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PROMISCES

Preventing **R**ecalcitrant **O**rganic **M**obile **I**ndustrial chemical**S** for **C**ircular **E**conomy in the soil-sediment-water **S**ystem**S**

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D2.3 – Toolbox fate & transport modelling of PMTs in the environment

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Executive Summary

The "Toolbox Fate & Transport Modelling of PMTs in the Environment" is a key deliverable from the H2020 PROMISCES project. This toolbox is a demonstrator that includes a collection of models developed in the PROMISCES project which are designed to assess the fate and transport of persistent, mobile, and toxic substances (PMTs) across various scales (local, regional) and conditions (e.g., urban run-off, bank filtration, unsaturated zone, groundwater).

This toolbox presents the basic information with links to the software and model input files with which the models can be run. This deliverable is intended for qualified modellers. It is complementary with the Guidance document, deliverable D2.4 (Zessner et al., 2025) which describes how to apply modelling tools in a tiered way as part of predictive risk assessment.

This report provides an overview of innovative approaches for fate, transport, and exposure to persistent, mobile, and potentially toxic (PM(T)) chemicals, presenting model results from the PROMISCES project. It includes:

- Models for identifying PM(T) properties using *in silico* approaches (QSPR/QSAR, Artificial Intelligence, machine learning).
- Screening level models for PM(T) exposure assessment.
- Models for soil-groundwater interaction.
- Fate and transport models for bank filtration sites.
- Fate and transport models in urban contexts.
- Emission models on a catchment scale.

Each model includes a technical description, followed by an explanation of how the models were improved and links to executable files and input data.

An overview of the model improvements is presented below.

Models for identifying PM(T) properties using *in silico* approaches.

Significant improvements were made to the **predictive QSPR models** designed to assess the properties and environmental behavior of PFAS compounds, enhancing their accuracy, applicability, and predictive power:

- 2 new QSPR models for predicting n-octanol-water partition coefficient (LogKow), and Bioconcentration Factor (BCF));
- 2 improved QSPR models (for predicting Water Solubility (logSW) and Vapor Pressure (logVP)) expanding the applicability domain for PFAS compounds;
- 1 model for predicting Melting Point (MP) was adapted conducting a detailed applicability analysis which confirmed its use for predicting the melting points of PFAS compounds.)

As part of **in silico predictive tools (other than QSPR/QSAR)** for identification of PM(T) a new predictive model has been developed. The final developed model is based on XGboost on a large diverse dataset of chemicals and species. The innovative character is in its ability to learn patterns from this wide range of chemicals and species, as well as the model architecture which closely resembles current risk assessment practices.

Screening level models for PM(T) exposure assessment.

In comparison to the earlier **SimpleBox** (4.01) version, the following improvements were added to the SimpleBox - Aquatic Persistence dashboard (SB-AP):

- Additional model routines to express aquatic persistence of emitted substances across surface water bodies at regional, continental and global scales.
- A macro function has been developed to enable the user to insert input values as ranges instead of single fixed values. As such, the SB-AP Dashboard is able to present the level of uncertainty inserted in the input values -emission volumes and physicochemical properties of the substance- as well as resultant ranges of uncertainty in the model outcomes.
- An option is added for the user to perform probabilistic sensitivity analyses to investigate the relationship between physicochemical properties of the substance and aquatic persistence of dissolved and sorbed species. The user is as such served with a new tool to evaluate the extent to which a persistent and mobile substance resides in surface waters and displaces to different spatial scale.
- The applicability of the SB-AP Dashboard as a tool for dedicated environmental fate studies is demonstrated with a case study in which the aquatic persistences have been expressed for eight different PFASs and how these compare to the current criteria for (very) persistent and (very) mobile substances (Zessner et al., 2025).

The **operational approach for deriving generic risk limit in a leaching situation** makes use of existing models Hydrus 1D and Modflow 6. Whereas these models are commonly applied to predict leaching and transport at local scale, in this application the models are parametrized in order to underpin generic risk limits for leaching. In the Guidance document, (deliverable D2.4, chapter 2.3, Zessner et al. 2025), sample calculations for the 'Dutch situation' have been included as well as pointers to decide on parametrization of the models in different areas.

The **probabilistic human health risk assessment for four reuse pathways** (HHEA) is built on Bayesian principles, which enable assessment of risk under conditions of low data availability and high uncertainty. This is particularly useful for evaluation of substances such as PFAS and other industrial persistent, mobile and potentially toxic (iPMT) substances, the removal of which in treatment processes is not yet well studied in literature. To date, Bayesian principles have been applied for assessing human health risks from microbial contaminants in water, but this framework has not yet been successfully adapted for chemical substances, due to their generally more chronic human health effects in comparison to acute effects from microbial contaminants. Therefore, the Bayesian principles were applied in a new model to enable assessment of literature, site specific, and modelled data to quantify the exposure risk for human health.

Models for soil-groundwater interaction.

In order to develop a **model train** for the soil-groundwater interaction the existing model codes of **Hydrus-1D, Modflow and MT3DMS** were coupled to model transport of PFAS in the unsaturated and saturated zone. The Hydrus-1D and MODFLOW are fully coupled considering the interaction between the unsaturated and saturated zone for water flow. For the coupling of the mass transport a post processing tool was developed to process the time-variant water and mass fluxes at the water table interface using input files for MT3DMS.

The presented approach is the combination of two complementary already-existing subsurface modelling codes: MODFLOW/MT3D and HYDRUS1D. The coupling consist in a single concatenation in the execution of both models. Therefore, no addition or modification to the original codes has been performed. The objective of this **python-based model train** is to provide a simple but effective modelling approach to estimate transport of PFAS in soil and groundwater, which can be used by operators as a first attempt to characterise PFAS polluted sites with scarce field data.

Fate and transport models for bank filtration sites.

The **small- and large-scale 3D numerical (iMOD/MT3DMS) models** employ pre-existing, well-established codes for groundwater flow and reactive solute transport. The novelty of the approaches with respect to their application to PMT substances is embedded in the use of experimentally derived sorption rates. The functionality of the chosen reactive transport code (MT3DMS) to deal with the occurring sorption kinetics was already satisfactory, and the field monitoring data did not warrant even more complex kinetics.

The **generic bank filtration model** translates a one-dimensional analytical model for calculating the sorption and degradation of chemicals traveling through groundwater into the R language. It also offers two visualization options that can be used with minimal R knowledge. This model enhances the usability and accessibility of generic analytical model approaches for PMT substances and other chemicals traveling through groundwater.

Fate and transport models in urban contexts.

The existing **emission model in an urban context** (urban mass balance/load model for Berlin) has been adapted with some updates and new features. In particular, the model was adapted to include 31 PMT- and PFAS-substances. Furthermore, the model's temporal resolution has been improved from an annual to a monthly scale, allowing for a more precise representation of pollutant loads by accounting for the seasonality of rainfall. In addition, the Berlin-specific input data have been updated ensuring a more accurate representation of the current hydrological and pollution dynamics in Berlin's surface waters.

The suite of programs that is used for the Berlin urban water system and development of the **DELWAQ/SOLUTIONS model**, consists of several pre-existing programs. The novelty is that these programs with a different background have been combined into a program suite for a complex surface water system by combining:

- An estimate of the loads from urban sources, using stochastic approaches.
- A hydraulic model system (water balance model) that provides the flow field and the geometrical information.
- A general water quality model that can combine the information on loads and water balance into a program suite for a complex surface water system.

The surface water system is first modelled via a hydrodynamic or hydraulic program that has been developed in close cooperation with the water quality program. In this case, the most important step was the estimation of the loads from the various wastewater treatment plants and the incorporation into the set-up for water quality calculations. The water system was schematised on the basis of the pre-existing water balance model. In a complex water system like that of Berlin where actually data on water quality are scarce, it is advantageous to have a tool that can be adapted to the situation with relatively little effort. The model suite was applied to a more or less generic PFAS type, as no information was available on the actual compounds.

Emission models on a catchment scale.

The existing **Modelling of Regionalized Emissions (MoRE) model** was adapted for modelling of PFAS. Additional emission pathways were implemented, which might be significant for PFAS and other pathways with less significance for this substance group were simplified and grouped together. The model now contains the following pathways: point sources and diffuse pathways.

Three model variants for the current state were implemented to represent the uncertainty in the model input data: base variant / best-case / worst-case.

The **PROMISCES watershed model for PM substances (PPM) model** is an application of a pre-existing set of interlinked tools to a new application domain. The novelty lies in the application to a larger group of 10 PFAS substances. These substances constitute a significant share of the 24 PFAS substances that are included in the proposed Environmental Quality Standard under the Water Framework Directive. As such, the results have a direct relevance for chemicals policy and risk assessment. Another novelty of the current implementation is the simulation of a precursor-end product combination (PFOS and precursor N-EtFOSAA) at the scale of a large watershed. Here, two separate emission models (one for the precursor and one for the end-product) have been set up to feed into a combined aquatic transport and fate model. This set-up presumes that the transformation of the precursor proceeds only (to a significant degree) in the surface water compartment. It leads to a noticeably better agreement between the simulated and observed concentrations of the end-product.

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List of abbreviations

Abbreviation	Definition
ADONA	4,8-dioxa-3H-perfluorononanoic acid
AFFF	Aqueous film forming foam
AI	Artificial intelligence
AI/ML	Artificial intelligence/Machine learning
AR	Activity rate
BCF	Bioconcentration factor
BF	Bank Filtration
CCC_{EXT}	Concordance correlation coefficient
CE	Circular Economy
CSO	Combined sewer overflow
CV	Cross validation
EC50	Half maximal effective concentration
ECHA	European Chemicals Agency
HFPO-DA / GenX	hexafluoropropylene oxide dimer acid /perfluoro-2-propoxypropanoic acid
f_{OC}	Fraction of organic carbon
GW	Groundwater
HC5	Hazardous concentration effecting 5% of species
HHEA	Human health exposure assessment
IMOD-WQ	iMOD-Water Quality; graphical User Interface + an accelerated Deltares-version of MODFLOW (see below)
iPMT	Industrial persistent, mobile and potentially toxic substance
K_d	Linear adsorption isotherm for soil or sediment
KGE	Kling-Gupta model efficiency coefficient
KIT	Karlsruhe Institute of Technology
K_{oc}	organic carbon-water partition coefficient
K_{ow}	octanol/water partitioning coefficient
LC50	Lethal concentration 50
LOQ	Limit of quantification
ML	Machine learning
MP	Melting point
MPC	Maximum permissible concentration
MoRE	Modelling of Regionalized Emissions
MODFLOW	Modular three-dimensional finite-difference ground-water flow model
MODPATH	A particle-tracking postprocessing package that was developed to compute three-dimensional flow paths using output from steady-state or transient ground-water flow simulations by MODFLOW
MT3DMS	Modular Three-Dimensional Multispecies Transport Model for Simulation
MW	Monitoring Well
NOEC	No observed effect concentration
NSE	Nash-Sutcliffe model efficiency coefficient
N-EtFOSAA	N-ethyl perfluorooctane sulfonamido acetic acid

Abbreviation	Definition
PC	Personal computer
PFAS	Per- and polyfluoroalkyl substances
PFBA	perfluorobutanoic acid
PFBS	perfluorobutane sulfonic acid
PFHpA	perfluoroheptanoic acid
PFHxA	perfluorohexanoic acid
PFHxS	perfluorohexane sulfonic acid
PFOA	perfluorooctonoic acid
PFOS	perfluorooctane sulfonic acid
PFPeA	perfluoropentanoic acid
PKS	Parallel Krylov package
PM	Persistent and mobile chemicals
PMT	Persistent, mobile and toxic chemicals
POC	Point of compliance
PPM	PROMISCES watershed model for PM substances
QMRF	QSAR model reporting format
QSAR	Quantitative Structure-Activity Relationship
QSPR	Quantitative Structure Property Relationship
R^2	Coefficient of determination
REACH	Regulation concerning the Registration, Evaluation, Authorisation and Restriction of CHemicals
$RMSE_C$	Root mean squared error
$RMSE_{EXT}$	Root mean squared error
SB-AP Dashboard	SimpleBox - Aquatic Persistence dashboard
SPM	Suspended particulate matter
SSDs	Species-sensitivity distributions
Sw	Water solubility
VP	Vapor pressure
WFD	Water Framework Directive, EU regulatory instrument for water management
WWTP	Waste Water Treatment Plant

1. Introduction

PROMISCES identifies how industrial pollution prevents the deployment of the circular economy (CE) in the EU and which strategies help overcome key bottlenecks to deliver the ambitions of the European Green Deal and Circular Economy Action Plan.

This project considers specific CE routes including (i) semi-closed water cycles for drinking water supply at urban and catchment scale; (ii) wastewater reuse for irrigation in agriculture; (iii) nutrient recovery from sewage sludge; (iv) material recovery from dredged sediment and (v) land remediation for safe reuse in urban areas.

To reach its goals, PROMISCES:

a. Develops new analytical methods and toxicological tools to provide data on persistent, mobile (PM) substances (i.e. PFAS and other industrial chemicals) in complex environmental matrices.
b. Explores sources and environmental pathways of PM substances released from (i) soil; (ii) sediment; (iii) landfills; (iv) wastewater treatment plants and via (v) urban runoff into relevant environmental compartments (soil, sediment, surface water, groundwater).
c. Assess fate and transport pathways within the different CE routes and evaluate the impacts of corrective measures.
d. Improves the assessment and management of human health risks from drinking water and agricultural products.
e. Develops and demonstrate cost-efficient and sustainable technologies for the removal of PM substances from different media.
f. Translates PROMISCES results into guidance for efficient and feasible management of PM substances and recommendations for the implementation of relevant EU policy strategies and directives.
g. Integrates the results into a decision support framework which considers resource recovery and water reuse and supports chemical management decisions with regards to i) stakeholders and societal demands; ii) PM chemical properties iii) technical solutions to prevent, mitigate and remediate industrial pollution and iv) the whole life cycle of current and future chemicals.

The toolbox “Fate & transport modelling of PMTs in the environment” contributes to achieve the goals b, c, d and f.

This deliverable “Fate & transport modelling of PMTs in the environment”, is a product from the H2020 PROMISCES project. The toolbox (a demonstrator) is a collection of (model)trains for the assessment of fate and transport of contaminants at different scales (local, regional) and under different conditions (e.g. urban run-off, bank filtration, groundwater).

Scope and structure of the toolbox

The toolbox presents an overview of the developed and improved knowledge on innovative approaches for fate, transport and exposure to PM chemicals. It is a collection of the model results produced in PROMISCES project. This toolbox is complementary to the Guidance document, deliverable D2.4 (Zessner et al., 2025) which describes how to applied model trains in a tiered way as part of predictive risk assessment. The toolbox presents the basic information with links to the software and model input files with which the models can be run. This deliverable is designed for

qualified modellers. For more information on how to use the software we refer to the information provided by the specific software developers websites.

The structure of the toolbox follows that of the Guidance document by presenting:

- models for identification of PM(T) properties using *in silico* approaches (QSPR/QSAR and AI and machine learning), chapter 2;
- screening level models for the assessment of exposure to PM(T)s, chapter 3;
- models for soil – groundwater interaction, chapter 4;
- fate & transport models for bank filtration sites, chapter 5;
- fate & transport models in an urban context, chapter 6;
- Emission-models on catchment scale, chapter 7.

For all models, a short technical description is given, followed by an explanation of how the models are improved and links to the executable files and model input files.

2. Models for identification of PM(T) properties using in silico approaches

2.1. QSPR models for PM properties identification

2.1.1. Technical description of the model

To develop valuable predictive models, a set of endpoints containing physicochemical properties of PFAS/PMT compounds was selected. Existing predictive models (i.e. models needing individual physicochemical properties) dedicated to PFAS were searched in the literature and evaluated. Available models were verified if they were scientifically valid and could be easily applied for the prediction of the properties of new compounds.

Two existing QSPR models for water solubility (Sw) and vapor pressure (VP) were adopted and improved to predict these endpoints for PFAS in PROMISCES. Additionally, two new QSPR models were developed to predict the octanol-water partition coefficient (K_{OW}) and bioconcentration factor (BCF) of PFAS. Given the limited data availability, a novel approach combining physics-based methods with data-driven models was applied for developing the models for Sw, VP, and K_{OW}.

The available QSPR model for melting point (MP) was evaluated for its applicability to PFAS and selected for use in PROMISCES. All details of the improved and newly developed in silico models for predicting PFAS physicochemical properties are presented in the standardized QMRF (QSAR Model Reporting Format), and the associated datasets and codes are available on Zenodo.

The details of the improved/developed/adopted in PROMISCES *in silico* models for predicting the physicochemical properties of PFAS are presented in Table 1.

Table 1: Equations of the developed predictive models.

Endpoint	Model equation and statistics	References
Water solubility (S_W)	$\log S_W$ = 1.049 (±0.178) – 1.981 (±0.204) x T(F..)F + 1.042 (±0.204) x SIC1 T(F..F) - sum of topological distances between F..F (T(F..F)) SIC1 - structural Information Content index (neighbourhood symmetry of 1-order) R^2 = 0.85 $RMSE_C$ = 1.13 Q^2_{LOO} = 0.83 $RMSE_{EXT}$= 1.327 Q^2_{F1} = 0.71 Q^2_{F2} = 0.71 Q^2_{F3} = 0.79	Publication: Sosnowska et al., 2023, Zenodo. https://doi.org/10.5281/zenodo.11446922 Model: Mudlaff, M., 2024. Datasets from deliverable 2.1. on the physicochemical properties of PFAS compounds [Data set]. Zenodo. https://doi.org/10.5281/zenodo.13330024 Streamlit app: https://physchempfas.streamlit.app/

Table 2: Equations of the developed predictive models (continued).

Endpoint	Model equation and statistics	References
Vapor Pressure (VP)	logVP = - 0.8314 (±0.143) – 2.2117 (±0.149) x F03[C-F] – 0.2274 (±0.180) x nDB – 1.8076 (±0.175) x AAC F03[C-F] - Frequency of C – F at topological distance 3 AAC - Mean information index on atomic composition nDB - Number of double bonds R^2 = 0.92 $RMSE_C$ = 0.86 Q^2_{LOO} = 0.90 $RMSE_{EXT}$ = 0.86 Q^2_{F1} = 0.91 Q^2_{F2} = 0.91 Q^2_{F3} = 0.92	Publication: Sosnowska et al., 2023. Zenodo. https://doi.org/10.5281/zenodo.11446922 Model: Mudlaff, M., 2024. Datasets from deliverable 2.1. on the physicochemical properties of PFAS compounds [Data set]. Zenodo. https://doi.org/10.5281/zenodo.13330024 Streamlit app: https://physchempfas.streamlit.app/
Octanol water partition ($LogK_{OW}$)	$logK_{OW}$ = 6.341 (±0.097) + 1.639 (±0.122) x T(F..F) - 1.854 (±0.122) x gmin T(F..F) - sum of topological distances between F..F Gmin - minimum atom E-state value in a molecule R^2 = 0.95 $RMSE_C$ = 0.75 Q^2_{LOO} = 0.93 $RMSE_{EXT}$= 0.87 Q^2_{F1} = 0.92 Q^2_{F2} = 0.92 Q^2_{F3} = 0.93	Publication: Mudlaff et al., 2024. https://doi.org/10.5281/zenodo.11382313 Model: Mudlaff, M., 2024. Datasets from deliverable 2.1. on the physicochemical properties of PFAS compounds [Data set]. Zenodo. https://doi.org/10.5281/zenodo.13330024 Streamlit app: https://physchempfas.streamlit.app/
Bioconcentration Factor (BCF)	log BCF = 3.01 (±0.141) + 1.78 (±0.182) x GATS2v - 0.7 (±0.182) x P_VSA_e_5 - 0.8 (±0.169) x E3m + 1.27 (±0.163) x nCp GATS2v–Geary autocorrelation of lag 2 weighted by van der Waals volume (2D – Autocorrelation) P_VSA_e_5–P_VSA-like on Sanderson electronegativity, bin 5 (2D – P_VSA_like descriptor) E3m–3rd component accessibility directional WHIM index / weighted by mass (3D – WHIM) nCp–number of terminal primary C(sp3) (2D – Functional group counts) R^2 = 0.92 $RMSE_C$ = 0.58 Q^2_{LOO} = 0.88 $RMSE_{EXT}$= 0.72 Q^2_{F1} = 0.89 Q^2_{F2} =0.89 Q^2_{F3} =0.88	Publication: Kowalska, D., Sosnowska, A. & Puzyn, 2024. [under revision] Model: will be public (code and datasets) on Zenodo after acceptance of the publication Streamlit app: the model will be implemented to the app after acceptance of the publication. https://physchempfas.streamlit.app/

Table 3: Equations of the developed predictive models (continued).

Endpoint	Model equation and statistics	References
Melting Point (MP)	MP= - 209.04 (±139.9) + 132.95 (±22.63) x ACC + 3.04 (±0.97) x F02[C-F] - 18.97 (±7.98) x C-013 +209.04 (±139.9) x RBF ACC - 'information indices' which characterizes mean information index on atomic composition F02[C-F] - frequency of C-F at topological distance 2 C-013 - carbon connected to at least three electronegative atoms (X) CRX3 RBF - rotable bond fraction R^2 = 0.81 $RMSE_C$ = 0.40 Q^2_{LOO} = 0.78 $RMSE_{EXT}$= 0.27 Q^2_{F1} = 0.83 Q^2_{F2} = 0.43 Q^2_{F3} = 0.93	Publication: Bhhatarai, B. et al., 2011. CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. *Mol. Inform.* **30**, 189–204 (2011).

The predictive models developed within the PROMISCES project for physicochemical properties were implemented using Python 3.9, in conjunction with the sklearn package. The descriptors incorporated into the models were calculated using the AlvaDesc program, which employs SMILES codes for all compounds. In instances where experimental data for properties such as water solubility, vapor pressure, and the n-octanol/water partition coefficient were scarce or unavailable, these values were estimated through the COSMO-RS method.

The performance of the QSPR models was assessed using required metrics: the coefficient of determination (R^2) and root mean squared error ($RMSE_{CV}$). A 1:X data split was applied to each model. External validation was carried out using Q^2EXT (Q2F1, F2, F3) coefficients, $RMSE_{EXT}$, and the concordance correlation coefficient (CCC_{EXT}). To confirm the models' applicability domains, a Williams Plot was used to visualize standardized residuals from leverage.

All models developed, improved, or adopted in PROMISCES are presented in the QSAR Model Reporting Format (QMRF), which includes essential information and validation results, as detailed below.

Additionally, a toolbox for the physicochemical properties of PFAS has been developed which is reported as deliverable D2.1 of the PROMISCES-project (Sosnowska et al., 2024). The toolbox is a summary of the in silico models that were improved, newly developed, and adopted for predicting the physicochemical properties and aquatic toxicity of PFAS.

The toolbox in which the models for physicochemical properties are implemented is available as a browser application. This app allows users to predict and visualize properties by inputting descriptors generated using the Ochem software. The app is freely available online at https://physchempfas.streamlit.app/.

2.1.2. Model improvements

The following significant improvements were made to the predictive models designed to assess the properties and environmental behavior of PFAS compounds, enhancing their accuracy, applicability, and predictive power.

2 new QSPR models for predicting n-octanol-water partition coefficient (LogKow), and Bioconcentration Factor (BCF):

- The objective for logKow was to address gaps in PFAS bioaccumulation data by combining quantum-chemical based methods with data-driven models. COSMO-RS was used to predict n-octanol/water partition coefficients ($logK_{OW}$) for over 4,000 PFAS compounds, resulting in a highly accurate QSPR model. This model divided the compounds into OECD categories and confirmed the role of fluorine atoms in bioaccumulation. Additionally, the study predicted other critical physicochemical properties such as Henry's Law constant (k_H), air-water partition coefficient (K_{AW}), octanol-air coefficient (K_{OA}), and soil adsorption coefficient (K_{OC}).
  The addition of over 4,000 PFAS compounds from the NORMAN database extended the model's coverage. The integration of COSMO-RS calculations helped fill experimental data gaps, enabling predictions for compounds with limited data. The model achieved high accuracy with an R^2 of 0.95 and predictive power ($Q^2_{LOO} = 0.93$). Along with $logK_{OW}$, the model predicted other important properties like logSw, logVP, k_H, K_{AW}, K_{OA}, and K_{OC}, which are essential for assessing the transport and dispersion of PFAS in the environment.
  This effort resulted in the development of a new QSPR model specifically for predicting PFAS bioaccumulation potential ($logK_{OW}$), utilizing the NORMAN database to expand the scope of PFAS predictions.

- A new QSPR model was created to predict the log BCF for fish based on experimental data from 33 representative PFAS compounds. This model was then applied to a larger dataset of 2,209 PFAS compounds. The model was also able to classify PFAS compounds into bioaccumulative, non-bioaccumulative, and very bioaccumulative categories, a feature does not present in previous tools.
  The new model advanced predictions by predicting log BCF for a broader dataset and classifying compounds based on their bioaccumulation potential. The model showed high predictive accuracy with an R^2 of 0.844, correlating well with experimental BCF values for 13 compounds, demonstrating the reliability of the model in predicting bioaccumulation potential.

2 improved QSPR models for predicting Water Solubility (logSW) and Vapor Pressure (logVP):

- The main improvement focused on expanding the applicability domain (AD) of two existing QSPR models for predicting water solubility (logSw) and vapor pressure (logVP) of PFAS compounds. This was achieved by incorporating quantum-chemical calculations (COSMO-RS) to fill gaps in experimental data, thereby improving prediction reliability. Additionally, external validation, which was previously absent, was conducted to ensure the improved models robustness.
  The improvements included extending the applicability domain by broadening the range of compounds the models could predict, incorporating COSMO-RS calculations to address data gaps, and applying external validation to ensure the models reliability for a wider range of

compounds. The models were also applied to a larger dataset of 4,519 PFAS compounds from the NORMAN Database, reducing the number of compounds outside the domain.
In terms of development, a new extension strategy was applied by integrating COSMO-RS calculations to extend the applicability domain. Tools were also developed to expand the training set using structural descriptors, which enhanced the model's accuracy.

1 adapted model for predicting Melting Point (MP):

- For the MP model, instead of developing a new one, a detailed applicability analysis (AD) was conducted on the existing QSPR model. This analysis confirmed that the existing model could reliably predict the melting points of PFAS compounds.

In summary, these developments significantly enhanced the predictive tools for assessing the environmental behavior of PFAS, expanding the applicability and improving the accuracy of predictions for a broader range of compounds.

2.1.3. Link to executables

The toolbox improved in silico models for identification of PMT properties (deliverable D2.1) is available on Zenodo: https://zenodo.org/records/14800915

The models, along with data from the training and validation sets, can be accessed on Zenodo https://doi.org/10.5281/zenodo.13330024. This data includes endpoints such as water solubility, vapor pressure, logP, melting point, and bioconcentration factor.

The app is available on site: https://physchempfas.streamlit.app/

2.2. In silico predictive tools (other than QSPR/QSAR) for identification of PM(T) properties of classes of substances

2.2.1. Technical description of the model

Introduction

The AI/ML-based model developed for prediction of aquatic toxicity takes account of the limited number of toxicity data typically available for PFAS compounds. One of the key issues in this respect is to use the data as efficiently as possible, and to supplement this data with additional information on the impact of chemical structure on toxicity (transfer learning). By far most data are available on PFOA and PFOS with relatively little information available on other PFAS compounds. It is therefore essential to use the scarcely available information on other PFAS compounds as efficiently as possible.

The first step in AI/ML-based modelling was the development and validation of a classification as well as a quantification model for the prediction of aquatic toxicity of organic compounds in general, including PFAS chemicals. The classification model is suited to classify PFAS compounds in a set of toxicity classes in line with the requirements for classification and labelling within REACH. The initially developed quantitative ML model can predict the aquatic toxicity of PFAS compounds for different aquatic species. Amongst others, the options for species-species interpolation were exploited and it was specifically considered how in the future it can be demonstrated that models based on AI/ML approaches have an added value as compared to other *in silico* models. A manuscript has been published on this activity (Viljanen et al., 2024).

In addition to the initially developed model, the best-performing model was developed using quantitative and qualitative transfer learning approaches (including Random Forest and XGboost). This was done by using a set of algorithms and 10-fold Cross Validation (CV). The developed model (i.e. the initially developed model + transfer learning) predicted PFAS better after transfer learning, especially when equally weighting PFAS and non-PFAS to get better predictions for PFAS. More details on the statistics of the model can be found in Deliverable 2.1 (Sonosnowska et al., 2024).

Model description

The final AI/ML-based model allows to generate predictions of effect levels for PFAS congeners for any of the aquatic species for which toxicity data are available in the database used for model development. Options for endpoints include LC50-, EC50-, and NOEC-values and predictions of the toxicity of PFAS congeners can be generated for any of these endpoints. The model is integrated into an application for environmental risk assessment of PFAS congeners. The basic approach towards chemical risk assessment, for instance advocated in the REACH legislation, is to use toxicity data on different aquatic organisms to generate so-called species-sensitivity distributions (SSDs). The Maximum Permissible Concentration (MPC) for the environment is defined as the concentration which protects at least 95% of the species in an ecosystem, thereby protecting the functioning of the ecosystem. The MPC is also termed ‘HC5’ to indicate the Hazardous Concentration that affects 5 % of the species. The AI/ML-based model is used as the basis for the generation of predictions of HC5-values for PFAS chemicals for which toxicity data are available, as well as for non-tested PFAS. This allows, amongst others, for ranking PFAS chemicals according to their predicted HC5-values. Subsequently, these predictions of HC5 can for instance be used for identifying PFAS chemicals that

are Safer by Design than currently commercialized PFAS chemicals. Examples of SSDs generated for a random set of PFAS chemicals are provided in Figure 1.

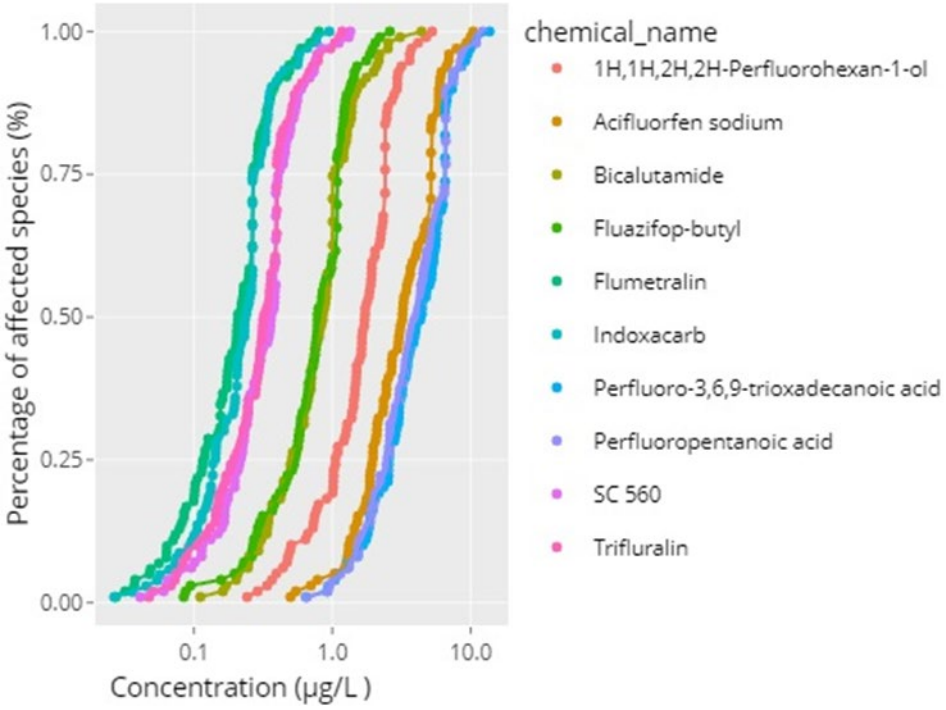


Figure 1: Examples of XGBoost SSDs for 10 randomly chosen PFAS chemicals.

2.2.2. Model improvements

As part of this work a new predictive model has been developed. The final developed model is based on XGboost on a large diverse dataset of chemicals and species. The innovative character is in its ability to learn patterns from this wide range of chemicals and species, as well as the model architecture which closely resembles current risk assessment practices.

2.2.3. Link to model input/executables

The underlying model code for the calculation of HC5-values has been stored in a repository on GitHub (https://github.com/rivm-syso/predictive_toxicology.git) and can be accessed via Zenodo (https://zenodo.org/records/14929053). This repository also contains the code needed to run a user-friendly interface. Although this repository is currently not accessible to outside collaborators, we aim to make this repository public as soon as all code and documentation is ready.

3. Screening level models for the assessment of exposure to PM(T)s

3.1. SimpleBox model for PM(T)s

SimpleBox is a model to predict environmental concentrations of substance across different compartments of air, water, soil and sediment at different spatial scales, e.g. local, regional, continental and global. The model has served as 'regional distribution module' in the European Union System for the Evaluation of Substances (EUSES). It is currently used as part of the CHESAR tool, hosted by the European Chemicals Agency (ECHA) to demonstrate possibilities for 'safe use' of chemicals, which is required for registration of chemical substances under the Registration Evaluation Authorization and Restriction of Chemicals (REACH) framework (ECHA, 2016). SimpleBox also serves as fate module in Life Cycle Impact Assessment models (Rosenbaum et al., 2011). The SimpleBox Aquatic Persistence (SB-AP) Dashboard has been developed within PROMISCES as an additional module to SimpleBox, so that users can screen the extent to which substances persist in surface water compartments at a regional, continental or global scale (Meesters, 2024).

3.1.1. Technical description of the model

SimpleBox is a multimedia mass balance model that simulates the environmental fate of chemicals as fluxes (mass flows) between a series of well-mixed boxes of air, water, sediment and soil on regional, continental and global spatial scales. The model does so by simultaneously solving mass balance equations for each environmental compartment box in the model (rivm.nl/simplebox 2024). The input that SimpleBox needs for its simulations refer to physicochemical properties of the substance, landscape characteristics, and emission volumes. The model then delivers exposure concentrations in the environment as output. The SB-AP Dashboard is developed as an additional module to SimpleBox operated as a Microsoft Excel spreadsheet, supported by numerical computations in R, which are linked to the spreadsheet via RExcel (rivm.nl/simplebox 2024). The SB-AP Dashboard demands the same input parameter as the SimpleBox model and calculates the aquatic persistence for substance emissions. The dashboard is as such added to the SimpleBox version 4.01 as new worksheets that link with SB's emission and landscape scenarios, substance data, the simulation of environmental fate processes and the derived chemical mass in the water compartments. Detailed information how to use the SB-AP Dashboard can be found in deliverable 2.6 (Meesters, 2024b). Additional information about the application of the model can be found in the Guidance document, deliverable 2.4, chapter 2.2 (Zessner et al., 2025).

3.1.2. Model improvements

In comparison to the earlier SimpleBox 4.01 version, the SB-AP Dashboard includes additional model routines to express aquatic persistence of emitted substances across surface water bodies at regional, continental and global scales. A macro function has been developed to enable the user to insert input values as ranges instead of single fixed values. As such, the SB-AP Dashboard is able to present the level of uncertainty inserted in the input values -emission volumes and physicochemical properties of the substance- as well as resultant ranges of uncertainty in the model outcomes. A button is added for the user to perform probabilistic sensitivity analyses to investigate the relationship between physicochemical properties of the substance and aquatic persistence of dissolved and sorbed species. The user is as such served with a new tool to evaluate the extent to which a persistent and mobile substance resides in surface waters and displaces to different spatial

scale. The applicability of the SB-AP Dashboard as a tool for dedicated environmental fate studies is demonstrated with a case study in which the aquatic persistences have been expressed for eight different PFASs and how these compare to the current criteria for (very) persistent and (very) mobile substances (Zessner et al., 2025). Moreover, the case study includes before mentioned sensitivity analyses to demonstrate that uncertain degradation rate constants and uncertain octanol-water or organic carbon-water partitioning coefficients yield the largest uncertainties in predicted aquatic persistence of PFASs.

3.1.3. Link to executables

The SimpleBox Aquatic Persistence Dashboard is available as an MS Excel Spreadsheet model at Zenodo (https://zenodo.org/records/13752192).

3.1.4. Link to model input

The SimpleBox model is available at GitHub at which different versions are available as MS Excel Spreadsheet and R programming script, see https://github.com/rivm-syso/SimpleBox

References on the SB-AP Dashboard: ECHA, 2016, Meesters, 2024, Rivm.nl/simplebox, 2024, Rosenbaum et all., 2011.

3.2. Operational approach for deriving generic risk limits in a leaching situation

3.2.1. Technical description of the model

Introduction

In this study, environmental quality criteria for PFAS in groundwater and surface water, e.g. based on WFD quality targets or drinking water protection, are the starting point for the calculation of corresponding concentrations in the soil or dredged material (sediment) to be used for the derivation of generic risk limits. Conceptual models have been drawn up for two main variants:

1. Groundwater. This main variant assumes that PFAS that are carried along with infiltrating rainwater end up completely in the groundwater.
2. Surface water. This main variant assumes a relatively shallow aquifer in which complete mixing takes place of PFAS originating from the topsoil layer.

Modelling approach

The groundwater variant is modelled using a Hydrus and Modflow model train whereas the surface water scenario is calculated using a simple dilution calculation based on the assumption of instantaneous mixing in the aquifer and a flux through POC2 that is equal to the net infiltration. For information about the application of the model the Guidance document, deliverable D2.4, chapter 2.3 (Zessner et al. 2025) should be consulted.

Transport of PFAS in the unsaturated zone was performed with the software 1D-HYDRUS. The subsequent transport of PFAS through the aquifer was modelled using MODFLOW 6. A general description of the software of 1D-Hydrus, MODFLOW and MT3DMS can be found in the manuals: Šimůnek et al., 2013, Harbaugh, 2005 and Zheng and Wang, 1999 respectively.

Parametrization of 1D-Hydrus

1. Geometry soil profile and spatial discretization

The profile has a length of 5 meters and consists of six materials, corresponding to different soil layers. The materials have unique soil physical and soil chemical properties. The thickness of the material depends on the scenario). For the simulations performed, cells of 1 cm are used. This discretization leads in all cases to minimal errors in the mass balance.

2. Time discretization

A simulation time of 500 years was used for this study. The initial time step for all simulations is 9.9E-4 days. The minimum and maximum allowed time steps are 9.9E-6 days and 5 days, respectively. The actual time step used is determined by HYDRUS-1D (Rassam, 2018; Šimůnek et al., 2013).

3. Hydrology

For the hydrological aspect of the model, an atmospheric boundary condition was used for water input. The same daily precipitation and evaporation data were used for this as in Verschoor et al., (2006) which was based on an average year for the period between 1980 and 2000. The average year was used repeatedly for the simulated period of 500 years. The second boundary condition concerns the groundwater level. Namely, it is assumed that the groundwater level is constant for the simulated period.

4. Soil physical and hydraulic parameters

The soil physical properties are based on a standard sandy soil (Verschoor et al., 2006). In this study, no preferential flow paths were assumed and the single porosity Van Genuchten-Mualem model (Van Genuchten, 1980) was used. For hydrodynamic dispersion one tenth of the distance covered by water was assumed. This is defined per layer in HYDRUS-1D.5. Soil chemical parameters

In HYDRUS-1D, initial concentrations must be described as total concentrations (mass per volume soil) or pore water concentration (mass per volume pore water). For this study, soil concentrations are set equal to total concentrations and are calculated with total concentrations. A Kd must be entered in HYDRUS-1D. It is therefore necessary to convert a K_{OC} to a Kd. This can be done with the following formula:

$K_d = K_{OC} \times f_{OC}$

In this formula, f_{OC} gives the fraction of organic carbon in the soil. Because organic matter concentrations are often reported and not organic carbon concentrations, it is necessary to determine what fraction of soil organic matter consists of organic carbon. In this study, it is assumed that 58% of organic material consists of organic carbon.

Parametrization of Modflow 6

A simplified schematization was chosen for the model. The model calculates the transport of PFAS in the groundwater that infiltrates during the application to the right-hand side of the model, where the Point of Compliance (POC) is located. Infiltration takes place at the surface of the model. The infiltration is, just like in the 1D modeling, set equal to 300 mm/year. On the location of the application, the infiltration is given a time-dependent concentration, equal to the results of the 1D modelling. Outside the application, the concentration in the so-called recharge (supply of groundwater) is set equal to 0 ng/l. The flow from left to right is imposed by means of fixed-head

cells (fixed boundary conditions) on the left and right sides of the model. The fixed-head cells are set so that the groundwater velocity is 5.1 m/year near the application. This is equal to the median groundwater velocity in groundwater protection areas with a well-permeable soil in the Netherlands. In addition to the imposed gradient, the flow in the model is also influenced by the replenishment of the groundwater, which means that there is no uniform flow velocity in the model. As a result, the flow velocity increases further away from the application. No flow occurs through the bottom of the model. The model includes sorption of PFAS. For the sorption, values were assumed equal to the 1D modelling, namely a K_{OC} equal to the 10th percentile in Dutch conditions and a percentage of organic matter of 0.6%.

3.2.2. Model improvements

This study makes use of existing models Hydrus 1D and Modflow 6. The innovative aspect lies in the application at a higher level of abstraction. Whereas these models are commonly applied to predict leaching and substance transport on al local scale, in this application the models are parametrized much more generically in order to underpin generic risk limits for leeching. In the Guidance document, deliverable D2.4, chapter 2.3 (Zessner et al. 2025), sample calculations for the 'Dutch situation' have been included as wel as pointers to decide on parametrization of the models in different areas.

3.2.3. Link to executables

Hydrus 1D is available at: https://www.pc-progress.com/en/Default.aspx?hydrus-1d

Modflow 6 is available at: https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic-model.

3.2.4. Link to model input

Input files for Hydrus 1D and Modflow are available at Zenodo:
https://doi.org/10.5281/zenodo.14755349

3.3. Probabilistic human health risk assessment for four reuse pathways

3.3.1. Technical description of the model

A risk-based human health exposure assessment (HHEA) was developed to evaluate the exposure for humans in 4 circular economy (CE) routes investigated in 6 of the 7 case studies in the project PROMISCES. The HHEA is a probabilistic tool evaluating the risk posed to human health. The HHEA was applied to the following routes: 1) semi-closed drinking water cycle; 2) groundwater remediation; 3) water reuse for agricultural irrigation; and 4) nutrient recovery. Each of these exposure routes results in a product – drinking water or lettuce – which can be consumed by humans. For some routes, the exposure is purely theoretical, while for others, the entire process chain is investigated in the PROMISCES case study. The HHEA is built on Bayesian principles, which enable assessment of risk under conditions of low data availability and high uncertainty. This is particularly useful for evaluation of substances such as PFAS and other industrial persistent, mobile and potentially toxic (iPMT) substances, the removal of which in treatment processes is not yet well studied in literature.

As the results from the experimental sites are not yet available, the current deliverable (D2.5 – Open source model for probabilistic human health risk assessment (version 0.4)) had to be based purely on removal of substances reported in literature. The deliverable explains the different treatments, environmental matrices, and substances which were the focus of the initial assessment. It describes the construction of the HHEA tool, with explanations of how different data types – literature data, site specific data, and modelled data – are used to update the prior probability of the removal factor for substances in a process. It also describes how non-technical processes, such as mixing or evaporation, have been included into the treatment trains evaluated. Finally, individual reference quotients for the substances are established, which are used to assess the relative risk of the final concentrations in the products which could be consumed by humans.

A preliminary discussion of the results of the 4 CE routes is available as of October 2024. However, a detailed evaluation or scenario assessments of the routes will be provided by April 2025, in an updated version of D2.5 once all experimental data is ready. This final version will report on a full evaluation of the routes in the HHEA tool.

3.3.2. Model improvements

The HHEA is built on Bayesian principles, which enable assessment of risk under conditions of low data availability and high uncertainty. This is particularly useful for evaluation of substances such as PFAS and other industrial persistent, mobile and potentially toxic (iPMT) substances, the removal of which in treatment processes is not yet well studied in literature. To date, Bayesian principles have been applied for assessing human health risks from microbial contaminants in water, but this framework has not yet been successfully adapted for chemical substances, due to their generally more chronic human health effects in comparison to acute effects from microbial contaminants. Therefore, the Bayesian principles were applied in a new model to enable assessment of literature, site specific, and modelled data to quantify the exposure risk for human health.

The HHEA tool stores intermediate results after every treatment step, which enables a transparent assessment of the changes occurring after every treatment step. This has the advantage that there are no restrictions imposed by external standards, however, the files cannot be opened by other applications. These intermediate results are only meant for further analysis (i.e. visualisation, establish a Bayesian networks) in Python.

3.3.3. Link to executables

To run the model, users need to download Python (https://www.python.org/). A list of packages and scripts needed to run the model is provided for more streamlined use.

3.3.4. Link to model input

The open source model for probabilistic human health risk assessment (PROMISCES deliverable D2.5 - final version) as well as the GitHub repository for the code will become available at: https://doi.org/10.3030/101036449.

4. Models for soil – groundwater interaction

4.1. Model train Hydrus/MODFLOW/MT3DMS (1D/2D/3D)

4.1.1. Technical description of the model

Introduction

The transport of PFAS in de the soil-groundwater continuum zone can be modelled using a model train coupling the software 1D-HYDRUS (vertical water flow and solute transport in the unsaturated zone), MODFLOW (3D water flow in the saturated zone) and MT3D or MT3DMS (3D transport in the saturated zone).

A general description of the software of 1D-Hydrus, MODFLOW and MT3DMS can be found in the manuals: Šimůnek et al., 2013, Harbaugh, 2005 and Zheng and Wang, 1999 respectively. The application of the model train for the transport of PFAS in the soil-groundwater continuum zone is described in detail in chapter 3 of deliverable D2.4 (Zessner et al., 2025).

A dedicated framework has been developed to use the model train. This framework is divided in the following steps:

- Develop 1D vertical model dedicated to unsaturated zone using 1D-Hydrus software. In the case, the unsaturated zone properties and associated boundary conditions of the simulated domain are heterogeneous, the unsaturated zone of the simulated domain has to be splitted in different zones. The number of zones need to be defined by the modellers. For each zone, a 1D-vertical model has to be developed.
- Develop a 3D groundwater flow model using MODFLOW software. According to the option selected to couple the models, these two steps can be conducted iteratively (option 1) or simultaneously (option 2). In the case, the unsaturated zone of the simulated domain is divided in several zones, the groundwater flow model has to account for the same number of recharge zones. Information exchange is performed between each 1D-vertical model and the corresponding recharge zone,
- Develop a 1D-reactive solute transport model dedicated to unsaturated zone using 1D-Hydrus solute transport module. In the case, unsaturated zone is divided in several zones, a 1D-reactive solute transport model has to be built for each zone.
- Develop a 3D solute transport model for saturated zone using MT3DMS software. In the case, several recharge zones are defined in the 3D groundwater flow model, the same discretization has to be used in the 3D solute transport model.

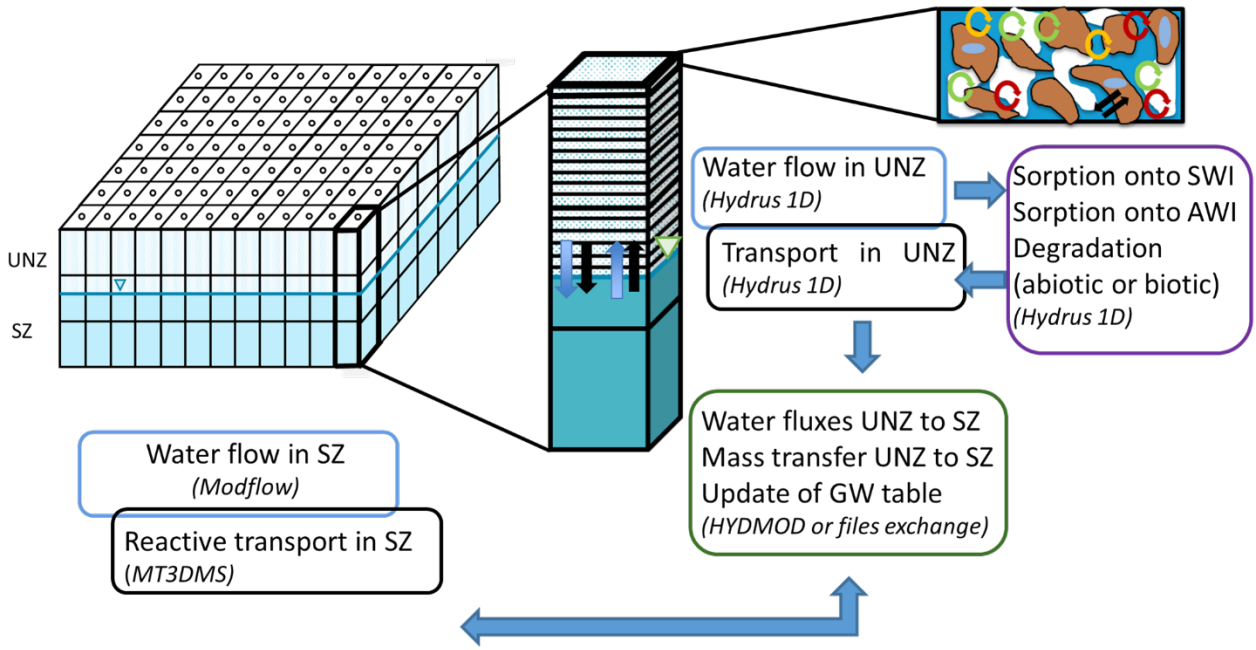


Figure 2: Sketch of the model train developed to simulate fate and transport of PFAS in soil-groundwater continuum.

Two different set-ups have been developed to couple the software.

The first set up is easiest and is based on running the software sequentially starting with simulations of water flow and solute in the unsaturated zone with 1D-HYDRUS. The calculated water flow and mass flux at the bottom of the unsaturated zone is used as input values for recharge (both for water and mass transfer) in the models developed using MODFLOW and MT3DMS, respectively. This set-up is best being used when the water table depth remains stable during the simulations time length, hence the impact of water table depth variations on water flow and mass transfer in the unsaturated zone can be neglected. Input/output data exchange between software is performed by using scripts programmed in Python.

The other set-up uses a coupled version of 1D-HYDRUS with MODFLOW. In this set-up, the effect of a time varying-water table on water flow and mass transfer in the unsaturated zone can be simulated without spurious errors. Input/output data exchange between 1D-HYDRUS with MODFLOW software is performed directly by implementing 1D-Hydrus software in a modified version of MODFLOW 2005. For solute transport, data exchange between solute transport module of 1D-Hydrus and MT3DMS is done using a dedicated post-processing tool.

For the two set-ups, heterogeneities of the unsaturated zone in the simulated domain, leading to spatial changes in terms of vertical water and mass transfers from surface to groundwater, can be simulated by considering simultaneously several 1D-vertical water flow and solute transport models using 1D-Hydrus. The version of the 1D-Hydrus used in the model train does not simulate explicitly PFAS sorption on the air-water interface. PFAS sorption on both soil-water interface and air-water interface are therefore lumped together and can be simulated using either an equilibrium approach or a non-equilibrium approach. The modelling work done in the PROMISCES project suggest that the use of the non-equilibrium approach must be used to contain a good model fit. One should also note that some processes impacting PFAS transport cannot be simulated using the model train such as the reduction of pore volume due to presence of foam in the pore network of soil contaminated by aqueous film-forming foam (AFFF), reducing considerably the hydraulic conductivity.

1D- Hydrus/Modflow

1D-Hydrus software was implemented in MODFLOW 2005 as a new package. Almost all the previously existing packages can be used in this modified version of MODFLOW 2005, allowing to maintain MODFLOW capabilities to build model simulating complex hydrosystem from contaminated scale to watershed scale. Furthermore, a numerical scheme using an algorithm developed by Beegum et al., 2008 is also implemented to eliminate inaccurate simulations of water flux at the bottom of the unsaturated zone due to sudden water inflow or outflow when the groundwater table depth changes. The algorithm updates the pressure head at the bottom of the 1D-vertical model for unsaturated zone at the beginning of the time step of the groundwater model by accounting for an equivalent pressure head profile that would exist if there was a continuous change in the water table elevation. In consequence, no unrealistic changes in flow rate are simulated preventing erroneous simulations of water flow, hence PFAS transport in the soil-groundwater continuum. In case of such changes in water saturation at the bottom of the unsaturated zone is simulated, solute concentrations are correspondingly adjusted to preserve mass balance. This is done by either lowering (diluting) or increasing (concentrating) solute concentrations. This tool is programmed in Fortran and both source code and executable, with the documentation for the coupled software are available on Github (see below).

Postprocessing 1D-HYDRUS/MODFLOW output to MT3DMS input.

The coupled 1D-HYDRUS-MODFLOW simulates both water flow in the unsaturated and saturated zone as well as solute transport in the unsaturated zone. MT3DMS simulates solute transport in the saturated zone. To combine both models in a model train, the outflowing solute flux at interface between the model domains of 1D-Hydrus and MT3DMS needs to be communicated. A post-processing tool was therefore written that reads the relevant data from the 1D-HYDRUS-MODFLOW model to input data of MT3DMS. The relevant output data of 1D-HYDRUS-MODFLOW is the water flux and concentration at the bottom boundary of the Hydrus part of the model domain. The corresponding input data for MT3DMS is the recharge flux and the concentration of the recharge. The tool is programmed in Fortran and both source code, executable and documentation are available in GitHub (see below).

4.1.2. Model improvements

The existing model codes of Hydrus-1D, Modflow and MT3DMS were coupled to model transport of PFAS in the unsaturated and saturated zone. The Hydrus-1D and MODFLOW are fully coupled considering the interaction between the unsaturated and saturated zone for water flow. For the coupling of the mass transport a postprocessing tool was developed to process the time-variant water and mass fluxes at the water table interface to input files for MT3DMS.

4.1.3. Link to model input

3D simulations of PFAS transport in the soil-groundwater continuum. Model input can be found at: https://zenodo.org/records/14812135.

Process-1D-HYDRUS-MODFLOW-to-MT3DMS. This tool processes output of a coupled 1D-HYDRUS-MODFLOW model to input files for Mt3DMS.
The model input can be found at Zenodo: https://zenodo.org/records/14929813 and Github: https://github.com/JohanValstar/Process-1D-HYDRUS-MODFLOW-to-MT3DMS

4.2. Python-based model train

4.2.1. Technical description of the model

Since recent years both MODFLOW/MT3D and HYDRUS1D have their own respective Python libraries. This allows parametrization, execution, and result interpretation while scripting, providing higher flexibility in the way models are built.

Phydrus is the Python library written by R.A. Collenteur, G. Brunetti and M. Vremec (Collenteur et al., 2021) that runs HYDRUS-1D unsaturated zone model developed by Šimůnek, J., M. Th. van Genuchten, and M. Šejna (Šimůnek et al., 2013). FloPy is the Python package that allows to create, run and post-process MODFLOW-based models (Bakker et al. 2024, Hughes et al., 2023, Bakker et al., 2016, Langevin et al., 2017 https://doi.org/10.1111/gwat.13327. Using both models allows to consider PFAS transport from its release point at the soil surface, travelling towards the unsaturated and saturated zones towards an exfiltration surface water body.

In this case, linear absorption has been assumed the main process driving PFAS transport in the subsoil. Moreover, the groundwater level is assumed to be static, thus, effect of drying and rewatering in PFAS transport is neglected. These, of course, are strong simplifications of the PFAS behaviour in the subsurface. Therefore, this approach may only be used for a first approximation of the PFAS fate and transport, especially useful when the data available is limited.

Both models are executed concatenated, meaning that the output leakage generated by the unsaturated zone 1D model (Phydrus), is injected into the fully saturated 2D model (FloPy) as a recharge flux at the location where pollution is expected to occur.

4.2.2. Model improvements

The presented approach is the combination of two complementary already-existing subsurface modelling codes. The coupling consists in a simple concatenation in the execution of both models. Therefore, no addition or modification to the original codes has been performed. The objective of this python-based model train is to provide a simple but effective modelling approach to estimate transport of PFAS in soil and groundwater, which can be used by operators as a first attempt to characterise newly discovered PFAS polluted sites with scarce field data.

4.2.3. Link to executables

General information and examples of FloPy package can the developer's website: https://flopy.readthedocs.io/en/stable/index.html.

FloPy can be installed using conda or pip Python functions. Additionally, MODFLOW-based model executables are freely available at USGS website: https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic-model .

Information on how to install Phydrus can be found at the developer's website: https://phydrus.readthedocs.io/en/latest/index.html.

Phydrus package can be installed using pip, while HYDRUS-1D executable needs to be compiled, or downloaded together with the HYDRUS-1D user interface from the developer's website: https://www.pc-progress.com/en/Default.aspx?Downloads .

1D-HYRDUS Software can be obtained from: https://www.pc-progress.com/en/Default.aspx?h1d-downloads.

MODFLOW 2005 software can be obtained from: MODFLOW-2005: USGS Three-Dimensional Finite-Difference Ground-Water Model | U.S. Geological Survey

The MT3DMS software can be obtained from: https://www.usgs.gov/software/mt3d-usgs-groundwater-solute-transport-simulator-modflow.

4.2.4. Link to model input

del Val, L., Valstar, J., Jou Claus, S., & Martínez del Álamo, M., 2025. Python-based model train to model PFOS transport in the subsoil.

Files on Zenodo: https://zenodo.org/records/14916566

Files on Github: https://github.com/laura-del-val-Eurecat/promisces_gw_model_cs7/tree/main

5. Fate and transport models for bank filtration sites

5.1. Small- and large-scale 3D numerical (iMOD/MT3DMS) models

5.1.1. Technical description of the model

The 3D physically distributed transport models are modelled with MODFLOW 2005 and MT3DMS (physically based models for flow and transport, respectively), implemented in iMOD-WQ (iMOD Water Quality) (Zheng & Wang, 1999, Harbaugh, 2005, Vermeulen & Roelofsen, 2024. MT3DMS uses the flow field as calculated by MODFLOW and calculates the reactive PFAS transport along this flow field, which allows for transient simulation.

iMOD-WQ was developed by Deltares in 2012 as a way of combining the then-existing iMOD environment with additional MODFLOW packages such as MT3DMS, RT3D and SEAWAT. The advantage of this is that everything can be run within the iMOD-environment, using iMOD-formatting (e.g. IDF- and IPF-files) for input and output. It allows for SEAWAT calculations, including reactive transport, on top of MT3DMS water flux simulations. Furthermore, parallel simulations can be carried out with the Parallel Krylov Package (PKS) to reduce calculation times (Verkaik et.al., 2015). The modelling approach and software were used at smaller scale (the Vienna case, see below) and at larger scale (the Budapest cases, see below).

For employing the 3D transport modelling approach at the larger scale (Budapest cases, Figure 3), a regional groundwater flow model of the entire Danube island of Szentendre in Budapest was constructed in iMOD, as described in Annex F of the Guidance Document (Zessner, 2025). This model was employed as 3D MODFLOW model consisting of 6 model layers of variable thickness with a horizontal cell size resolution of 50x50 m. The groundwater flow model was calibrated against head measurements in the pumping wells on the island for the monitoring period (2022-2024). This regional groundwater flow model provides the data basis as well as the boundary conditions for the two local cut-out models (the actual bank filtration models) located at the two monitored sites (Tahi and Surany), which were further calibrated on water levels in the monitoring wells at both sites. Like their parent model, both models have 6 layers, but have a higher resolution of 5x5 m. The Surany cut-out is 1.2x1.6 km, containing 460.000 cells, and the Tahi cut-out is 1.0x1.1 km, containing 396.000 cells. The higher resolution allowed all the pumping wells within the two domains to be modelled in more detail, including a vertical shaft and five horizontal adits of 15-35 m length, arranged in a star shape. The small-scale Vienna model was constructed without a separate regional model, and is 1.4x1.3 km, containing 915.776 cells with a resolution of 4x4 m. For more information on the bank filtration models, see chapters 4.4.4 and 4.6.3 in the Guidance Document (Zessner (2025)). Although the Vienna model extent is comparable to that of the Budapest models, the transport takes place over much smaller distances.

The three models are used to study the reactive PFAS transport during the bank filtration process using the RCT package within iMOD-WQ, which allows for one-site non-equilibrium sorption. A daily time-step was implemented for the groundwater flow model. For the reference period, normally distributed daily PFAS concentrations in the Danube River were generated on the basis of statistical data from the monitoring period (minimum, mean, standard deviation, maximum) using the Python-command np.random.normal (Harris et al., 2020).

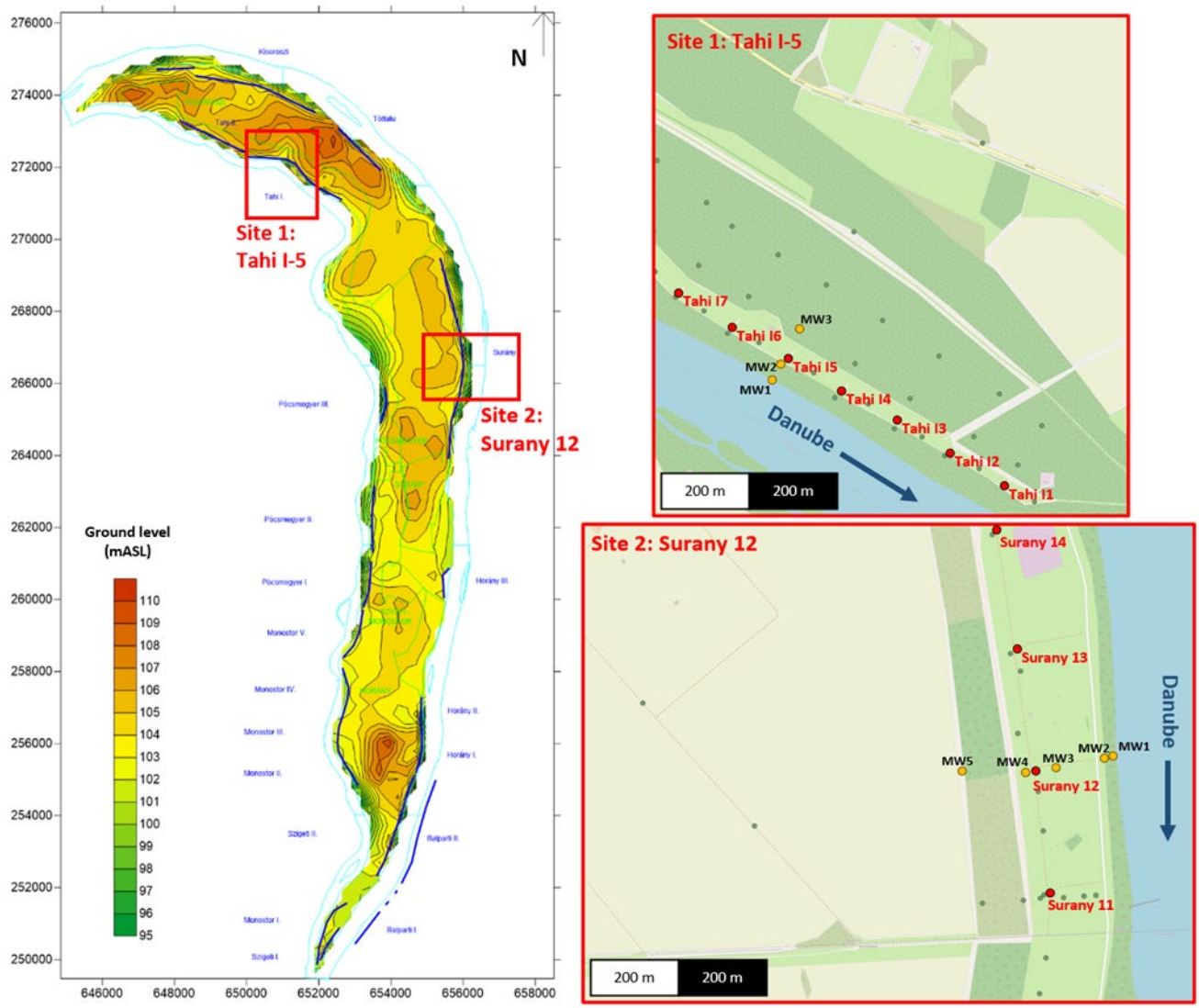


Figure 3: Map of bank filtration sites at Budapest. Left: ground level [m a.s.l.], Right: detailed map of Site 1 (Tahi I-5) and Site 2 (Surany 12). Extraction wells in red, monitoring wells (MW) in orange, unused monitoring wells in green.

5.1.2. Model improvements

The models employ pre-existing, well-established codes for groundwater flow and reactive solute transport. The novelty of the approaches with respect to their application to PMT substances is embedded in the use of experimentally derived sorption rates. The functionality of the chosen reactive transport code (MT3DMS) to deal with the occurring sorption kinetics was already satisfactory, and the field monitoring data did not warrant even more complex kinetics.

2.1.1. Link to executables

The models can be run by using the iMOD Graphical User Interface (GUI) or by using the iMOD Python package (freely available at https://gitlab.com/deltares/imod/imod-python, documentation at https://deltares.github.io/imod-python/). With the latter, one is able to make quick changes to the models (e.g. changes to hydraulic conductivities, pumping rates, etc.) by editing the runfile directly. The input files for the models are already structured correctly for use with the iMOD Python package.

The output of the models consists of IDF-files with water levels and concentrations of each species, for each layer at every timestep (i.e. daily). These can be read either with the iMOD GUI or programming software like Python. Because the models are computationally taxing (especially on the CPU), a strong computer is advised.

More information on how to use iMOD-WQ and iMOD-python can be found in the manual: https://content.oss.deltares.nl/imod/imod56/iMOD_User_Manual_V5_6.pdf

5.1.3. Link to model input

Link to model input on Zenodo: https://zenodo.org/records/14931007

Link to model input on TU Wien Research Data Repository:

https://researchdata.tuwien.ac.at/records/bank filtration models for PFAS

5.2. Generic bank filtration model

5.2.1. Technical description of the model

This Generic bank filtration model is designed as a tool for the initial assessment of PMTs including PFAS contamination at riverbank filtrate sites. The model was developed using an analytical equation for solute transport in porous media. The one-dimensional analytical solution accounts for advection, dispersion, linear isothermal sorption, and first-order decay as described in Bear, 1979, solution given in (West et al., 2007). For more information and a demonstration, please read chapter 4.4.2 and 4.6.3 of the PROMISCES deliverable D2.4 Guidance document (Zessner et al., 2025).

The model is available as an R package. Model use is demonstrated in two R markdown vignettes. The first demonstrates a generic riverbank filtrate scenario, and another presents results from Promisces case study 2 data. It is possible to run your own model simply using the package functions, or by altering parameter values in the vignette itself. The code can be applied to any fate and transport problem fitting at least two criteria: (1) long-term exposure, and (2) travel times of the bank filtrate are known.

The model creates data frames used for two plot outputs – substance Breakthrough curves and a Heat map of equilibrium resulting concentrations for a range of Koc and Half-life parameters. Output options for the combined breakthrough curve include the possibility of plotting multiple Koc and half-life values at the same time, and the option to change the frequency of the line breaks on the x axis. For the heatmap plot, it is possible to create a second box inside the plot representing parameters of interest (for example a range of koc and half-life values for a given substance). Along with that, it is possible to plot a line where a given substance attenuation would lie in the heatmap's parameter space.

The model is intended as an early assessment tool for PMTs and PFAS and may be used before development of more detailed fate and transport models.

5.2.2. Model improvements

This model translates a one-dimensional analytical model for calculating the sorption and degradation of chemicals traveling through groundwater into the R language. It also offers two visualization options that can be used with minimal R knowledge. This model enhances the usability and accessibility of generic analytical model approaches for PMT substances and other chemicals traveling through groundwater.

5.2.3. Link to software / model input

The software and model input files can be found on:

Zenodo: https://zenodo.org/records/13767204

Github: https://github.com/KWB-R/kwb.1dbear or use remotes::install_github("KWB-R/kwb.1dbear") in an Rstudio / R console. / R console.

6. Fate & transport models in an urban context

The model train assesses the rain-related PMT/PFAS pollution of surface waters caused by urban drainage inputs through source-pathway and process descriptions. An emission model calculates monthly pollutant loads entering surface waters via stormwater discharges, combined sewer overflows (CSOs) and wastewater treatment plant (WWTP) effluent, using measured and/or literature data with monthly resolution. These loads are then integrated into a surface water model to simulate the fate and transport of the substances. The surface water model considers the potential adsorption of contaminants to particulate organic matter, which can lead to sedimentation in areas or periods of low flow. Variations in adsorption behaviour between PMTs are also taken into account to ensure more accurate predictions.

6.1. Emission model in an urban context

6.1.1. Technical description of the model

The emission model is a tool developed specifically for urban catchments to calculate the loads of specific substances - such as PFAS (per- and polyfluoroalkyl substances) and PMT (persistent, mobile and toxic substances) - entering surface waters. This model uses measured and /or literature data to determine monthly substance loads. It focuses on three main pathways of urban water systems: stormwater discharges from separate sewer systems, effluent from wastewater treatment plants and combined sewer overflows. The model's calculations are based on data with a monthly resolution, allowing detailed temporal analysis of substance emissions. By integrating hydrological and chemical data sets, the model estimates the quantities of pollutants discharged to surface waters, providing valuable insights into the contribution of each pathway.

Input Data

The calculation of pollutant loads requires a variety of input data, integrating both measured and simulated datasets, as well as supplementary literature-based information when local data is unavailable. Key inputs should be in csv format and include:

Concentration data; measured concentrations of pollutants in stormwater runoff, wastewater, and treated wastewater (WWTP effluent).

Volume data; local data on effluent volumes from WWTPs, stormwater runoff volumes entering surface waters, CSO discharge volumes (with storm- and wastewater shares).

Calculation methodology

The emission model uses a probabilistic approach to deal with uncertainties in the input data. First, the probability distributions of pollutant concentrations and effluent volumes must be determined. A Monte Carlo simulation is then performed, generating, for example, 1000 random data points for each input parameter. These random data points are used to calculate 1000 monthly pollutant loads, with the results summarized in statistical measures such as means, medians and percentiles. This approach ensures that the outputs capture the underlying variability and uncertainty of the input data, providing a more realistic and comprehensive estimate of pollutant loads than deterministic methods.

Results and applications

The outputs of the model include both the total monthly discharge volumes and the corresponding pollutant loads to watercourses, broken down by source (stormwater or wastewater) and pathway (separate sewer system, CSO or WWTP effluent). The results are summarized in a list in R and can be exported in various file formats, such as csv or Excel tables. Primary applications include identification of main pollution sources, uncertainty analysis, temporal and spatial analysis, urban drainage and infrastructure planning.

For more information and a demonstration, please read chapter 4.3.2 and 4.5.2 of the PROMISCES D2.4 Guidance document (Zessner et al., 2025).

6.1.2. Model improvements

The existing emission model (urban mass balance/load model)

has been adapted with some updates and new features. In particular, the model was adapted to include 31 PMT- and PFAS-substances. Furthermore, the model's temporal resolution has been improved from an annual to a monthly scale, allowing for a more precise representation of pollutant loads by accounting for the seasonality of rainfall. In addition, the Berlin-specific input data have been updated, as the previous input dataset of urban runoff volumes, wastewater volumes and WWTP effluent has not been updated for about 10 years, ensuring a more accurate representation of the current hydrological and pollution dynamics in Berlin's surface waters.

6.1.3. Link to executables

The model can be run using the software R or R Studio:

https://cran.r-project.org

https://posit.co/download/rstudio-desktop/

6.1.4. Link to model input

The emission model and an exemplary model input (from the Berlin case) can be downloaded by using the following links:

Zenodo:https://zenodo.org/records/14931210

Github: https://github.com/KWB-R/kwb.promisces-emission-model.git

or by using remotes: install_github("KWB-R/kwb.promisces-emission-model") in an Rstudio / R console.

6.2. DELWAQ/SOLUTIONS model

6.2.1. Technical description of the model

The DELWAQ model is a general software program that is used to simulate water quality in a wide variety of situations, both with respect to the type of water system and to the type of water quality issues. General information can be found at https://www.deltares.nl/en/software-and-data/products?types=Water%20quality%20and%20ecology. Note that the program is distributed as part of the Delft3D 4 and the Delft3D FM packages and is the computational core of the Delft3D-WAQ and D-Water Quality modules. It is also used as part of SOBEK and Delft3D FM 1D2D.

As such the program solves coupled advection-diffusion-reaction equations using the finite volume approach. It is flexible in a number of important ways:

- The geometry of the water system is described by means of a connectivity table rather than a structured or unstructured grid. This allows DELWAQ to be used in network applications, like for the urban water system of Berlin but also for coastal and estuarine regions.

- The user defines what substances to use and what water quality processes to include from a built-in library. There is therefore no need to programme this yourself, though it has a feature that allows the addition of new processes without having to change the program code itself.

For the urban context two different schematisations were devised:

- A network of channels and lakes to model the Berlin surface water system.

- A 1D vertical schematisation to represent the lake “Flughafensee", which is a more or less separate lake in Berlin with no significant connections to the rest of the surface waters, but with noticeable discharges from surrounding activities.

In many cases the schematisation and the accompanying hydrodynamic or hydrological data are provided via a hydrodynamic or hydrological model, but in this case there was no suitable model available (that is, a hydrological model that can be coupled directly to DELWAQ, like output from SOBEK-FLOW or D-Flow FM). For this reason, the hydrological information from the BIBER model (Schumacher, 2023) was used to set up an ad hoc model schematisation. This was done via an auxiliary program, called mknetwork. The schematisation for the Flughafensee was set up using the Berlin water atlas, which publishes detailed information about all the urban lakes.

For more information and a demonstration, please read chapter 4.3.3, 4.5.3 and 4.5.4 of the PROMISCES D2.4 Guidance document (Zessner et al., 2025).

6.2.2. Model improvements

The suite of programs that is used for the Berlin urban water system and development of the DELWAQ/SOLUTIONS model, consists of several pre-existing programs. The novelty is that these programs with a different background have been combined into a program suite for a complex surface water system. This was done combining:

- An estimate of the loads from urban sources, using stochastic approaches.
- A hydraulic model system (water balance model) that provides the flow field and the geometrical information.

- A general water quality model that can combine the information on loads and water balance into a program suite for a complex surface water system.

The surface water system is first modelled via a hydrodynamic or hydraulic program that has been developed in close cooperation with the water quality program. In this case, the most important step was the estimation of the loads from the various wastewater treatment plants and the incorporation into the set-up for water quality calculations. The water system was schematised on the basis of the pre-existing water balance model. In a complex water system like that of Berlin where actually data on water quality are scarce, it is advantageous to have a tool that can be adapted to the situation with relatively little effort. The model suite was applied to a more or less generic PFAS type, as no information was available on the actual compounds. Also, the water system has a short residence time, which means that for such persistent substances as PFAS the accumulation in the sediment layer may be the most important aspect, and not so much the presence in the water itself.

6.2.3. Link to executables

The DELWAQ program is available as part of the Delft3D 4 or Delft3D FM suite - https://www.deltares.nl/en/software-and-data/products?types=Water%20quality%20and%20ecology&types=Hydrodynamics%20and%20morphology

The source code is available via the Deltares GitLab repository – https://git.deltares.nl/oss/delft3d. Note: you need to contact Deltares for access. It is part of the complete set of modules that comprise the Delft3D FM suite.

The documentation is available via the documentation site - https://content.oss.deltares.nl/

The auxiliary program mknetwork is available via: https://zenodo.org/uploads/14772635

6.2.4. Link to model input

The model input for both water quality models and a description of this input is available via: https://zenodo.org/records/14772635

7. Emission-models on catchment scale

7.1. Modelling of Regionalized Emissions (MoRE) model

7.1.1. Technical description of the model

The model system MoRE (Modelling of Regionalized Emissions) was initially developed by the Karlsruhe Institute of Technology (KIT) in cooperation with the German Federal Environment Agency. It is based on the MONERIS model system. MoRE was developed as a tool in an open-source environment for modelling substance emissions into surface waters for a wide range of substances with relevance for water quality (Fuchs et al., 2017).

The modelling in MoRE is carried out as a regionalized pathway analysis. The substance emissions are modelled with temporal and spatial differentiation via various emission pathways**,** as indicated in the EU Guidance Document No 28 (EC, 2012) for tier 3 for establishing an inventory of emissions. The temporal resolution of the model are annual time steps, and the spatial resolution is 526 sub-catchments with a size of 354 ± 352 km².

In the PROMISCES project the model was adapted for modelling of PFAS, which means additional emission pathways were implemented, which might be significant for PFAS and other pathways with less significance for this substance group were simplified and grouped together. Thus, the model contains now the following pathways:

- **Point sources:**
  - Municipal wastewater treatment plants
  - Industrial direct dischargers

- **Diffuse pathways:**
  - direct atmospheric deposition onto water surface
  - surface runoff from unsealed areas
  - soil erosion
  - Groundwater with contribution from
    - legacy pollution from PFAS production site (in case of PROMISCES CS#2, the industrial park at Gendorf, Germany)
    - legacy pollution from aerodromes caused by fire-fighting training activities
    - legacy pollution from municipal landfills
  - sewer systems

Due to the **flexible structure** of MoRE, new substances and emission pathways can be integrated at any time, provided that the necessary input data are available, and modelling can be carried out in a reasonable way. In addition, MoRE offers the possibility to modify existing calculation approaches and to test different input data sets by comparing them. For this purpose, different **variants** can be created. In the PROMISCES project three model variants for the current state were implemented to represent the uncertainty in the model input data:

- Base variant: Based on the median evaluation of environmental concentrations this variant should present the most likely model outcome. If more than 80% of the environmental

concentrations were measured as below the analytical limit of quantitation (LOQ), or less than 3 concentrations were observed above the LOQ, half value of the LOQ was used as input data.
- Best-Case: This variant is based on the 25th percentile of environmental concentrations and represents a best-case evaluation with rather low pollution. If more than 80% of the environmental concentrations were measured as below the LOQ, or less than 3 concentrations were observed above the LOQ, 0 was used as input data.
- Worst-Case: This variant is based on the 75th percentile of environmental concentrations and represents a worst-case evaluation with rather high pollution. If more than 80% of the environmental concentrations were measured as below the LOQ, or less than 3 concentrations were observed above the LOQ, the value of the LOQ was used as input data.

The MoRE model system is based on an Open Source PostgreSQL or SQLite database, a generic calculation engine and the MoRE Developer user interface, which can be used to read, modify and extend the contents of the database. All computations are performed by the calculation engine, which is controlled via the user interface. The modelling results can be exported as tables via the MoRE Developer user interface and the results can be used in GIS for mapping. Users can work with MoRE in two different ways: on the basis of multi-user access in a PostgreSQL database via the Internet or as a stand-alone application on the PC (SQLite version).

More information on how to use MoRE can be found in the manual: https://more.iwu.kit.edu/wiki-en-neu.

7.1.2. Model improvements

The existing MoRE model was adapted for modelling of PFAS. Additional emission pathways were implemented, which might be significant for PFAS and other pathways with less significance for this substance group were simplified and grouped together. The model now contains the following pathways: point sources and diffuse pathways.

Three model variants for the current state were implemented to represent the uncertainty in the model input data: base variant / best-case / worst-case.

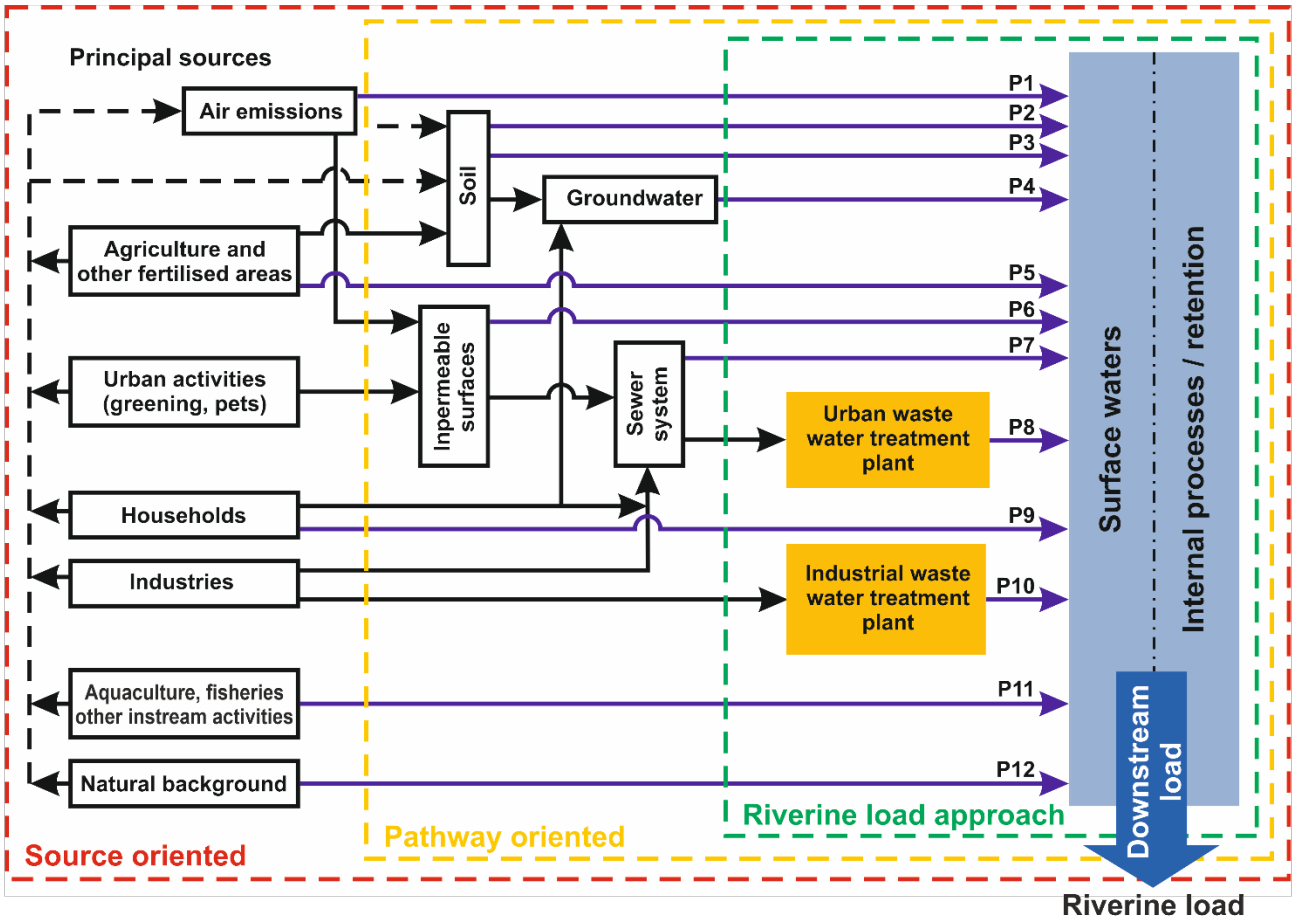
7.1.3. Link to executables / input data

The modelling guidance document (D2.4) in Chapter 4.2 and 4.6 (Zessner et al., 2025) provides an example of the application of the model in the Upper Danube region. The model itself including all necessary input data is available for download under https://doi.org/10.48436/wg9dy-r9r31..

7.2. PROMISCES watershed model for PM substances (PPM) model

7.2.1. Technical description of the model

The PPM model conceptually relies on the Technical Guidance on the Preparation of an Inventory of Emissions, Discharges and Losses of Priority and Priority Hazardous Substances (European Commission (2012)). This Guidance defines sources as "all processes and activities that are likely to contribute to the input of pollutants into the environment". Pathways are "the means or routes by which specific substances can migrate or are transported from their various sources to the aquatic environment". The PPM models follow the "source oriented" approach, see Figure 4.



Pathways			
P1	Atmospheric deposition directly to surface water	P7	Storm water outlets and combines sewer overflows + unconnected sewers
P2	Erosion	P8	Urban wastewater treated
P3	Surface runoff from unsealed areas	P9	Individual – treated and untreated – household discharges
P4	Interflow, drainage and groundwater	P10	Industrial wastewater treated
P5	Direct discharges and drifting	P11	Direct discharges from aquaculture, fisheries and other instream activities
P6	Surface runoff from sealed areas	P12	Natural background

Figure 4: Schematic representation of source-oriented approach towards emission modelling and key pathways (source: European Commission, 2012).

The PPM was applied to a set of 10 PFAS substances: PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFBS, PFHxS, PFOS (including its precursor N-EtFOSAA), ADONA and HFPO-DA /GenX. The model was implemented on a regular grid consisting of 81,217 cells (about 1500 x 1500 m), see Figure 5. It was set up for the period 2011-2022 and runs dynamically with a timestep of 1 day. The model therefore resolves individual weather events, intra-annual differences and inter-annual differences within the simulation period.

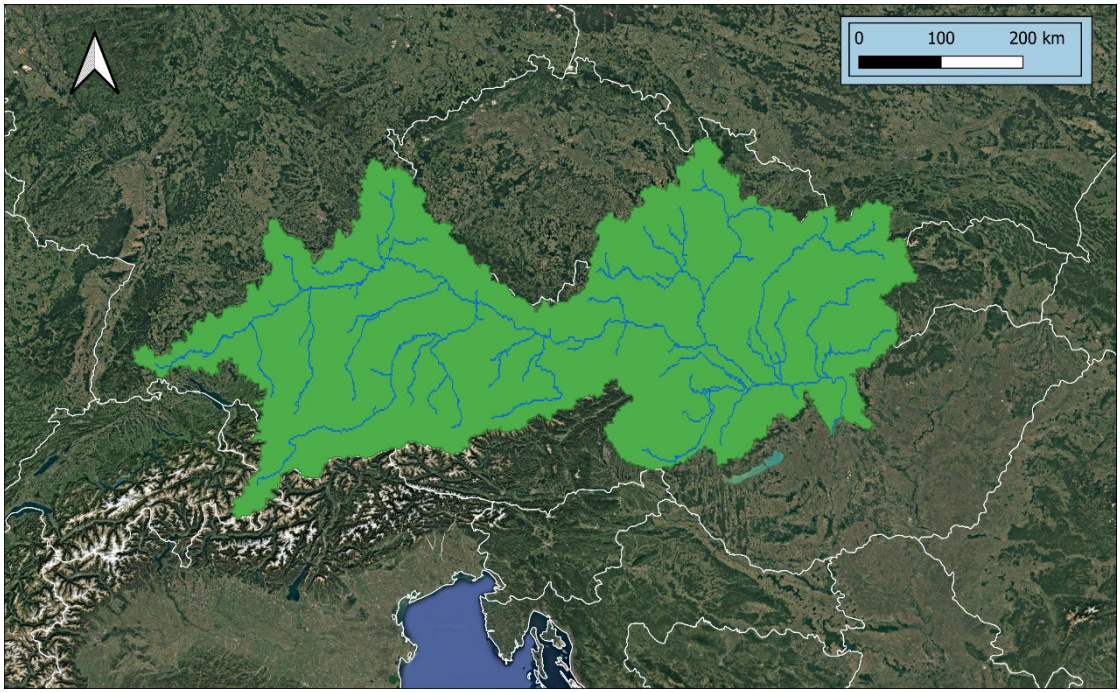


Figure 5: PPM model domain.

The losses of PM substances associated to the various sources were quantified by the emission factor method (Deltares, 2024). Losses (L) of a pollutant "p" for a certain socio-economic activity "a" are the product of an activity rate (AR_a) and an emission factor for this activity and pollutant ($EF_{p,a}$): $L_{p,a} = AR_a \times EF_{p,a}$. Losses were distributed in space, typically by specifying a spatially variable AR, and sometimes by a spatially variable EF.

The PPM explicitly distinguishes the following sources: households (domestic wastewater), industry, atmospheric deposition and construction materials. In addition, a collection of unspecified urban diffuse sources was implemented as a locally elevated concentration in soils.

The quantified losses are allocated to initial receptors and routed through connected compartments towards the surface waters (as shown schematically in Figure 4 (Deltares, 2024). To this end, the model uses spatial input to define wastewater and stormwater management practices (P7 and P8 in Figure 4). These pathways, as well as the pathways associated to soils (P2, P3 and P4 in Figure 4), are driven by hydrological processes.

Hydrological processes are represented on the model grid cells with their own local physical characteristics (elevation, soil, land use and landcover) (van Verseveld et al., 2024). Meteorological forcing data are used to calculate the generation of runoff and infiltration, which is then routed through the catchment river system, taking into account the presence of natural lakes and reservoirs. The routing process accounts for both surface and subsurface flows. Snow related processes are

included. A specific component calculates erosion and sediment delivery to the river network (Boisgontier and van Gils, 2020).

The PPM includes a dynamic fate & transport model that covers the river network. This combines the results from the hydrology model and the emissions model, and includes various processes (Deltares, 2024a; Smits and van Beek, 2013):

- Partitioning between the freely dissolved phase and the suspended particulate matter (SPM), using an equilibrium partitioning concept.
- Net settling of the fraction associated with SPM.
- Degradation by various processes (biodegradation, hydrolysis, photolysis), represented by a temperature dependent first order decay process.
- Transformation of precursors of specific PM substances.

The PPM fate and transport component simulates time dependent water concentrations that allowed a validation of the model by a comparison to observed in-stream concentrations.

A full account of the implementation is included in Annex E of the Guidance document (D2.4) (Zessner et al., 2025).

7.2.2. Model improvements

The PPM is an application of a pre-existing set of interlinked tools to a new application domain. The novelty lies in the application to a larger group of 10 different PFAS substances. These substances constitute a significant share of the 24 PFAS substances that are included in the proposed Environmental Quality Standard under the Water Framework Directive. As such, the results have a direct relevance for chemicals policy and risk assessment. Another novelty of the current implementation is the simulation of a precursor-end product combination (PFOS and precursor N-EtFOSAA) at the scale of a large watershed. Here, two separate emission models (one for the precursor and one for the end product) have been set up to feed into a combined aquatic transport and fate model. This set-up presumes that the transformation of the precursor proceeds only (to a significant degree) in the surface water compartment. It lead to a noticeably better agreement between the simulated and observed concentrations of the end product.

7.2.3. Link to executables

The PPM model consists of three components:

1. The Wflow distributed hydrological modelling framework (https://www.deltares.nl/en/software-and-data/products/wflow-catchment-hydrology)
2. The D-Emissions (EM) emission modelling framework.
3. The D-WaterQuality (WQ) water quality modelling framework.

The EM and WQ model components both make use of the Delft3D-WAQ open source water system modelling software (https://oss.deltares.nl/web/delft3d).

7.2.4. Link to model input

The input files can be found at: https://zenodo.org/records/14764569.

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