hilly terrain.

The soils in the catchment are predominantly Cambisols and Stagnosols on the slopes and higher elevations. In the floodplain of the Martinicky potok and its tributaries, Gleysols and Fluvisols are common. The Cambisols have moderate fertility, while the Stagnosols and Gleysols are characterized by waterlogging in certain periods, which can influence agricultural practices and nutrient runoff. The permeability of these soils plays a crucial role in the transport of pollutants from the surface to the water bodies.

Land use

The basin is primarily used for agriculture (Figure 2). However, the upper regions of the basin are predominantly forested, mainly with coniferous trees, with spruce being the dominant species. A significant part of the forest was damaged and partly harvested after bark beetle outbreak following the 2015-2018 period of serious hydrological drought.

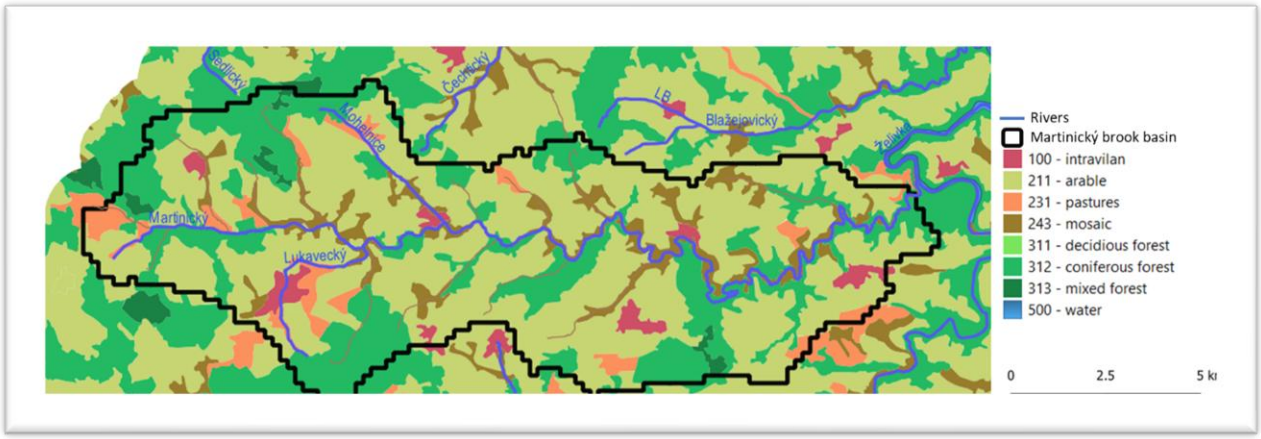


Figure 2 Landuse of Martinicky creek

Land use enters the model indirectly in the form of Leaf Area Index (LAI, Figure 3) distributed in time and space derived from MODIS, product of Terra satellite survey. Accompanied by Crop Coefficient and Root Depth, LAI serves as the main parameter for actual evapotranspiration estimation as a function of vegetation properties and soil moisture.

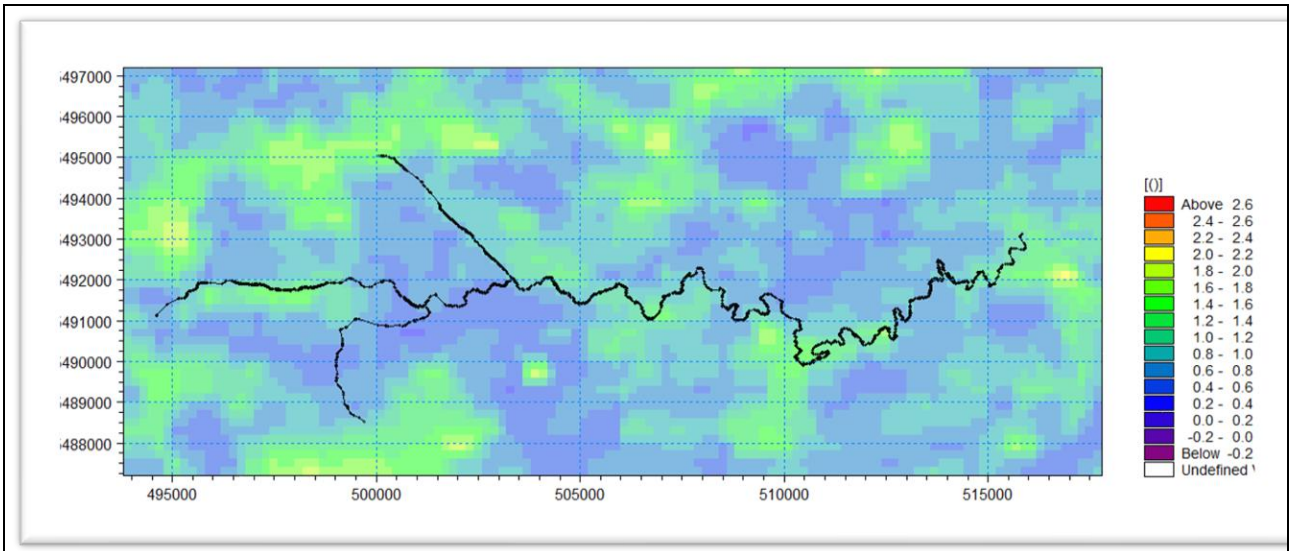


Figure 3 Leaf area index – main parameter describing vegetation in MIKE SHE

Soil types

The soil of Martinicky creek is mostly uniform. The main soil type is Cambisol (Figure 4) with a smaller extent of Pseudogley. The soils were characterized based on their retention properties, utilizing Van Genuchten parameters obtained from laboratory analyses of in-situ soil samples.

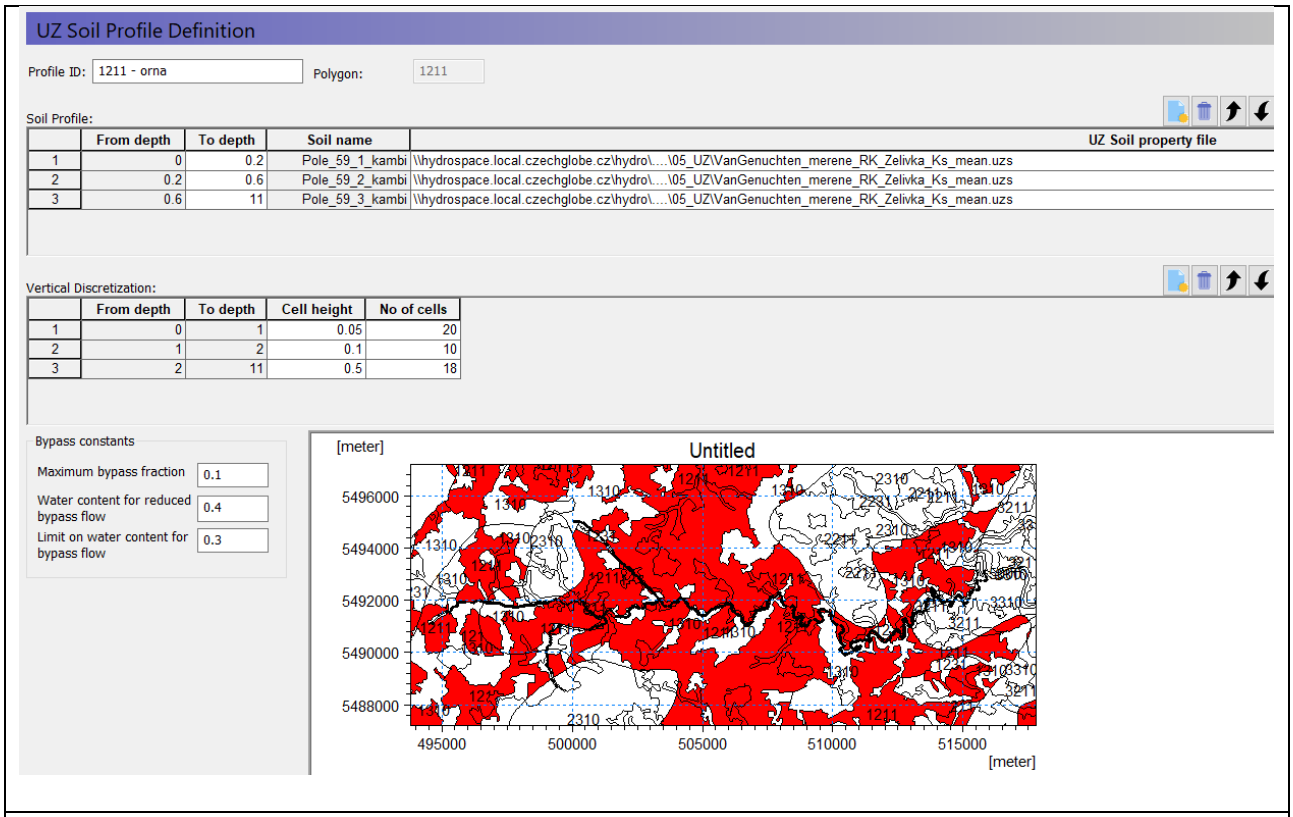


Figure 4 Extent of Cambisol, main soil type of Martinicky creek

Geological structure of the basin consists mainly of crystalline and metamorphic rocks with highest water storage and movement in a thin layer of regolith (< 30 m). Aquifers are shallow with fast exchange and transmissivity decreases with altitude.

Hydraulic properties of the shallow saturated zone (0-5 m) were derived from multiple measurements of saturated hydraulic conductivity, Kh. Highest values (Kh = $6e^{-5}$ m/s) were set at forested parts of the basin meanwhile lowest values were set at arable lands (Kh = $1e^{-5}$ m/s). However, the differences in values are quite minor (Figure 5).

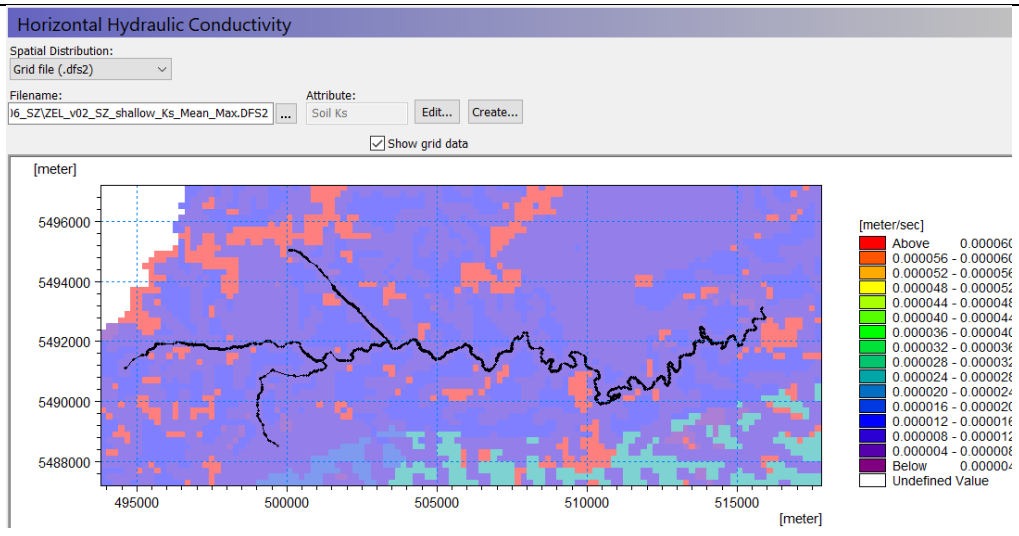


Figure 5 Soil and shallow saturated zone hydraulic properties

Fast runoff response on rainfall events is simulated by overland and saturated zone drainage. Those paths are simulated separately but react similarly to conceptualized drains triggered after crossing a threshold level of overland water or groundwater level. The physical parameters of those conceptual drains (rate of outflow and level of drain) were set as a function of altitude, slope, landuse and site-specific information of artificial drainage systems.

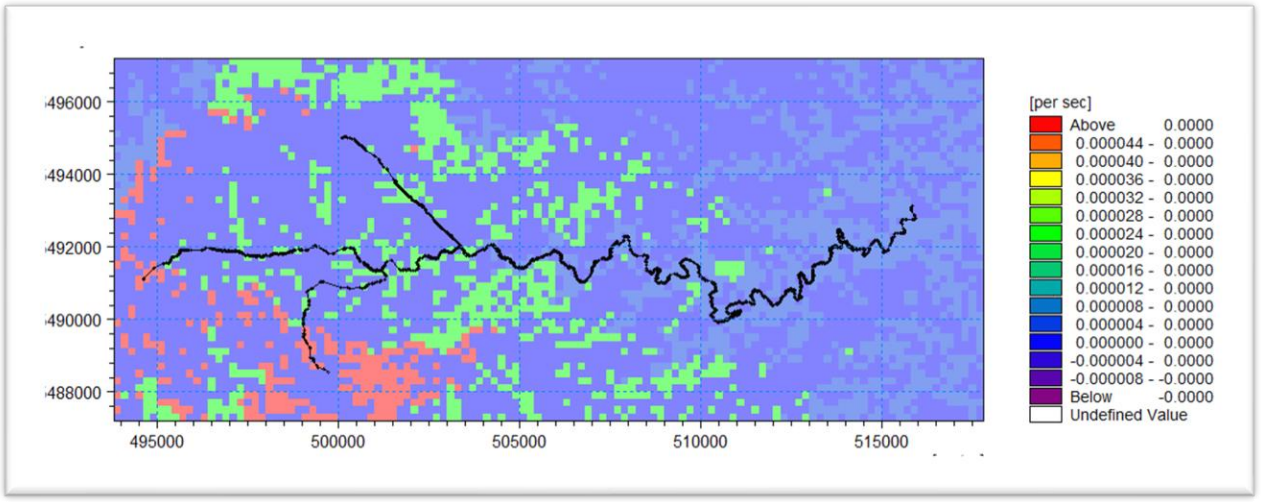


Figure 6 Outflow rate of saturated zone conceptual drainage

Cascade of basins in the Martinicky creek basin selected for PHISHES project – as a test site with specific data sets and detail monitoring

The Martinicky creek basin was selected as a specific test site, because it represents the unique combination of the data (in some parts) of the precise record of agricultural techniques being applied, but also the load of fertilizers and load of protective chemical compounds in the past period, and monitoring of water quantity and water quality in the basin. For this reason, a cascade of sub-catchments was selected as the platform for establishing, calibrating, and verifying simulation chains focused on water and substance transport processes in the soil – water system. The cascade of sub-catchments is seen in Figure 7, Figure 8, and Figure 9. The “Basin A” – Cernici belongs to the experimental field, where monitoring and experiments have been carried out for more than a decade. Basin A will serve as a laboratory test site. A new profile B (Figure 8) is under construction and the final version of the measuring station should include a bio filter from wooden chips and biochar.

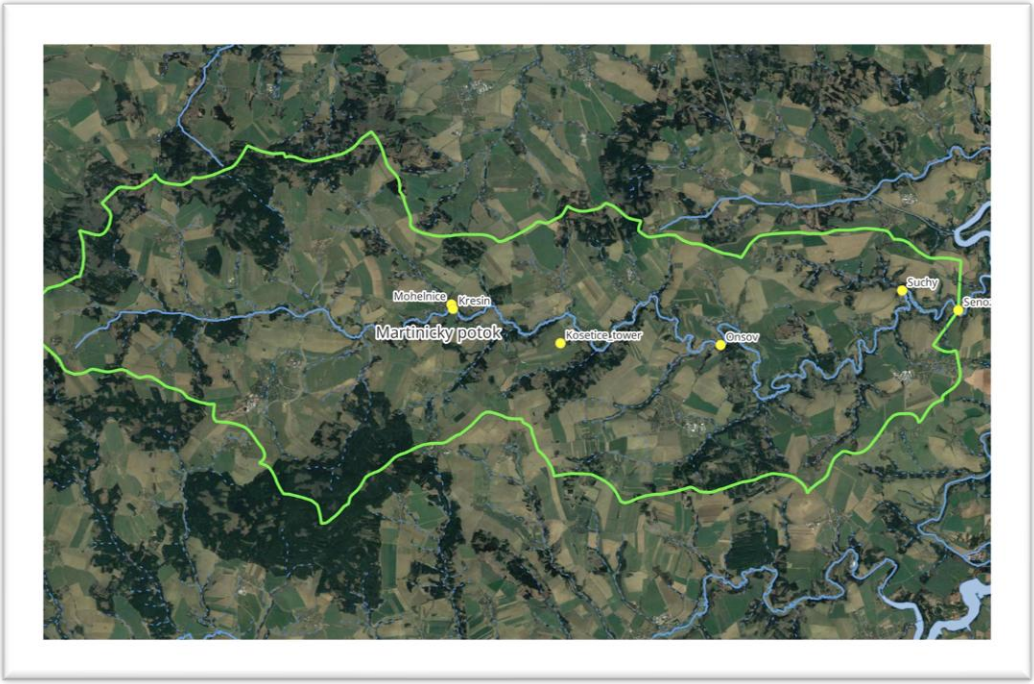


Figure 7 Martinicky creek – orthophoto map with existing and new monitoring profiles used for project execution

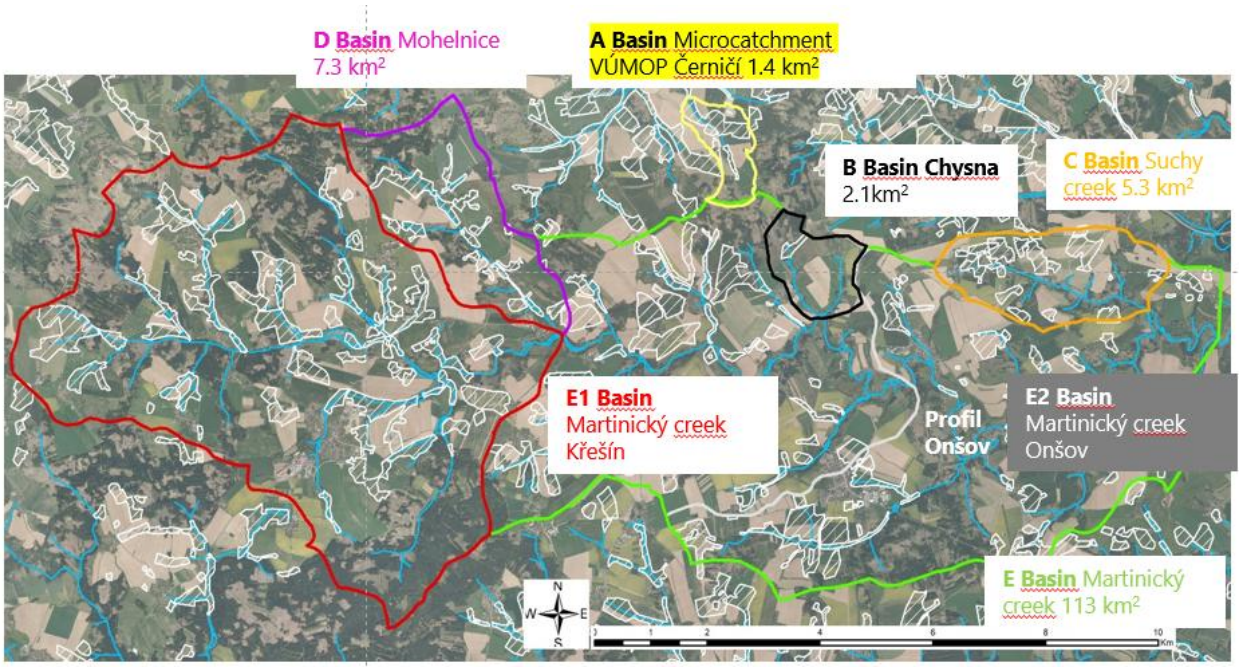


Figure 8 Cascade of sub-basins in the Martinicky basin. White fields are drainage systems built in the last century

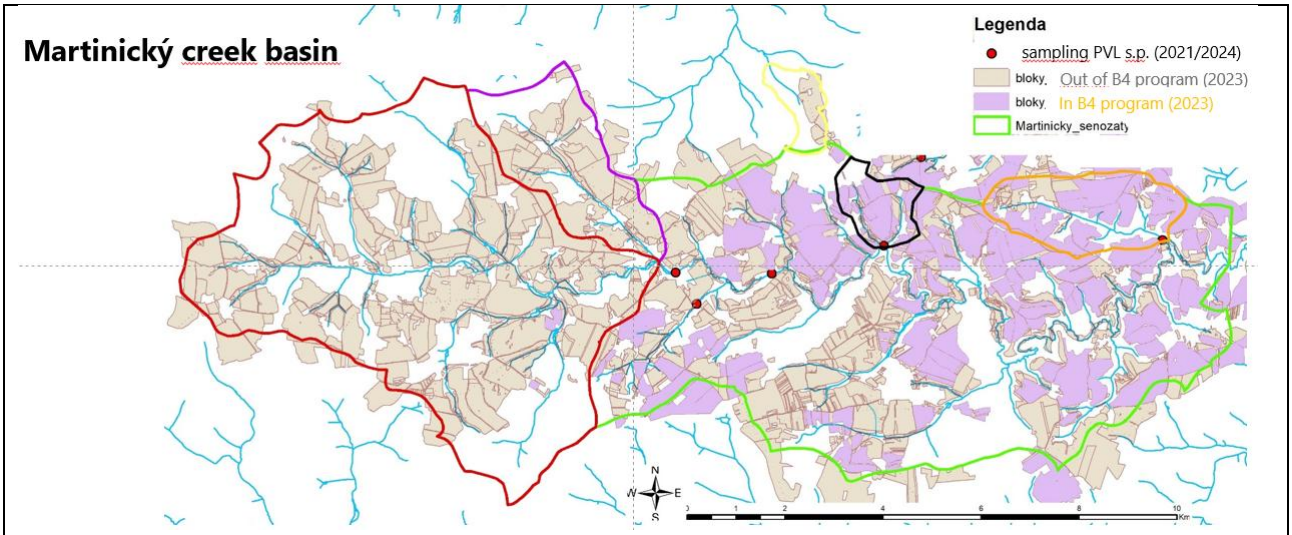


Figure 9 PVL s.p. has data available for the period 2019-2023 from reports on the application of treatment substances on plots within the B4 program. Data is not commonly available on other plots. This information is a key input for all analyses and models – calibration and verification.

Sub-basin A - Cernici has been mentioned as a laboratory field test site for researchers. The catchment is under the management of VUMOP v.v.i. Although VUMOP is not directly involved in the PHISHES project, it has kindly granted permission to use the data for project purposes. This sub-catchment is very limited in area, but rich in all types of experiments and monitoring efforts. That is why this "field laboratory" is essential for testing the model trains to describe the processes in the system of soil and water transport processes. The sub-basin itself is presented in the Figure 10.

A set of basins and sub-basins serves as a reference for defining the scenarios to be tested in the Zelivka Basin as part of the PHISHES project.

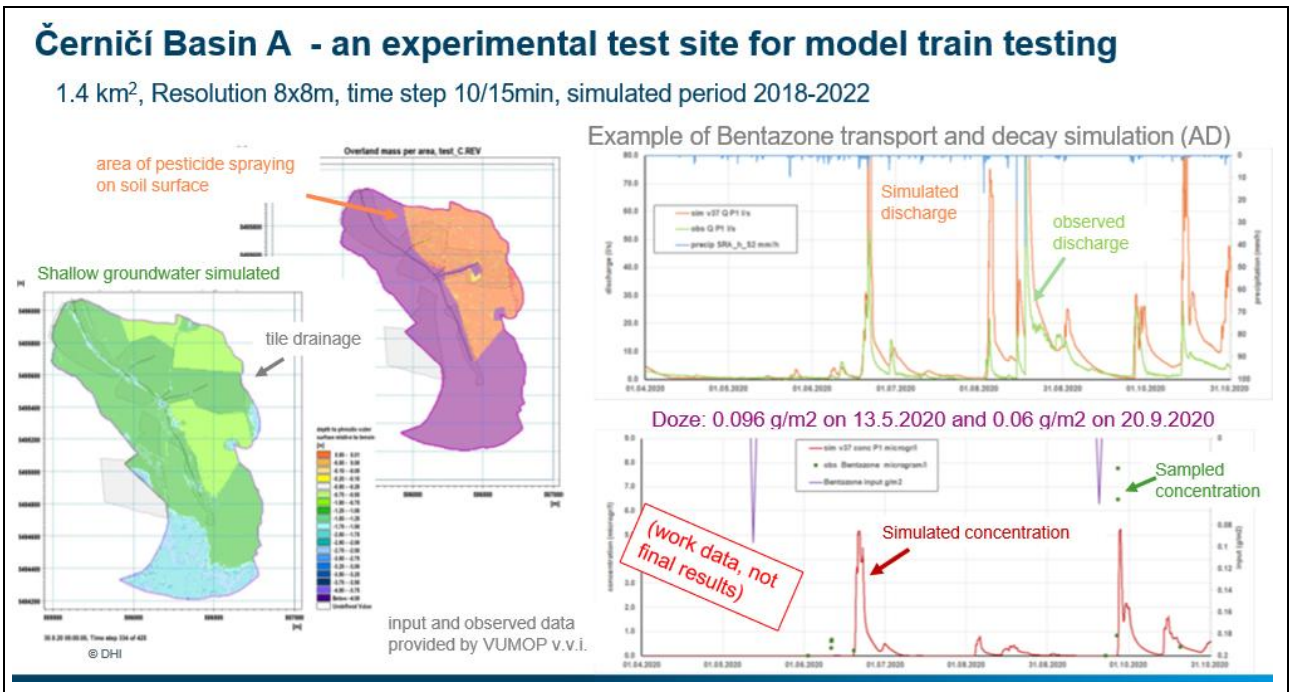


Figure 10 Cernici Basin A included specific drainage and permanent monitoring sites

Land Use and Anthropogenic Pressures

The Martinicky creek catchment is predominantly an agricultural landscape. Arable land constitutes most of the land use, with a significant portion dedicated to the cultivation of cereals, oilseed rape, and maize. This intensive agricultural activity is a primary source of anthropogenic pressure on the creeks, and their water quality. The remainder of the catchment consists of forests, permanent grasslands, and scattered rural settlements, the largest being Martinice u Onsova. The land use pattern directly influences the types and sources of pollution impacting the Martinicky creek.

The utilization of water generally represents human activity with varying degrees of impact on water status and quality. From sub-basin management plans, it's possible to identify these impacts, assess their significance and effect on water status, and propose appropriate measures to eliminate adverse impacts. The goal is to achieve a balance between the requirements for achieving good water status and the benefits that water utilization provides.

Generally, four main categories of impacts can be identified:

- Point source pollution
- Diffuse source pollution
- Hydrological alteration of watercourses (abstractions, transfers, peak flows, and water accumulation)
- Hydromorphological alteration of riverbeds and floodplains

While point source pollution and hydrological alterations can be identified with relative precision, diffuse source pollution and hydromorphology exhibit considerable uncertainties for certain indicators. The effects of these impacts are reflected in the assessment of water body status. Impact identification is an integral part of the sub-basin management plans. The water quality of the Martinicky creek is influenced by a combination of point and non-point source pollution.

The main point sources of pollution are municipal wastewater from settlements within the catchment, including Martinice u Onsova and other smaller villages. While information on the specific level of wastewater treatment for all settlements is not readily available, untreated or insufficiently treated wastewater can introduce significant loads of nutrients (nitrogen and phosphorus), organic matter, and pathogens into the creeks.

Non-point source pollution, primarily from agriculture, is the most significant threat to the water quality of the Martinicky potok. This includes:

- Nutrient Runoff: The application of nitrogen and phosphorus fertilizers on arable land leads to their leaching and runoff into the creek, contributing to eutrophication. This process, characterized by excessive algal and plant growth, can lead to oxygen depletion and negatively impact aquatic ecosystems.
- Pesticide Contamination: The use of herbicides, insecticides, and fungicides in intensive agriculture results in their presence in the water. Studies conducted in the broader Zelivka reservoir basin, including the Martinicky creek, have detected various pesticide residues. These substances, even at low concentrations, can have adverse effects on aquatic organisms and pose a risk to the drinking water supply.
- Soil Erosion: Agricultural practices on sloping land can lead to increased soil erosion, resulting in higher turbidity and sedimentation in the creek. Sediments can carry adsorbed pollutants, such as phosphorus and pesticides, further degrading water quality.

- Atmospheric Deposition: Studies in the wider region have indicated that atmospheric deposition of pollutants, such as heavy metals and polycyclic aromatic hydrocarbons (PAHs), can also contribute to the overall pollution load in the catchment.

Overall Water Quality and Quantity Status

The overall water quality (WQ) of the Martinicky creek is classified as moderate to poor, primarily due to the pressures from agricultural activities. The creek is a significant contributor of nutrients and pesticides to the Zelivka Reservoir. As the reservoir is a critical source of drinking water, the quality of the inflowing water from tributaries like the Martinicky creek is of paramount concern. The water management authorities, including the Vltava River Basin Authority, have implemented various measures to mitigate these impacts, including the establishment of protection zones and the promotion of more sustainable agricultural practices.

In terms of water quantity, the Martinicky creek, like many watercourses in the region, faces the dual challenge of potential flood events and periods of low flow, which can be exacerbated by climate change. Maintaining a stable water quantity regime is essential for the ecological health of the creek and for ensuring a reliable inflow to the Zelivka Reservoir.

2.1.3. Existing data available

Existing data for basin and land use descriptions were partly presented in the general basin description. The data availability is summarized in Table 3. The data about agriculture practices and load of fertilizers and also chemicals used for the protection of crops is not generally available - this data is not found in open sources. Thanks to the projects (like reduction program B4, Methodology for Management in the OPVZ VN Svihov 2020) of MoA (Ministry of Agriculture) of the Czech Republic, some of the tributaries of the Martinicky creek sub-catchments have unique information about the fertilizer load and protective chemicals at least during a certain period. The Water Authority and CzechGlobe have adopted a program for extraordinary monitoring focused on pesticides and fertilizers and their forms in surface waters. These data on both sides of the system soil - ground water - surface water provides a reasonable condition for applying modelling techniques in order to simulate the transport processes of the substances of fertilizers and protective chemicals in the defined systems and try to find best practices or adaptation measures, which can improve transport processes under changing climate conditions.

Climate Projections and Scenario Design

Future climate development is based on using General Circulation Model (GCM) projections from the CMIP6 (Coupled Model Intercomparison Project Phase 6) dataset. Four Shared Socioeconomic Pathways (SSPs) were selected to capture different trajectories of global development:

SSP1: "Sustainability" – a pathway focusing on sustainable practices

SSP2: "Middle of the road" – environmental degradation offset by improvements in resource and energy efficiency

SSP3: "Regional rivalry" – limited economic development due to geopolitical fragmentation

SSP5: "Fossil-fueled development" – rapid economic growth driven by intensive use of fossil fuels

In parallel, four Representative Concentration Pathways (RCPs) were used to represent varying degrees of anthropogenic greenhouse gas and aerosol emissions:

RCP2.6 – Radiative forcing increase limited to 2.6 W/m² by 2100 (compared to 1750 levels)

RCP4.5 – Radiative forcing increases up to 4.5 W/m² by 2100

RCP7.0 – Radiative forcing increases up to 7.0 W/m² by 2100

RCP8.5 – Radiative forcing increases up to 8.5 W/m² by 2100

Seven GCMs were selected for modeling future scenarios. This selection is based on the recommendation from CzechGlobe scientists focusing on climate change and modelling of this phenomenon in the CEE region.

As a result of the modeling process, climate change scenarios up to 2100 were developed for the entire Zelivka test site, focusing on key meteorological variables. These included projections of air temperature, precipitation, relative humidity, solar radiation, and wind speed. The scenarios were derived from selected combinations of global circulation models (GCMs) and representative shared socioeconomic pathways and concentration pathways in line with the CMIP6 framework. These outputs serve as the foundation for assessing future hydrological responses and potential shifts in the water balance under different climate conditions.

Models related data

Data collection for the PHISHES project spanned an extended period, primarily due to the challenge of acquiring such a large and comprehensive dataset. A significant achievement of the project has been the establishment of strong collaborative relationships, not only with the Vltava River Basin Authority but also with the Research Institute for Soil and Water Conservation (VUMOP).

Although neither organization is a formal partner of the PHISHES project, their willingness to support the initiative has proven invaluable. Their contribution goes beyond mere consultation; it includes expert guidance, access to otherwise restricted land areas, and, most importantly, the provision of essential data along with formal consent for its use in the project. This level of cooperation has greatly enhanced the scope and quality of the research, enabled a more thorough understanding of the monitored systems and strengthened the overall impact of the PHISHES project.

The following is a basic list of the available data for the Martinicky creek basin:

- Weather related data
    - Precipitation
    - Radiation
    - Wind
    - Basic information about measuring instruments
- Hydrological data
    - Drainage system flow (for Cernici, A basin only)
    - Discharge
    - Water table level below surface
- Nitrogen deposition for Zelivka test site
- Management (Cernici, A basin only)
    - Fertilizer – type, dose, date of application etc.
    - Pesticides – type, dose, date of application etc.
    - Crop rotation with dates
- Pesticides in water

- Monitoring data from sampling
- Soil profile
  - Retention curves
  - Conductivity curves
  - Data from in situ measurement
- Soil chemistry
  - Nutrient data from sampling
- GIS data
  - Catchment borders
  - Drainage system, location, depth, capacity
  - Measuring station location
  - Land use
- Geodetic data
  - DTM
  - Rivers with cross section profiles

As already mentioned, the whole modelling concept in the Martinicky creek basin is based on the division into sub-basins. One of the main reasons for this division is the diversity in the quality and quantity of data for individual sub-basins. The following Table 3, in a simple form, shows the availability of each key data for the individual sub-basins.

Table 3 Data overview in Martinicky creek basin

Data category	Data description	Zelivka basin	Martinicky basin **E**	Martinicky sub-basin **E1**	Mohelnice sub-basin **D**	Suchy sub-basin **C**	Chyšná sub-basin **B**	Cernici sub-basin **A**
Data about basin	dtm	X	X	X	X	X	X	X
	land use	X	X	X	X	X	X	X
	drainage systems locations	X	X	X	X	X	X	X
	river network and reservoirs	X	X	X	X	X	X	X
meteorological data	base line time series	X	X	X				
	climate change 3x30 years	X	X	X	X	X	X	X
	short time series continous		X	X	X	X	X	X
Hydrological data	base line time series	X	X	X				
	short time series continous		X	X	X	X	X	X
Method of agricultural cultivation and crop rotation, protection	Agricultural cultivation					X	X	X
	Crop rotation					X	X	X
	Load of fertilisers					X	X	X
	Load of pesticides and herbicides					X	X	X
WQ data	point source data	X	X	X	X	X	X	X
	non point source data					X	X	X
	WQ monitoring long term 12/y	X	X					
	WQ monitoring short term continous			X	X	X	X	X
CC adaptation measures	Changes on arable land	X	X	X	X	X	X	X
	Changes in forested area	X	X	X	X	X	X	X

2.1.4. Additional – optional – monitoring within the project frame

Monitoring of Selected Substance Concentrations in the Martinicky creek and Cernici (A) Catchments

The state enterprise Povodí Vltavy s.p. has been conducting long-term monitoring of the occurrence of pesticidal, herbicidal, and other agricultural treatment substances at selected sites on

the watercourses within the Martinicky creek basin area (basin E). Sampling is performed using instantaneous grab samples 12 times per year (typically once per month, independent of the instantaneous flow rate). In the adjacent research micro-catchment of Cernici (basin A), managed by the Research Institute for Soil and Water Conservation, research sampling is carried out as dictated by the needs of ongoing projects, employing a combined approach: discrete samples are collected both regularly (approximately once per month) and during rainfall-runoff events in response to elevated flow rates. The scope of evaluated substance concentrations largely overlaps with the list of substances monitored in the Martinicky creek catchment.

In 2024, based on the indicative by CzechGlobe, VUMOP and Povodi Vltavy s.p., the sampling system was expanded at selected profiles of the Martinicky creek: namely Suchy creek, station Syrov, Martinicky creek, station Onsov and Mohelnice, station Kresin - to include automated WQ samplers. This enabled the capture of changes in substance concentrations during rainfall-runoff episodes.

In 2024, the occurrence of 33 substances (selected from a comprehensive list due to their repeated detection in previous years at the Senozaty profile and in some sub-catchments of the Martinicky Creek) was monitored and analyzed at five profiles within the Martinicky Creek area. For further, more detailed analysis, the profile (P1) from the neighboring Cernici catchment (basin A) will also be included.

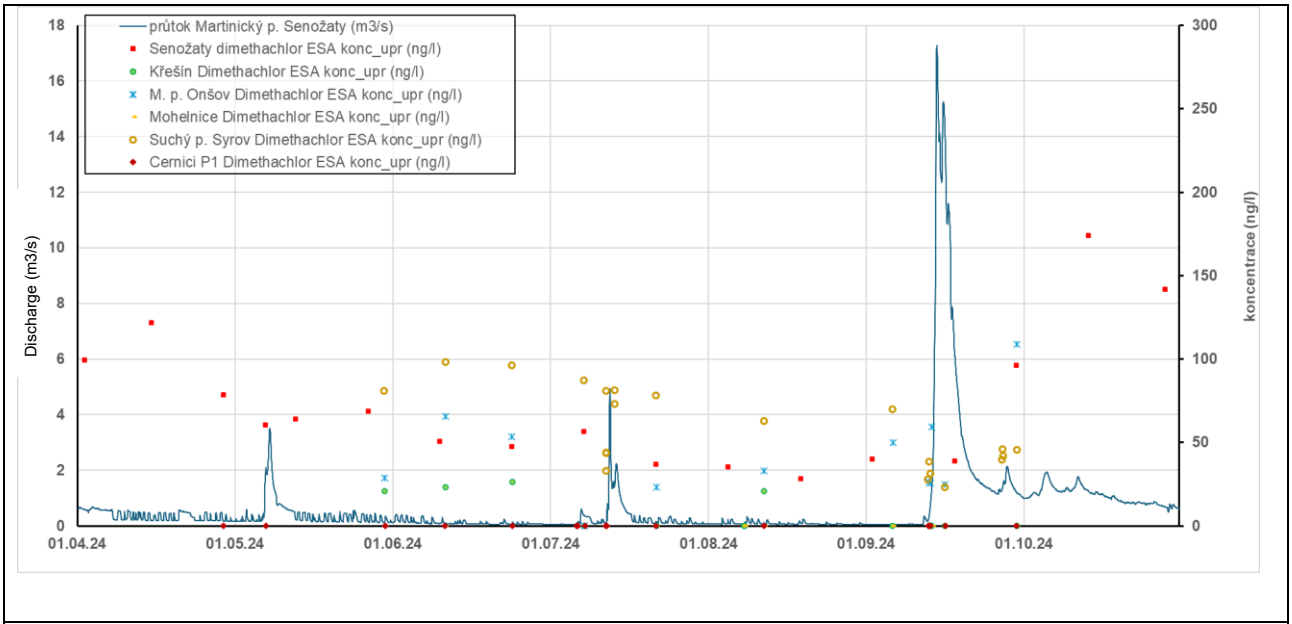


Figure 11 An Example of the results of sampling in Martinicky creek and concentration of some metabolites in the basin, year 2024 - left Y axis shows discharge, right concencration and X axis time. Blue line represents discharge at Senozaty station and colored points represent Dimethachlor (as an example) concentration at various sampling places along Martinicky creek.

2.1.5. Tools, model trains, scenarios expected to be employed or utilized

Healthy soil and its properties affect water quality parameters, both surface and groundwater. In the case of Zelivka basin this integrated process of movement of water is even more important, because a potable reservoir is located on the lower parts of the basin and all waters are collected from the basin itself. The modelling trains were selected carefully and consist of: MIKE SHE + ECOLAB and DAISY.

MIKE SHE: Integrated Hydrological and Water Quality Modeling

DHI's MIKE SHE is a powerful, physically based modeling platform that provides a comprehensive framework for simulating the entire land phase of the hydrological cycle. Its modular structure allows for the integrated simulation of surface water and groundwater systems, making it a

valuable tool for a wide range of water resource management and environmental applications. This technical overview delves into the core modules of MIKE SHE for hydrological parameter simulation, its advanced capabilities for addressing water quality issues, and the practical application of the software for water quantity and quality mass balance assessments.

Hydrological Modules

At its core, MIKE SHE is designed to simulate the intricate movement of water through the various components of a watershed. This is achieved through a suite of interconnected modules that represent the key hydrological processes:

- Overland Flow (OL): This module simulates the flow of water across the land surface, typically using a 2D finite difference grid. It accounts for factors like surface roughness, topography, and the exchange of water with other components, such as rivers and the unsaturated zone. This is crucial for understanding surface runoff generation and flood dynamics.
- Unsaturated Zone (UZ): The UZ module models the movement of water in the soil layer between the land surface and the groundwater table. It can employ various methods, from simple water balance approaches to the more complex, physically based Richards's equation, to simulate infiltration, evapotranspiration, and deep percolation to the saturated zone.
- Saturated Zone (SZ) / Groundwater: This module simulates the flow of water within the aquifer system. It is a fully 3D finite difference model that can handle complex hydrogeological settings, including multiple aquifers and aquitards. It is essential for assessing groundwater resources, well capture zones, and the interaction between groundwater and surface water bodies.
- Channel Flow (CF): River and channel networks are simulated using the integrated 1D hydrodynamic model, MIKE HYDRO River (formerly MIKE 11). This module calculates flow, water levels, and can simulate various hydraulic structures like weirs, culverts, and bridges. The dynamic coupling with the other modules allows for a realistic representation of river-groundwater interactions, floodplains, and the overall basin hydrology.
- Evapotranspiration (ET): This module calculates the loss of water from land and water surfaces to the atmosphere. It can utilize various methods, from simple empirical equations to more data-intensive, physically based approaches that account for vegetation type and soil moisture conditions.

The WQ Module, Advection-Dispersion, and MIKE ECO Lab

Beyond water quantity, MIKE SHE offers robust capabilities for simulating the fate and transport of contaminants and other water quality constituents. The primary tool for this is the Water Quality (WQ) module, which is fundamentally based on the Advection-Dispersion (AD) equation. This allows for the simulation of the movement of dissolved substances in both the surface and subsurface domains. The AD module accounts for:

- Advection: The transport of solutes with the bulk movement of water.
- Dispersion: The spreading of solutes due to variations in flow velocity and molecular diffusion.

This standard AD functionality is suitable for modeling conservative tracers and simple, first order decay processes.

For more complex water quality issues involving multiple interacting species, biogeochemical transformations, and ecological processes, MIKE SHE can be dynamically coupled with MIKE ECO Lab. MIKE ECO Lab is a flexible and powerful numerical laboratory for defining and simulating aquatic ecosystem models. It allows users to define their own water quality models by specifying the

state variables, transformation processes, and kinetic reaction rates. This opens the door to simulating a wide range of complex phenomena, including:

- Nutrient cycling: Simulating the fate of nitrogen and phosphorus species.
- Contaminant fate and transport: Including processes like sorption, biodegradation, and chemical transformations.
- Heavy metal transport
- Metabolites transport

The integration with MIKE ECO Lab allows for a holistic approach to catchment management, where the hydrological model provides transport pathways and water fluxes, and MIKE ECO Lab simulates the biogeochemical reactions occurring within the water.

Furthermore, as part of the PHISHES project, a new two-way coupled dynamic vegetation module for MIKE SHE is planned to be developed, utilizing the capabilities of MIKE ECO Lab. The integration of MIKE SHE and MIKE ECO Lab will form a model train designed for application in the Zelivka basin.

Mass Balance Assessments

The integrated nature of MIKE SHE makes it an ideal tool for performing detailed water quantity and water quality mass balance assessments at the catchment scale.

Water Quantity Mass Balance

By simulating all the major components of the hydrological cycle, MIKE SHE provides a comprehensive water balance for any defined control volume (e.g., a sub-catchment, an aquifer, or the entire basin). The model outputs detailed information on all the fluxes in and out of the system, including:

- Inputs: Precipitation, irrigation, climate parameters.
- Outputs: Evapotranspiration, surface runoff to rivers, groundwater recharge, and discharge to rivers (baseflow).
- Changes in Storage: In the snowpack, soil moisture, and groundwater.

This detailed water balance is crucial for:

- Water resource assessment: Quantifying available surface and groundwater resources.
- Impact assessment: Evaluating the effects of land-use change, climate change, or new water management strategies on the water balance.
- Model calibration and validation: Ensuring the model accurately represents the hydrological processes in the catchment.

To perform a water quantity mass balance in MIKE SHE, users can extract the time-series or spatially distributed results for each hydrological component and sum the fluxes over a specified period. The model output files provide a detailed breakdown of these components.

Water Quality Mass Balance

Similarly, when the WQ module and/or MIKE ECO Lab are utilized, MIKE SHE can perform a mass balance for any simulated water quality constituent. This involves tracking the inputs, outputs, and transformations of the substance throughout the model domain. A water quality mass balance can account for:

- Inputs**:** Point sources (e.g., wastewater treatment plant outfalls) and non-point sources (e.g., agricultural runoff).
- Transport: Advection and dispersion in overland flow, rivers, and groundwater.
- Transformations: Decay, degradation, and biogeochemical reactions simulated by MIKE ECO Lab.
- Outputs: The mass of the constituent leaving the catchment via the river network or other defined boundaries.
- Changes in Storage: The mass of the constituent stored in the soil, groundwater, or river channel.

This capability is invaluable for:

- Pollution source apportionment: Identifying the major sources of contamination in a catchment.
- Evaluating best management practices (BMPs): Assessing the effectiveness of measures to reduce pollutant loads.
- Total Maximum Daily Load (TMDL) development: Determining the maximum amount of a pollutant that a waterbody can receive and still meet water quality standards.

To conduct a water quality mass balance, users need to define the sources of the constituent, specify the relevant transport and reaction parameters, and then analyze the model outputs for fluxes and concentrations in the different hydrological compartments. The detailed output from the WQ and MIKE ECO Lab modules provides the necessary data to quantify the fate and transport of the substance and construct a comprehensive mass balance.

In conclusion, MIKE SHE's integrated and physically based approach provides a robust platform for simulating both the quantity and quality of water resources within a catchment. Its modular design, coupled with the advanced capabilities of the WQ module and MIKE ECO Lab, empowers water managers and scientists to address a wide array of complex hydrological and environmental challenges.

Daisy Agro-Ecosystem Model

The Daisy model, developed at the University of Copenhagen, is a process-oriented, one-dimensional simulation model designed to analyze the intricate dynamics of agro-ecosystems. It operates on a daily time step and simulates the physical, chemical, and biological processes occurring within the soil profile and the crop canopy. Its primary application is to study the fate of water and nutrients (particularly nitrogen) in agricultural systems under various management scenarios.

The model is structured in a modular fashion, with a central "manager" that calls upon specialized sub-modules to simulate different processes. The core of the model revolves around the simulation of soil water dynamics, which directly influences almost all other processes.

Module for Soil Water Simulation

The simulation of water movement in the soil is the engine of the Daisy model. It is handled by a sophisticated physics-based module that solves water flow in a variably saturated porous medium.

- Governing Equation: The vertical, one-dimensional movement of water in the soil profile is described by the Richards equation

- Soil Hydraulic Properties: To solve the Richards equation, the model requires the soil's hydraulic properties, which define the relationship between water content, pressure head, and hydraulic conductivity. Daisy primarily uses the Mualem-van Genuchten functions
- Numerical Solution: The soil profile is discretized into a finite number of layers (typically 10-50), and the Richards equation is solved numerically using a finite difference scheme.
- Boundary Conditions:
    - Upper Boundary (Surface): Flux is governed by precipitation, irrigation, and potential evapotranspiration. The model computes actual evaporation from surface moisture and allocates remaining ET to crop transpiration. Excess water beyond infiltration capacity becomes surface runoff.
    - Lower Boundary: User-defined options include free drainage, zero flux (impermeable layer), or fixed/fluctuating groundwater table.

Modules for Simulating Dynamic Soil Properties

The term "soil properties" in the context of Daisy refers not just to static parameters like texture, but to the dynamic properties that change over time, primarily soil temperature and biogeochemical composition.

Soil Temperature Module:

This module simulates soil thermal dynamics by solving the heat conduction equation. Daily temperatures are calculated for each soil layer based on surface energy input (affected by air temperature and vegetation) and soil thermal properties, which depend on moisture content from the water module. Soil temperature is vital for crop growth, root function, and microbial activity.

Soil Organic Matter (SOM) and Nitrogen Cycling Module:

One of Daisy's core features is simulating carbon and nitrogen cycling through conceptual pools and key soil processes.

Pools:

- Added Organic Matter (AOM): Fresh inputs like crop residues or manure, split by decomposition rate.
- Soil Microbial Biomass (SMB): Active microbes decomposing organic matter.
- Soil Organic Matter (SOM): Stabilized matter, divided into fast (labile) and slow (resistant) pools.

Processes:

- Decomposition & Mineralization: SMB decomposes AOM and SOM, releasing ammonium (NH_4^+).
- Immobilization: Microbes absorb NH_4^+ for growth.
- Nitrification: $NH_4^+ \rightarrow NO_2^- \rightarrow NO_3^-$ under aerobic conditions.
- Denitrification: $NO_3^- \rightarrow N_2O/N_2$ under anaerobic conditions.

Process rates depend on soil temperature (heat module) and moisture (water module).

Solute Transport Module:

This module simulates the movement of dissolved substances, primarily nitrate (NO_3^-) and ammonium (NH_4^+), through the soil profile.

- Governing Equation: one-dimensional Advection-Dispersion Equation (ADE).
- Integration:
  - Water flux (q) comes from the Richards equation.
  - Source/sink terms (Φ) are supplied by the nitrogen cycling and crop modules (e.g., nitrification, root uptake).
  - This strong coupling enables realistic simulation of key processes like nitrate leaching.

In summary, Daisy provides a powerful, vertically integrated framework where soil water simulation form the foundation upon which dynamic soil properties like temperature and nutrient concentrations are built. The interplay between the water, heat, and biogeochemical modules allows for a detailed and mechanistic investigation of soil-plant-atmosphere interactions in agricultural settings

Scenarios for application of model trains in the cascade of experimental field sites – sub-catchment of the River Zelivka basin

The modelling trains will be used in pre-agreed sets of scenarios, which are schematized in Table 4.

Table 4 Scenarios on the River Zelivka Basin – cascades of experimental sites – broad overview and preliminary scenarios set-up, where "x" indicates the scenario is considered relevant and is planned to be addressed within the given test case, and "o" indicates the scenario is not planned for that test case or is lower priority, for example because it is not relevant to the site, the required data are not available, or the respective modelling approach is not applicable.

		Measures											
		No measures	Spatial reduction in agricultural activity	Shift to conservational agriculture	Shift to no-till agriculture	Permament soil organic cover	Crop rotation and diversification (more legumes)	Decrease pesticide usage	Shift to conservational agriculture x Spatial reduction in agricultural activity	Increased water retention through modification of landuse	Increased water retention through modification of landuse x Spatial reduction in agricultural activity	Increased water retention through modification of landuse x Conservational agriculture	Increased water retention through modification of landuse x Spatial reduction in agricultural activity x Conservational agriculture
Drivers	Baseline (curent situation)	x	x	x	x	x	x	x	x	x	o	o	o
	Climate scenario SSP1-2.6	x	x	x	o	o	o	x	x	x	o	o	o
	Climate scenario SSP5-8.5	x	x	x	o	o	o	x	x	x	o	o	o

2.1.6. Activities executed on site up to date

Main activities carried out at the Zelivka test site within the PHISHES project have been described in previous chapters. Therefore, only a summary of the individual activities is given here.

- Collecting of all relevant data for Martinicky creek catchment and its sub-catchment, including water quality data

- Collecting rich data from experimental micro catchment Cernici (A), including water quality data and agro-management data. Essential part of this sub-task was to deepen cooperation with the research organization VUMOP, as owner of the A basin and its data
- Development, calibration and validation of the MIKE SHE models for Martinicky creek and its sub-catchments
- Adding water quality (Advection-Dispersion) module to the hydrology models
- Identification of source pollution and first basic WQ simulations for the A catchment
- Preparation and handover of data needed for development of DAISY model on the A catchment
- Setting up new measuring stations and processing the first measured data

Short description of Daisy model setup and data used during first year is described below. For a more detailed description please refer to Deliverable 3.1.

Subcatchment Cernici– Daisy Model Setup and Preliminary Results (1st year)

The Cernici (A) catchment (1.4 km²) consists of approximately four agricultural fields with crop rotations managed by two farmers. Soil data is available for multiple profiles in three of the fields. Daisy models will be established for 2–3 profiles in these fields, as well as one model representing the low-lying parts of the catchment with permanent grass, if management data for the grasslands becomes available. The upper part of the catchment is dominated by forest, which is outside Daisy's modelling scope and is therefore not represented.

For now (Year 1), three 1-dimensional models with a soil simulation depth of 0–200 cm have been established using soil data from profiles representing the upper, middle, and lower parts of field, respectively.

The Daisy models simulate water, nitrogen (N), carbon (C), and pesticide dynamics over a 12-year period (2012–2024), driven by measured weather data (weather station S2 in Cernici and Kosetice weather tower) and management practices reconstructed from farmer records.

An overview of the model inputs and setup is provided below, along with highlights of the preliminary results. For detailed information on model setup, input choices, and results, please refer to Deliverable 3.1.

Model Inputs and Setup

- Weather Data: Combined local measurements (precipitation, air temperature and reference evaporation from Cernici station and regional data (global radiation) from the Kosetice weather tower (~5 km away) were used. Precipitation was corrected using monthly factors from the Myjava weather station (Slovakia). Nitrogen deposition data is based on older measurements (1993–1994) from Kosetice and should ideally be updated.
- Soil Data: Profiles were parameterized using measured texture, organic carbon, bulk density, and hydraulic conductivity. Hypres pedotransfer functions were used for hydraulic properties. The properties of the lowest measured horizons was extent to represent the soil down to 200 cm depth.
- Management: Crop rotations, fertilization, and pesticide applications were reconstructed from farmer records. Fertilizers and agrotechnical operations were parameterized using Daisy defaults and parameterizations established as part of the FertOrgaNic Eu project, also modelling Czech agriculture.

- Pesticides: Bentazone was selected for initial pesticide simulations due to its repeated application (spring 2018–2021) and frequent detection in drain (S2) and surface water (P1). In addition is the formation and fate of the metabolite N-methyl bentazone simulated.

Preliminary Results

- Crop Yields: During the simulation period, winter wheat, maize, winter rape, peas, and winter barley were grown. Simulated dry matter and N yields varied across profiles and years. Yields appear reasonable, except for maize, which may require parameter adjustment. A comparison with measured or average yields in the Czech Republic should be carried out.
- Water Balance: Annual average corrected precipitation was 568 mm. Simulated annual average actual evapotranspiration ranged from 430–448 mm, highest in the lower profile (1645). Annual average percolation was 137 mm and 116 mm in the upper (1640) and middle (1641) profiles, respectively, both simulated with free drainage. The lower profile (1645), simulated with an aquitard and a drain at 110 cm depth, showed only 21 mm percolation to groundwater and 85 mm drain flow annually.
- Nitrogen Dynamics: Average annual N input was ~266 kg N ha^{-1} (mineral, organic, and deposition). Simulated average annual downwards N leaching was 14, 67 and 94 kg N ha^{-1} for the lower, middle and upper part, respectively. Drain leaching in the lower profile averaged 35 kg N ha^{-1}. Simulated N_2O emissions ranged from 6–8 kg N ha^{-1} annually.
- Carbon Dynamics: Total soil carbon varied between profiles, with the lowest content in the lower profile (1645), reflecting measured values. Both total soil carbon and microbial biomass carbon showed temporal variation linked to management and weather. Microbial biomass carbon dynamics can serve as a proxy for soil health.
- Pesticide Fate: Bentazone leaching was simulated for all three profiles following application, with the highest concentrations occurring during the winter months. In the lower profile, downward leaching was minimal (maximum annual average: 3.2 g ha^{-1}), as most of the leached Bentazone exited the soil profile via drainage (maximum annual average: 24 g ha^{-1}). Decomposition accounted for the majority of pesticide loss in all profiles (203-653 g ha^{-1} in the years of application, 2018-2021). Between 11–45 g ha^{-1} of the metabolite N-methyl bentazone was formed from Bentazone degradation in the years of application. Of this, the majority (18–29 g ha^{-1}) was further decomposed, and no leaching, neither downward nor via drains, was simulated.

2.1.7. Planned activities for the upcoming period

The CzechGlobe team plans to continue the activities that started in the previous period. The main effort, in the modelling part of the project, will be directed at completion, calibration and validation of the WQ models on all watersheds within the Zelivka test site. There should be enough measured and collected data to build "simple" qualitative models on most of the test sub-catchments. The detailed data from micro-catchment A (Cernici) will also allow for the construction of a Daisy growth model that will be linked to the hydrological and water quality model constructed in the MIKE SHE environment for the same A basin.

Another important task is to maintain all previously established measuring stations, check the quality of measurements, and evaluate the measured values. This task, simple as it may seem, requires sufficient time and flexibility. Flood discharges on such small creeks are often tens to hundreds of times the normal discharges and pose a threat to these small gauging stations and their equipment.

One of the challenges in the upcoming period is the establishment and operation of an experimental biofilter at the B basin (Chysna). Along with this biofilter, new measurements will be

installed at the inlet and the outlet of the biofilter in order to obtain, if possible, relevant data to evaluate the effectiveness of this measure on improving water quality on the small creeks.

Finally, in the upcoming period, the focus will be on trying to establish clear connections between soil management changes and their impacts on specific soil functions and services (e.g., water quality, runoff).

2.2. River Koprzywianka (PL)

The studies on hydrologic aspects and water quality of the Koprzywianka river were envisaged due to mainly drought and water shortage issues in the wide regions of southern Poland. Water balance analyses became a basis for any activities to be planned there, in particular groundwater abstractions and irrigation for agriculture. On the other hand, a scientific interest was developed into that catchment due to complex nature of hydrodynamic and hydro structural conditions, nonuniform aquifer setting and variable surface water- groundwater interactions. All these issues also incorporate surface water quality as shaped by current use of groundwater resources for potable water production, irrigation requirements and the mining industry. Koprzywianka was selected as one of the pilot basins for high priority drought threats, included into State Drought Mitigation Plans of Poland. The case study of significant hydrogeological complexity, and on the other hand, a variety of possible measures to increase soil water retention, create an ideal situation for it to be one of the core basins for application of integrated hydrologic modelling. One of the most emerging problems is the management of land cover and soil in such a way that their functions remain supported and can sustain soil health.

2.2.1. Purpose of the sites within the PHISHES project

The main goals of the project studies on Koprzywianka river involve:

1) Overall impacts of point source and aerial pollution in the river basin on the current situation considering baseline time series;

2) Impact of adaptation measures related to soil treatment, improvements in soil condition, and changes in agricultural practices, as well as the impact of adaptation measures on the ecocycle;

3) Mitigation strategies for heavy metal concentrations in particular, which are monitored in the streams by the Water Authority at their gauging stations of the regular monitoring network;

The main research challenge becomes the capacity of an improved MIKE ECO Lab module in the MIKE SHE model to simulate heavy metals leaching from soils.

2.2.2. Description of the basin/site

The River Koprzywianka basin is a typical agricultural landscape without any special arrangement. The land-use in the basin can be characterized as typical, regular agricultural one. The area is located in the south-eastern part of Poland, in the southern part of the Swietokrzyskie Voivodship. The prevailing land use forms involve rural areas: arable land and grasslands – around 50% of the catchment area, orchards – approximately 25 %, and forests – approximately 15%. The River Koprzywianka is a left tributary of the Vistula of the II order, 65.9 km long and with a catchment area of 707 km^2 and mean slope of 3.3‰.

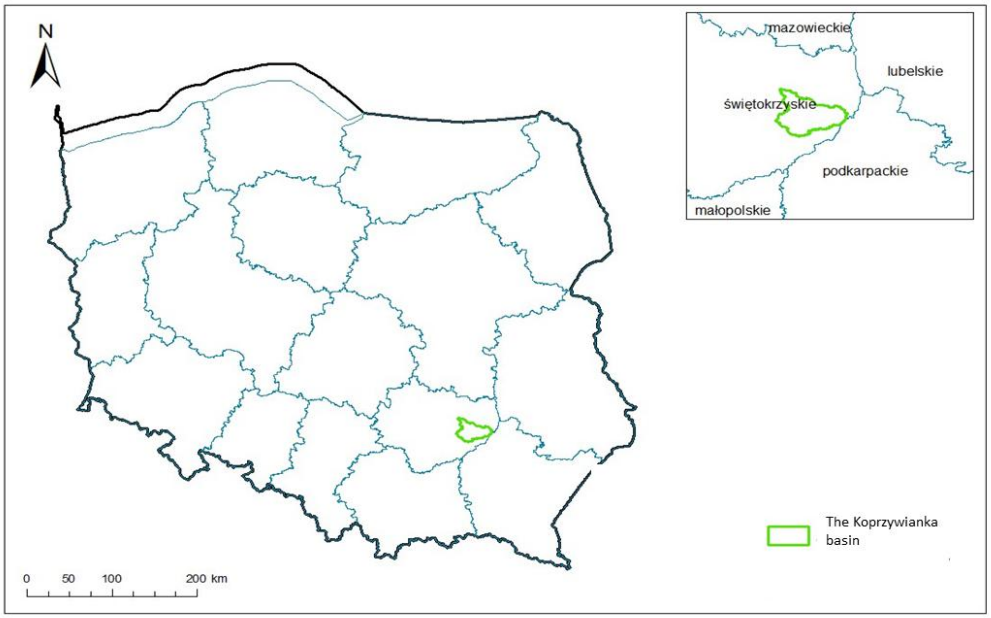


Figure 12 Location of Koprzywianka catchment within Poland territory

Most of the watershed area is characterized by hilly landscapes. The average slopes of the land range from 15% to 30% and induce a high or moderate erosion susceptibility. Average elevations range from 200 to 300 m above sea level (67% of the total area). Areas higher than 300 m above sea level (about 12% of the total) are found only in the Swietokrzyskie Mountains. Areas below 200 m above sea level (21% of the total) lie in the lower parts of river valleys and at the confluence with the Vistula. The highest points are located in the Main Range of the Swietokrzyskie Mountains - about 554 m above sea level. The lowest points are at the confluence of Koprzywianka with the Vistula - 141 m above sea level.

The hydrogeological conditions in this area are complex due to the varied geological structure. Five usable aquifer levels have been identified in the area, which occur in fragments and are often not hydraulically connected. These are the levels (from the surface):

Table 5 Aquifer system within Koprzywianka basin

Aquifer stratigraphy	Lithology	Thickness [m]	Hydraulic conductivity [m/day]
Quaternary	sands, sandy gravels and gravels	5 —35	0.003 — 0.36
Neogene (Tertiary)	limestones, marls, sandstones, and sands	10 —100	0.005 — 1.0
Cretaceous	upper chalk marls with a fissured structure	80 —100	0.003 — 0.40
Jurassic	limestones and marls with a fissured-karst structure	70 —150	0.001 — 0.35
Triassic	Middle Triassic limestones with a fissured-karst structure	80 —150	0.003 — 0.20

In the area of the Koprzywianka catchment there are the most fertile soils in the country. The dominant types are fertile brown and chernozem (about 40% of the catchment area). Locally, there are brown soils formed on glacial clays, rendzina on carbonate rocks and riverine heavy clays (developed mainly from loess and loess formations) - in river valleys. Loess and alluvials are part of the highest quality classes, they are characterized by good physical and chemical properties: permeability, water absorption, water capacity and abundance in macro- and microelements.

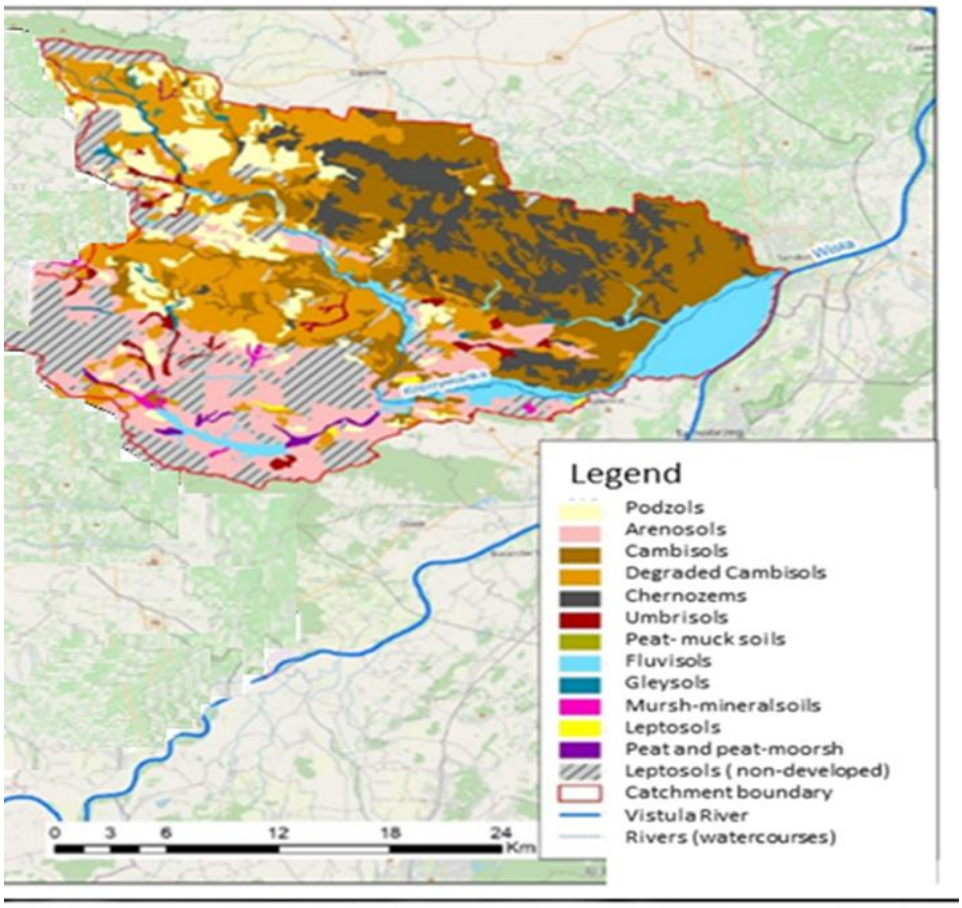


Figure 13 Soil types in the Koprzywianka catchment

The main factors that define the soil cover in the studied watersheds are the variations in terrain and lithogenetic conditions. On the flat elevated surfaces of the area (especially in the Koprzywianka watershed), typical brown soils, leached brown soils, acidic soils, and chernozems have developed (Figure 13). On the moderately sloping deluvial slopes of the highlands the Podzols and pseudopodzolic soils (pale soils) as well as sandy soils of various genetic types have developed. The bedrock materials of these soils are sandy deposits with different grain size compositions.

The main land uses in the area are orchards, grass and arable land, forests and bushes (Figure 14). Dominant sources of pollution in the Koprzywianka catchment include runoff from areas used for cultivation and domestic wastewater from municipal treatment plants. In addition, the susceptibility of soils to erosion causes pollution. Old excavations and mining areas are also considered potential pollution sources.

According to data from the Institute of Meteorology and Water Management in Poland for the years 1991-2020, the climatic parameters in the catchment area were as follows: average temperature in January: -3 – -1°C, average temperature in July: 19-20°C, average annual temperature: 8-10°C, average annual precipitation: 500-650 mm, average annual sunshine duration: 1800-1850 hours, average number of days with snow cover: about 65.

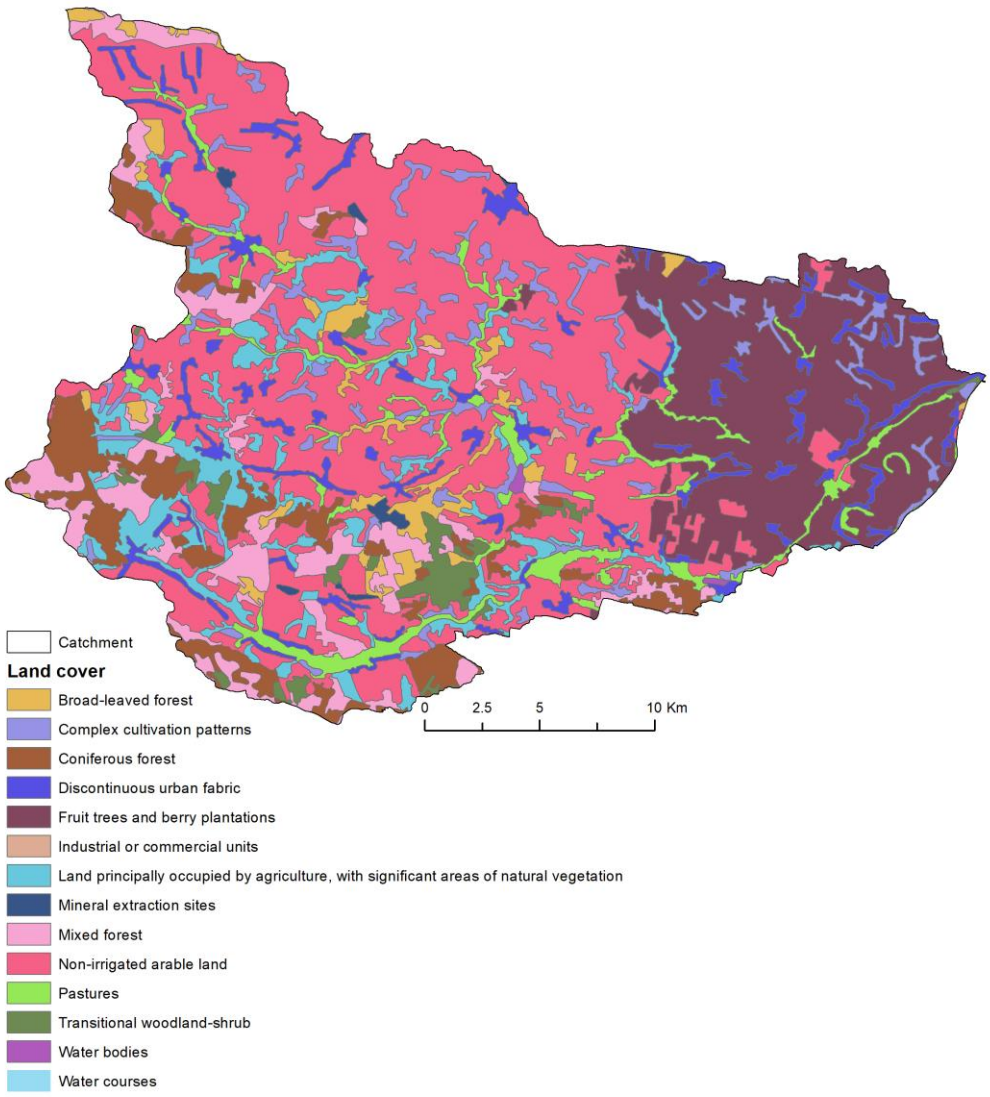


Figure 14 Land use classes of Koprzywianka catchment.

2.2.3. Existing data available

The available data for the Koprzywianka river was compiled for the needs of the primary Polish planning document relating to the phenomenon of drought. It was called the 'Drought Impact Mitigation Plan', adopted under the regulation of the Polish Ministry of Infrastructure on July 15, 2021. Another significant document with a similar theme and scope is the 'Water Shortage Counteraction Program', which is to be adopted as part of a resolution by the Council of Polish Ministers. The sets of actions detailed in both documents were created as a result of a global analysis of the availability of water resources and retention on a national scale, considering the range of actions proposed in numerous preceding documents and plans developed for Koprzywianka at the national Water Management Plans and Flood Risk Management Plans.

Neither of the documents contain detailed analysis of measures on a local level but provide a framework for the determination and implementation of relevant measures to improve drought resiliency and water quality Special emphasis was placed on searching for optimal solutions for agriculture, involving soil protection through proper dosage of fertilizers and pesticides in orchards and arable lands.

All data utilized for soil pollution estimation and modelling in the Koprzywianka catchment are available from the following sources:

- Numerical Terrain Model (NTM) Numeric Terrain Model with a resolution of 1 m 2017-2019 Main Bureau of Geodesy in Poland,
- Geological and hydrogeological data Datasets from CBDG - Central Geological Database (borehole cards, location data, etc.) 1985-2022 Polish Geological Service, Datasets from CBDH - Central Hydrogeological Database (groundwater level reports, performance reports, etc.) 1985-2022 Polish Geological Service Datasets on Main Groundwater Reservoirs status in 2022.
- Data on Uniform parts of surface waters status – Hydrographic Map of Poland 2022
- Data on groundwater levels and chemistry monitoring 1985-2022, Polish Geological Institute
- Hydrogeological Map of Poland at a scale of 1:50,000 1996-2018 Polish Geological Institute
- Detailed Geological Map of Poland, 1956-2009 Polish Geological Institute, Lithogenetic Map of Poland 2006-2022, Data on groundwater extraction 2005-2022.
- Meteorological Measurement data (precipitation, temperature, sunshine, etc.) from rain, synoptic, and climate stations 1985-2022, Polish Institute of Meteorology and Water Management
- Hydrological data and Measurement data on water levels and flow rates at gauging stations within the catchment area 1985-2022, Polish Institute of Meteorology and Water Management
- Hydrological models MIKE 11 (MIKE Hydro River) implemented in the projects 2014-2022 of National Water Management Authority in Poland, Hydrographic Division Map of Poland, Retention action program as part of flood risk management in the Upper Vistula and Upper Eastern Vistula region
- Soil data: Spatial database of soil data 2022- Polish Institute of Fertilization and Soil Science
- Water use data (discharges and abstractions) Identification of pressures in water regions and basins (Part I - 2017, Part II - 2018) National Water Management Authority Water in Poland
- Data on selected water quality indicators of Koprzywianka river from the State Monitoring of Poland and the research by polish universities, conducted on a weekly and biweekly basis in years 1991-2024 including: Total Phosphorus, Phosphates, Total Nitrogen, Ammonia, Nitrites, Nitrates, Arsenic, Nickel, Cadmium, Zinc, Mercury and Aluminum.

2.2.4. Additional – optional – monitoring within the project frame

Three monitoring points were established in the basin for water level, discharge rates and water quality parameters recording (Figure 15):

1) at a catchment - closing gauge

2) the other gauge on the main river in the center of the catchment

3) on a side river (ditch of around 80 km^2 catchment area)

At those points the monitoring of water quality was started in October 2024, and it is expected to continue it for at least two years (October 2024 - October 2026) with the sampling frequency of 4 days on average and with special emphasis on high water periods. As already indicated, the other aim is to control the concentrations in total suspended substance, not only in a dissolved form, including: Total Phosphorus, Phosphates, Total Nitrogen, Ammonia, Nitrites, Nitrates, Arsenic, Nickel, Cadmium, Zinc, and Aluminum. At the same time, the water level and discharge recording and climatic data (precipitation, air temperature, air relative humidity, wind speed and solar radiation) will be downloaded from automatic stations. All the collected data will serve to better understand the mechanisms of metal leaching from the soil in various conditions.

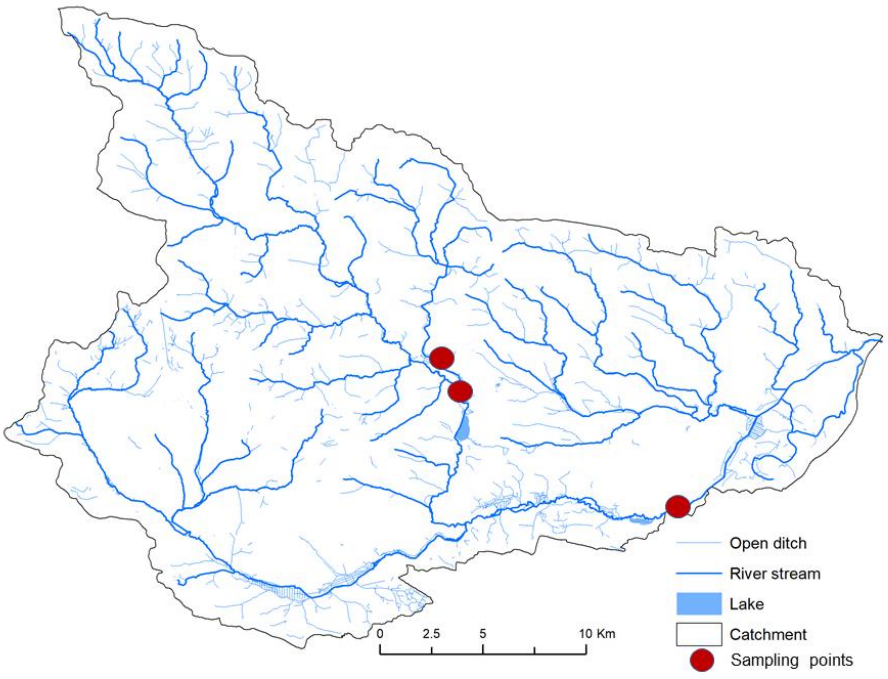


Figure 15 Water sampling and gauging points.

The water quality indicators will be analyzed at the laboratory of the Faculty of Civil and Environmental Engineering of Warsaw University of Life Sciences and also at a state-owned Environmental Inspectorate Laboratory in Warsaw. In case of more frequent measurement campaigns, possibly at a span of less than four days (1-2 days), due to a higher number of samples it is also foreseen to use the laboratories of Mineral and Metallurgical Academy in Poland.

2.2.5. Tools, model trains, scenarios expected to be employed or utilized

MIKE SHE: Integrated Hydrological and Water Quality Modeling framework was selected for the development of the Koprzywianka catchment model. The data used in the model, as was already mentioned, included:

- the topography of the land surface considering its anthropogenic transformations,
- bedrock maps and charts of hydraulic conductivity of distinguished computational layers,
- river and ditch routes, data on channel geometry, gauging data,
- location and parameters of drains affecting the amount of drained water,
- time-variable precipitation and potential evaporation,
- time-dependent parameters of vegetation affecting evapotranspiration,
- time-variant volumes of water intake/discharge,
- parameters of the unsaturated zone affecting flows: retention curves and relationships between moisture and hydraulic conductivity for different types of soils present in the model area.

DHI's MIKE SHE is a physically based modeling platform that provides a comprehensive framework for simulating the entire land phase of the hydrological cycle. Its modular structure enables integrated simulation of surface water and groundwater systems, providing a valuable tool for a wide range of water resource management and environmental problems.

Hydrological Modules

At its core, MIKE SHE is designed to simulate the intricate movement of water through the various components of a watershed. This is achieved through a suite of interconnected modules that represent the key hydrological processes:

- Overland Flow (OL): This module simulates the flow of water across the land surface, typically using a 2D finite difference grid. It accounts for factors like surface roughness, topography, and the exchange of water with other components, such as rivers and the unsaturated zone. This is crucial for understanding surface runoff generation and flood dynamics.
- Unsaturated Zone (UZ): The UZ module models the movement of water in the soil layer between the land surface and the groundwater table. It can employ various methods, from simple water balance approaches to the more complex, physically based Richards's equation, to simulate infiltration, evapotranspiration, and deep percolation to the saturated zone.
- Saturated Zone (SZ) / Groundwater: This module simulates the flow of water within the aquifer system. It is a fully 3D finite difference model that can handle complex hydrogeological settings, including multiple aquifers and aquitards. It is essential for assessing groundwater resources, well capture zones, and the interaction between groundwater and surface water bodies.
- Channel Flow (CF): River and channel networks are simulated using the integrated 1D hydrodynamic model, MIKE HYDRO River (formerly MIKE 11). This module calculates flow, water levels, and can simulate various hydraulic structures like weirs, culverts, and bridges. The dynamic coupling with the other modules allows for a realistic representation of river-groundwater interactions, floodplains, and the overall basin hydrology.
- Evapotranspiration (ET): This module calculates the loss of water from land and water surfaces to the atmosphere. It can utilize various methods, from simple empirical equations to more data-intensive, physically based approaches that account for vegetation type and soil moisture conditions.

The WQ Module, Advection-Dispersion, and MIKE ECO Lab

Beyond water quantity, MIKE SHE offers capabilities for simulating the fate and transport of contaminants and other water quality constituents. The primary tool for this is the Water Quality (WQ) module, which is fundamentally based on the Advection-Dispersion (AD) equation. This allows for the simulation of the movement of dissolved substances in surface and subsurface domains. The AD module accounts for:

- Advection: The transport of solutes with the bulk movement of water.
- Dispersion: The spreading of solutes due to variations in flow velocity and molecular diffusion.

For more complex water quality issues MIKE SHE can be coupled with MIKE ECO Lab. This is a flexible tool for defining and simulating aquatic ecosystem models. It permits users to define own water quality models by specifying the state variables, transformation processes, and kinetic reaction rates. The EcoLab module for the Koprzywianka basin will be applied for a better insight in plant species impact on heavy metals mobility in soils and the significance of groundwater table fluctuations to their leaching.

2.2.6. Activities executed on site up to date

A MIKE SHE model was developed and calibrated for the catchment of Koprzywianka river as part of the Polish, national drought mitigation plans and projects to counteract water shortages. In this respect a range of measures was proposed, and their effectiveness was examined by means of the applied model. Technical actions to increase retention in the catchment area included partial restoration of the river channel- revitalization of the floodplains and meanders, increasing channel

retention by repairing existing weirs. Preliminary analysis showed that the scope of these actions is too small and localized to have an impact on the hydrodynamic conditions of the catchments where these actions are proposed. They can only increase channel retention locally. To achieve a noticeable effect, continuous riverbed revitalization has been proposed. In the model, the effect of revitalization was obtained by manipulating roughness coefficients in the riverbed. The recommended direction for renaturation may be to restore meanders in this section. From the perspective of hydrological processes, it is expected that the speed of water will slow down and increase surface water flow in the riverbed, as well as greater exchange with groundwater in floodplain areas along the riverbed. In the model, this effect was achieved by changing the roughness coefficient in the channel from n=0.035 (earth, silt) to n=0.1 (channel with riparian vegetation). Additionally, the flow between the channel and the groundwater in the surrounding cells was modified to unrestricted conditions, simulating the absence of channel embankment in reality. Simulations of the impact of these actions were conducted for the period from January 1, 1986, to June 29, 2009. From the long-term water balance, it can be inferred that the exchange between groundwater and surface water in the riverbed has changed. The total amount of water flowing into the riverbed has decreased by about 35% due to the increased amount of water replenishing groundwater resources, which seeps from the riverbed into the surroundings. Part of this water moves through floodplain areas, while another part is used by vegetation along the riverbed for evapotranspiration. The absolute amounts of stored water are rather small (a few mm per year) and are distributed evenly along the riverbed, thus no specific areas showing noticeable changes in groundwater levels have been defined.

In addition to the scenario analyses, mainly related to water shortage issues, current activities in the catchment involved the determination of water quality sampling points, gathering all historical records of water quality data, downloading the data from existing network of hydrometeorological stations and preparations for discharge measurements at gauging cross-sections. Furthermore, the considerations with the Polish Water Authorities were carried on, regarding the elaborated hydrological model and possible scenarios for the catchment from the perspective of local users and governments.

2.2.7. Planned activities for the upcoming period

The monitoring of surface water quality at three locations will be continued in the upcoming period. It is particularly important to capture relationships between the water levels, discharge rates and pollutants (mainly heavy metals) concentrations. Empasis is laid on high water events to determine the moments of peak concentrations of analysed pollutants.

Additional monitoring points are being considered, particularly in the vicinity of mining sites and exploitation areas so as to capture the difference in metals concentrations in waters in the direct vicinity of these industrial locations. Relating to this issue, the discussions with local authorities would be helpful to better understand and cover all “hot-spots” of pollutants emission to soils. This also pertains to actual applied dosage of fertilizers and pesticides over the areas of different use, and the techniques of their application. The number of sampling points will also depend on the labolatories’ availability.

Next, the continuous recording of water levels and discharges at gauging points will be realized along with control discharge measurements to ensure the validity of rating curves. It is also expected to perform model validation on water quality data gathered by the end of 2025.

2.3. BRGM Test Facility - Soil Laboratory (FRA)

The BRGM Test Facility, known as the **PRIME platform**, is dedicated to conducting experiments under controlled conditions, ranging from laboratory scale to semi-real scale. It addresses challenges related to the monitoring of water flows and pollutant transfer in water, soil, and the subsurface, while also supporting the development and testing of remediation and mitigation solutions. PRIME serves as an intermediate link between laboratory-scale studies and fully

contaminated site-scale applications. It enables refinement of conceptual understanding of the main drivers of pollutant migration, the development of various remediation/mitigation technologies, and the testing of monitoring devices for analyzing contamination in water, soil, and the subsurface.

2.3.1. Purpose of the sites within the PHISHES project

In the **PHISHES project**, the BRGM Test Facility is primarily used to address challenges associated with soils contaminated by emerging pollutants such as per and polyfluoroalkyl substances (**PFAS)**, and their impacts on soil functions that support ecosystem services. The following challenges are addressed:

- Enhancing the understanding of key processes governing PFAS fate and transport from soil to groundwater and surface water at the contaminated site scale, in particular by better characterizing the forces controlling PFAS sorption at the air–water interface.
- Bridging current knowledge gaps that hinder the conceptualization of PFAS migration pathways at contaminated sites. This includes addressing unknowns such as source terms due to the use of multiple Aqueous Filming-Forming Foam (AFFF) formulations, the role of the unsaturated zone as a long-term emission source, and the impact of capillary fringe variations on PFAS remobilization to groundwater associated with fluctuations in the groundwater table.
- Scaling up laboratory findings to contaminated site conditions in order to determine a robust PFAS mass balance over the long-term contamination history of the site.
- Evaluating the impact of PFAS contamination on various soil functions related to ecosystem services.
- Updating existing models used to simulate soil functions to incorporate PFAS fate and transport, notably by implementing physically-based modelling of PFAS sorption at the air–water interface, with a focus on competition and facilitation reactions among PFAS compounds.
- Identifying the minimal set of input parameters required for physically-based models in order to simulate contaminant transport and soil functions.
- Developing a conceptual framework to describe the effects of the most promising remediation technologies on soil properties and functions, enabling the prediction of potential impacts at contaminated sites where these technologies may be deployed.
- Providing the datasets needed to initialize, calibrate, and validate the model train used to simulate the effects of remediation technologies on soil functions.

It is important to highlight that several remediation technologies have been tested at the BRGM Test Facility in the context of past research activities, including in situ flushing with non-Newtonian fluids (NNF), in situ chemical reduction, on-site chemical oxidation, and on-site biological treatment (some of which are mentioned in the PHISHES Grant Agreement). However, not all of these are relevant to the PHISHES project. During the initial months of the PHISHES project, a synergy has been developed between the BRGM Test Facility test case and the Örnsköldsvik Airport test site (section 2.4) in view of the complementarity between these test cases in the context of the PHISHES scientific objectives (i.e. establishing linkages between contaminated soil land management and soil functions and associated ecosystem services). During the discussions between BRGM and SGI, it appeared that the remediation technology tested at the BRGM test facility that is most relevant for the Örnsköldsvik Airport test site is **in situ flushing using** NNF. Application of this technology will be included in the simulation scenarios defined as part of WP5. These scenarios are being developed to assess the most suitable land-use management options for maintaining or enhancing soil functions at contaminated sites. Actions at the BRGM Test Facility (see section 2.3.4) are tailored for the needs of these scenarios.

Given the similarities between the BRGM Test Facility and the Örnsköldsvik Airport test site (Sweden), a collaborative effort has been initiated between the two sites to strengthen the results obtained at each. Special attention will be given to demonstrating the upscaling of knowledge and findings generated under controlled conditions at the BRGM Test Facility to the Airport site. Since the start of the project, several collaborative themes have been identified:

- Advancing the understanding of key processes controlling PFAS fate and transport at the Airport test site by combining data on the transformation/degradation of precursors into terminal PFAS (from the Airport site) with BRGM results on PFAS sorption onto air–water and solid–water interfaces.
- Addressing the challenges in estimating PFAS mass balances at the Airport site by leveraging insights from the BRGM Test Facility regarding PFAS distribution from soil to groundwater.
- Identifying results from BRGM laboratory-scale experiments that can be used to parameterize the model train designed to simulate contamination plumes and soil functions at the Airport site.
- Assessing the potential application of **in situ flushing using NNF**—whose effectiveness has been demonstrated under controlled conditions—at the Airport test site.
- Predicting the impact of NNF on soil properties and contamination plumes at the Airport site using a site-specific model parameterized with experimental data from the BRGM Test Facility.

2.3.2. Description of the basin/site

The **BRGM Test Facility** addresses practical needs and challenges related to monitoring contamination plumes from soil to groundwater and surface water, as well as to developing and testing innovative technologies for the remediation of contaminated soil and subsoil. By enabling the design and execution of experiments under controlled conditions at scales ranging from centimetres to several meters, the BRGM Test Facility serves as a crucial intermediate link between laboratory research and operational applications on contaminated sites.

To meet these objectives, various tools and methods are developed, qualified, and validated at different scales, including:

- **An environmental monitoring system** that combines sampling devices with advanced analytical tools to detect and quantify pollution in soil, subsurface, and water, while delivering robust mass balance data during experiments.
- **Datasets to parameterize and validate modelling tools**, which: i) characterize the key processes controlling contaminant fate and transport within the soil–groundwater continuum (e.g., degradation, storage, transfer), as well as the relationship between soil properties and soil functions; ii) simulate the spatio-temporal patterns of soil properties and contamination plumes; iii) forecast short- and long-term changes in soil properties, including contamination evolution.
- **Development of innovative, environmentally friendly remediation methods**, including physical, chemical, and biological processes.

The BRGM Test Facility is a purpose-built, 1,000 m² hall that allows for the maintenance of controlled conditions during experiments. It houses multiple experimental devices capable of operating from laboratory scale to multi-meter (plurimetric) scale. Experiments have been conducted on various types of contaminants (both inorganic and organic) and media (soil, sediment, water, and subsoil solids). For example, the facility has been used to enhance understanding of contaminant fate and transport, and to test the effectiveness of several remediation technologies for pollutants such as hydrocarbons, chlorinated solvents, pesticides, heavy metals, and PFAS.

The facility allows experiments at different scales, from small-scale (a few kilograms or cubic centimetres of soil, sediment, or water) to plurimetric-scale (several tons or tens of cubic meters), enabling semi-realistic conditions that closely simulate those encountered in field applications. A brief description of the available experimental platforms is provided below:

- **Sub-metric Platform**

  This platform allows for experiments under fully controlled conditions using **small-scale setups**, including 1D columns (Figure 16), 2D tanks (Figure 17), and centimetre-scale vats. These setups are used to precisely characterize and quantify the forces and mechanisms governing **physical and biogeochemical processes related to soil functions**, particularly those influencing pollutant migration. By simplifying environmental variables, these experiments provide a detailed understanding of processes that cannot be isolated in larger-scale, more variable conditions.

  Advanced monitoring systems — such as imaging and geophysical techniques — are used alongside standard physical, chemical, and biological measurements, applied to both solid and aqueous phases. Dedicated devices are also available to monitor interfacial forces at solid–water and air–water interfaces**,** in the presence of both synthetic solutions (containing single chemical species) and real-life environmental samples.

  Experiments have been carried out to study the key physical and biogeochemical processes controlling the fate and transport of various contaminants (both inorganic and organic). For example, advection and dispersion properties have been measured in various porous media (soil, subsoil solids, geological materials or sediments). Sorption reactions at the solid–water interface have been studied under the influence of multiple factors, including pH, aqueous phase concentration, sorption site competition, surface properties of solids, ionic strength**,** and temperature**.**

  The platform is also used to study physically-induced transformations **and** microbially-mediated degradation processes. Additionally, experiments aimed at designing and optimizing remediation strategies are conducted, including tests on pollutant recovery and degradation under varying temperature conditions and with the application of flushing agents (e.g., surfactants, foams**).**



Figure 16 Illustrative examples of 1D column set up to assess transport properties of the porous medium and fate and transport of inorganic contaminants



Figure 17 Illustrative example of an experiment on Light non aqueous phase fluid filtration in a sandy material in the 2D tank set up

- **The metric platform** consists of a set of large stainless-steel columns (100 cm in diameter and 145 cm high), known as lysimeters (Figure 18), designed to simulate vertical mass and water transfer at an intermediate scale over long-term experiments, under conditions as close as possible to those of real soils. Each lysimeter can be equipped with multiple sensors and samplers, allowing the monitoring setup to be tailored to the specific objectives of each experiment.

  Furthermore, the lysimeters can be interconnected — the outlet of one lysimeter serving as the inlet for another — enabling the simulation of a multi-meter soil–groundwater continuum. For this purpose, water circulation is fully controlled and automated, allowing the reproduction of natural flow variations such as seasonal fluctuations in groundwater table levels.

  The lysimeters are located in a temperature-controlled room. The tops of the columns are designed to replicate real topsoil conditions: horticultural LED lights simulate day/night cycles, and a sprinkler system connected to a water reservoir simulates rainfall. This setup allows for plant growth on the surface of the lysimeter columns. A closed water and mass balance is achieved by collecting the outflows in stainless-steel tanks, where volumes are precisely measured using weighing scales.

  Over the past five years, this platform has been used to conduct experiments focused on: pollutant migration from soil to groundwater, changes in soil properties in response to seasonal variations in natural recharge, testing environmentally-optimized mitigation technologies, such as assisted phytostabilization of historical mine tailings, and evaluating their effects on soil properties and pollutant mobility.

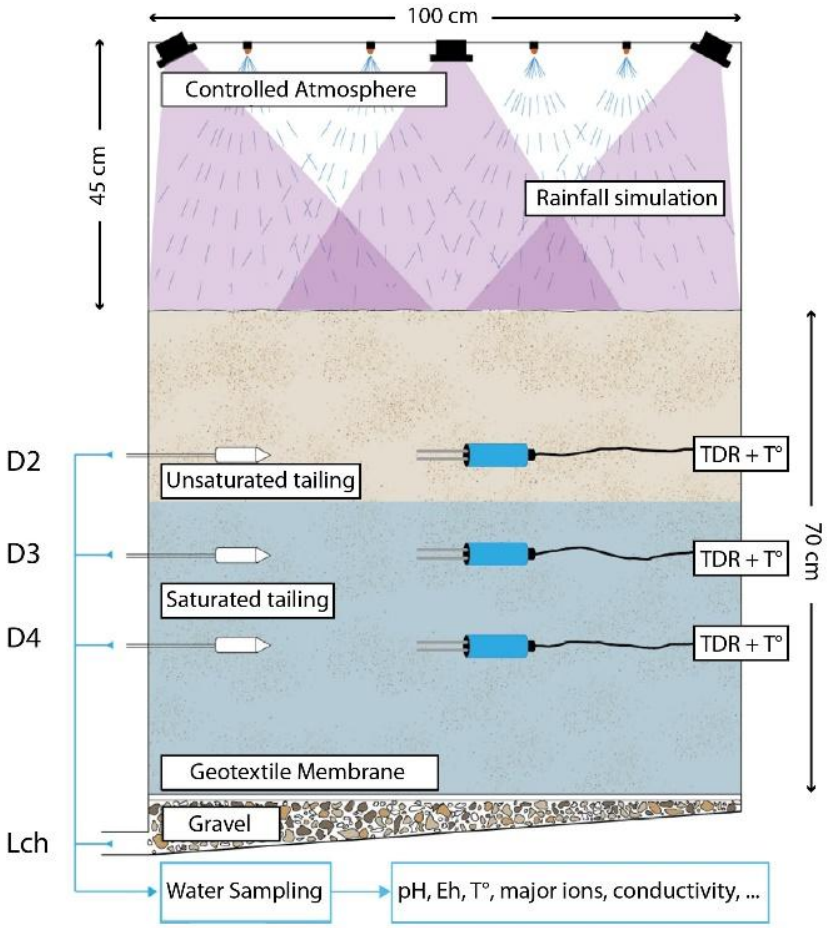


Figure 18 Schematic sketch of the lysimeters used in the metric platform

- **The plurimetric platform** is a large-scale facility designed to simulate soil and subsoil environments, from the surface soil layer down to the groundwater, for studying pollutant transport as well as the physical, chemical, and biological properties of the medium and the changes it undergoes during experimentation (Figure 19). The pilot plant is highly modular, allowing users to implement customized monitoring setups by freely selecting the spatial locations of sensors and samplers throughout the facility.

  It is specifically designed to enable experiments that closely replicate real-life environmental conditions, while retaining the key advantage of controlled experimental settings. This control notably enables the establishment of a robust water and mass balance, which significantly enhances the validity and reliability of the experimental results.

  The facility consists of a large experimental tank measuring 10.40 m in length, 3.6 m in width, and 4 m in height, with an effective volume of approximately 120 m³. Both unsaturated and saturated conditions can be maintained in any spatial configuration, depending on the experimental objectives. As a result, full 4D monitoring (three spatial dimensions plus time) of the soil–groundwater continuum can be achieved, allowing for precise investigation of contaminant migration, spatial distribution, and temporal evolution of specific soil functions.

  The tank walls are equipped with numerous access ports, offering high flexibility for installing sensors and sampling devices at various depths and locations.

  This platform has already been used for two long-term experiments (each lasting more than one year), focusing on the fate and transport of pollutants from soil to groundwater and on the evaluation of remediation technologies aimed at the recovery and degradation of contaminants. These include LNAPLs (Light Non-Aqueous Phase Liquids) in the

MOBILMOUSSE project and PFAS in the PROMISCES project (Grant Agreement N°101036449).

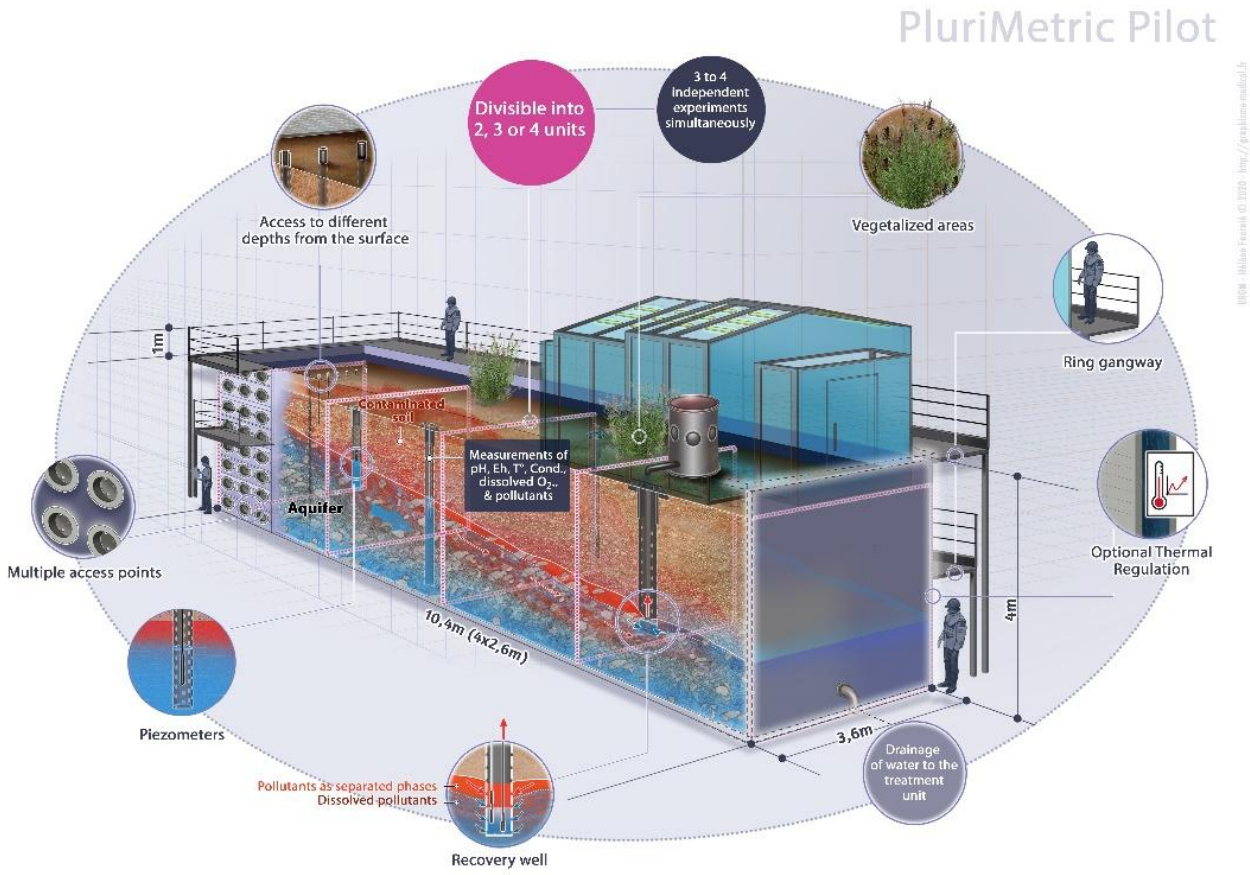


Figure 19 Schematic sketch of the plurimetric pilot.

2.3.3. Existing data available

The PHISHES project will benefit in part from publicly available data acquired during a long-term, large-scale experiment conducted as part of the PROMISCES project on the Plurimetric Platform. The main results provided by the experiment enable us to:

- Improve the understanding of the key processes governing PFAS behavior, particularly precursors, and their transport from soil to groundwater at large scale;
- Identify frameworks for upscaling lab-scale data for use in large-scale studies and modelling;
- Compare targeted PFAS analysis with total fluorine measurements to assess the spatial extent and temporal evolution of PFAS plumes;
- Develop and apply a model train to simulate the fate and transport of major AFFF constituents and derived precursors from soil to groundwater;
- Provide proof of concept for several remediation technologies, both in situ (using non-Newtonian fluids) and on-site (PFAS destruction using DMSO/alkaline additives and sonocavitation).

The experiment was designed to replicate, as closely as possible, contamination of the soil–groundwater continuum by AFFF, as observed at real-world contaminated sites, and to test the efficiency of PFAS recovery and destruction technologies under semi-realistic conditions. The setup was selected to closely mimic a real aquifer. The water table depth was maintained at one meter below the surface of the Plurimetric Platform PMP, resulting in unsaturated and saturated zones of

one meter and two meters thickness, respectively. Water flow and mass transport boundary conditions were tightly controlled throughout the experiment. Three boundary conditions were implemented for water flow:

- **In the saturated zone**, the two boundary conditions are: i) a hydraulic barrier on one side of the PMP maintained a constant hydraulic head, ii) a pumping well located on the opposite side operated at a constant flow rate of 4×10^{-2} m³/h, ensuring steady-state conditions. The two remaining sides of the PMP were designated as no-flow boundaries
- **In the unsaturated zone**, transient boundary conditions are fixed by performing weekly infiltration of 120 L. Water recharge and PFAS injection were carried out using a sprinkler system installed over a 2.25 m² infiltration square, allowing infiltration into the unsaturated zone. This area represents approximately 10% of the total surface at the top of the PMP. The infiltration square was positioned closer to the side where the hydraulic head was maintained constant (1.5 m between the center of the square and the boundary), and further from the pumping well (3 m downstream from the center of the square to the well).

The PMP was filled with a porous medium consisting of 92% sand, 5% clay, and 3% organic matter. The characteristics of the porous medium were as follows: porosity (ϕ): 39±1% and permeability (k): 93 (±20) $\times 10^{-12}$ m^2. The filling and equipping operations of the PPM took place over approximately 1 month.

The AFFF used during the PMP experiment mainly contains PFAS with an eight carbon chain length. The main PFAS found in the AFFF are 6:2 FTSA, 6:2 FTAB and 6:2 FTSAam (1525.0 mg/L, 3409.0 mg/, 780 mg/L, respectively) and, in a lesser extent, PFHxA, 8:2 FTSA, 4:2 FTSA and 10:2 FTSA (8.9 mg/l, 3.8 mg/L, 3.4 mg/L, 1.7 mg/L). Other chemical compounds as also part of the AFFF formulation such as polyethylene glycol or ionic salts (SO_4^{2-} and NH_4^+). This AFFF formulation is similar to the one reported in literature for products developed during the 2000's. Homogeneity and stability of the product has been assessed by performing multiple sampling and analysis on the stored solution during the experiment.

The monitoring set up in PMP is based on probes and sampling devices allowing us to monitor water table depth, soil moisture and soil water potential in the vadose zones as well as sample water in vadose and saturated zones. Water table level has been monitored by using an automatic pressure transducer installed in 9 piezometers. Capillary pressure and water content in the vadose zone have been monitored using 15 tensiometers and 95 TDR. To collect water samples, 80 suction cups were positioned along the main flow lines in different locations in the PMP and at different depths from -0.5m to -2.5m. Water samples were also collected in the 9 piezometers. Sensors and probes are distributed according to a regular grid at the surface and at different depths within the PMP. This grid has been selected to ensure robust calculations of PFAS distribution in the PMP at the end of the experiment.

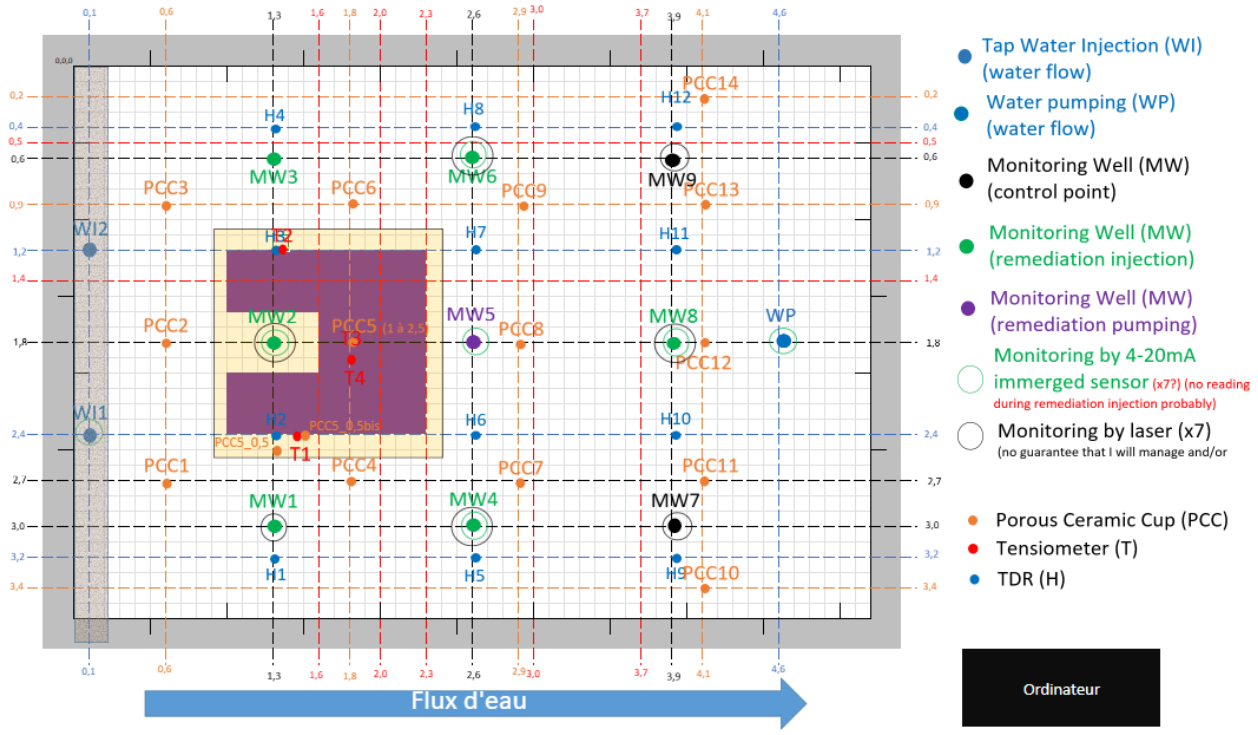


Figure 20 Implementation of the monitoring tools of the PMP

The experiment ran for eleven **months**, with eight **months** dedicated to monitoring PFAS migration and three **months** to assessing the performance of remediation technologies at semi-real scale (Figure 21). It was structured into four key stages:

- **Baseline stage.** This stage was devoted to acquired baseline of the PMP prior to AFFF contamination. The flow rate in the saturated zone was kept at the fixed value. Weekly recharge events have been performed by infiltrating 120 L of PFAS-free water (tap water issued from the domestic water supply was used) on the infiltration square at the top of the PMP. The length of this stage is 2.5 months (from mid-February 2024 to mid-April 2024). Prior to this stage, a stabilisation stage of four months was applied. A sampling campaign has been conducted at the beginning and the end of this stage. Water was sampled in each sampling point in the PMP.
- **PFAS infiltration stage**. This stage was conducted for three weeks (from mid-April 2024 to mid-May 2024). A diluted solution of AFFF (3% w/w) was infiltrated from an injection square corresponding to a fraction of the surface at the top of the PMP. The total volume of input solution is equal to 1.6 m^3. This volume has been selected to reach PFAS concentration in pore solution and a sorbed PFAS concentration in the range of the concentrations measured in highly contaminated site mentioned in literature. To prevent saturation of the unsaturated zone, the total volume of diluted AFFF solution was infiltrated in 14 infiltration periods. During each infiltration period, 120 L of diluted AFF solution was infiltrated during 3h. A non-reactive tracer (Br) was also added to the input solution to characterize the transport properties of the PMP during PFAS migration. The flow rate in the saturated zone is maintained at the value fixed in the first stage. A monitoring campaign was conducted after each PFAS injection step at the sampling points located below the infiltration square and in its vicinity.
- **PFAS leaching stage.** This stage was performed to induce PFAS migration from the infiltration square to the unsaturated and saturated zones as it can be induced by natural recharge on a real AFFF-contaminated. During this stage, PFAS-free water has been infiltrated on a weekly basis for five months (from mid-May to October 2024) in the injection

square. The infiltrated volume is equal to 120 L. Each week, water samples have been collected in each sampling point in the PMP.

- **Test of remediation technologies stage.** This stage has focused on demonstrating a proof-of-concept for a set of remediation technologies consisting of in situ flushing using non-Newtonian fluids (NNF), in situ chemical reduction, on site chemical oxidation (PFAS destruction using DMSO/alkaline additives and sonocavitation) and on-site biological treatment. Two types of shears thinning NNF were investigated: a xanthan-based polymer and a surfactant foam. The injection of non-Newtonian shear thinning liquids (e.g. foams and gels) makes it possible to sweep the entire medium, using the notion of "front flattening", which is the relatively homogeneous progression of the injected fluid in the form of a flat front, by attenuating the permeability contrasts of the media crossed (the NNF becomes less viscous when it crosses the less permeable zones). Several experimental conditions (air flow rate, water flow rate and water table depth) have been tested to assess the efficiency of this technology for removing PFAS from the saturated and unsaturated zones. For in-situ chemical reduction, on site chemical oxidation and on-site biological treatment, batch experiments have been conducted using contaminated water issued outlet of the PMP for designing the most suitable features for performing PFAS degradation.

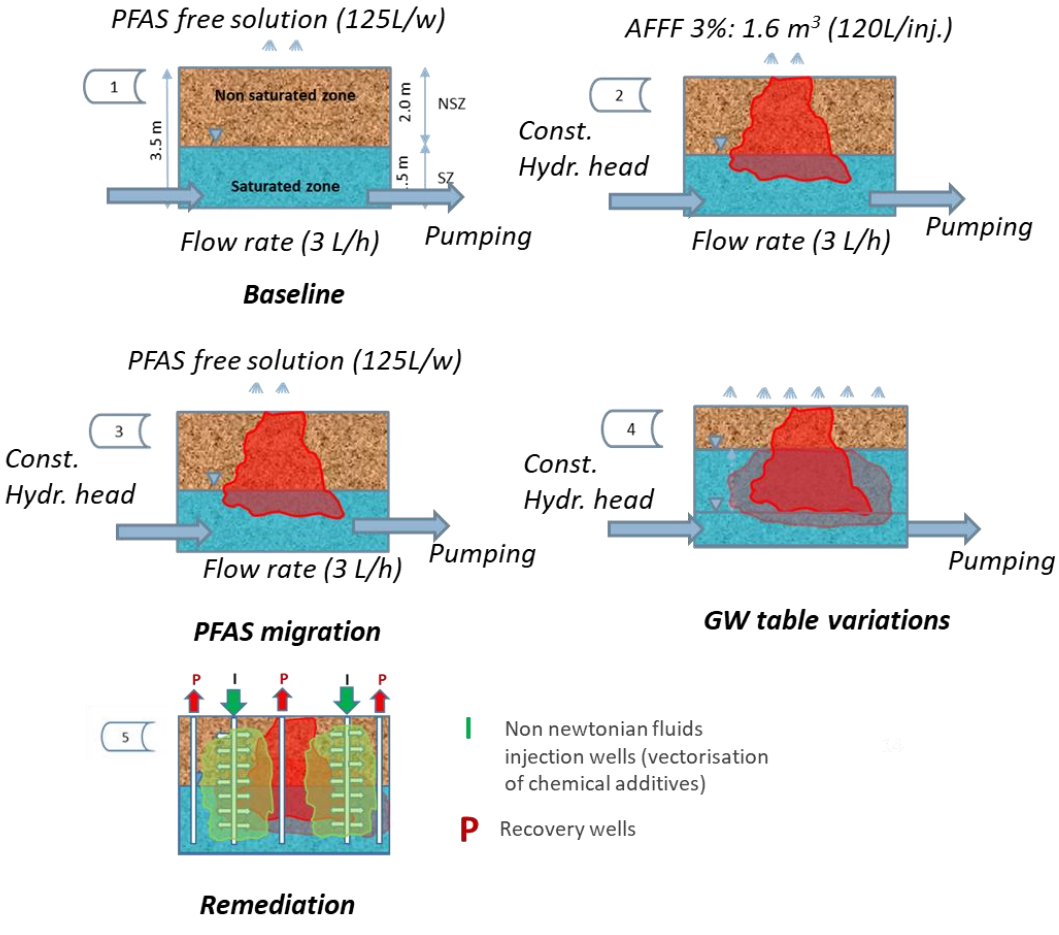


Figure 21 Conceptual design of the PMP experiment (modified from Zessner et al., 2025)

During this experiment, a broad range of physical and chemical parameters have been measured on solid and water samples. This data is summarized in the following Table 5.

Table 5 Table summarizing the data issued from the PMP experiment

Data Type	Description
Soil and sub-soil properties	XRD analysis on man-made media used to fill the PMP (5 points)
	Grain size analyses (10 points)
	Total chemical analysis (5 points)
	Total organic carbon (5 points)
	Soil core after PFAS injection, prior remediation phase and post remediation phase
Hydrogeological	12 Monitoring wells equipped with transducers probes (divers) every hour
	95 TDR (water content) every hour
	10 tensiometers (water pressure) every hour
	Transport properties issued from column experiments
Hydrogeochemical	pH, redox, temperature and electrical conductivity on each water sample
	Total organic fluorine by combustion ionic chromatography. Every 15 days during the 3 first stages on selected samples (250 points) and two time by weeks during the remediation phase on selected samples (250 points)
	8 PFAS by LC/MS/MS (every 3 weeks during the 3 first stages, two time by weeks during the remediation phase)
	Major cations and anions, trace metals and bromide every month
	Dissolved organic carbon every month

Considering similarities between the PMP experiment conducted in the BRGM Facility test site and the Airport test site, collaborative work between SGI and BRGM is planned to enhance the synergies between the two sites. This will improve our capability to use these datasets to parameterize and test the capabilities of the model train developed during the project to simulate soil functions in contaminated soil by PFAS and the impact of the use of remediation technologies as an option of land-use management. One should note that the design of the PMP experiment is kept controlled considering spatial heterogeneities of soil properties as well as maintaining steady-stade hydrodynamic conditions during a large part of the experiment. Hence, this dataset is not suitable to assess spatial and temporal heterogeneity of soil functions as can be expected in a natural environment. Despite the length of the experiment, it is not suited for assessing long-term (decades) processes occurring in C or nutrient cycles that can be monitored in long-term studied test sites such as the Airport test site. environment.

By allowing calculation of a robust mass balance, the PMP experiment is suited to assess the main processes controlling the fate and transport of PFAS along the soil-groundwater continuum, overcoming the unknowns that a rise in a real contaminated site due to the complexity to establish a water budget and mass balance as mentioned for the Airport test site. Furthermore, an accurate estimation of the recovery yields by using non-Newtonian fluids to flush PFAS can be gained due to performing the experiment in controlled conditions, which is not the case in the field. Based on these datasets, one can use them to parameterize a model train to forecast the impact on another contaminated site. This is one of the scenarios envisioned for the Airport test site. The framework developed for this purpose is generic and allow its application on other contaminated sites.

2.3.4. Additional – optional – monitoring within the project frame

The existing data provided by the aforementioned PMP experiment will be supplemented with additional experiments. This new data will primarily aim to address one of the objectives of the PHISHES project: assessing the impact of remediation technologies used in land-use management

on key soil functions. Specifically, the experiments will contribute new knowledge related to the Örnsköldsvik Airport test site, in particular by providing conceptual understanding and model parameters needed to develop simulations modeling the efficiency of non-Newtonian fluids in removing PFAS contamination—a remediation technique identified as particularly promising during the PMP experiments—and their impacts on soil functions. This data will be especially valuable for developing the scenarios in PHISHES Work Package 5 (WP5), which will be tested at the Örnsköldsvik Airport test site. To this end, experiments will be carried out at the BRGM Testing Facility. These experiments will use core soil samples collected from the Örnsköldsvik Airport test site, representing at least the main soil types found in the contaminated areas of the site. The resulting data will be used to parameterize the model being developed for this location. Furthermore, additional insights into the main processes explaining the impacts of non-Newtonian fluids (NNFs) on soil functions—not only their ability to reduce PFAS contamination, as previously observed during the PMP experiment—will be gained by performing further experiments on the same soils used in the PMP study. For both soil types, the following types of experiments will be conducted: batch tests, 1D column tests, and 2D tank tests. These are described in more detail below.

First, a batch experiment will be conducted to refine our understanding of the sorption of the PFAS contained in the diluted AFFF solutions on the man-made soil and the soils from the Örnsköldsvik Airport test site. The batch experiment will be carried out in 50 mL polypropylene centrifuge tubes. The solid-liquid ratio will be kept as close as possible to the one encountered in real-life environment to promote the use of these data at larger scale. The tubes will be mixed to optimize the interaction between the soil and the solution containing PFAS. To assess the time-dependency of the sorption reaction, water samples will be collected at different time steps. Temperature will be controlled. All water samples will be analyzed by liquid chromatography-tandem-mass spectrometry (LC-MS/MS) according to the analysis protocol developed at BRGM. For the desorption experiments, the residual wet soil from sorption tests will be utilized. PFAS-free water is introduced to the wet soil using the same liquid-solid ratio as in the sorption test. Subsequently, the suspensions are mixed, centrifuged, and analyzed using the same procedure as that used for sorption.

Then, several one-dimensional (1D) column experiments will be conducted. The columns will be filled with the man-made soil used in the PMP experiment and one or two representative soils from the Örnsköldsvik Airport test site. Briefly, the columns—borosilicate glass with an inner diameter of 4 cm and a length of 50 cm—will be used in a standard column setup (including tubing, inlet/outlet pumping system, and pressure transducers). A weighing scale will be placed under the inflow container to monitor the mass of injected solution.

Each column experiment will follow four stages:

1) Injection of a 3% AFFF solution for at least six pore volumes (PV);
2) Injection of the non-Newtonian flushing solution, identical to that used in the PMP experiment, for at least eight PV;
3) Injection of one PV of methanol;
4) Injection of one PV of PFAS-free input solution.

Foam for the flushing solution will be prepared by mixing air with SDBS (Sodium Dodecyl Benzene Sulfonate) at the correct concentration, using a dedicated foam generator designed to produce foam qualities suitable for the porous medium and targeted radius of influence. Different foam qualities will be tested. Additional batch experiments will assess the impact of non-Newtonian fluids on interfacial tension at both the solid–water and air–water interfaces. The last two steps are included to assess the PFAS mass balance at the end of the experiment. The choice of the number of PVs is based on previous experimental results.

Several soil properties, including permeability, porosity, and longitudinal dispersivity will be evaluated before and after the experiment to quantify the impact of the remediation method. These parameters are related to critical soil functions such as water retention, infiltration, and the soil's buffering capacity against pollutants. Hydrodynamic properties will be assessed via permeability

tests, based on measuring pressure changes in response to increased inflow rate, according to Darcy's law. Non-reactive tracer experiments will be conducted to estimate transport-related properties (porosity and longitudinal dispersivity). Experiments will be conducted under both saturated and unsaturated conditions to closely replicate field conditions at contaminated sites, thus improving the accuracy of predictions for the Örnsköldsvik Airport test site.

Based on the column experiment results, two-dimensional (2D) tank experiments will be conducted to better approximate real environmental conditions. The 2D tank is made of polyvinylidene difluoride (PVDF), with dimensions: 50 cm length, 30 cm height, and 7 cm width. The front face is made of glass for visual monitoring of fluid flow. The tank includes a central reservoir for the porous medium and two lateral counter-channels used for water level regulation. These counter-channels are connected to the central reservoir via a metallic grid that allows fluid flow but retains solid particles. The tank is thermoregulated using internal double-walled ducts located between the glass panels. Peristaltic pumps are used to inject and extract both PFAS-containing water and non-Newtonian fluids. Liquid volumes are measured using graduated cylinders and monitored using a stainless-steel balance (Sartorius Cubis MSE8201S-000-D0) with automatic data acquisition.

Several 2D tank experiments will be performed using the same man-made soil from the PMP experiment and another using the soil and solid materials coming from the Örnsköldsvik Airport test site based on the core samples taken on site. Experiments will be conducted under fully saturated conditions and under variably saturated conditions, where the top of the tank remains unsaturated and the bottom remains saturated, simulating real-world subsurface environments.

As with the 1D experiments, the 2D tank experiment will have four stages. First, the five bottom lines will be used to saturate the porous medium from the bottom up—fully for saturated conditions and up to a targeted height for variably saturated conditions. In the latter case, inlet and outlet pipes in the counter-channels will regulate the water level to maintain the desired unsaturated-saturated interface. Next, a diluted AFFF solution will be injected from the top of the 2D tank to simulate a contamination event. During the flushing stage, four additional injection and pumping lines placed in the counter-channels will deliver non-Newtonian fluids under steady-state conditions, mimicking in situ injection wells. The central line will act as an extraction well.

As in the column experiments, the same soil properties related to water flow and transport will be measured before and after the experiments. Hydrodynamic behavior will be studied by inducing flow between the tank sides via a hydraulic head difference. Non-reactive tracer tests will also be performed to evaluate transport-related parameters.

These results will provide key data for characterizing the mechanisms by which flushing fluids, depending on their quality, alter soil properties related to water flow and contaminant transport. They will also inform the parameterization of models used to simulate these processes. These soil properties are crucial to understanding functions such as water retention, pollutant buffering, nutrient cycling, and carbon dynamics.

2.3.5. Tools, model trains, scenarios expected to be employed or utilized

For the PHISHES project, a modelling framework has been developed that couples a one-dimensional (1D) model—used to describe water flow and reactive solute transport in the soil and subsoil—with three-dimensional (3D) groundwater flow and transport models. This approach has proven effective for simulating various soil functions, including pollutant transfer from the soil to the groundwater.

This framework avoids the main limitations commonly encountered with fully 3D variably saturated flow and transport models, especially when applied to large domains that include the unsaturated zone. The core principle behind coupling independent models for the unsaturated and saturated zones lies in exchanging information about the recharge flux from the unsaturated zone to the saturated zone, as well as the water table elevation, at a given time step. The time step will be selected during the building of the model according to the type of processes that will be considered.

Solute transport requires a similar numerical framework, except that the exchanged information consists of solute concentration fluxes at the bottom of the unsaturated zone and solute concentrations at the top of the saturated zone (i.e., the water table).

A modelling chain combining several software tools has been implemented and updated to simulate soil functions and PFAS transport. This modelling chain includes the following software: **1D-Hydrus**, **MODFLOW**, **MT3DMS**, and **PHREEQC** (see Figure 22). The coupling scheme is kept as simple as possible and is based solely on input/output data exchange between the models.

Specifically, the water flux at the bottom of the unsaturated zone, calculated at time step *n–1*, is used as the recharge input for the groundwater flow model at time step *n*. Conversely, the water table depth computed by the groundwater flow model at time step *n–1* serves as the bottom boundary condition in the 1D vertical model of the unsaturated zone at time step *n*.

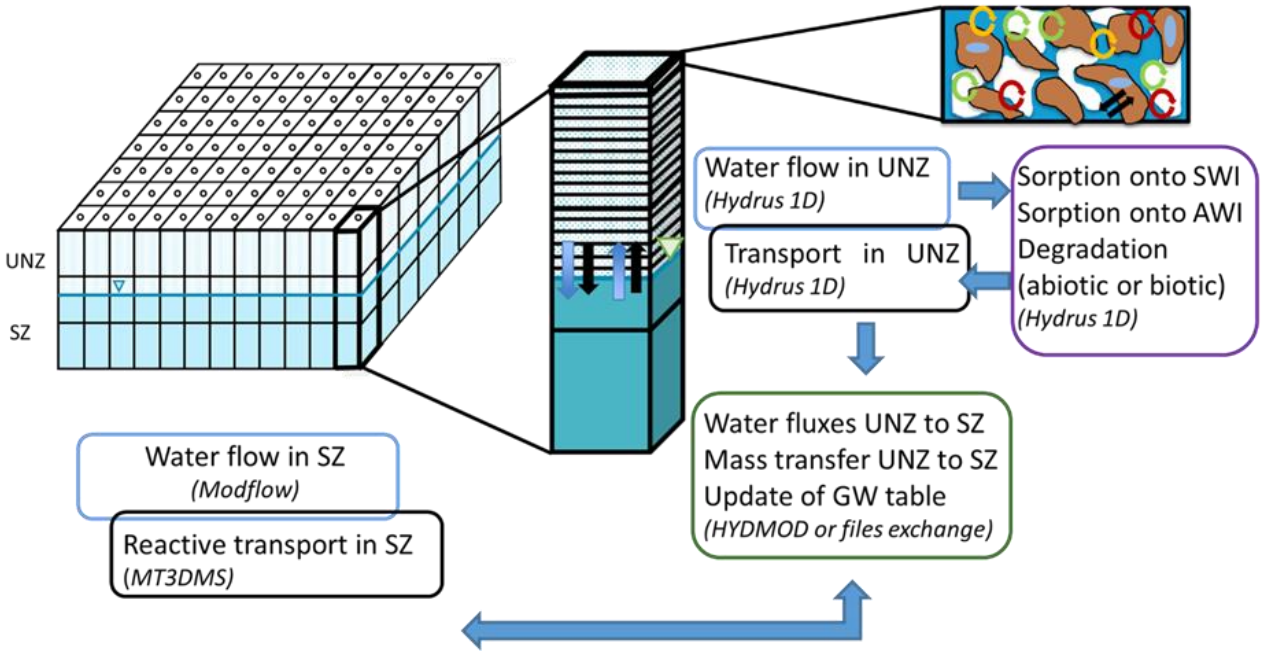


Figure 22: Sketch of the model train developed to simulate fate and transport of PFAS in soil-groundwater continuum.

A dedicated framework has also been developed to use the modelling chain for simulating the fate and transport of PFAS along the soil–groundwater (SGW) continuum at large spatial and temporal scales. This framework consists of the following four steps:

1. **Building, calibrating, and validating 1D variably saturated flow models** in the unsaturated zone using the 1D-Hydrus model for each recharge zone to be considered in the groundwater flow model (developed using MODFLOW). The number of recharge zones is determined by dividing the recharge area into several subzones based on similarities in soil hydrological properties, topographic features, and depth to groundwater. The outputs from this model are used to simulate water flow associated with each soil unit.
2. **Building, calibrating, and validating the groundwater flow model** using MODFLOW, while accounting for the key hydrogeological processes relevant to the domain. The coupling is kept as simple as possible by using the water flux outputs from the 1D-Hydrus simulations as recharge inputs to the MODFLOW model.
3. **Building, calibrating, and validating the solute transport model** for each recharge zone in the domain using the 1D-Hydrus–PHREEQC solute transport module. The PHREEQC software enables the simulation of various soil biogeochemical processes associated with

the following soil functions: nutrient cycling, carbon cycle, pollutant buffering and microbially-mediated transformations. Several biogeochemical models can be developed using the PHREEQC software to simulate the soil processes supporting the aforementioned soil functions. A key step will be to select the model the best suited to simulate them while keeping the data needed to parametrize them as limited as possible.

4. **Building, calibrating, and validating the solute transport model in the saturated zone** using MT3DMS. Depending on the coupling option selected between 1D-Hydrus and MT3DMS, steps 3 and 4 may be conducted iteratively to ensure consistency and convergence in the simulated solute fluxes and concentrations at the interface between the unsaturated and saturated zones.

As previously mentioned, a synergy has been established between the BRGM Test Facility test case and the Örnsköldsvik Airport test case. This means that SGI and BRGM have chosen to use a similar modelling framework and model train to simulate soil functions at both test sites, as well as to assess the impacts of PFAS contamination and the application of targeted remediation technologies. The same coupling scheme—linking the outputs of 1D-Hydrus-PHREEQC to the inputs of MODFLOW and MT3DMS—will be maintained.

Particular attention will be paid to eliminating computational errors in water fluxes at the bottom of the unsaturated zone, especially those caused by sudden inflows or outflows due to changes in the groundwater table depth. Given the dependency of solute transport on water flow, solute concentrations will be adjusted accordingly to preserve mass balance. A specific strategy will be developed to update the inputs and outputs of the four models in the model train, in order to prevent unrealistic variations in flow rates and mass transport within the soil–groundwater continuum. From BRGM's side, the model train will be adapted to simulate and forecast the effects of using non-Newtonian fluids as a land management option to update the inputs and outputs of the four models in the model train, in order to prevent unrealistic variations in flow rates and mass transport within the soil–groundwater continuum. From BRGM's side, the model train will be adapted to simulate and forecast the effects of using non-Newtonian fluids as a land management option for treating contaminated soils.

As already noted, the dataset generated from the PMP experiment is highly suitable for parameterizing and validating the model train developed to assess the impact of land management on PFAS-contaminated soils and their inherent soil functions. Building on this initial step, simulation scenarios will be carried out (in WP5), representing theoretical simulations of an AFFF-contaminated site under hydroclimatic conditions similar to those found in the northern part of France—comparable to the setting of the BRGM Test Facility hall.

For this purpose, European and national-level data on soil properties, geology, climate, and hydrogeology will be analysed and selected to parameterize the model train. The scenarios will be designed to simulate spatial and temporal changes in several soil functions under the influence of climate change. Two RCP scenarios will be tested, combined with various land management strategies. Three options will be considered: i) bare soil; ii) greening, i.e., planting vegetation (likely grass) on part of the contaminated soil and iii) application of non-Newtonian fluids for in situ flushing of the contamination.

2.3.6. Activities executed on site up to date

Although no experimental activities have been carried out since the start of the project, the design of the upcoming activities has been finalized. The types of experiments conducted prior to the start of the project and the information available from these experiments, are detailed above in the description of the test facility and available existing data. Experimental conditions have been reviewed in preparation of the upcoming experiments within PHISHES.

2.3.7. Planned activities for the upcoming period

BRGM plans to carry out batch experiments and the first 1D column experiments during the remaining months of 2025, in accordance with the experimental protocol described above.

In parallel, BRGM will develop a first version of the model train capable of simulating water flow, multispecies mass transport, and biogeochemical reactions, in order to assess the following soil functions: water infiltration and recharge, pollutant buffering—with a particular focus on PFAS fate and transport—nutrient cycling, and the carbon cycle.

The next steps will involve designing the modelling framework required to parameterize the model train for simulating the impact of using non-Newtonian fluids on soil functions.

2.4. Airport in Örnsköldsvik (SWE)

2.4.1. Purpose of the sites within the PHISHES project

The current purpose of the Örnsköldsvik Airport test site within PHISHES is to provide a real-world test-case for model trains and to understand the implications of different remediation measures as well as changes in land-use targeting PFAS on soil health and function . As the site is well-characterized and limited in scope, it provides a framework for exploring which data is necessary in evaluating different scenarios in order to best inform policy decisions. As the site is currently the focus of a pilot-scale test of an in situ PFAS remediation strategy employing a permeable barrier of colloidal activated carbon (CAC), an ongoing characterization of hydrogeological setting, source zone as well as retention parameters and transport through both unsaturated and saturated media is being carried out in order to evaluate the efficacy and longevity of in-situ remediation techniques (activated carbon) as well as their impacts on downstream soil and aquatic recipients. As such, the detailed data which is available from the site, both in the saturated and unsaturated zone, allows for an extrapolation of the different modelling approaches employed under more controlled conditions (see section 2.3) to a real-world site. Coupling of different models (mainly 1D Hydrus and MODFLOW/MT3D) will be evaluated to assess their efficacy in providing data for assessment of soil health and function parameters under different remediation measures.

2.4.2. Description of the basin/site

Örnsköldsvik Airport is located roughly 450 km north of Stockholm, Sweden and 13 km from the coast of the Baltic Sea. The airport was inaugurated in 1961 and expanded in 2004. Regular fire drills were conducted at the fire training site using PFAS-containing extinguishing agents until 2008. The fire training site remains active today, but now only water is used as the extinguishing agent. Örnsköldsvik airport has been the subject of several environmental studies from the 2010's onwards with regards to PFAS contamination arising from AFFF use between 1993 and 2008. The site is located on the terminus of a glacial esker and is characterized by a complex hydrogeological environment of glacial and postglacial clays, sands and gravels, crystalline bedrock and glacial till with both confined and unconfined conditions.

The primary case area is a roughly 2 km^2 groundwater recharge area which then outflows as a 1st order intermittent stream from glaciofluvial deposits to local peat layers. Near-surface groundwater flows (as well as intermittent surface flows) have PFAS concentrations on the scale of 10^4 to 10^5 ng/l. The local sub watershed area is 11.6 km^2.

The area consists of both glacial and postglacial deposits, with varying thickness within the region. The fire training site itself is located on postglacial sand with a thickness of approximately 8-10 m. Just north of the fire training site is the airport, which is constructed on glaciofluvial sediments, deposits which are likely uniform to the crystalline bedrock beneath. Under the AFFF site and overlying the glaciofluvial sediments is a clay layer separating the fluvial sediments from overlying postglacial sand. Glacial till, bedrock, and clay make up most of the surrounding geology, where peat layers may cover the clay. The clay layer is interpreted as continuous under the fire training site with the exceptions being near the glacial deposits at the airport and towards bedrock and moraine southwest of the fire training site. South of the fire training site, the clay becomes more superficial

(NIRAS 2019), which likely explains the less extensive peatland south-southwest of the fire training site. The postglacial sand deposits become thinner towards the southeast and northwest, where they are situated under the peat. The thickness of the glacial deposits varies in the area but can be at least 20 meters. At the fire training site, the glacial deposits under the clay layer are approximately 5 meters thick (NIRAS 2019).

The vegetation of the area is mostly comprised of boreal forest, with frequent pine and spruce as well as various lower vegetation types covering the area. Northwest, directly south, and southeast lie water-saturated peatlands. The peatland south of the fire training site is interpreted to arise due to less permeable layers, which is supported by geophysical ground radar surveys from the area (Figure 23) where the upper surface of the clay layer is interpreted to be very shallow just south of the fire training site.

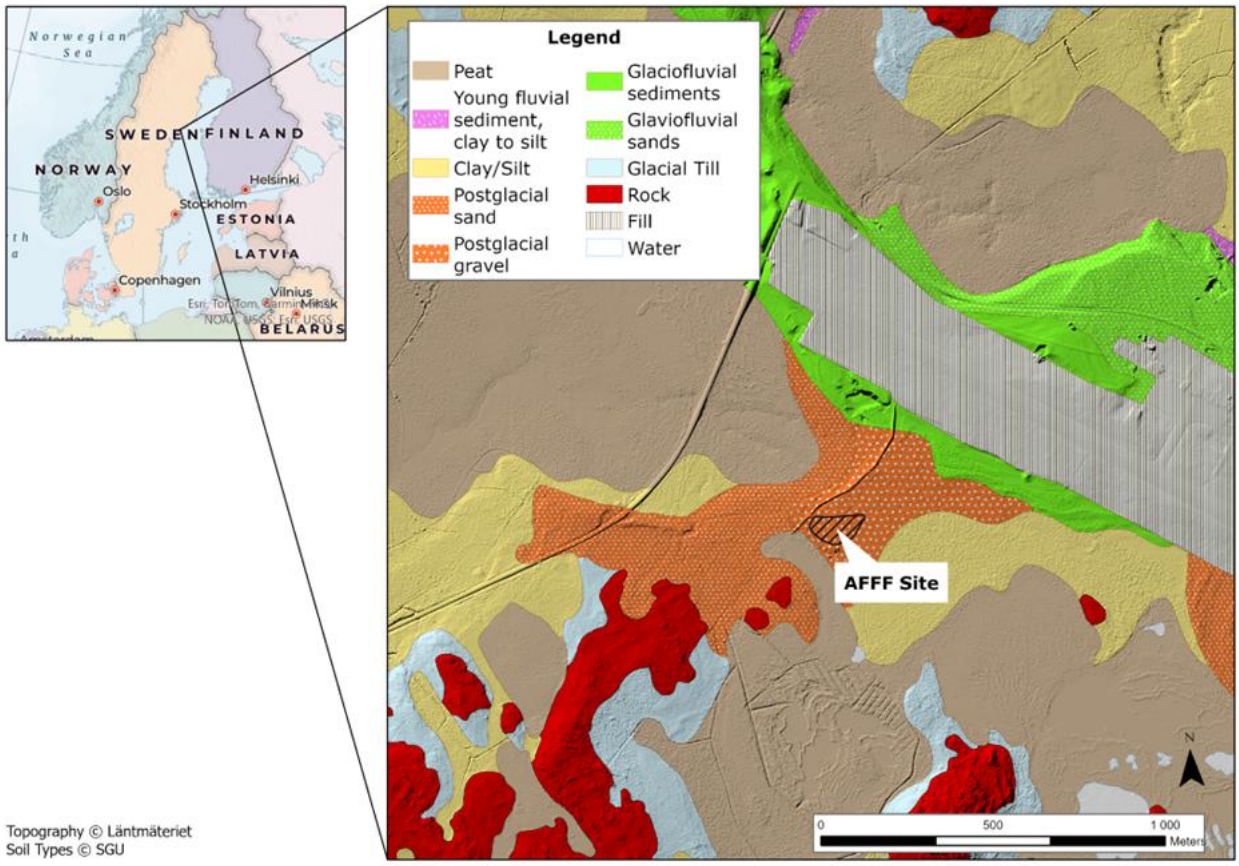


Figure 23 Soil types according to the Geological Survey of Sweden's 1:25 000 – 1:100 000 Soil types map.

The postglacial sand under the fire training site primarily consists of a homogeneous fine sand in the upper reservoir. Analysis of grain size distribution in 22 extracted cores showed a median value of 83.9% with a grain size between 0.063 and 0.25 mm, ranging from 67% to 91.2% (Figure 24). However, single-hole interpretations of sonic cores showed the presence of layers rich in mica with coarser grain size, just above the underlying clay layer. The clay layer varies between 1-2 meters thick and was blue gray to brown and showed laminations of about 2-5 mm. The presence of silt and sand lenses was common. The underlying reservoir, likely glaciofluvial sediments, showed finer sand directly under the clay that became coarser with increasing depth.

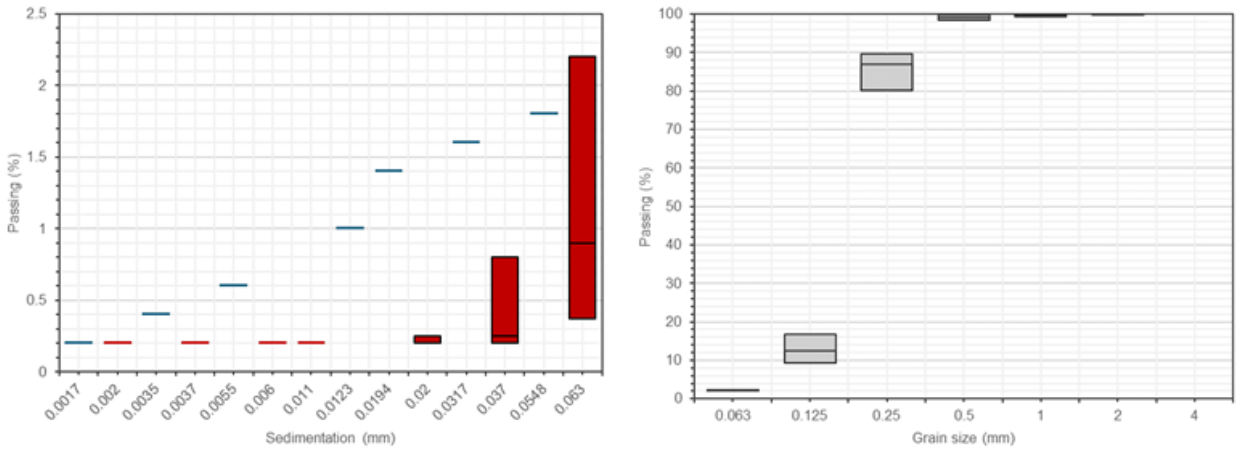


Figure 24 Summary of sedimentation analyses (left, n=16) and 28 sieve analyses (right, n=22). Sedimentation analyses were performed using the hydrometer method (blue, n=6) and pipette method (red, n=10).

The groundwater in the upper, unconfined aquifer is significantly impacted by PFAS predominantly originating from the AFFF site. Concentrations of PFAS-32 in the groundwater exceed 200 000 ng/l, with representative concentrations in the groundwater plume of roughly 40 000 ng/l. PFOS comprises the vast majority of the concentration of PFAS, with significant concentrations of PFHxS, PFOA and 6:2 FTS.

A summary of the general groundwater chemistry is presented in Table 6 and Figure 25.

Table 6 Median chemical concentrations from groundwater samples collected during 2018 (NIRAS)

TYPE	UNIT	MEDIAN
ALKALINITY, HCO3	mg/l	8.65
CHLORIDE	mg/l	1.8
SULPHATES, SO4	mg/l	2.8
CALCIUM, CA	mg/l	3.1
POTASSIUM, K	mg/l	2.7
MAGNESIUM, MG	mg/l	0.85
SODIUM, NA	mg/l	1.9
PH	mg/l	5.8

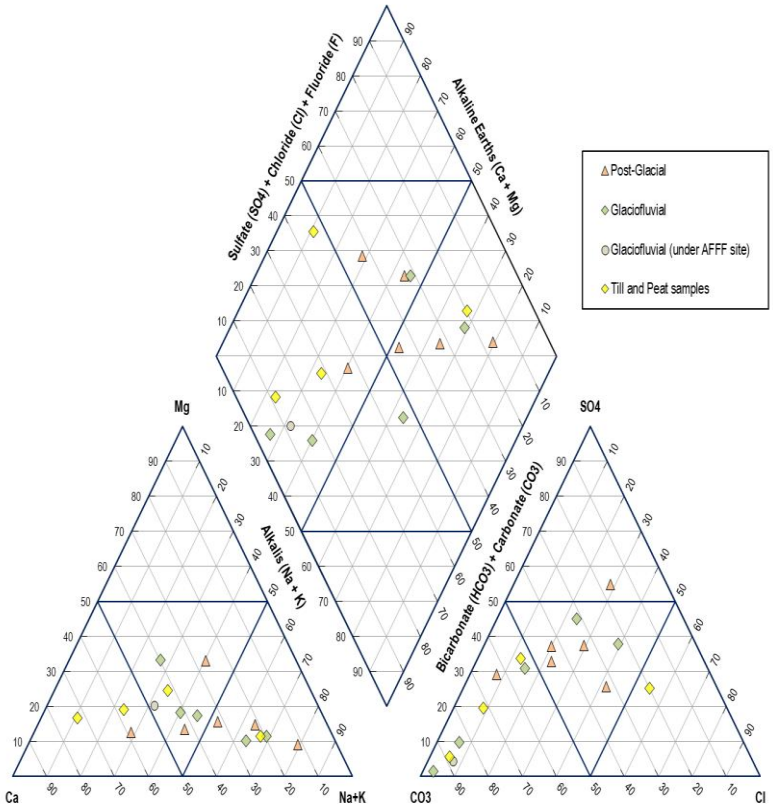


Figure 25 Piper plot of proportional chemistry data prior to the installation of the CAC barrier. Points represent the relative ion composition of groundwater samples collected in the vicinity of the AFFF site at Örnsköldsvik Airport during 2022.

The average temperature in Örnsköldsvik is 4.3°C since 2000, with snow cover from approximately the beginning of November to mid-April. The representative length of the growing season is about 158 days (Figure 26). This implies that groundwater recharge usually occurs in two periods: in October and during the snowmelt from mid-April to mid-May.

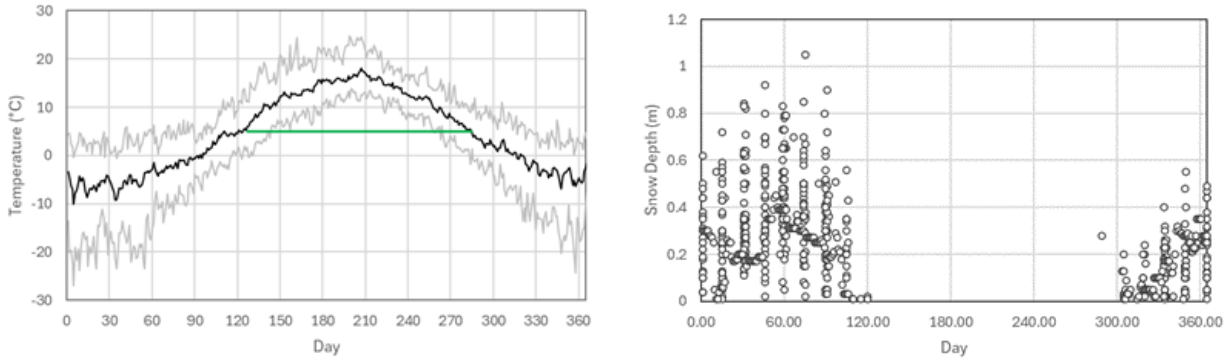


Figure 26 Minimum, average and maximum daily temperature 2000-2024 (left), Örnsköldsvik's airport (SMHI station 138240) and snow depth observations 1947-2024, Örnsköldsvik (SMHI station 138180). Average length of the vegetation period (158 days) shown with green line.

Groundwater recharge, estimated as the sum of effective precipitation in the Swedish Meteorological and Hydrological Institute's (SMHI's) S-Hype model, shows an average of 450 mm/year (2010-2023). This corresponds with hydrograph analysis from 2023-2024, which shows an annual groundwater recharge of 440 to 470 mm/yr over this period (Figure 27). Median yearly precipitation measured at SMHI's Örnsköldsvik station (138180) is 637 mm and 641 mm for the period 1945-2000 and 2001-2024, respectively. It is relatively common for days with high

accumulated precipitation to occur; for example, an accumulated daily precipitation of 36 mm has a return period of one year (Figure 28).

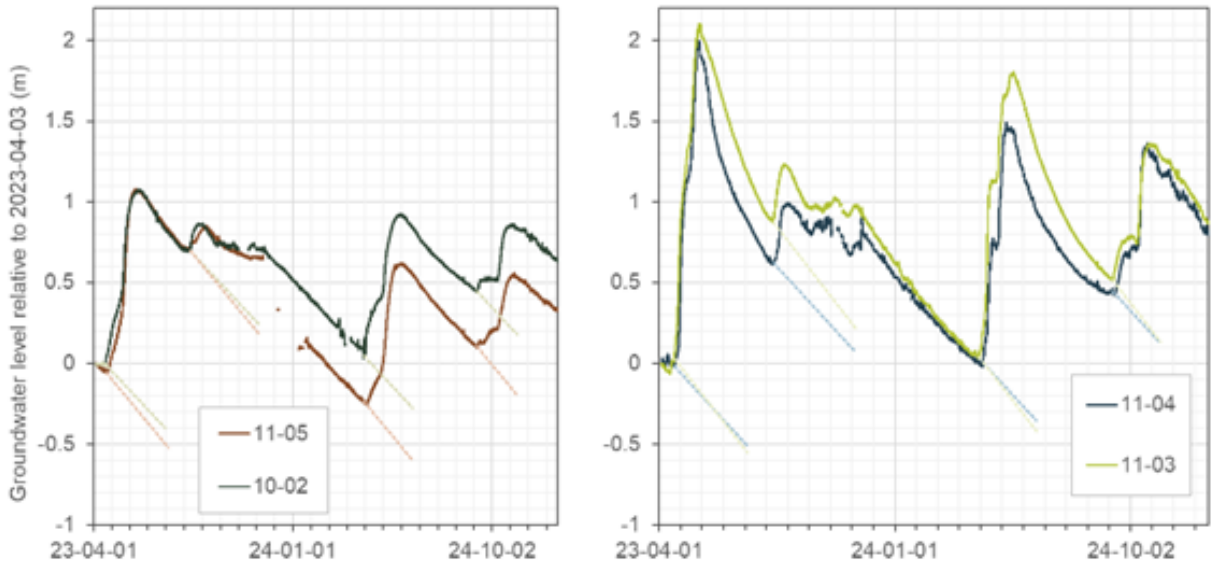


Figure 27 Relative groundwater level to April 2023 measured at selected wells at the AFFF site, 2023-2024. Dashed lines indicate extrapolated groundwater decline (assuming no recharge) during groundwater recharge events.

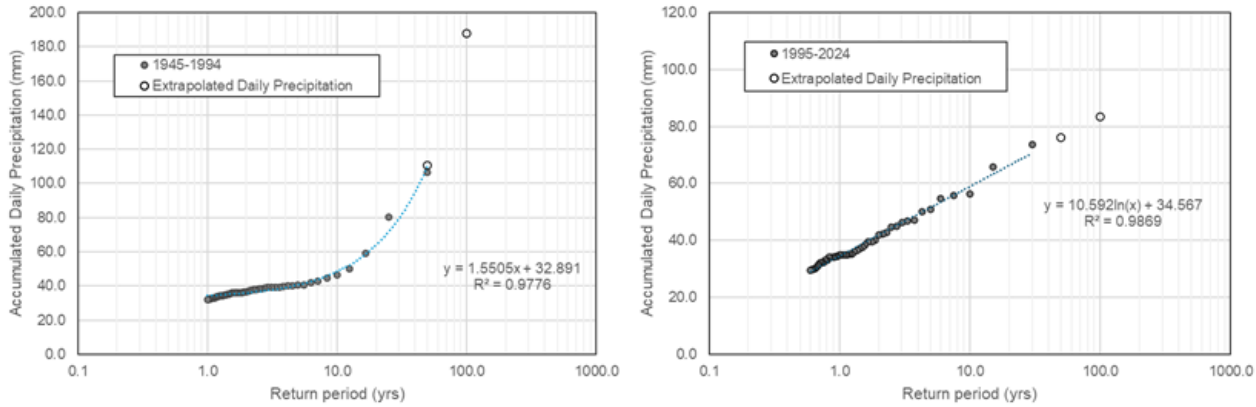


Figure 28 Example of return period for accumulated daily precipitation, SMHI station 138180 Ornsköldsvik. Period 1945-1994 (left) and 1995-2024 (right).

Extensive hydrogeological characterization of the site has been carried out during 2023-2024. Hydrogeological investigations include measurements with the hydraulic profiling tool (HPT), slug tests, passive measurements of flow using iFLUX cartridges, tracer monitoring downgradient of the injection site, grain-size analyses, groundwater level observations and time series, and numerical modelling. Groundwater level observations indicate a local groundwater flow direction towards the north-northwest (Figure 29), which corresponds with numerical modelling and the conceptual understanding of the site. The conceptual understanding of the major transport pathways is a slow transport through the unsaturated zone beneath contaminated areas (limited by sorption to the air-water interface, where lab, field and modelling results indicate that $K_{d,awi} >> K_{d,soil}$), followed by a relatively rapid transport in the saturated groundwater aquifer followed by an ouflow of part of the PFAS plume via a non-seasonal spring to a stream (exhibiting the characteristics of a wetland and stream at different locations). It is likely that a portion of the PFAS plume flows through the organic soils and may emerge downstream, possibly delayed by sorption to the organic soils.

Numerical groundwater modelling (steady state, MODFLOW) has been calibrated against groundwater level data in the area, and current transport models (MT3D-USGS) show promising descriptive capacity of plume characteristics.

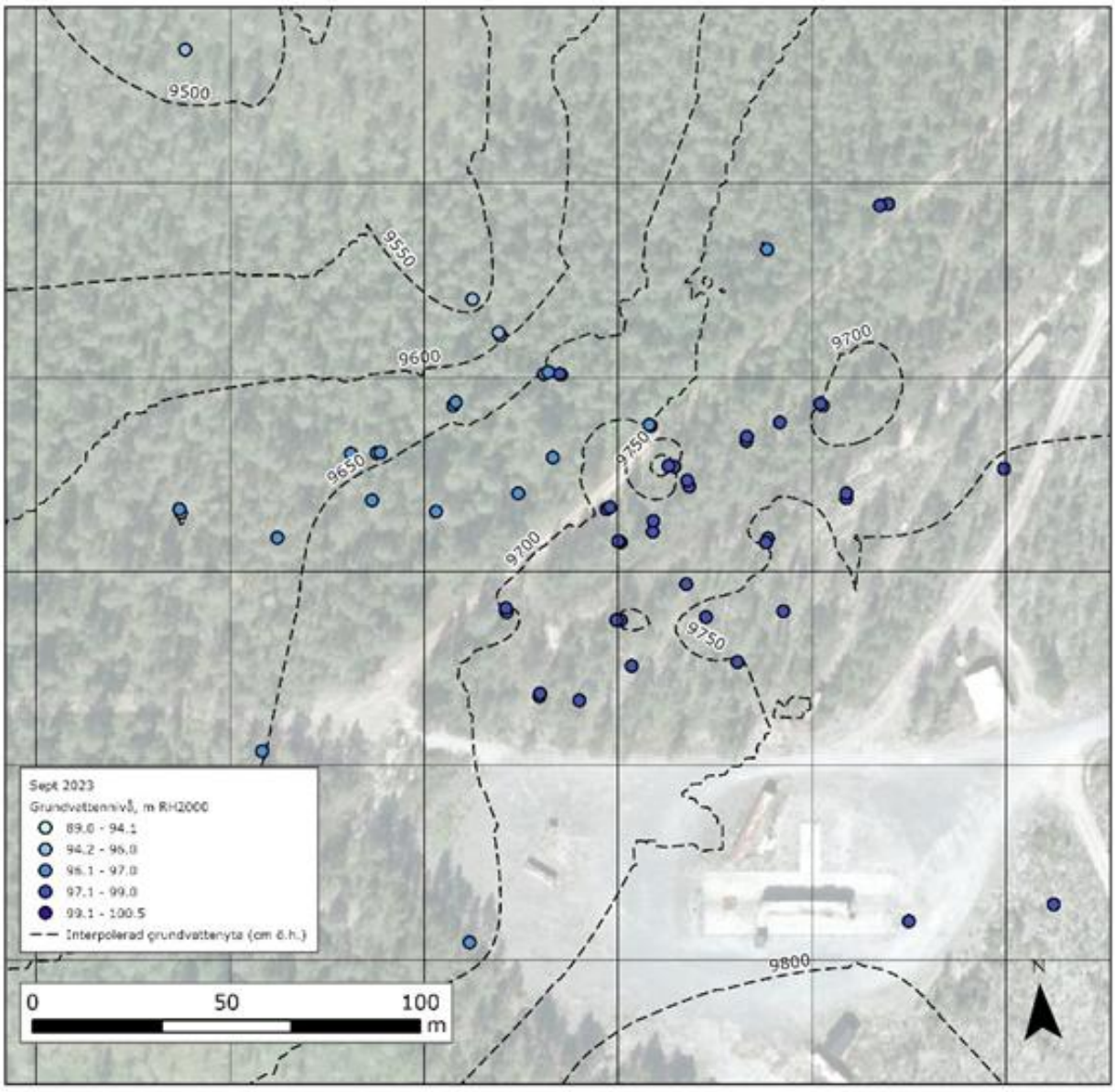


Figure 29 Groundwater level September 2023 (m.a.s.l.). Interpolation of the groundwater surface using kriging (cm a.s.l., Ordinary, Spherical) is shown.

Hydraulic conductivity values of the difference hydrogeological units are illustrated in Figure 30. The hydraulic conductivity of cohesive soils estimated from HPT measurements likely provides an overestimated view of a representative hydraulic conductivity for this type of soil (e.g., clays) due to the measurement method. The horizontal hydraulic conductivity in the hydrogeological unit can be significantly affected by silt and sand layers, but the vertical hydraulic conductivity is likely much lower (Sparrenbom and Jepsson 2022) and dominated by the lower part of the distribution. It is also likely that HPT measurements of glaciofluvial sediments are influenced by the upper measurement limit, which would give rise to the anomalous shape of the distribution and imply the existence of high-permeability layers of thus preferential flow pathways.

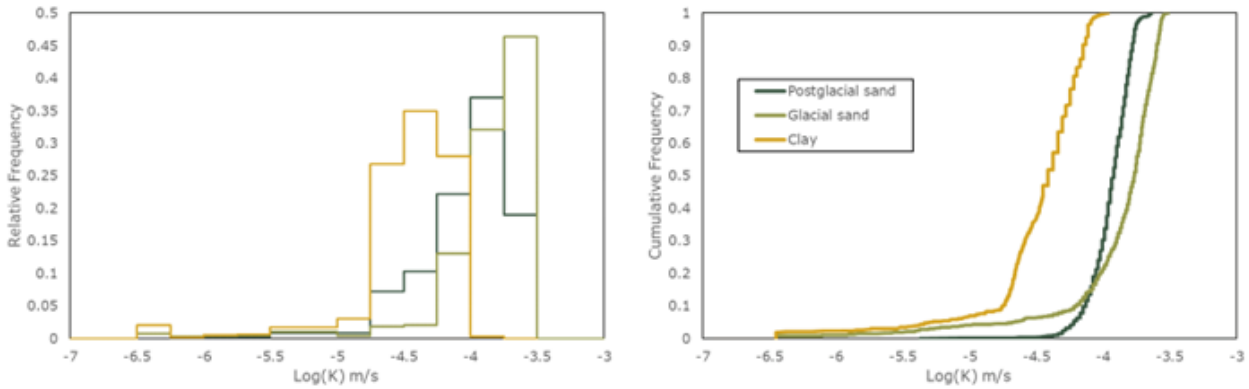


Figure 30 Relative frequency of Log(K) data (a) and cumulative frequency of Log(K) data from different hydrogeological units measured using the HPT.

The advective transport velocity at the site varies significantly under the AFFF site and further towards the groundwater spring, estimated using manual sounding as between 0.17 m/day and 0.85 m/day under AFFF site and up to 1.2 m/day closer to the groundwater outflow (Figure 29). However, gradients obtained by comparing the pressure levels at different points measured using pressure transducers show that the gradient north of AFFF site near the spring is usually about 5 times greater than under AFFF site (Figure 31), and thus a representative flow under the AFFF site is likely about 0.2 m/day and the flow in the aquifer at the groundwater outflow is about 1 m/day.

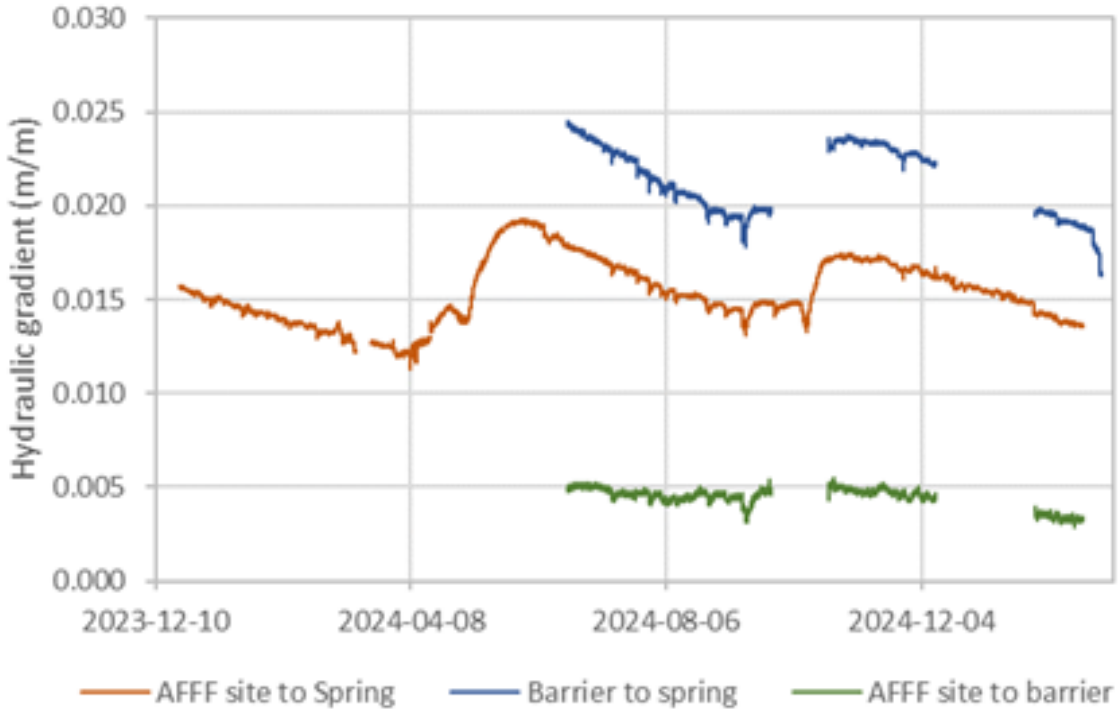


Figure 31 Hydraulic gradient calculated from groundwater level time-series measurements from selected wells.

2.4.3. Existing data available

Sampling of groundwater regarding PFAS has been carried out in and around Örnsköldsvik airport since 2009. Two primary source areas for PFAS contamination have been identified, with the currently relevant fire training site south of the airport being one of them. Extensive sampling regarding PFAS has been performed in stages within and around the fire training site. Environmental

investigations and supporting technical documents have been produced by external consultants in 2010, 2011, 2015, 2016, and 2019.

The Swedish Geotechnical Institute (SGI) has, since selecting the site in 2023 for their in-situ test of stabilization of PFAS using a CAC barrier of colloidal activated carbon, conducted an extensive site characterization campaign. The pilot-test of the CAC barrier was installed September to November 2023, and an extensive monitoring campaign has been implemented in order to study the effects of the remediation measure.

Table 7 Overview of the data collected at Örnsköldsvik within the Swedish Geotechnical Institute's governmental assignment regarding PFAS.

Data Type	OER Data and models, overview
Geological	Sonic drilled points (17 points)
	Grain size analyses (22)
	Geophysics (Electrical resistivity and induced polarization + ground penetrating radar)
Hydrogeological	HPT Measurements (7 points)
	Divers (11; 4 CTD-divers which measure EC since Nov 2024)
	Slug tests (2)
	Monitoring wells (85)
Hydrogeochemical	Passive GW measurements (4 points, flow + $PFAS_{11}$)
	Dynamic groundwater sampling (29 points with 3 depths)
	$PFAS_{32}$ + 6:2 FTAB + TOP + chloride/metals
	Seasonal ultra short PFAS analyses (3 times yearly)
In situ pilot test	CAC barrier completed Nov 2023, 70 m x 5.5 m x 4.5 m
	Soil cores from barrier and source zone (14 near-barrier)
Source zone investigation	Soil cores, groundwater wells installed using Geoprobe (Aug 2024)
	Suction lysimeters installed at three cells and 6 depths (Aug 2024)

Current available groundwater data includes groundwater chemical analyses of PFAS-32 as well as TOP-assay analyses, chloride and metal analyses from selected wells. Additionally, groundwater level observations (manual) and time series (pressure transducers) have been accumulated. As mentioned previously, hydraulic characteristics of the site have been studied in detail using slug tests, tracer monitoring, measurements with the HPT, grain size analyses, three dimensional numerical models (steady state and transient), and soil core data. Passive measurements of groundwater flow and PFAS-4 have been collected during 2023 using iFLUX cartridges.

Dynamic groundwater sampling using a Geoprobe has been carried out at 31 points with 92 independent measurement sections providing important spatial data regarding the plume's characteristics. Comprehensive sonic soil profiling with accompanying geological single-hole interpretations, geophysical data (GPR and CVES) and drill logs provide a good basis for geological characterization.

In the vadose zone of the AFFF site, soil core data has been analyzed for PFAS-32 and TOP-assay with 1 m homogenized intervals at more than 20 points, with data of soil concentrations collected during previous environmental investigations also available. Additionally, dual installations of suction lysimeters at 6 depths and three points have been used to sample soil water concentrations of PFAS-32 and TOP-assay during the fall of 2024.

Weather and climate data are available from weather stations and models from the Swedish Meteorological and Hydrological Institute, although these stations are not specific to the airport with the exception of temperature measurements. A precipitation gauge has been installed during the summer of 2024.

2.4.4. Additional – optional – monitoring within the project frame

While use of PFAS on the site has ceased, relatively high concentrations (tens of thousands of ng/l) of PFAS have been reported in down-gradient groundwater springs connected to the site. Retention within the approximately 4 m unsaturated zone is thus a significant research topic. Site descriptive modelling based on new data and data from previous environmental investigations has been carried out within the scope of an ongoing governmental assignment to investigate the efficacy of in-situ remediation strategies and dissemination of these results.

Current monitoring of the groundwater chemistry of the area includes monthly sampling from 62 groundwater observation wells and 5 surface water points, as well as an additional 23 groundwater observation wells and 5 surface water points sampled three times yearly. The monitoring will continue during 2025 but may be adjusted during 2026. Additionally, at three locations within the source zone suction lysimeters at 6 depths sample the soil water in the vadose zone, roughly eight times per year during the warmer months.

Groundwater sampling includes PFAS-32, TOC and TOP-Assay analyses, as well as analyses of the PFAS precursor 6:2 FTAB. Measurements of electrical conductivity of the groundwater, pH and REDOX potential among other chemical parameters are collected in the field at the time of measurement. Chloride and metal analyses of the groundwater are collected from selected wells, but sampling of these parameters will likely not continue after 2025.

Groundwater level measurements from 62 observation points are sampled either monthly or 3 times yearly, depending on their frequency of sampling within the site-specific monitoring plan. Time series data for groundwater pressure and temperature are collected with hourly frequency from eight monitoring wells, with an additional four monitoring wells having multi-divers which are capable of measuring pressure, temperature, and electrical conductivity of the groundwater. Air temperature and barometric pressure are collected at all locations with a diver present. Data collection relating to pressure and temperature will continue throughout the entirety of 2025 and 2026.

2.4.5. Tools, model trains, scenarios expected to be employed or utilized

The primary model train to be employed at the Airport test site is MODFLOW/MT3D and Hydrus 1D/PHREEQC in order to capture the transport of PFAS within the unsaturated (HYRDRUS/PHREEQC) and saturated (MODFLOW/MT3D) zones. Local and Regional 3D numerical groundwater flow and transport models have been developed at the site within SGI's ongoing governmental assignment. Cross-sections (2D) from the 3D models can be employed as an initial step in coupling the models.

Modelling scenarios include a baseline, business-as-usual, meaning a scenario with no changes to land use or remediation within the simulated time period. Three remediation scenarios are envisaged to be examined within the project: the first illustrating a stabilization of PFAS within the unsaturated zone using activated carbon or comparable sorbent, and the second a natural reclamation of the site with remediation activities implemented within the saturated zone with little to no direct changes to the soil characteristics within the source zone, but noticeable changes to downstream soil chemistry, and finally a remediation strategy applying a non-Newtonian fluid (NNF) in order to flush contaminants from the source zone.

Realization of the remediation strategies will be implemented within the model trains mentioned above via adjustment of model hydrogeochemical parameters, such as porosity, permeability, partitioning coefficients and root zone depth.

All scenarios with the exception of the NNF-scenario are planned to be run under different climate scenarios, a baseline scenario as well as two scenarios under different climatic conditions.

These scenarios can be modelled using existing models from SMHI which predict, for example, changes to precipitation or length of vegetation period, or by assigning specific values more skewed to a specific end of a statistical distribution from existing data sets. Scenarios will be primarily implemented via adjusting model drivers, such as groundwater recharge or infiltration or boundary conditions within the model such as a static hydraulic head.

The output of the model trains above is primarily focused on hydraulic and chemical properties of the soil, namely porosity, hydraulic conductivity, soil moisture, and contaminant concentration.

2.4.6. Activities executed on site up to date

As of the time of writing this report and in addition to the activities mentioned in the preceding sections, activities have been focused on defining scenarios, initial parameterization, and exploration of model packages. Preparation for coupling of model trains has also been underway. These scenarios have been defined to provide the basis for evaluating realistic remediation measures. Current scenarios are delineated to bridge the gap between the BRGM plurimetric pilot data (see section 2.3) and the field case afforded by the Örnsköldsvik data.

The testing of Hydrus 1D has involved conceptual modelling of input parameters and the impacts of discretization. This step is critical to ensure that the models accurately reflect the complexities of the real-world scenarios and provide meaningful insights into the behavior of contaminants and water fluxes under varying conditions. By identifying how different scenarios will impact model drivers such as hydraulic conductivity, porosity, and recharge, the team can better predict the long-term outcomes of various remediation strategies. The insights gained from these tests will be invaluable in refining the models and ensuring their robustness.

Additionally, ongoing efforts are focused on determining which indicators may be extracted from the model to inform soil function and soil health tools. This involves a detailed examination of the hydraulic and chemical properties of the soil, including porosity, hydraulic conductivity, soil moisture, and contaminant concentration. By understanding these parameters, researchers can develop more effective remediation strategies that address the specific challenges posed by PFAS contamination. This comprehensive approach ensures that the models not only provide accurate predictions but also contribute to the development of practical solutions for soil and groundwater remediation.

2.4.7. Planned activities for the upcoming period

Evaluation of Hydrus and MODFLOW water fluxes and boundary conditions is a critical step in understanding the dynamics of water movement and distribution within our study areas. This involves detailed assessments of how water fluxes, such as infiltration and groundwater recharge, interact with various boundary conditions set within the model. By comparing the outputs from HYDRUS and MODFLOW simulations, the research team can identify discrepancies and refine the models to ensure accurate representations of the study site conditions. This evaluation is essential for predicting the long-term impacts of remediation strategies and for guiding decision-making processes.

Assessing the fluxes of PFAS in HYDRUS 1D /PHREEQC, with varying partitioning coefficients in both the unsaturated and saturated zones, provides insight into the behavior and movement of these contaminants. This assessment allows researchers to simulate different scenarios to see how PFAS interacts with soil and groundwater under varying conditions. By adjusting partitioning coefficients, which influence how PFAS is retained or transported within the soil, the team can better understand the potential spread and concentration of these contaminants over time. This information is crucial for developing effective remediation strategies and for mitigating the risks associated with PFAS contamination.

The comparison of results between 1D and 2D models is another important step. While 1D models, such as HYDRUS 1D /PHREEQC, are valuable for understanding the vertical distribution of contaminants and water fluxes, 2D models provide a more comprehensive view by incorporating horizontal and vertical interactions. By comparing the results from both types of models, the researchers can validate their findings and ensure that the simulations accurately capture the complexity of the real-world scenarios. This dual approach enhances the robustness of the study and helps in refining the models to better predict the outcomes of various remediation strategies.

Establishing a framework for coupling HYDRUS 1D/PHREEQC with MODFLOW/MT3D is a significant advancement in the modeling process. This coupling allows for the integration of detailed soil moisture and contaminant transport simulations from HYDRUS 1D /PHREEQC with the comprehensive groundwater flow modeling capabilities of MODFLOW. By combining these two powerful modeling tools, the research team can create a more holistic and accurate representation of the subsurface environment. This integrated approach is essential for evaluating complex remediation scenarios where both soil and groundwater interactions play a critical role. The framework will serve as a foundation for future studies and for the development of more effective remediation strategies.

2.5. The Rotterdam Urban Area (NL)

2.5.1. Purpose of the site within the PHISHES project

The city of Rotterdam is the second largest city in The Netherlands and is situated in the Rhine-Meuse delta in the southern part of the Netherlands. It is a key economic city due to its strategic location along the Maas river. In urban areas, complex environmental challenges emerge from the interaction between new developments and issues such as urban greening, biodiversity, groundwater recharge, salinization, soil health, ecosystem services, groundwater quality, water management, the unsaturated zone, and land-use change. The Municipality of Rotterdam is addressing the challenges posed by climate change and biodiversity loss. Various programs have been developed to be implemented at the street and neighbourhood level. The presence of contaminants such as organic pollutants and heavy metals in soil and groundwater may hinder efforts to achieve soil health objectives. At the same time, these circumstances offer opportunities to integrate measures with nature-based solutions. Gaining insight into these factors is essential. This initiative aims to assess the cumulative effects of environmental measures—both across the city as a whole and within the specific areas where they are applied.

The urban area of Rotterdam will act as a real-life testcase for evaluating the effects of various nature-based solutions on soil health parameters. At this moment, various nature-based measures are being implemented, and effects are evaluated in a quantitative way. Examples of already implemented measures are underground urban water buffers, green-blue schoolyards, and bioswales (Toolkit - Rotterdams Weerwoord). The main reason for implementing these various measures is to reduce peak discharge in heavy rain events and increase greening to deal with temperature rise due to climate change. The municipality is interested in how these measures would affect soil health parameters as well. Especially as the goal to reduce (the spread of) soil pollution might conflict with the goal to promote infiltration of rainwater instead of all rainwater going into the sewage system.

In urban areas several different interests interact in a small area. Currently, our understanding of soil health in urban areas is limited. Increasing our understanding of urban soil health, and how climate change and changing land use influence soil health will aid in creating sustainable urban environments. Additionally, in urban areas space is usually limited, which might complicate the suitability of certain measures. The advantage of including the Rotterdam urban area as a test site in the PHISHES project is that the test site will help understand soil health in urban environments, and aids in determining relevant measures that not only serve soil health but also other relevant interests in urban areas, like stable soil for infrastructure.

2.5.2. Description of the basin/site

Rotterdam consists of a large harbor area and urban area (see Figure 32). The urban area of Rotterdam is situated in a polder area; the largest part is between 2 and 6 meters below sea level. To protect these areas from flooding, dike rings are in place to keep river and seawater out. Within these dike rings, all net precipitation must be drained out, upward to the river and/or sea level. This is achieved through drainage systems and pumps. The city is divided into two divisions by the 'Nieuwe Maas' river, which is a distributary of the Rhine River, and a former distributary of the Maas River. Rotterdam is situated in the southwest of the Netherlands.

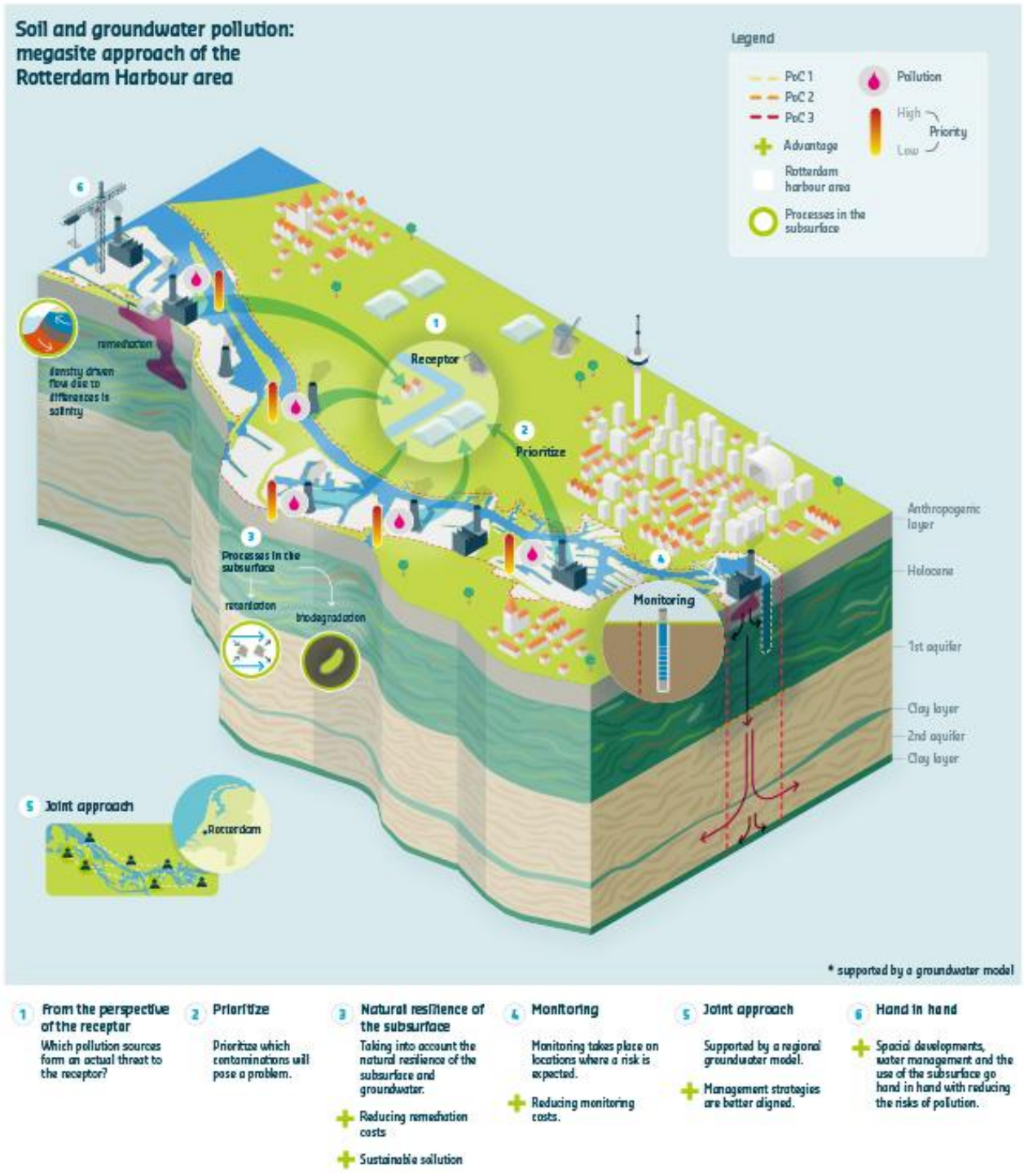


Figure 32 Location of Rotterdam in the Netherlands (bottom left) and cross section of harbour and urban area.

The soil consists of a maximum two-meter-thick anthropogenic top layer of sand and rubble (see Figure 32). The rubble originates from the bombing of historical buildings during WWII. This

layer is not always present and varies in thickness. Below are the Holocene deposits consisting of sandy clay, clay and peat. This layer is approximately 15 -20 meters thick. Below these are the sandy deposits from the Pleistocene Kreftenheye formation. This is the first (regional) aquifer. The 'Nieuwe Maas' river cuts through the Holocene deposits and has a direct connection with this regional aquifer. For most parts, the urban area is situated on top of the Holocene deposits. This means that the local urban (ground) water system is relatively isolated from the regional groundwater system.

Traditionally precipitation infiltrates to the groundwater and is drained by local surface waters. These local surface waters are discharged into the river via various pumping stations. Due to urbanization the amount of paved areas increased, and local surface waters were removed. Within this paved area, precipitation is now mainly discharged via the sewage system. Currently, this causes flooding problems during intense rainfall events. With future climate change and increased urbanization, these problems are expected to become more severe.

The increased paved area also reduced the amount of vegetation. Both gave positive feedback on the urban heat island effect. Studies show that this reduces the quality of living for its inhabitants, especially considering future climate changes.

In 2023, 663,500 people lived in the Rotterdam urban area (Rotterdam | 2024 | Wijkprofiel Rotterdam). Over the years the population of Rotterdam is slowly increasing. The people of Rotterdam live on a small surface area with on average around 5100 people per km^2. Almost 55% of the surface area in Rotterdam is paved (Buurtdashboard - Klimaateffectatlas). Compared to other parts of the Netherlands people in Rotterdam are relatively vulnerable to the negative effects of climate change. Due the relatively high percentage of older people (65+) with poor health, people with a small social network, and people living in poverty, people in Rotterdam are more vulnerable to heat (Buurtdashboard - Klimaateffectatlas). Additionally, a large part of Rotterdam is currently vulnerable to significant flooding, with more than 60% of Rotterdam facing flood depths of more than 50 cm, of which 22% could face flood depths of over 2 m (Buurtdashboard - Klimaateffectatlas). The vulnerability to climate change has compelled the municipality of Rotterdam focus on climate adaptation. Current measures focus on local water buffers and urban greening.

2.5.3. Existing data available

Water quantity

The Municipality of Rotterdam operates an extensive monitoring network for groundwater levels. These data are disseminated via the GIS web service of the Geological Survey of the Netherlands (TNO) through Ondergrondgegevens | DINOloket. The spatial distribution of the monitoring wells is presented in Figure 33.



Figure 33: Locations of the available groundwater level monitoring wells

The dataset comprises both historical and contemporary monitoring series, with measurement periods varying substantially; in several instances, observations commenced prior to 1950. The average temporal resolution of these data is one observation per month. An illustrative example of such a time series is presented in Figure 34.

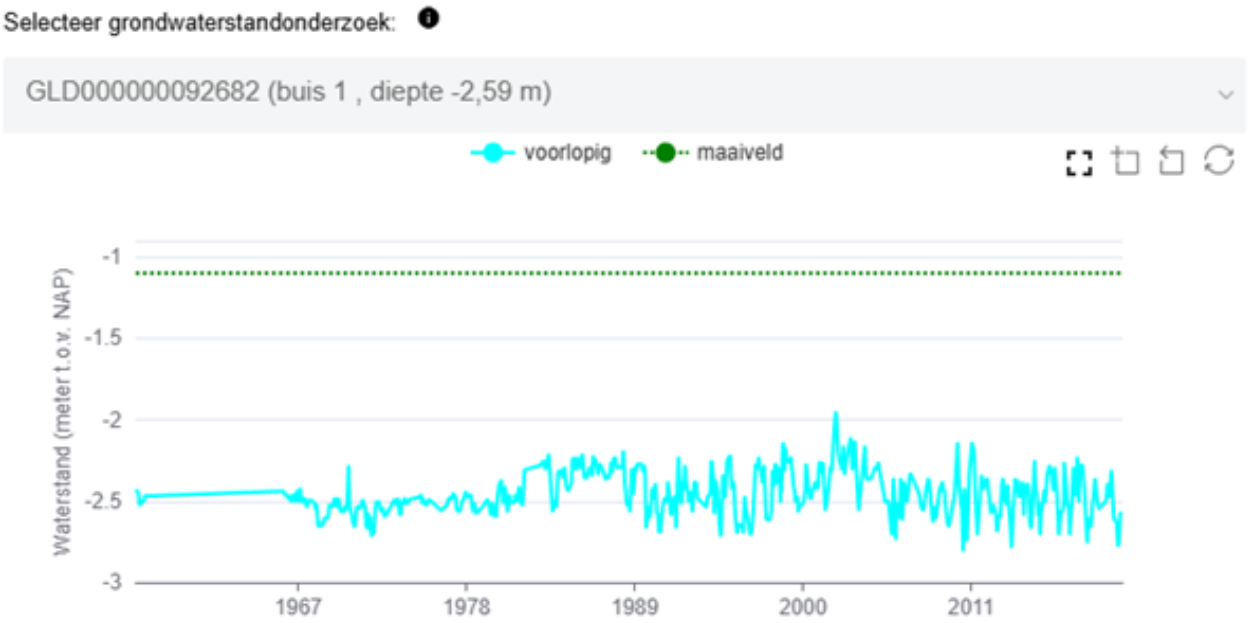


Figure 34: Timeseries of groundwater levels for a specific location in Rotterdam at a depth of NAP –2.59 m. NAP stands for 'Normaal Amsterdams Peil', the national reference level for the Netherlands. This approximately corresponds to the geoid.

In addition to these publicly accessible data, the Municipality has collected high-frequency (10-minute interval) time series of groundwater levels and drainage discharge in the context of various applied projects. Within these projects, experimental infiltration events were implemented in engineered infiltration facilities. These high-resolution datasets have previously been employed, among other purposes, for the validation of modelling workflows and will again be incorporated in the present study.

Water and soil quality

The average quality of the soil and groundwater within the phreatic aquifer is well documented. These data are synthesised in the official soil quality map that is available in Annex 2 of the Soil Management Memorandum (Nota bodembeheer Rotterdam)

Figure 35 depicts the quality classification of the uppermost section of the phreatic aquifer (to a depth of 1 m below ground level).

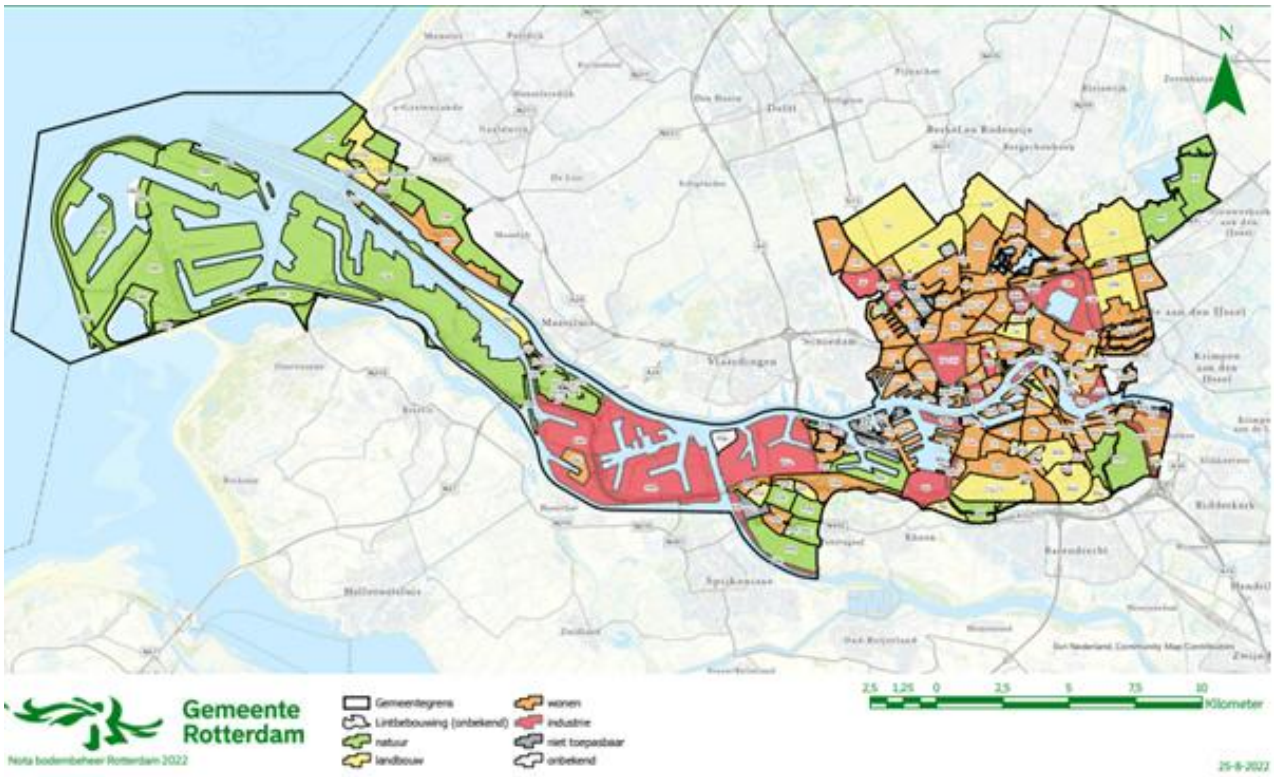


Figure 35: Soil quality classification of up to 1 m below ground level for the city of Rotterdam. Within the urban area, the classifications residential (orange), industrial (red), agriculture (yellow) and nature (green) are present. The black lines represent the boundaries between various neighbourhoods.

The predominant classification within the urban area of Rotterdam is “residential.” This designation corresponds to the reference values for a standard soil composition (10% humus, 25% clay) for both soil and groundwater. Annex 2 of the Soil Management Memorandum (Nota bodembeheer Rotterdam) specifies the relevant water quality parameters, including metals, organometals, inorganic compounds, aromatic hydrocarbons, and PFAS. In Table 8, an example for Metal parameters is shown, for the various classifications shown in Figure 35. The residential area in Figure 35 (orange) correspond to the column ‘(L) MW Wonen’ in Table 8.

Table 8: Reference values for metal parameters, for the soil quality classifications 'soil quality map'. In the Rotterdam Urban area the class '(L)MW Wonen' is dominant (residential areas in orange).

Parameter	AW	LMW Landbouw	(L)MW Wonen	(L)MW Industrie	I-Waarde	Opmerkingen
metalen:						
aluminium	**30.000**				**70.000**	
antimoon	4,0	**5**	15	22	22	
arseen	20	**30**	**40**	76	76	
barium	190	**280**	550	920	920	antropogeen
beryllium	1,5	**1,9**	**3,4**	30	30	
cadmium	0,60	**1,0**	**3,7**	**13**	13	
chroom(III)	55	**80**	**120**	180	180	
chroom(VI)	**0,5**	**0,5**	**0,5**	**78**	[78]	
kobalt	15	**25**	**50**	190	190	
koper	40	**60**	**100**	190	190	
kwik	0,15	**2,0**	4,8	4,8	36	
lood	50	**200**	**300**	**530**	**530**	Bij gevoelig gebruik zie §3.2.2
molybdeen	1,5	**10**	88	190	190	
nikkel	**60**	**60**	**75**	100	100	
seleen	**3,0**	**9,0**	**50**	**100**	[100]	
thallium	**1,0**	**2,6**	**8,0**	15	[15]	
tin	6,5	**40**	**200**	900	[900]	
vanadium	80	**100**	**150**	250	[250]	
zilver	**2,5**	**5**	**7,5**	**10**	[15]	
zink	140	**200**	**350**	720	720	

The reference values have been spatially aggregated to a neighbourhood scale, illustrated in Figure 35. Greater spatial resolution, down to the level of point-specific data, is available through Rapportage via zoeken op adres op kaart.

In accordance with regulatory requirements, soil investigations are mandatory prior to undertaking any subsurface interventions in Rotterdam. The substances to be tested depend on the nature of the proposed activities. Reports from both historical and recent investigations are publicly accessible via the online reporting system, which allows address-based queries on a geospatial interface. The locations of these investigations are visualised in Figure 36 as red markers.

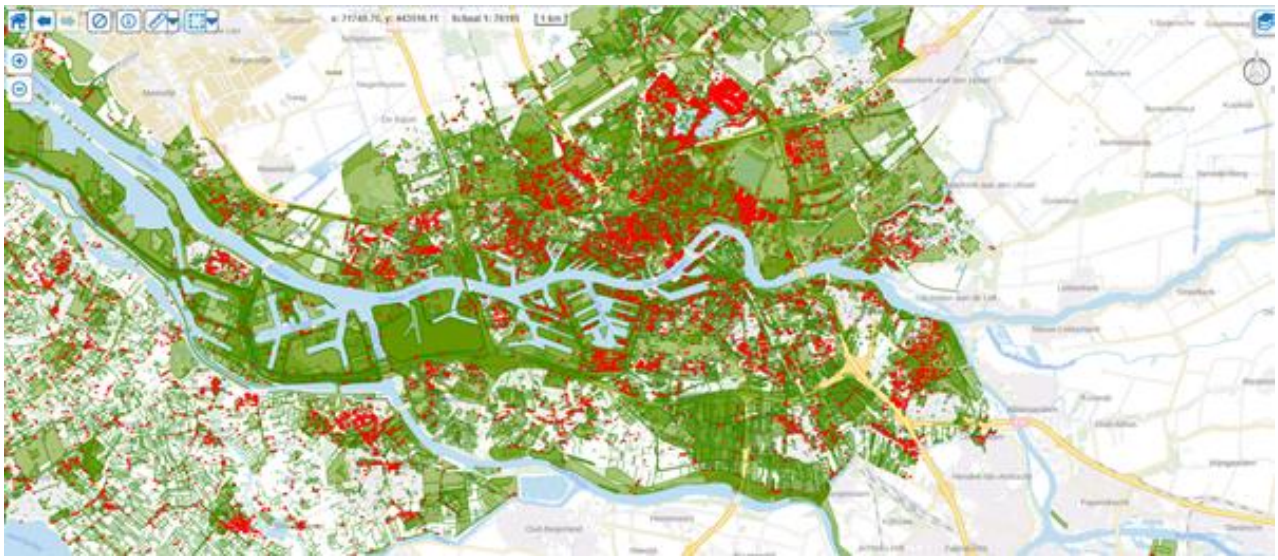


Figure 36: In red the locations of available (historical) soil investigations

Soil type

Various types of data are available regarding subsurface composition. Borehole and cone penetration test (CPT) profiles can be accessed via Ondergrondgegevens | DINOloket. Figure 37 shows the locations of the available data.



Figure 37: Location of borehole profiles (light brown) and CPT profiles (dark brown).

Figure 38 presents an example of an available borehole profile for a specific point location.

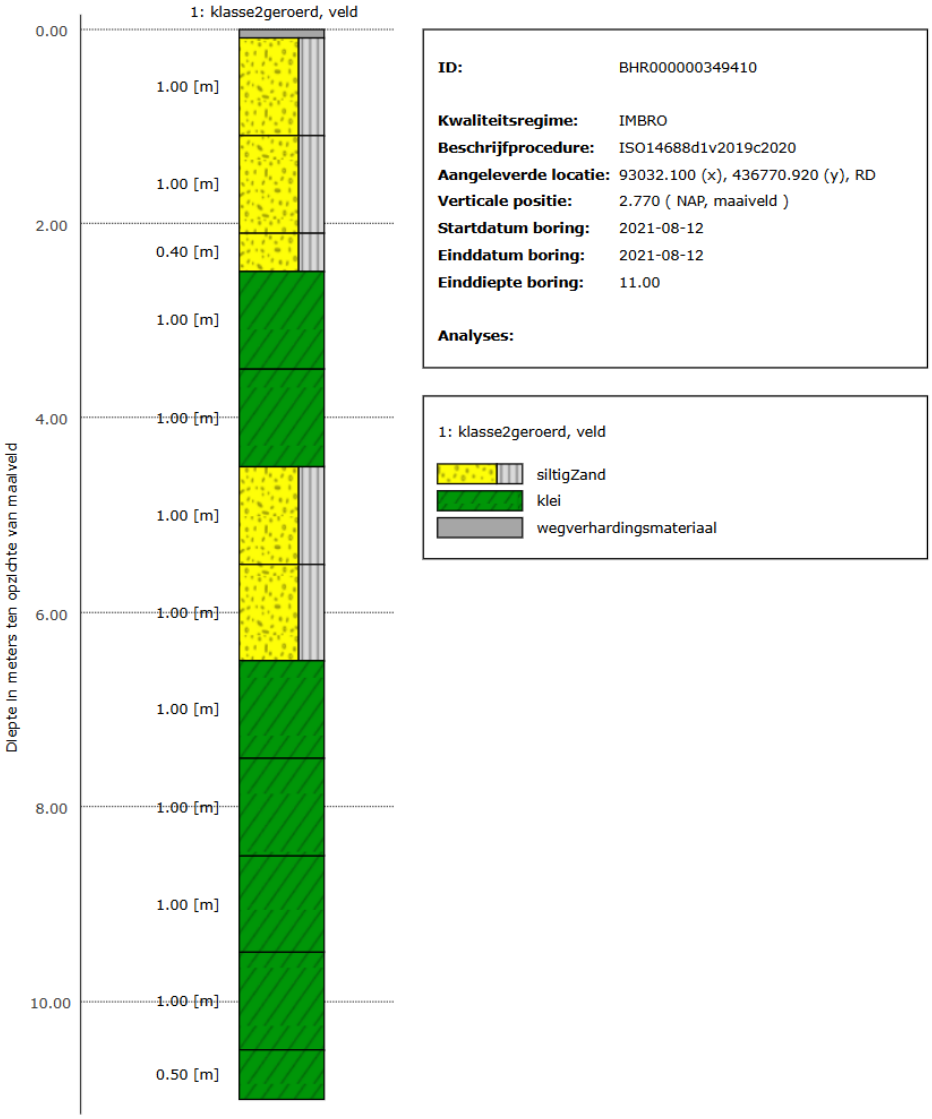


Figure 38: Borehole profile for a specific location.

In addition, several subsurface models provided by TNO are available for the Rotterdam area. For the phreatic aquifer, the **GeoTOP model** is the most relevant. This voxel model provides a detailed description of the upper 50 meters of the subsurface. The model has a vertical resolution of 0.5 meters and a lateral resolution of 25 meters. Figure 39 illustrates, as an example, a north–south cross-section displaying the most probable lithological classes.

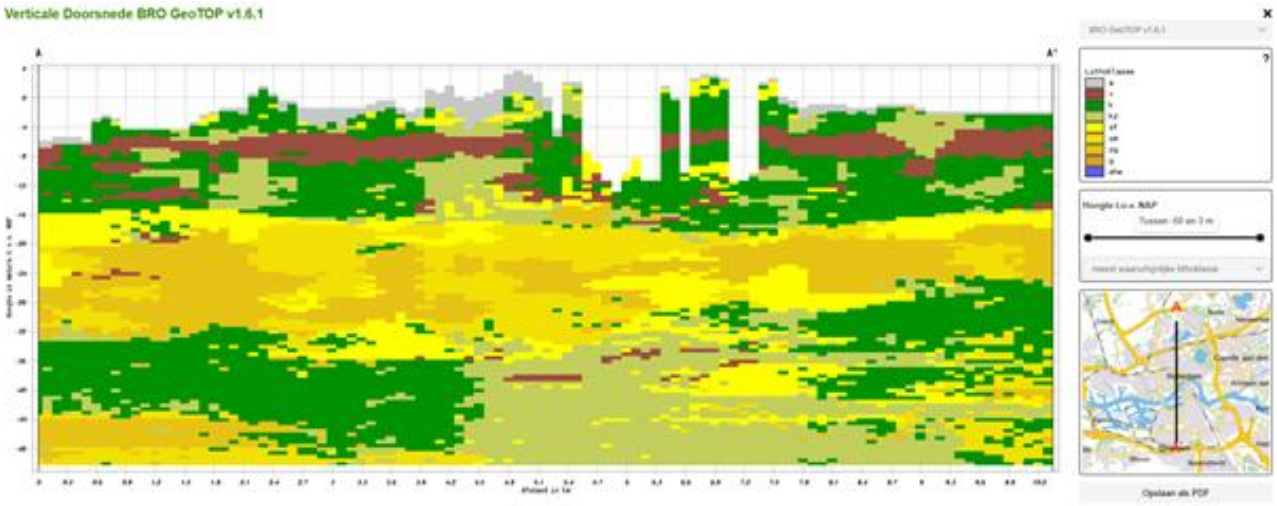


Figure 39: A north–south cross-section of GeoTOP (TNO) showing the most probable lithological classes. In grey: anthropogenic fill; in yellow: sandy deposits; in brown: peat; and in green: clay.

Meteorological data

Meteorological data are available for the airport located on the northern side of Rotterdam (*Rotterdam The Hague Airport*) and at the most western side (*Hoek van Holland*) of Rotterdam. For these stations, variables such as precipitation and Makkink reference evapotranspiration are available.

The observational records extend from 1970 (Hoek van Holland) and 1956 (*Rotterdam The Hague Airport*) up to the present, with data available at a daily time step.

Climate change data

The Royal Netherlands Meteorological Institute (KNMI) has translated the AR6 IPCC climate scenarios to local conditions in the Netherlands. These scenarios have been converted into key indicators for four scenarios and 4 time horizons. The indicators are available per season via KNMI Klimaatscenario's. Based on these data, transformed time series are available for, among others, the Hoek van Holland station. For each scenario and time horizon, it is thus possible to generate, for example, precipitation and reference evapotranspiration series.

2.5.4. Additional – optional – monitoring within the project frame

During the course of this project, a study will be conducted on the relation between various land use types (e.g. paved and various types of vegetation) and various soil health parameters. The outcome of this study can be used to relate model outcome to soil health parameters. In a “living lab-site setting”, a large-scale experimental soil pilot study is set up at the campus location of Deltares in Delft (see Figure 40). The expected output of this study is knowledge on indicators that are usable for determining urban soil health. The pilot study creates knowledge on the impact of spatial planning (or land use) on the performance of these indicators (or soil health). The pilot study consists of 4 test fields of 5x5 meter. The soil conditions are the same, but environmental conditions are different: 1. Covering 2. Planting and 3. Under water. Three rounds of measurements will be taken. A list of soil health indicators is based on existing knowledge on soil health indicators: carbon content, biodiversity, nutrients, physical conditions, texture, water content, stability.



Figure 40. Pilot field soil health experiments.

The municipality of Rotterdam is planning a detailed monitoring of water quality in drain discharge and groundwater around a newly realized drainage pond. This monitoring is not part of this project, but the outcome will be used to validate the model workflow.

2.5.5. Tools, model trains, scenarios expected to be employed or utilized

Deltares developed a model workflow for the quantitative evaluation of the effect of various nature-based solutions. This workflow is based on the MODFLOW 6 (MF6) framework. For surface

water ponding, a water balance model was developed by Deltares. This model keeps track of the water balance at the subsurface and relates this to a ponding water level and inundation zones. This is online coupled to the Unsaturated Zone Flow (UZF) package via the available API. The coupling scheme is shown in Figure 41.

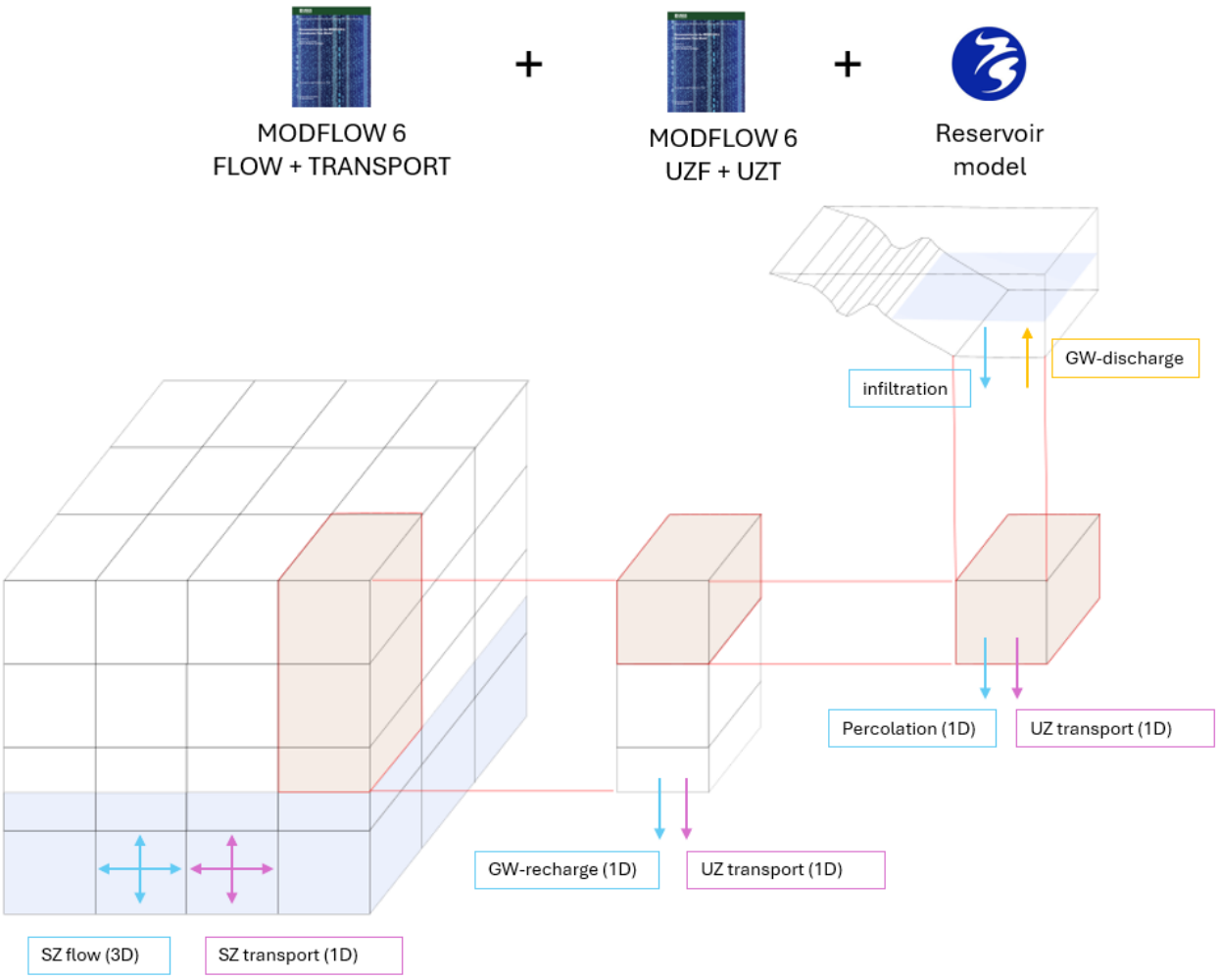


Figure 41: coupling scheme for MF6 – UZF - Reservoir-model.

The UZF-package is a 1D Richards based model taking only the gravitational potential into account. This is done by removing the diffusive term from the Richards equation and solving the resulting two differential equations via the Method of Characteristics.

The first equation describes the velocity of a wetting or drying front as

$$\frac{dz}{dt} = \frac{\delta K(\theta)}{\delta \theta} = v(\theta),$$

where $\delta K(\theta)$ is the change of the unsaturated hydraulic conductivity due to a change in water content, $\delta \theta$ the change in water content and $v(\theta)$ the wave velocity.

The second equation describes the change of water content due to evapotranspiration as

$$\frac{d\theta}{dt} = -iET,$$

Where $-iET$ is the evapotranspiration rate. It is assumed that evaporation is removed from the soil profile immediately.

For evaluating $K(\theta)$, the Brooks-Corey model is used as

$$K(\theta) = K_{sat}\left[\frac{\theta - \theta_{resid}}{\theta_{sat} - \theta_{resid}}\right]^{\epsilon},$$

Where ϵ is the Brooks-Corey exponent, K_{sat} is the saturated hydraulic conductivity, θ_{sat} and θ_{resid} the saturated and residual water content respectively.

The UZF-package is internally coupled to the saturated zone in the MF6-framework by exchanging the recharge flux at the bottom of the unsaturated zone. To keep the water balance consistent, the Specific Yield (SY) used for the saturated zone is computed via

$$Sy = \theta_{sat} - \theta_{resid}.$$

For the saturated zone MF6 solves Darcy's equation for saturated and constant density groundwater flow. To deal with the wetting and drying of cells in the phreatic aquifer, the Newton formulation is used.

The workflow is already validated using field measurements for experimental infiltration events. For these experimental events both the inflow rate, ponding water levels, groundwater levels and drain discharge from the ponding reservoir were measured and compared to the model output.

Within this project this workflow will be updated with transport functionalities to simulate the transport of contaminants in the unsaturated and saturated zone.

2.5.6. Activities executed on site up to date

The workflow was extended with solute transport functionalities. This was done by using the available groundwater transport models in the MF6 framework. This deals with both advection and diffusive transport in the unsaturated (1D) and saturated zone (3D). A first technical validation of the results was was carried out. The results appear plausible, as they show continuous transport from the unsaturated zone (1D) toward the saturated zone (3D) and into a fixed boundary condition.

2.5.7. Planned activities for the upcoming period

For the upcoming period the work from current period will be finalised. This means that the work on the workflow will be finalised and further validated. This still will be a technical validation using standardised reference test models. Actual validation with field measures will take place later.

Together with the municipality a first concept of scenarios will be derived. The scenarios will describe the type of measures and under which conditions these will be evaluated. The type of measures could be the implementations of various infiltration measures. This can be evaluated under different future climatological condition and urbanisation trends.

In addition to the scenarios and the technical validation of the workflow, specific local test sites will be selected for validation and effect evaluation using the model workflow.

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