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Soil-sediment-water system - Solutions to deal with PMT/vPvM substances

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Foreword

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Introduction

Over the past decades, concerns have been growing about chemicals which do not degrade ((very) persistent substances; (v)P), can easily spread throughout the aqueous environment ((very) mobile substances; (v)M) and are suspected to harm organisms (toxic substances; T).[1] However, various challenges concerning the detection, risk assessment, remediation, and prevention of these PMT/vPvM substances from entering the soil-sediment-water system still exist and need to be addressed. To collectively focus on developing solutions to address these upcoming challenges, this CEN Workshop Agreement (CWA) was proposed and supported by the Horizon 2020 research projects PROMISCES [2], ZeroPM [3], and SCENARIOS [4]. Additionally, this CWA also integrates insights, methodologies, and innovations from other stakeholders not affiliated with these initiatives, ensuring a comprehensive and inclusive approach to tackling the challenges posed by PMT/vPvM substances. These contributions enrich the CWA, offering a broader range of strategies and reinforcing the collaborative effort necessary for effective PMT/vPvM management.

During the development of this workshop, a particular focus was placed on per- and polyfluoroalkyl substances (PFAS), a group of compounds that is especially relevant in the context of PMT/vPvM substances. With forthcoming EU legislations, which could potentially demand stakeholders to address these compounds in their field of work, the development and implementation of appropriate solutions is of utmost importance for the compliance with new regulations. Therefore, throughout this document various action fields were divided into five different categories, starting with their prevention and substitution, remediation measures, co-creation and prioritization, monitoring as well as hazard and exposure assessment to address these PMT/vPvM substances, whether they are directly used or formed as metabolites. These categories provide different ways to approach PMT/vPvM substances and aim to present a holistic and feasible approach for their management. In the following paragraphs these categories are explained with a focus on PFAS.

The **prevention of PFAS** entering the soil-sediment-water system relies on a reduction in manufacture, use, and release. Tools such as policy development, a transition towards safe and sustainable chemicals, materials and products as well as the identification and use of alternatives are needed. To support this, tools are being developed that allow companies to identify whether they have PFAS in their supply chains and provide a database of alternatives to support the **substitution of PFAS**. In addition, the development process includes tools that can assess the impact of unregulated PFAS and their transformation products, as well as methods for non-animal based toxicity testing to avoid regrettable substitution. This CWA identifies opportunities and constrains in current PFAS policy.

The **monitoring of PFAS** is complex but also developing continuously. Currently, standardized methods exist for only a limited number of PFAS and other emerging PMT/vPvM substances. These methods often require specific detection techniques, with which analytical laboratories are equipped. They can be applied routinely in laboratories, especially as they have been developed and published in the form of standards, as is the case of the standardized method for drinking water (EN 17892). In other cases, methods for analysing wastewaters, surface, ground waters, as well as complex solid matrices (such as sewage sludge, sediment, fertilisers, or stack emission) are under development to ensure maximum interlaboratory comparability. Additionally, (bio)analytical tools are being advanced to analyse toxic relevant PFAS as well as PFOA-toxic equivalents based on *in vitro* tests. Analytical methods for specific PFAS parameters and testing methods such as for soil, water, and sludge are being validated and assessed by e.g. national and international standardisation bodies and organisations. Guidance documents are also being developed to support sampling, risk assessments, and remediation suitability assessments.

Concerning **hazard and exposure assessment**, crucial toxicological, persistence, and mobility data gaps exist. Currently, *in vitro* bioassay test batteries and *in silico* models are under development to assess not only individual PFAS compounds – many of which are unknown - but also entire substance classes and complex (water) samples. The goal is to fill these gaps in knowledge for PMT/vPvM substances and also to address them in the present inventory. Moreover, both internal and external, human, and environmental exposure are considered in advanced risk assessment models and are a part of this CWA. The application of a PFAS modelling software, consisting of a sequence of procedures for developing predictive models, is also described in this document. On the one hand, the numerical tools enable the predictive mapping of the spatial-temporal evolution of PFAS pollution in the vadose zone and underlying aquifers. On the other hand, the numerical tools allow the design and assessment of the efficiency for in-situ/ex-situ remediation technologies. Moreover, the PROMISCES project has created a risk assessment toolbox in the form of an improved and optimized toxicological model platform for developing a risk assessment framework for PFAS.

The interest in new insights and technologies for **PFAS remediation measures** is increasing, particularly as industrial sites contaminated by PFAS have been identified as primary sources responsible for soil and (ground)water contamination. Additionally, wastewater serves as another source of PFAS, often containing these substances in a range of concentrations. Many PMT/vPvM substances, including PFAS, are poorly removed in conventional wastewater treatment plants. The inefficient removal of PMT/vPvM limits the circularity in the water cycle, for instance by complicating nutrients recovery from sewage sludge for fertilizer use. Up to date recommendations on selecting sludge treatment technologies to deliver ‘PFAS free’ fertilisers are missing. Furthermore, no comprehensive mass flow analysis exists for the fate and degradation of PFAS during treatment aimed at material recovery from dredged sediments, soil, water and other materials. PFAS removal is essential for drinking water, especially in urban areas with semi-closed water cycles where legacy pollutants and high chemical concentrations create challenges for sustainable drinking water provision. Efforts include developing novel treatment approaches for contaminated soils and groundwater as part of a broader solutions inventory. Innovative solutions for water and sludge are being developed, focusing on the removal efficiency, and sustainability of the solutions.

Co-creation strategies and guidance documents are being formulated for contaminated soil management, encompassing risk assessment, socio-economic assessment, resilience assessment, and stakeholder concerns. Furthermore, several PFAS removal technologies, including one for PFAS destruction, are being validated. This CWA addresses results on combined drinking water treatment, advanced wastewater treatment, and landfill leachate treatment, with a particular focus on PFAS removal from these matrices - wastewater, sediments, sludge. Remediation efficiency will be monitored by a combination of single compounds chemical testing and total PFAS by effect-based bioanalysis tools.

1 Scope

This document defines best practices, solutions, and guidelines concerning the management of (very) persistent ((v)P), (very) mobile ((v)M) and toxic (T) (PMT/vPvM) substances, not only assessing their behaviour in the soil-sediment-water system but also their possible prevention at source as well as end-of-pipe solutions. These solutions are clustered into categories (e.g. prevention and substitution, remediation measures, co-creation and prioritization, monitoring, hazard and exposure assessment) in order to reach various stakeholders working within the soil-sediment-water system. As part of the categorized solutions, a special focus is placed on the following five circular economy routes:

a) Semi-closed water cycle for drinking water supply

b) Wastewater reuse for agricultural irrigation

c) Nutrient and energy recovery from treated sludge for fertilizers

d) Material recovery from dredged sediment for eco-materials

e) Groundwater and soil remediation to protect water cycle

This document is applicable to researchers, public authorities, problem owners, NGOs, water utilities, chemical manufacturers and users, soil/brownfield actors or companies developing market-ready solutions.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at http://www.iso.org/obp/

— IEC Electropedia: available at http://www.electropedia.org/

3.1
persistent substance
P substance
substance with a degradation half-life in marine water higher than 60 days and/or a degradation half-life in fresh or estuarine water higher than 40 days and/or a degradation half-life in marine sediment higher than 180 days and/or the degradation half-life in fresh or estuarine water sediment higher than 120 days and/or the degradation half-life in soil higher than 120 days

[SOURCE: CLP regulation, 2008 [5]]

3.2
Very persistent substance
vP substance
substance with a degradation half-life in marine, fresh or estuarine water higher than 60 days and/or a degradation half-life in marine, fresh or estuarine water sediment higher than 180 days and/or a degradation half-life in soil higher than 180 days

[SOURCE: CLP regulation, 2008 [5]]

3.3
mobile substance
M substance

substance where common logarithm of the organic carbon-water partition coefficient log Koc is less than 3

Note to entry 1: For an ionisable substance, the lowest value for the common logarithm of the organic carbon-water partition coefficient log Koc for pH between 4 and 9 is less than 3.

[SOURCE: CLP regulation, 2008 [5]]

3.4
very mobile substance
vM substance

substance where the lowest organic carbon-water coefficient log Koc is less than 2

Note to entry 1: For an ionisable substance, the lowest value for the common logarithm of the organic carbon-water partition coefficient log Koc for pH between 4 and 9 is less than 2.

[SOURCE: CLP regulation, 2008 [5]]

3.5
Toxic substance

substance where the long-term no-observed effect concentration (NOEC) or ECx (e.g. EC10) for marine or freshwater organisms is less than 0,01 mg/l and/or the substance meets the criteria for classification as carcinogenic (category 1A or 1B), germ cell mutagenic (category 1A or 1B), or toxic for reproduction (category 1A, 1B, or 2) and/or there is other evidence of chronic toxicity, as identified by the substance meeting the criteria for classification as specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) and/ or the substance meets the criteria for classification as endocrine disruptor (category 1) for humans or the environment

[SOURCE: CLP regulation, 2008 [2]]

3.6
Hazardous substance

product or chemical that has properties which are explosive, flammable, oxidising, toxic, corrosive or toxic to the environment

[SOURCE: ISO 24252: 2021-11]

3.7
Co-creation

participatory and collaborative problem-solving approach that enables the generation of socio-economic value by involving a diverse range of stakeholders at all stages of the project

[SOURCE: Dervojeda et al., 2014 [12]]

3.8
Zero pollution

reducing air, water, and soil pollution to levels that no longer pose a risk to health and natural ecosystems while staying within the earth's capacity, thereby creating a toxin-free environment

[SOURCE: [30]]

4 Abbreviated terms

For the purpose of this document, the following abbreviated terms apply:

AhR	Aryl hydrocarbon receptor
BEQ	Bioanalytical equivalents
BS	Binding score
CAA	Chemical alternatives assessment
CAS number	Chemical abstracts service number
CW	Constructed wetlands
EAOP	Electrochemical advanced oxidation process
EAT	Estrogenic, androgenic, thyroidal
EBT	Effect-based trigger value
EC50	50 % effect concentration
ECVAM JRC DB	EURL ECVAM dataset on alternative methods
EQ	Analytical equivalent
ER	Estrogen receptor
FHxSA	Perfluorohexane sulfonamide
FOSAA	N-[(1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Heptadecafluorooctyl)sulfonyl]glycine
FTAB	Fluorotelomer sulfonamide alkylbetaine
FTSA	Fluorotelomer sulfonic acid
FTSaAM	Fluorotelomer sulfonamido N,N-dimethyl amine
SGW	Soil-groundwater
INCHI key	International chemical identifier key
KPI	Key performance indicator
LCA	Life cycle assessement
LCIA	Life cycle impact assessment
LOQ	Limit of quantification
MIE	Molecular initiating events
MLR	Multiple linear regresion
MW	Molecular weight
NAM	Non-animal method
NF	Nanofiltration
NGO	Non-governmental organization
NOEC	No-observed-effect concentration
OECD	The organization for economic cooperation and development
PAH	Polycyclic aromatic hydrocarbons
PCB	Polychlorinated biphenyls

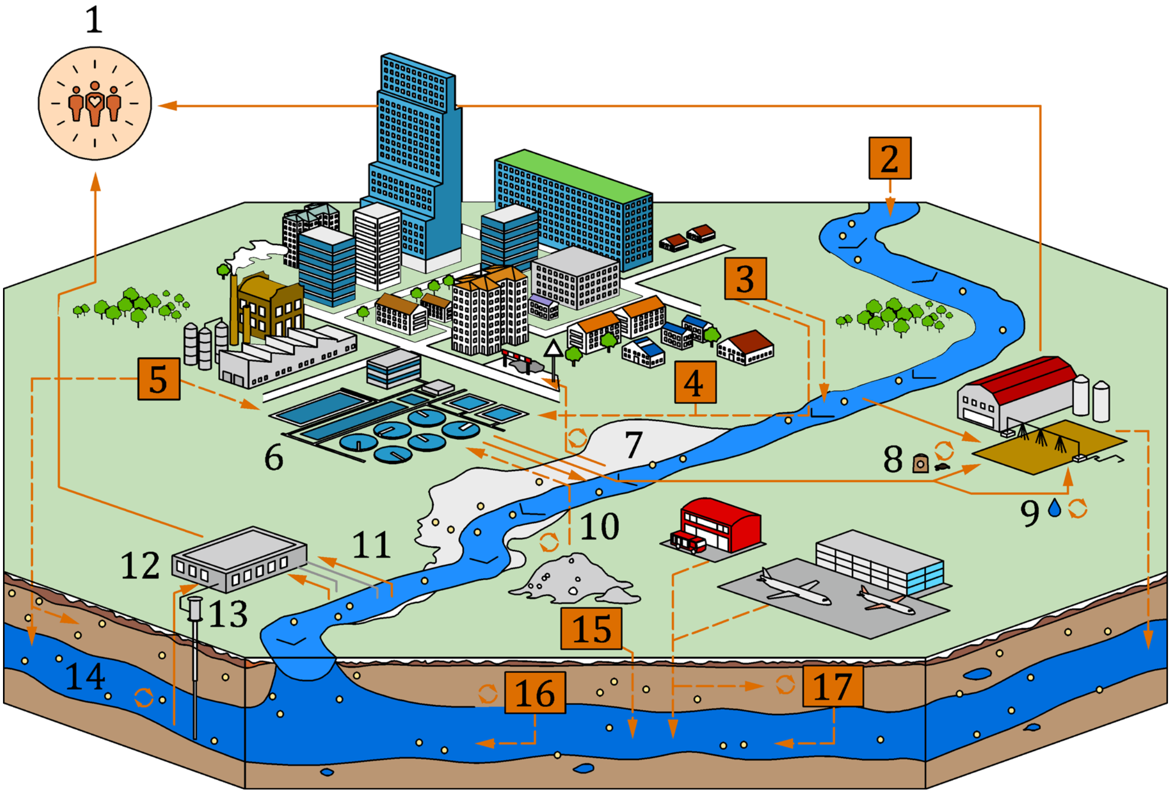
PFAS	Per- and polyfluoroalkyl substances
PFBA	Perfluorobutanoic acid
PFBS	Perfluorobutanesulfonic acid
PFDA	Perfluorodecanoic acid
PFDoDA	Perfluorododecanoic acid
PFDoDS	Perfluorododecane sulfonic acid
PFDS	Perfluorodecane sulfonic acid
PFHpA	Perfluoroheptanoic acid
PFHpS	Perfluoroheptane sulfonic acid
PFHxA	Perfluorohexanoic acid
PFHxS	Perfluorohexane sulfonic acid
PFHxSAM	Perfluorohexane sulfonamido amine
PFNA	Perfluorononanoic acid
PFNS	Perfluorononane sulfonic acid
PFOA	Perfluorooctanoic acid
PFOS	Perfluorooctane sulfonic acid
PFOSA	Perfluorooctane sulfonamide
PFPeA	Perfluoropentanoic acid
PFPeS	Perfluoropentane sulfonic acid
PFPrS	Perfluoropropane sulfonic acid
PFTrDA	Perfluorotridecanoic acid
PFTrDS	Perfluorotridecane sulfonic acid
PFUnDA	Perfluoroundecanoic acid
PFUnDS	Perfluoroundecanoic sulfonic acid
PMT	Persistent, mobile and toxic
PPAR	Peroxisome proliferator-activated receptors
PPARg	Peroxisome proliferator-activated receptors gamma
PS	Persulfate
PXR	Pregnane-X-receptor
QSAR	Quantitative structure-activity relationship
RE	Responsive element
REACH	Registration, evaluation, authorization and restriction of chemicals
RO	Reverse osmosis
RPF	Relative potency factor
SAFF	Surface active foam fractionation
SMILES	Simplified molecular input line entry system

SSD	Species sensitivity distribution
TAT	Turn around time
TBT	Tributyltin
TCDD	Tetra-chlor-dibenzo-para-dioxin
TEQ	Toxic equivalency
TG	Test guideline
TH	Thyroid hormone
TPO	Thyroid peroxidase
TRL	Technology rediness level
TTR	Transthyretin
UV	Ultraviolet
UNZ	Unsaturated zone
vPvM	Very persistent, very mobile
WFD	Water framework directive

5 Circular Economy Routes

5.1 General

This document addresses five Circular Economy routes (A – E) that have a focus on the soil-sediment-system. The pathways of those routes are shown in Figure 1. Critical issues and potential solutions for (bio)monitoring and remediating industrial PMT shall be identified to enable safe circularity of resources. The solutions described in the following Clause 6 focus on solutions developed by the participating projects and external stakeholders to enable dealing with PMT/vPvM substances and by doing so contribute to safe circularity of resources.



Key

1 Human exposure
2 upstream watershed contribution
3 urban runoff
4 municipal wastewater
5 industrial activities
6 wastewater treatment plant
7 dredged sediments
8 sewage sludge / fertiliser
9 irrigation
10 leachate
11 surface water
12 drinking water treatment plant
13 bank filtrate
14 groundwater
15 landfill
16 PM(T) release from soil contamination
17 legacy contamination

⇢ Discharge/release
🟧 Stressors
°∘°∘ Contamination
→ Circular economy routes
⟳ Treatment

Figure 1 — Depicted are five Circular Economy Routes

5.2 Route A: Semi-closed water cycle for drinking water supply

Drinking water is produced in drinking water treatment plants by treating raw water sources such as groundwater, surface water, and/or a combination of both. Additionally, water treatment plants can pump surface water through various soil layers – known as bank filtration – to supplement the raw water needed to produce new drinking water. Once drinking water has been produced, distributed and used by consumers, it is discharged as wastewater and is transported via the sewer system to wastewater treatment plants. There it is treated physically, chemically, and biologically to ensure nutrient removal and environmental protection which are otherwise discharged to rivers or other surface water bodies. Such a semi-closed water cycle not only recycles water but can also transfer persistent chemicals, such as PFAS or PMT/vPvM substances in general, to water consumers.

5.3 Route B: Wastewater reuse for agricultural irrigation

In areas where surface water or groundwater quantities are lacking, treated municipal or industrial wastewater can be reused to irrigate farmland. The reuse of wastewater for irrigation can be accomplished by applying additional treatment steps after its traditional wastewater treatment plant processing (tertiary or quaternary treatments). These additional treatment steps are designed/selected to remove any remaining contaminants, pathogens or harmful chemicals to ensure the water meets safety and quality standards. These water reuse schemes shall consider the water-to-crop transfer of compounds, potential human health risks associated with direct or indirect (e.g. via animal fodder) crop consumption and agricultural best practices for farmers when setting the water quality limits for reclaimed water.

5.4 Route C: Nutrient and energy recovery from treated sludge for fertilizers

Recovering nutrients and energy from treated sludge is a valuable process that transforms waste into resources. To enable safe resource reuse in the form of fertilizers produced from sewage sludge, treatment technologies and combinations for PFAS and PMT/vPvM removal are required. This approach supports agricultural productivity, contributes to circular economy and finally brings us closer to the goal of near zero pollution discharge from landfill leachate plants, and allows energy recovery (e.g. syngas, bio-oil) as an additional benefit.

5.5 Route D: Material recovery from dredged sediment for eco-materials

With increasing urbanization, demands for construction materials (e.g. bricks, cement and concrete, asphalt, etc.) are constantly rising. An alternative to continuous production of new materials is the manufacturing of such materials from reclaimed and/or waste products. One example of this is the reuse of dredged sediment extracted during the expansion and maintenance of harbours or shipping channels. Once properly treated and freed from harmful substances, including PFAS and PMT/vPvM, these sediments can be reused as ecological and sustainable building materials, for example in the construction of dams, embankments or roads.

5.6 Route E: Groundwater and soil remediation to protect water cycle

Safeguarding the water cycle requires the diligent protection and remediation of soil and groundwater. Contaminants like PFAS and PMT/vPvM can infiltrate through soil and reach groundwater via human activities such as industrial discharges, or when brownfields and landfills are poorly designed and managed. By actively (bio)monitoring and addressing pollution in both the soil and groundwater, the quality of the groundwater can be ensured. This proactive approach is essential for maintaining the integrity of the water cycle and safeguarding environmental and public health.

6 Categories of solutions

6.1 Prevention and substitution

6.1.1 General

To prevent PMT/vPvM substances from reaching the soil-sediment-water system, upstream, proactive solutions are needed. However, currently and in many cases, retrospective, downstream (end-of-pipe) solutions can be implemented to remedy a problem that has already occurred. By using preventative measures, it is possible to reduce the manufacture, use and emissions of PMT/vPvM substances to the environment. The Chemicals Strategy for Sustainability towards a Toxic Free Environment [1] and the toxic free hierarchy presented therein, show that prevention via safe and sustainable chemical production and use is preferred over minimizing and controlling the risks and over eliminating and remediating chemical pollution.

To achieve action aimed at prevention, a variety of policy based, market related or academic tools can be used to support the development and substitution of harmful PMT/vPvM substances with safer and more sustainable alternatives or that result in cleaner processes and technologies.

This section provides information about the prevention and substitution of PMT/vPvM substances.

6.1.2 Why Prevention

The importance of limiting the release of PMT/vPvM substances to the environment is based on strong evidence that these substances are increasingly accumulating over time and space, entering drinking water sources and re-circulating within anthropogenic and natural water cycles. Once a PMT/vPvM substance is ubiquitous in the environment, it can be too late to apply downstream solutions and remove it from the environment efficiently. However, if a PMT/vPvM substance is prevented from being manufactured and thus used, then there are no exposure or removal costs.

The European Green Deal states "Achieving a toxic-free environment requires more action to prevent pollution from being generated as well as measures to clean and remedy it". This is key when considering solutions related to prevention. The recent introduction of hazard classes for PMT/vPvM substances into the Classification, Labelling and Packaging Regulation (1272/2008) [5] represents a milestone in the legislative framework for these substances. Additional legislations are expected to be revised to include PMT/vPvM substances, an example being the possible introduction of the identification of PMT/vPvM substances as substances of very high concern under the REACH.

In many cases, companies are unaware of whether they have PMT/vPvM substances in their supply chains or products. Financial investment is needed to support companies as they transition away from PMT/vPvM substances. Avoiding regrettable substitution of one harmful PMT/vPvM substance for another is of paramount importance. Previous examples have shown that the replacement of one substance with another thought to be less harmful can lead to further environment problems (e.g. the substitution of perfluorooctanoic acid (PFOA) with GenX which is also harmful to the environment and humans).

6.1.3 Types of preventative actions

To prevent PMT/vPvM substances reaching the environment, a safer and sustainable approach is needed for the manufacture and use of chemicals where harmful PMT/vPvM substance manufacture and use is limited but replaced with suitable alternatives. This will ensure a transition to safer chemicals, materials, products, and processes. To support this transition information is needed on alternatives and their suitability for a particular use.

An example of this can be viewed in the ZeroPM Alternative Assessment Databases [7] which has been built for PFAS. The database takes a functional substitution approach [8] to look at the chemical functions, end-use functions, and functions as a service when defining the use of a certain PFAS. This means it is possible to link the technical functions of the substance with the actual service provided by the final product or process it is used in, which makes the identification of potential alternatives easier. The database is built around use, rather than around the specific PFAS given the vast number of individual PFAS. For each use category, the database has the following:

- A list of sub-use(s) and application(s) of PFAS;
- The chemical function(s), end-use function(s), and service(s) provided by PFAS for all applications identified.

A non-exhaustive list of substances used for each application, along with their CAS number and INCHI key if available, the type of alternative, and some basic information on the suitability of the alternative of the specific application, and whether it is already available/in use on the market.

The main source of information used to identify alternatives in the database was the proposal for restriction of all uses of PFAS under the REACH Regulation and the ChemSec Marketplace online tool [9].

Prevention can also take the form of a conducive policy framework, and stakeholders can play a role in supporting the development of the framework armed with expertise and knowledge. The current policy framework for PMT/vPvM substances spans a wide range of policies and legislation, including:

- those aiming to reduce pollution at the source, by banning or restricting the manufacturing, placing on the market and use of hazardous substances (chemicals and product legislation), or requiring industrial facilities or other sectoral activities to take preventive measures against pollution (industrial emissions legislation);
- those monitoring and controlling concentrations of hazardous substances in environmental compartments and food (water, air, food safety legislation);
- those establishing rules for the collection, treatment, reuse, recycling, decontamination, and disposal of certain types of waste or for water reuse (water and waste legislation);
- those establishing the polluter pays principle to prevent and remedy environmental damage.

6.1.4 Proactive nature of the solution

Prevention and substitution are proactive in nature. Both should be applied upstream to ensure that PMT/vPvM substances are prevented from reaching the environment in the first place. By identifying alternatives that are safer and then by substituting the PMT/vPvM substance with the safer alternative, the need for reactive, end-of-pipe solutions is reduced.

6.1.5 Implementation Time

Preventative solutions shall be implemented upstream, so their effectiveness is maximized. Implementation is not a fast process. However, the identification of alternatives can be time-consuming and any regulatory framework change have to go through many formal processes before entering force.

6.1.6 Cost-benefit aspects

The cost-benefit of the substitution of a harmful PMT/vPvM substance to a safer alternative can be assessed within the framework of the Chemical Alternatives Assessment (CAA), which incorporates full life cycle considerations via life cycle impact assessment (LCIA). CAA allows hazards and/or risks for a specific use to be compared to the original substance and its alternative. In CAA it is important to consider the full life cycle (manufacture, use and disposal) of the chemical product. By using LCIA, impact categories such as persistence, mobility, and toxicity can be added to the more traditional categories such as climate change and destruction of the ozone layer.

Cost-benefit aspects of policy changes are considered via both Inception Impact Assessments and Impact Assessments. Inception Impact Assessments aim to inform citizens and stakeholders about the Commission's plans allowing them to provide feedback on the intended initiative and to participate effectively in future consultation activities. Citizens and stakeholders are invited to provide views on the Commission's understanding of the problem and possible solutions and to make available any relevant information that they possibly have, including on possible impacts of the different options. Impact Assessments are carried out on initiatives expected to have significant economic, social or environmental impacts. The impact assessment report shall include a description of:

— the environmental, social, and economic impacts, including impacts on small and medium enterprises and competitiveness, and an explicit statement if any of these are not considered significant,

— who will be affected by the initiative and how the consultation strategy and the results obtained from it will be used.

6.2 Remediation measures

6.2.1 General

This section provides information on the remediation measures for PFAS and other PM(T) substances. Remediation measures relevant for the soil-sediment-water system include technological solutions, including physical, chemical, biological, and thermal methods and technologies involved in different types of removal (e.g. separation, destruction, etc.).

The remediation measures presented reflect the current state of research and practice in remediation, including technologies at varying stages of development—from early laboratory research to market-ready solutions (TRL 3 to 9). However, this section does not cover all existing technologies for PFAS and other PM(T) substance removal, as the field is very rapidly evolving.

While there are currently no standards for PFAS and PM(T) remediation, existing directives and regulations provide limit values which shall be achieved to ensure compliance, e.g. drinking water requirements for PFAS set in the Drinking Water Directive. The technologies discussed have a critical role in achieving these regulatory requirements.

6.2.2 Overview of technologies

Table 1 outlines the different technologies discussed in this solution category. Information on the category (method for removal), target pollutants, target media, and TRL are presented for each technology. Detailed information for the listed technologies are presented in individual factsheets in A.1.

Table 1 — Technologies for remediation measures

Technology	Category	Target pollutants	Target media	TRL [10]
Surface Active Foam Fractionation (SAFF ®) (see Table A.1)	Separation – physical	PFAS	Water	9
Membrane filtration (nanofiltration, reverse osmosis) (see Table A.2)	Separation – physical, Concentration - physical	PFAS, other PMTs	Landfill leachate, water	9
Sediment washing (see Table A.3)	Separation – physical	PFAS	Sediment	7
E-peroxone based electrochemical advanced oxidation process (EAOP) (see Table A.4)	Destruction - chemical	PFAS, other PMTs	Water	6
Plant uptake (constructed wetlands) (see Table A.5)	Separation – physical, Destruction – biological	PFAS, other PMTs	Water	6
Activated persulfate with ferrate (see Table A.6)	Destruction - chemical	PFAS	Water	6
Co-pyrolysis of membrane concentrates and sewage sludge (see Table A.7)	Destruction – physical, chemical	PFAS	Landfill leachate concentrate, sewage sludge	6
In situ non-newtonian fluid flushing (see Table A.8)	Separation	PFAS	Soil	6
Cold atmospheric plasma (see Table A.9)	Destruction - chemical	PFAS	Water	4
Plasma (see Table A.10)	Destruction - chemical	PFAS	Landfill leachate	4
Ultrasonic cavitation (see Table A.11)	Destruction - chemical	PFAS	Water	4
Vermichar (see Table A.12)	Separation - biological and physical	PFAS	Soil	3

6.3 Co-creation and prioritization

6.3.1 General

Solutions that are selected to deal with PMT/vPvM substances in the soil-sediment-water system may not fit the needs of all stakeholders, particularly in the common reality of multiple demands for land, sludge and water use, limited budgets and potentially conflicting interests. Often long-term solutions cannot be made by simple technical analysis. Ambiguity calls for involvement of all stakeholders involved with issues related to pollutants like PMT/vPvM substances. These stakeholders can include: local authorities, scientists and technical consultants, landowners, businesses, and civil society [14]. Co-creation is based on stakeholder engagement, which refers to all the activities, practices, and processes that engage the active participation of individuals, communities, associations, and public authorities identified by the project management team as entities that can potentially contribute to the achievement of the project's objectives.

Through co-creation with external end-users, along with those at authority/policy level, it is possible to prioritize solutions through stakeholder engagement to:

— better identify problems and challenges by integrating diverse perspectives (e.g. landowners, community members, authorities at different levels);

— customize solutions to meet specific needs and preferences with regards to decision making strategies (e.g. guidance and tools for remediation strategies);

— build trust and ownership among key stakeholders through a bottom-up approach;

— ensure sustainability and transferability of the main outputs.

6.3.2 Purpose

Environmental decisions, including those related to soil-sediment-water remediation and restoration, are complex and multifaceted as they require a comprehensive understanding of both scientific and local perspectives. Decisions regarding remediation should not solely rely on scientific expertise but should integrate the practical knowledge and experiences of stakeholders directly involved in soil-sediment-water management. At local level, a long-term and sustained environmental management would benefit from bottom-up decision-making approaches, which calls for collaborative models involving different types of stakeholders [19]. Insufficient stakeholder engagement will prevent the progress of remediation and rehabilitation [15]. Stakeholder behaviours are shaped by emotions, perceptions, habits, and practices. While solutions to soil-sediment-water contamination challenges clearly require a collective understanding and joint action, inadequate stakeholder engagement can pose substantial obstacles to the progress of remediation and rehabilitation.

The report “Communication and citizen engagement initiatives in line with the Horizon Europe Mission A Soil Deal for Europe” [13] offers an overview of activities and initiatives of public consultation that involved citizens as target groups or stakeholders implemented across diverse geographic and socio-economic contexts both in rural and urban areas. As highlighted in the report, the level of citizen involvement encompasses active participation and consultation facilitated through engagement activities such as surveys, focus groups, online platforms etc. Additionally, citizens are engaged in various activities such as citizens experiments and/or active practices of soil protection and restoration practices.

The practices and tools employed in remediation projects have facilitated the sharing of best practices and increased awareness regarding the substantial efforts needed for effective remediation and sustainable management. These instances underscore advancements in research, innovative technologies, stakeholder engagement, and public awareness, offering insights into how remediation plays a crucial role in mitigating soil and water degradation and ensuring the provision of essential ecosystem services.

6.3.3 Co-creation and risk governance of remediation projects

In addition to environmental concerns related to remediation projects, it is crucial to comprehend the socioeconomic implication of soil-sediment-water remediation efforts, including their impacts on community dynamics, relationships and overall well-being [21]. The broader social and economic implication of these impacts are not only reflected in their effectiveness in cleaning contaminated soil-sediment and water, but also in relation to other factors, such as the acceptance of these initiatives within the local community. This involves evaluating the economic costs versus benefits, discerning implications for local economies, and identifying opportunities for sustainable development that align with remediation and restoration goals (e.g. land use goals, water quality goals, nutrient recycling). The ongoing process of learning and applying insights from past remediation efforts forms a vital component of a continuous improvement cycle. This iterative approach, based on the Risk Governance Framework [14] contributes to the evolution of informed and effective strategies to address soil contamination, fostering the development of best practices in remediation (Figure 2). The framework utilizes co-creation to prioritize and monitor solutions at all stages of risk-governance [14] during the remediation effort, from pre-assessment, assessment, characterization and evaluation and management.

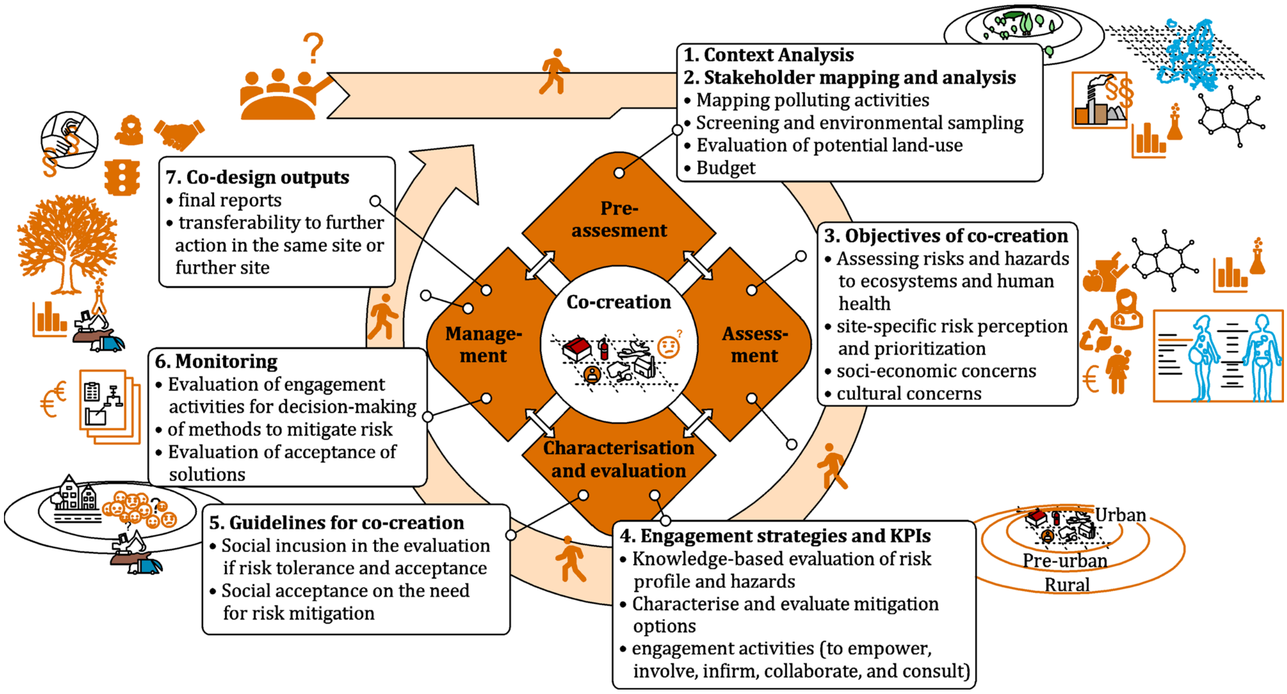


Figure 2 — The Risk Governance Framework as adopted by the Horizon project ARAGORN [14]

This iterative approach to a remediation effort can occur at smaller scales (pilot scales) and increase to larger scales as the remediation effort is expanded to optimize the volume of soil, sediment or water treated. All remediation technologies tend to come with challenges, be it energy consumption, water usage, chemical application or the potential degradation of ecosystems. These challenges can be identified by involving various stakeholders to ensure that acceptable solutions are identified to address such challenges.

As an example, in-situ chemical oxidation is a remediation approach relevant for PMT/vPvM sites, such as those containing chlorinated solvents [20]. This technique involves injecting chemical oxidants directly into the contaminated soil to break down or neutralize pollutants. This system is characterized by its efficiency in targeting specific contaminants and minimizing disturbance to the surrounding environment. In-situ chemical oxidation is particularly under discussion for addressing widespread substances without the need for extensive excavation. This can result in the formation of mobile degradation products and can lead to spread pollution. Therefore, the level of initial social acceptance for the use of chemical oxidants in the subsurface to treat contaminants can be low, due to concerns from local communities about the health and safety risks associated with the use of strong chemical oxidants, and risks to pollute drinking water from transformation byproducts. Expectations management and transparent communication are crucial factors to increase public trust and facilitate effective engagement, as well as ensuring a thorough understanding of the project's goal, its related safety measures and expected outcomes.

When opting for soil remediation strategies, effective decision-making requires a thorough understanding of the contaminants present at a given site, including not only the type of contaminant, but also their spatial distribution, concentrations, and potential migration pathways within the soil and surrounding environment. In this sense, to determine the most suitable remediation approach, studies on decision-making frameworks stress the need for robust risk assessments [16], which provide a systematic evaluation of the potential harm posed by contaminants to human health, ecosystems, and the environment supplemented by systematic socioeconomic analysis of risks, mitigation techniques and other concerns. The fundamental necessity of adopting a comprehensive solution-oriented perspective in soil and land management cannot be overstated. A crucial step entails embracing a systemic approach to innovation that tackles various societal challenges while mitigating adverse impacts on others [17]. Recognizing the interconnected nature of soil and land management, encompassing biophysical, economic, social, and political elements, underscores the importance of establishing a dynamic and location-specific/contextualized feedback system.

In this context, the potential of social innovation and the active involvement of local communities in the formulation and execution of soil management practices becomes highly significant. Such engagement contributes valuable insights into local conditions, priorities, and cultural considerations [18]. This approach aligns with the broader objective of promoting a nuanced understanding of the intricate relationships between soil management and various contextual factors, facilitating more effective and culturally sensitive solutions [18]. This underscores the potential of social innovation and stresses the importance of actively involving local communities in the formulation and execution of soil management practices. This active engagement is deemed essential as it enables communities to contribute valuable insights into local conditions, priorities, and cultural considerations. For instance, social innovation within soil management can encompass initiatives such as community-led monitoring programs, participatory soil remediation efforts or the development of educational campaigns aimed at raising awareness about soil health.

6.3.4 Approaching co-creation in practice

Figure 2 presents seven steps towards co-creation, as being used and developed in the project ARAGORN [75]. The steps are directed by methodological inquires and approaches. The identification of the problem(s) at stake is explored through a structured **context analysis (Step 1)** that draws on e.g. desk research on the contaminated sites (if available) and/or workshops, panel discussions, surveys that aim at both better understanding the context as well as identifying and categorizing the main stakeholders.

This leads to **stakeholder mapping and analysis (Step 2)**. The methodological inquires focus on defining the problem(s) and identifying who is involved or is affected. For large scale projects, this can imply deep dives into the geographical and socio-cultural aspect of the contaminated sites to explore what happened, when it occurred, whether and how the problem(s) has been addressed and who are the stakeholders impacted by contamination and those responsible for, inter alia, decision making, remediation strategies etc.

This systematic analysis is followed by discussing and agreeing with the site owners and with the key stakeholders, who are integral to the engagement activities on the **objectives of the co-creation**

(Step 3) activities. The objectives should encompass guidance documents and decision trees about the role and objectives of each stakeholder, but they could also relate to other aspects which are deemed of relevance in a specific context e.g. proposals for the development of effective risk and crisis communication management in case of soil contaminations.

Subsequently, methods and tools are selected based on the data collected in the previous steps. This entails deciding the **engagement strategies (Step 4)**, which can be the thought of as tools for consulting the stakeholders. The tools and methods are tailored to context and stakeholder-related information. In this step, key performance indicators (KPIs) can be set to evaluate whether the stakeholders involved in the engagement activities represent the interests, needs, and perspectives of the key stakeholders and to measure their level of engagement in the activities.

Key part of developing an engagement strategy is to identify how to consider the most important engagement level. A useful tool here is the **the ladder of engagement theory** [11], which ranks levels of engagement from highest to lowest as follows:

— **Empower**: stakeholders are the final decision-makers for prioritizing a solution. The goal is to support **decision-making and self-governance** among the community of stakeholders.

— **Collaborate**: stakeholders are a key partner in the design and prioritization process; activities are focuses on co-generating ideas, co-designing, co-creating, co-implementing solutions. The goal is to **integrate ideas** from stakeholders into the decision-making as much as possible.

— **Involve**: stakeholders are directly involved in the project; project decisions reflect their ideas and concerns. The goal is to **gather requirements, build consensus, co-design** of elements of a broader solution.

— **Consult**: stakeholders provide feedback on **alternatives or solutions**. **The goal is receiving actionable feedback** on available options by stakeholders.

— **Inform**: stakeholders are informed of the project and solutions. The goal is to **generate interest** and increase awareness among stakeholders.

The engagement strategies, based on consideration of the engagement level that is most desirable for activities with the stakeholders, will result in the formulation of **guidelines for co-creation (Step 5)** for the remediation project. As an example, an initial meeting can be to inform of plans, followed by a second meeting to consult, with an invitation for future involvement, collaboration or empowerment. The guidelines will be both general and context-specific, namely they will consist of general guiding principles to ensure e.g. social inclusion during workshops and other consultation activities with the stakeholders and of specific recommendations at site level, as necessary, based on the context and stakeholders' analyses. Templates to collect relevant information from the sites owners will be provided to ensure rigorous **monitoring (Step 6)** of the engagement strategies and activities while the project is ongoing. These steps will lead to the **co-design of the outputs (Step 7)**, specifically documents and reports that evaluate the success or outcome of the project, mindful of the objectives of the co-creation, and how this could be transferred into different projects.

Overall, the implementation of a structured co-creation framework in soil remediation and restoration projects has the objective of fostering collaboration and effective engagement between a vast array of stakeholders. Such a framework builds trust and ownership of the co-created results, creates active communication channels, and ensures tailored solutions that meet stakeholders’ needs and expectations. Lastly, it facilitates the achievement of more innovative and sustainable project outcomes that can be replicated in other contexts.

6.4 Monitoring

6.4.1 General

When talking about the Green Deal strategy for toxic-free water, it is usually referred to waters that are free from harmful chemicals or substances that can negatively impact human health, ecosystems, or both. In recent years, there has been a growing global emphasis on monitoring the mixture of the handful known and majority of yet unknown toxic PMTs from everyday waters by effect-based and non-animal-based diagnostic tools, driven by increased awareness about environmental and health risks.

In the context of the European Green Deal and sustainability movements, a "toxic-free" water approach involves several key aspects:

1) Chemicals and hazardous substances

   Many everyday waters contain chemicals that can be hazardous to health, such as certain endocrine disrupting chemicals (such as PFAS) and PMTs. Under the EU Green Deal, there are efforts to regulate and phase out the use of such substances in many products and to minimize them in the environment.

2) Circular economy and product design

   Eco-design: One focus is on designing products to be free from toxic substances from the outset and to be recyclable or reusable in the water cycle. The EU Circular Economy Action Plan promotes making products less harmful by encouraging the use of non-toxic materials and reducing waste.

3) EU regulations and standards

   REACH Regulation: The Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) is a key EU law that regulates the use of chemicals. It requires companies to register the chemicals they use, ensuring they are safe for human health and the environment by applying non-animal methods (NAMs) such as described in OECD IATA 320 guideline for endocrine disrupting chemicals (EDCs). The here applied NAMs are described in OECD (e.g. TG455, TG456), ISO standards (e.g. ISO 19040 and ISO 24295[1]), and the EU-ECVAM guideline (DB-ALM method Nr. 197).

4) Promoting safe substitution

   The EU and other regions are pushing for safer alternatives to toxic chemicals. For instance, companies are encouraged to use non-toxic, biodegradable ingredients in cleaning and personal care products, or safer alternatives to PMTs in products on the market and their impact to the environment.

5) Health and environmental impact

   Toxic-free products are especially important for reducing pollution, both as products (e.g. fire fighter foams AFFFs) as in the environment. They contribute to improved health outcomes by lowering exposure to chemicals that can cause cancer, hormonal disruptions, allergies or developmental issues in children.

Using cost-efficient, ethical friendly non-animal methods (NAM)-based and high-capacity toxicity testing (such as the human cell-based reporter gene assay panel) for a wide range of molecular initiating events (MIE) will help to shift toward toxic-free products, creating a healthier environment, improve personal well-being, and encourage companies to adopt safer and more sustainable practices.

For the Green Deal strategy for toxic free and zero pollution water covering many PMT a panel of NAMs such as for cytotoxicity, genotoxicity (e.g. p53 DNA repair, mutagenicity, micro nuclei), oxidative stress (e.g. Nrf2, ROS), early warning activities (e.g. PXR), PAH-like activities (e.g. Ah receptor ligands), obesity (e.g. PPARg) and endocrine disrupting activities (e.g. estrogenicity ER, inhibition androgenicity anti-AR, inhibition progestinicity anti-PR, thyroid-hormone transport inhibition TTR, TPO inhibition assay and inhibition thyroid-like activities anti-TR e.g. for PFAS-like compounds) can be applied based on human- and effect-based reporter gene assays (Table 2).

6.4.2 Purpose

New analytical *in vitro* and *in silico* toxicological methods are developed and applied to characterize PM substances of relevance to be applicable in different case studies. Non-animal methods (NAMs) are able to rapidly identify toxic hazards, irrespective of the chemical structure of the compound or chemical mixture. In combination with effect-directed analysis, powerful combinations can be made, enabling quantification of biological activity and identification of chemical structures involved. Reporter gene bioassays can be used to validate and further optimize the *in silico* QSAR models to better predict the toxic hazards of PFAS and related chemicals. The approaches using reporter gene technologies also enable the detection and hazard assessment of yet unknown and unidentified persistent and mobile chemicals and their complex mixtures and therefore provide a more comprehensive way of safety evaluation of drinking water and related production waters.

Effect-based results are used in risk assessments of both prioritised WFD compounds and their transformation products as well as applied in innovative water and soil removal technologies.

6.4.3 Overview of technologies

Table 2 outlines the different technologies discussed in this solution category. Information on the category (method for removal), target pollutants, target media, and TRL are presented for each technology. Technologies for which more detailed information could be compiled are presented in individual factsheets in A.2.

Table 2 — Technologies for monitoring

Technology	Target pollutants	Endpoints	Matrix
Non-animal methods (NAM) (see Table A.13)	PMTs	a) Cytotoxic Compounds [such as TBT-, several aromatic phenols/phosphates- and benzotriazoles-derivatives] b) Estrogenic compounds [such as estradiol-, several aromatic phenols/ phosphates-, benzotriazoles-and plastic additive-derivatives] c) Dioxin-like compounds [such as dioxins, PCBs and PAHs] d) Androgenic inhibiting compounds [such as many biocide, plastic additives and pharmaceuticals] Early Warning toxicants [such as nicardipine, aromatic phosphates and galaxolide]	Water/solid/sludge...
Chemical analysis based (see Table A.13)	Total PFAS (PFOA-CEQ)	Single PFAS concentration converted with NON-animal (PFAS reporter gene)-based RPFs	Water, sediments
Chemical analysis based (see Table A.14)	Total PFAS (PFOA-TEQ)	Single PFAS concentration converted with animal-based RPFs	Water, sediments
Surface Enhanced Raman Scattering (SERS) (see Table A.15)	PFAS (short and long chain)	Quantification of various short and long chain PFASs	Water /solid/human serum
Effect-based analysis (see Table A.14, Table A.18)	Total PFAS (PFOA-BEQ)	Thyroid-hormone transport competition	Water, sediments
***In silico* modelling** (see Table A.18)	PFAS	Endocrine Disrupting properties	PFAS pure chemical
Effect-based analysis (see Table A.20)	PMTs (BEQs)	Endocrine Disrupting Properties (EAT), AhR activation	Water, sediments

NOTE PFOA-BEQ (bioequivalency) is based on direct PFAS CALUX bioanalysis. PFOA-TEQ (total equivalency) is based on chemical concentrations converted with animal-based RPF values and PFOA-EQ (*in vitro* based equivalency) is based on chemical concentrations converted with non-animal (NAM)-based RPF values.

6.5 Hazard and exposure assessment

6.5.1 General

In case of pollution of the soil-sediment water system, an assessment of risks for the environment and for human health can be required. This clause provides different options on assessing the toxicity and/or the exposure of PFAS and other PMT substances with models and tools. It contains solutions for hazard and/or exposure assessment relevant for the soil-sediment-water system, including drinking water. The technologies considered in this chapter include *in vitro* methodologies for toxicological assessment of environmental media and *in silico* models for the prediction of substance properties or their behavior in the environment.

NOTE The solutions assess either hazard or exposure of PMT substances and not 'risks' as a whole. For this reason, risk assessment can only be done by combining solutions of hazard and exposure.

6.5.2 Technologies

There are three categories of technologies in this clause:

1) *In vitro* and *in silico* methodologies for toxicological assessment of PFAS

   - In this category, five solutions for the assessment of PFAS are presented. The first solution predicts physico-chemical properties of PFAS, while the other four are for the assessment of PFAS toxicity.

2) Model train for transport of PMT-substances in the porous media and groundwater

   - This model category contains one solution, namely the modelling train for reactive transport of PFAS in the unsaturated and saturated zone.

3) Novel exposure assessment models

   - This category contains two solutions, which are all newly developed or improved exposure assessment models.

In Table 3 the solutions are listed per category, which are presented in a factsheet in A.3. This list is not exhaustive as this is an evolving area, so there are other solutions that are still being developed.

Table 3 — Three categories for hazard and exposure assessment in which the solutions are divided in

Category	**Technology/ Solution**
Category 1: *In vitro* and *in silico* methodologies for assessment of PFAS	PFAS Physicochemical Predictions App
	QSAR models for predicting the binding score of PFAS to selected Nuclear Hormone Receptor
	Integrated *in silico* and *in vitro* approach TTR-TRβ PFAS
	Aquatic toxicity prediction tool
	Non-animal methods (NAMs) for *in vitro* toxicity testing of PMT compounds and complex mixtures
Category 2: Model train for transport of PMT-substances in porous media and groundwater	2/3D modelling train for reactive transport of PFAS in the unsaturated and saturated zone
Category 3: Novel exposure assessment models	SimpleBox Aquatic Persistence Dashboard
	Human Health Exposure Assessment model

Annex A
(informative)

Factsheets for the solutions of the different categories

A.1 Filled factsheets for solutions on remediation measures

Table A.1— Factsheet for SAFF

<table>
<tr><th colspan="3">Surface Active Foam Fractionation (SAFF®)</th></tr>
<tr><td colspan="3">General description of the remediation measure/technique
Surface active foam fractionation uses the active properties of short-chained PFAS to adsorb them onto rising air bubbles, forming a foam at the top of a fractionator. The PFAS rich foam is then harvested and treated separately.</td></tr>
<tr><td colspan="3">1. Fields of application</td></tr>
<tr><td>1.1 Target compounds</td><td>1.2 Receptors/media</td><td>1.3 Solution category</td></tr>
<tr><td>PFBA, PFBS, PFPeA, PFPeS, PFHxA, PFHxS, PFHpA; PFHpS, PFOA, PFOS, PFOSA, PFNA, PFNS, PFDA, PFDS, PFUnDA, PFUnDS, PFDoDA, PFDoDS, PFTrDA, PFTrDS</td><td>Water</td><td>Physical separation and concentration.</td></tr>
<tr><td colspan="3">2. Implementation Duration</td></tr>
<tr><td colspan="3">Treatment available full-scale on the market. Can be operated within a week from commissioning the system.</td></tr>
<tr><td colspan="3">3. Risks</td></tr>
<tr><td colspan="3">Less effective for short-chained PFAS, when only air is used. If additives are used, a higher reduction can be achieved for short-chained PFAS, although it is still difficult to remove PFBA.</td></tr>
<tr><td colspan="3">4. Innovation potential (vs classical technologies)</td></tr>
<tr><td colspan="3">This is a sustainable remediation technique. SAFF® contributes zero harm to the environment by using no consumables, minimal energy and labour, and producing no waste other than PFAS hyper-concentrate. By combining SAFF®'s ability to concentrate the PFAS waste together with a destruction method, a closed treatment system can be achieved (under development).</td></tr>
<tr><td colspan="3">5. Remediation yield</td></tr>
<tr><td colspan="3">Without additive: above 97% for PFHxS, PFHpS, PFOA, PFOS, 6:2 FTS, Sum of PFOA, PFOS, PFNA, PFHxS.
With additive: additionally above 90% for PFPeS, PFHxA, PFBS, PFHpA, Sum of 20 PFAS.</td></tr>
<tr><td colspan="3">6. Technology readiness level (TRL)</td></tr>
<tr><td colspan="3">TRL 9: SAFF® is a mature technology proven over many years at multiple sites globally, for the rapid removal of PFAS compounds from landfill leachate and other impacted waters.</td></tr>
</table>

7. Energy Aspects

0,7 kWh/m^3 treated water

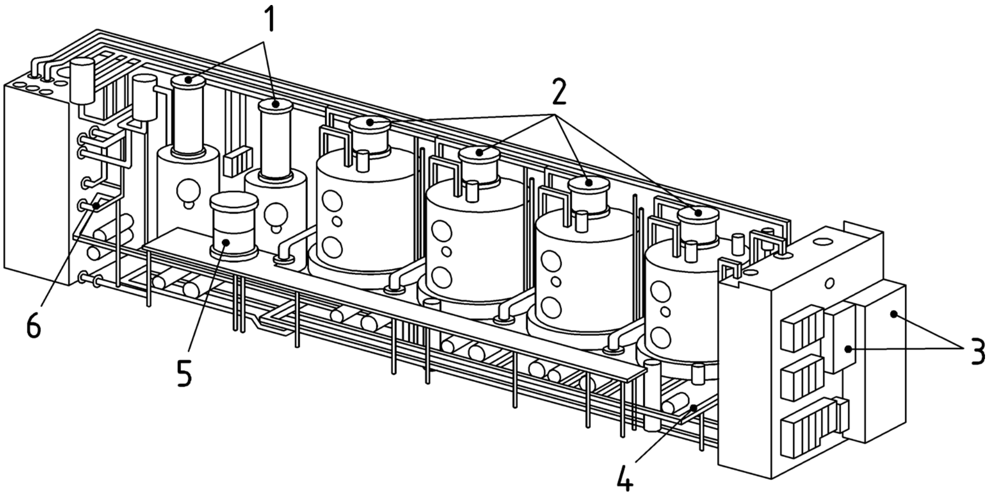
8. Cost aspects (€/ton or €/m^3)

Vary depending on the volume of treated water.

9. Environmental evaluation (if available: LCA, others)

Not available yet, currently being researched

10. Flow schematic/process description



Key

1	Secondary Fractionation Vessels
2	Primary Fractionation Vessels
3	Control Panel & Distribution Board
4	Contaminated Water Inflow and Recirculation
5	Surfactant Dosing System
6	Treated Water Outlet

SAFF® system [32]

11. Solution owner and contacts

EPOC Enviro [32]
ENVYTECH [29]

Table A.2— Factsheet for membrane filtration

Membrane filtration (nanofiltration, reverse osmosis)

General description of the remediation measure/technique

Compounds are filtered out of a solution by using membranes of different pore sizes.

1. Fields of application

1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFAS, other PMTs	Landfill leachate	Physical separation

2. Implementation Duration

Treated flow rate of 5 m^3/day with 50% of concentrate recirculation

3. Risks

The concentrate from this technology needs to be treated using destructive methods (e.g. using evaporation and subsequent pyrolysis).

4. Innovation potential (vs classical technologies)

Development of advanced treatment train to completely remove PFAS from landfill leachate.

5. Remediation yield

Removal by nanofiltration:

30 PFAS were analyzed and only 6 were detected. Observed removals were:

PFBA:from 81% to 95%

PFBS: from 74% to 94%

PFHpA: From 90% to 97%

PFHxA: From 87% to 98%

PFOA: From 89% to 98%

PFPeA: From 82% to 92%

Removal by reverse osmosis:

No PFAS were detected in the reverse osmosis permeate with a limit of quantification (LOQ) of 20 ng/l.

6. Technology readiness level (TRL)

TRL 9

7. Energy Aspects

Nanofiltration: 3 kWh/m^3 permeate (pilot data)

Reverse osmosis: 5,6 kWh/m^3 permeate (pilot data)

8. Cost aspects (€/ton or €/m^3)

Estimated operational treatment costs of Nanofiltration:

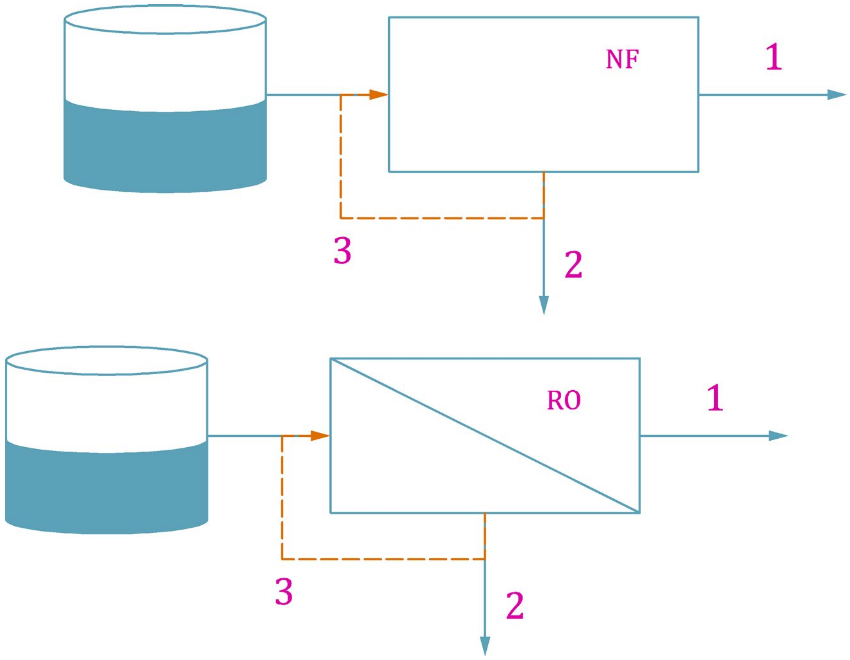
- Energy costs 0,22 €/m^3
    - operational costs (reagents and membranes) 6,0 €/m^3
    - concentrate disposal 3,6 €/m^3
- Reverse osmosis:

- Energy costs 0,32 €/m^3
    - operational costs (reagents and membranes) 6,2 €/m3
    - concentrate disposal 5,2 €/m^3

9. Environmental evaluation (if available: LCA, others)

LCA results are available for the full landfill leachate treatment train (NF/RO combined with pyrolysis) in PROMISCES deliverable D4.6. [31]

10. Flow schematic/process description



Key

1 Permeate
2 Concentrate
3 Recycle

Membrane filtration flow schematic [33]

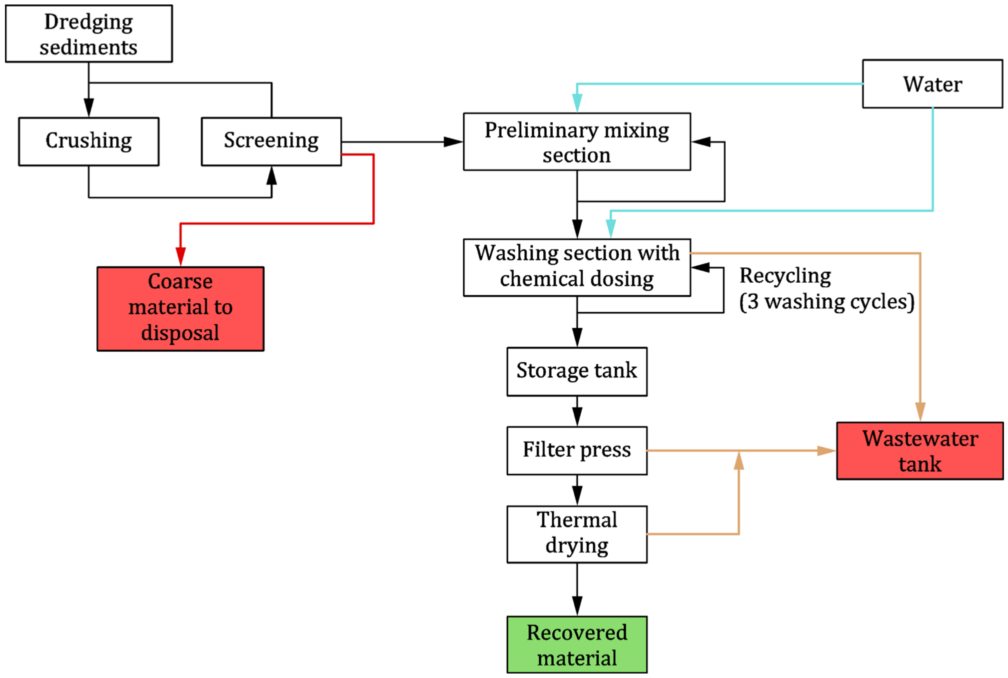
11. Solution owner and contacts

UNIVPM [33]
ACEA Infrastructure [34]
SIMAM [35]

Table A.3 — Factsheet for sediment washing

Sediment washing		
General description of the remediation measure/technique Washing sediments can remove the contaminated compounds from the sediments.		
1. Fields of application		
1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFAS	Dredged sediments	Physical-chemical separation
2. Implementation Duration		
200 kg/day for sediment washing		
3. Risks		
It is a separation method, so washing water containing all the removed PFAS needs to be treated later using destruction methods. Increase of PFBA concentration has been observed after mass balance analysis due to by-product transformation.		
4. Innovation potential (vs classical technologies)		
Soil/sediment washing treatment targeted to remove PFAS.		
5. Remediation yield		
Sediment washing with three washing cycles (acid washing, basic washing, neutral washing) Pilot scale tests with only basic washing and neutral washing Removal in sediments with low/medium contamination (sum of PFAS up to 1 000 ng/kg): PFBA 0%, PFOA 38% - non detectable in treated sediments, PFOS 73 – 80% Laboratory tests with three washing cycles. Removal in sediments with low/medium contamination (sum of PFAS up to 1 000 ng/kg): PFBA 67-74%, PFPeA >90% and non-detectable in treated sediment, PFOA complete removal and non-detectable in treated sediment, PFOS > 83% and non-detectable in treated sediment Removal in sediments with high contamination (Sum of PFAS > 2500 ng/kg): PFBA 20 – >60% and non-detectable in treated sediment, PFBS complete removal and non-detectable in treated sediment, PFOA 50 – 55%, PFOS 35 – 67%, N-MeFOSAA 0 – 41%, N-EtFOSAA 0 – 31%, PFDS 0 %		
6. Technology readiness level (TRL)		
TRL 7		
7. Energy Aspects		
Not available		
8. Cost aspects (€/ton or €/m3)		
Not available		
9. Environmental evaluation (if available: LCA, others)		
Not available		

10. Flow schematic/process description



Sediment washing flow schematic [33]

11. Solution owner and contacts

UNIVPM [33]

SO.GE.IN. [36]

ACEA Infrastructure [34]

Table A.4— Factsheet for EAOP

E-Peroxone based electrochemical advanced oxidation process (EAOP)

General description of the remediation measure/technique

Advanced oxidation processes, including an electrochemical cell, an ozone generator, and an ozone reactor, are coupled to oxidize compounds in water.

The electro-Peroxone (e-Peroxone) process merges electrochemical oxidation with ozonation, offering an advanced solution for wastewater treatment. This method efficiently degrades persistent toxic chemicals by generating hydroxyl radicals through an innovative, in-situ production of H_2O_2 via the cathodic oxygen reduction, enhanced by ozone gas sparging. Since hydroxyl radicals (E_0 = 2,80 V vs. SHE) are significantly stronger oxidants than ozone (E_0 = 2,07 V vs. SHE), they can rapidly degrade a wide range of organic pollutants at exceptionally high reaction rates ($\approx 10^{-8}$-10^{10} M^{-1} s^{-1}). During the e-Peroxone process, competing reactions at the cathode can hinder efficient H_2O_2 production. Key side reactions include the reduction of water to hydrogen, the further reduction of electro-generated H_2O_2 back to water, and the reduction of ozone to oxygen. To optimize H_2O_2 generation and enhance the overall efficiency of the process, reducing these competing reactions is crucial for advanced water treatment applications.

1. Fields of application

1.1 Target compounds	1.2 Receptors/media	1.3 Solution category
PFAS and PMTs	Water use for edible crop irrigation	Destruction-chemical treatment

2. Implementation Duration

Testing conducted between April to July 2024, in Montornès del Vallès WWTP, Barcelona Province, Spain, using the secondary-treated effluent as input to the EAOP. Around 60% of the inlet water to this WWTP comes from industries: pharmacy, organic chemistry, food industry, metal coating, leather and textile.

3. Risks

- Deposition of struvite on the boron-doped diamond electrodes, pipes, and pumps (maintenance required)
- Potential formation of inorganic ions (chlorate, perchlorate and bromate)
- Possible formation of byproducts (monitoring analyses required)
- Increase in the solution temperature resulting from the Joule effect in the electrochemical cell.

4. Innovation potential (vs classical technologies)

Superior oxidation rates lead to a significant improvement in the breakdown of highly persistent contaminants by enhancing the generation of hydroxyl radicals.

The H_2O_2 electro-generation overcomes the limitations of conventional methods, eliminating the need for high doses of H_2O_2 that pose safety risks during storage, transport, and handling. Furthermore, the e-Peroxone system addresses the limitations of traditional ozone treatments. By optimizing ozone mass transfer and utilization, this system boosts treatment efficiency and effectively prevents the unwanted formation of bromate, providing a powerful and reliable solution for advanced wastewater treatment. Therefore, this approach amplifies the oxidation efficiency, enabling contaminant breakdown and the quality of treated water [37].

5. Remediation yield

Ranging from 18% to 98% PMTs removal:
2-aminophenol (98±2) %
Carbendazim (67±27) %
Terbutryn (79±22) %
Venlafaxine (86±16) %
Carbamazepine (68±20) %
Ofloxacin (79±12) %
Caffeine (65±23) %
Flecainide (72±7) %
Diuron (47±24) %
1,2,3-Benzotriazole (47±15) %
Triethyl phosphate (30±3) %
Temazepam (22±4) %
Galaxolidone (34±6) %
Tributyl phosphate/triisobutyl phosphate (18±6) %
(4+5)-Methylbenzotriazole (63±19) %
N,N'-Diphenylguanidine (DPG) (93±7) %
Tributylamine (78±14) %
Dibutyl phthalate (75±31) %
Diethyl phthalate (74±23) %
Carbendazim (67±27) %
PFAS removal could not be observed in the EAOP system

6. Technology readiness level (TRL)

TRL 6

7. Energy Aspects

5,10 kWh/m^3

8. Cost aspects (€/ton or €/m^3)

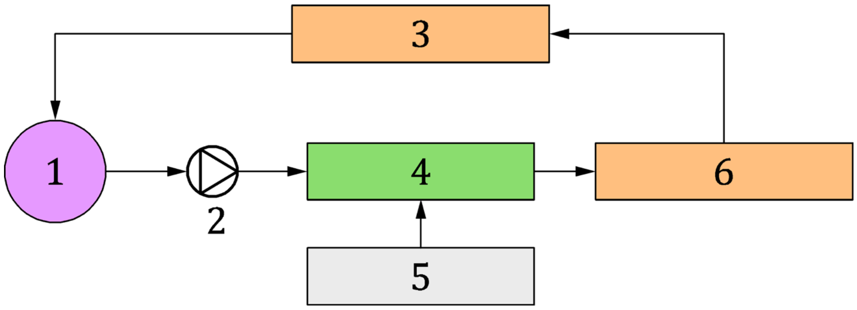
≈ 2,54 €/m^3
(EU average price for non-household consumers: 0,2008 €/kWh in second-half 2023)

9. Environmental evaluation (if available: LCA, others)

Toxicity testing was conducted using CALUX bioassays, which showed an overall 72,6% toxicity reduction

10. Flow schematic/process description

The EAOP prototype (APRIA Systems, Photobench LED275-8a) has been designed to integrate three advanced oxidation technologies, each engineered to operate independently or in combination with the others: (i) an ozone generation system equipped with an ozoniser and a Venturi tube, (ii) an annular UV-C LED photoreactor, and (iii) an electrochemical cell equipped with BBD (boron-doped diamond) electrodes. This flexible configuration enables for tailored operation depending on the treatment requirements, optimizing performance, and efficiency in the pollutant degradation.



Key

1 Feeding tank
2 Pump
3 Electrochemical cell/Photochemical unit
4 Ozone contact reactor
5 Ozone generator
6 Electrochemical cell/Photochemical unit

Schematic representation of the EAOPs prototype (APRIA Systems, Photobench LED275-8a)

11. Solution owner and contacts

EURECAT [38]

Table A.5 — Factsheet for plant uptake (constructed wetland)

Plant uptake (constructed wetland)

General description of the remediation measure/technique

Constructed wetlands (CWs) are engineered ecosystems designed to mimic filtration and purification functions of natural wetlands to enhance the water quality. These systems are composed of three key components: well-balanced substrates made of sand, gravel, and other materials; diverse populations of microorganisms; and hardy plant species selected for their capacity to absorb pollutants.

These artificial systems can be categorized based on three key criteria: i) hydrology, distinguishing between surface or subsurface flows, ii) plant species type, including emergent, submerged, or free-floating plants, and iii) flow direction, whether horizontal or vertical [39].

Horizontal subsurface flow constructed wetland (HSSFCW) is one of the most widely used CW systems across Europe. In this setup, wastewater flows gradually through a porous medium, reaching the plant substrate where many pollutants are filtered out before being discharged as treated effluent. The wetland features aerobic zones, populated by macrophytes and soil substrates, alongside anaerobic zones primarily composed of gravel and sand [40].

The selection of the appropriate vegetation is crucial for effective CW design. Two of the most used species are *Phragmites australis* and *Iris pseudacorus*, wetland macrophytes, which play a vital role in enhancing the system's performance. These species serve multiple functions including nutrient uptake, oxygen release in the rhizosphere, filtration, providing surfaces for microbial biofilm growth, stabilizing substrates, and aiding in pollutant treatment [41].

1. Fields of application

1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFAS and PMT	Water use for edible crop irrigation	Biological/physico-chemical treatment

2. Implementation Duration

Testing conducted between April to July 2024 in Montornès del Vallès WWTP, Barcelona Province, Spain. The wetland treated two types of effluents: secondary treated WWTP effluent and tertiary treated with EAOP (Table A.4).

Four weeks during the testing period experienced rainfall exceeding 20 mm, with a maximum of 51.1 mm recorded on April 29, 2024 (week 3). To prevent overflow, water input to the wetland is suspended during heavy rain events.

Temperature patterns revealed a temperate climate during the initial weeks (13–18ºC from weeks 1 to 7), rising to averages above 25ºC in July. Evapotranspiration rates, calculated by the Catalan meteorological network using temperature and solar radiation data, consistently exceed 30 mm per week.

3. Risks

- Water loss through evapotranspiration;
- Factors such as prolonged droughts or excessive rainfall affect assessment of treatment performance;
- Media saturation with contaminants, reducing the process efficiency;
- Limited understanding of the potential desorption of these pollutants accumulated in the roots after plant death.

4. Innovation potential (vs classical technologies)

- More sustainable/eco-friendly treatment, contributing to climate change mitigation by carbon sequestration;
- Long-term stability and low maintenance, making wetlands a reliable and environmentally friendly solution;
- Low power consumption:

5. Remediation yield

41 %±9 % PMTs removal in average with tertiary EAOP-treated wastewater as input:
Dibutyl phthalate (72±35) %
N,N’-DPG (56±6) %
Diethyl phthalate (52±18) %
Tributylamine (43±9) %
Tributyl phosphate / triisobutyl phosphate (35±10) %
2-aminophenol (34±19) %
1,2,3-Benzotriazole (29±16) %
(4+5)-methylbenzotriazole (14±5) %
36±20% PMTs removal in average with secondary-treated wastewater as input:
Dibutyl phthalate (80±29) %
Diethyl phthalate (43±40) %
2-aminophenol (40±15) %
1,2,3-Benzotriazole (32±26) %
Tributylamine (32±24) %
Tributyl phosphate / triisobutyl phosphate (28±13) %
N,N’-DPG (21±9) %
(4+5)-methylbenzotriazole (10±6) %
PFAS removal could not be observed in the CW systems
Removal of oxidation byproducts:
Chloride (17 %)
Chlorate (50 %)
Perchlorate (14 %)

6. Technology readiness level (TRL)

TRL 6

7. Energy Aspects

Minimal energy requirements (only for water pumping, 0,89 kWh/m^3).
Gravity-driven design is recommended to reduce energy consumption.

8. Cost aspects (€/ton or €/m^3)

≈ 0,18 €/m^3
(EU average price for non-household consumers: 0,2008 €/KWh in second-half 2023)

9. Environmental evaluation (if available: LCA, others)

Toxicity testing was conducted using CALUX bioassays, which showed a 64 % toxicity reduction for PFAS.

10. Flow schematic/process description

Two small wetland flumes, each 3 meters in length, were constructed. One wetland receives treated water from the E-Peroxone based electrochemical advanced oxidation prototype, while the other receives secondary wastewater effluent. Both wetland channels measure 74 cm in width, 47 cm in depth, and 3 meters in length, and two plant species, Iris pseudocorus and Phragmites sp., were used.

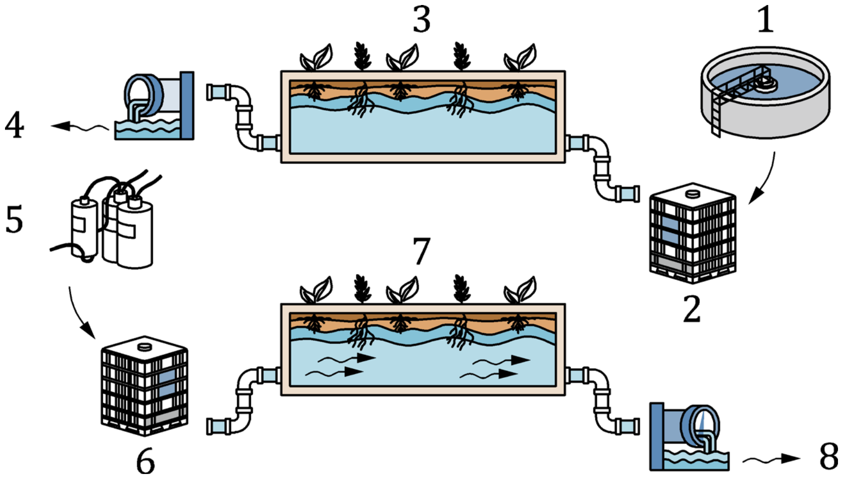
Two CW channels were thoughtfully designed to maximize their natural filtration capabilities, each measuring 74 cm in width, 47 cm in depth, and 3 meters in length, and employing a horizontal subsurface flow configuration. These artificial ecosystems incorporated a layered gravel system (1,5 cm diameter), enhancing water flow and filtration, along with the introduction of two macrophyte species: Iris pseudacorus and Phragmites australis.

One of the flumes received water directly from the outlet of the Montornès del Vallès WWTP, utilizing secondary effluent without prior filtration, and the second channel was supplied with water from the EAOP prototype outlet, which underwent both filtration and e-Peroxone process.

Both constructed wetlands were fed from the lower part of the flume and worked as subsurface horizontal flow where water flowed through a granular medium, with a depth that depends on the size and extent of plant roots.

Both constructed wetlands (CWs) operated under the same hydraulic conditions, with a flow rate of ca. 0,35 L/min (21 L/h).

The CWs had an effective porosity of 25 % (determined through granulometric analysis), and with the water filled to half depth, they hold an estimated water volume of approximately 250 litres. The average hydraulic residence time, based on the inlet flow rate and total volume treated, ranged between 16 and 17 hours. However, during peak flow periods (21 L/h), the residence time was reduced to 6 hours.



Key

1	WWTP Secondary effluent
2	Secondary effluent (buffer tank)
3	Control flume
4	Outlet WWTP
5	Filtration and e-Peroxone process
6	AOP outlet (buffer tank)
7	Promisces flume
8	Outlet WWTP

Experimental set-up design for the CW

11. Solution owner and contacts

CBT [42]

EURECAT [38]

Table A.6 — Factsheet for activated persulfate with ferrate

Activated persulfate with ferrate

General description of the remediation measure/technique

The combination of ferrate and persulfate produces reactive species which can further react and oxidize compounds of concern. This method can be used for in situ groundwater remediation by injection of activated persulfate with ferrate into the groundwater.

1. Fields of application

1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFAS	Groundwater	Destruction-chemical treatment

2. Implementation Duration

Tests conducted for one month (July 2024). First set of 3 injections of activated persulfate with ferrate into the groundwater body (at 0 h, 8 h and 24 h). Second set of 3 injections (at 0 h, 8 h and 24 h). Treatment time depends on the transmissivity of the soil – it will be dictated by the water flow, but 3 injections should be made, with the first one having the ideal/recommended dose of reagent based on the contamination concentration, with the second and third doses adjusted to ensure optimal in situ treatment.

3. Risks

Potential formation of transformation products.

Groundwater flow contingencies due to potential reagent precipitates.

4. Innovation potential (vs classical technologies)

When ferrate, a green and effective oxidant, is combined with persulfate, various highly reactive species are formed through a sophisticated activation process. Key reactive species, such as persulfate radicals (SO_4^-) and hydroxyl radicals (HO) are produced at a much faster rate than intermediate iron species. These radicals and formed iron species react with high-rate constants, resulting in a rapid abatement of different organic pollutants including PFAS.

5. Remediation yield

Maximum removals achieved after the first set of injections, ranging from 34 % to 95 %.

- PFBA: 81 %
- PFPeA: 34 %
- PFHxA: 92 %
- PFHpA: 53 %
- PFOA: 61 %
- PFNA: 73 %
- PFDA: 77 %
- PFBS: 74 %
- PFPeS: 78 %
- PFHxS: 79 %
- PFHpS: 56 %
- PFOS: 90 %
- PFNS: 87 %
- 6:2 FTS: 95 %

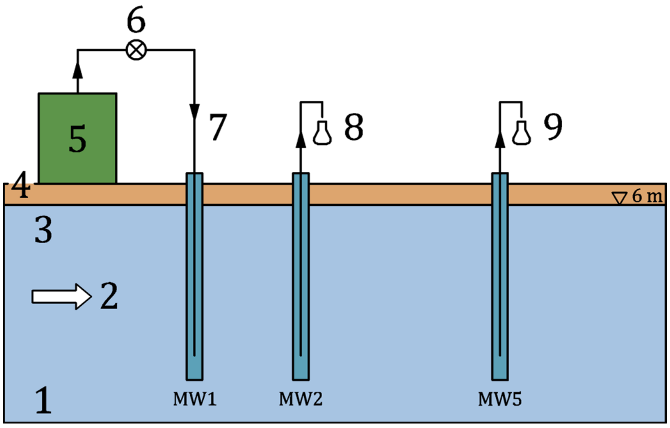
- 8:2 FTS: 86 % Maximum removals achieved after the second set of injections, ranging from 1 % to 97 %. PFPeA: 16 % PFHxA: 77 % PFOA: 40 % PFDA: 40 % PFHxS: 18 % PFHpS: 22 % PFOS: 97 % 6:2 FTS: 1 %
6. Technology readiness level (TRL)
TRL 6
7. Energy Aspects
Minimal energy requirements (only water pumping, 0,89 kWh/m^3).
8. Cost aspects (€/ton or €/m^3)
Considering only reagents costs 0,5 €/m^3 Considering reagents costs and other costs such implementation costs (employee wages and other materials) 4 €/m^3.
9. Environmental evaluation (if available: LCA, others)
Depending on the well, 50 % to 89 % toxicity reduction was achieved after the first set of injections, and 18 % to 70 % after the second injection.

10. Flow schematic/process description

The groundwater remediation consists of two series of 3 injections each (6 injections in total), carried out at 0 h, 8 h and 24 h in monitoring well 1 (MW1). PFAS concentrations were monitored in wells MW2 and MW5 at 0 h, 4 h, 8 h, 32 h, 2 weeks, and 3 weeks for well MW2, and at 0 h, 4 days, 2 weeks, and 3 weeks for well MW5.

In the first set of injections, a total volume of 200 L was prepared for each injection in a drum containing tap water with a 10 mM PS+1 mM Fe(VI) reagent mixture.

In the second set of injections, the same injection volume was used, but the dose of ferrate used was tripled, 10 mM PS+3 mM Fe(VI).



Key

1	Aquifer
2	GW flow direction
3	Saturated zone
4	Unsaturated zone
5	Tank with PS+Fe(VI)+ tap water; Total = 200 L
6	Injection at 0 h, 8 h and 24 h
7	Injection well
8	Sampling well
9	Sampling well

Flow scheme of the usage of activated persulfate with ferrate for groundwater remediation

11. Solution owner and contacts

EURECAT [38]

ESOLVE [43]

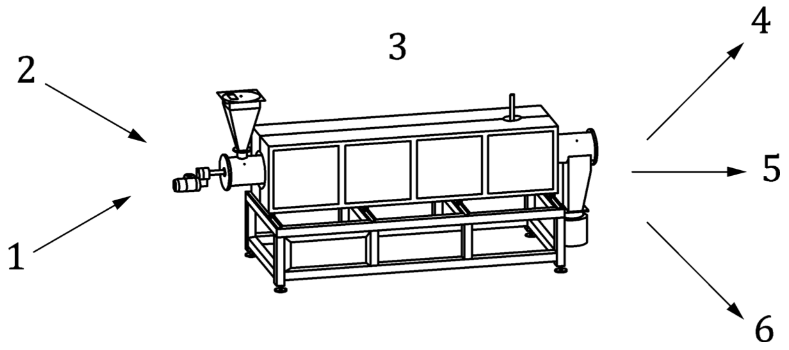
Table A.7 — Factsheet for co-pyrolysis of membrane concentrates and sewage sludge

Co-pyrolysis of membrane concentrates and sewage sludge		
General description of the remediation measure/technique Non-oxidative thermochemical treatment of reverse osmosis and/or nanofiltration concentrate and sludge at a high temperature (600 °C) ensures physical and chemical destruction of organic compounds.		
1. Fields of application		
1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFAS	wastewater treatment plant sludge, landfill leachate treatment plant sludge, nanofiltration/reverse osmosis dried concentrate	Physical-chemical destruction
2. Implementation Duration		
Treated material 9 kg/hour		
3. Risks		
Additional analysis should be carried out on the recovered products (i.e. biochar, biooil, and syngas) for a safe and profitable use.		
4. Innovation potential (vs classical technologies)		
Development of co-pyrolysis treatment of landfill leachate treatment plant sludge and nanofiltration/reverse osmosis dried concentrate for complete elimination of PFAS compounds. It is a compact technology that can be operated on site at the landfill leachate treatment plant.		
5. Remediation yield		
Pyrolysis reactor operated at 600 °C and with 20 min of reaction time: None of the treated 30 PFAS were found in the biochar (limit of quantification (LOQ) =1 µg/kg) PFAS are transformed during thermal treatment and trace level of PFAS were detected in the stack emissions and bio-oil. The main source of PFAS was from the NF/RO concentrate when compared to the sludge. When pyrolysis was operated under non-optimal conditions (lower temperature and different reaction times), PFAS were also detected in the biochar.		
6. Technology readiness level (TRL)		
TRL 6		
7. Energy Aspects		
Literature data: power consumption of 16 kWh for a treatment capacity of 100 kg/h Production of excess thermal energy of 1 125 000 kWh		
8. Cost aspects (€/ton or €/m3)		
Not available		

9. Environmental evaluation (if available: LCA, others)

LCA results are available for the full landfill leachate treatment train (NF/RO combined with pyrolysis) in PROMISCES deliverable D4.6. [31]

10. Flow schematic/process description



Key

1 RO/NF Concentrate
2 Leachate Sludge
3 Pyrolysis
4 Syngas
5 Bio-Char
6 Bio-Oil

Pyrolysis reactor, with treatment inputs and outputs [33]

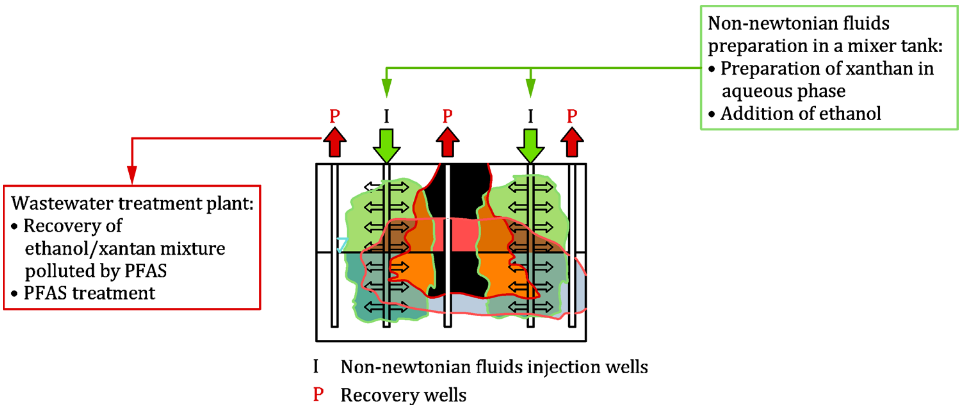
11. Solution owner and contacts

UNIVPM [33]
ACEA Infrastructure [34]
SIMAM [35]

Table A.8 — Factsheet for *in situ* non-newtonian fluid flushing

***In situ* non-newtonian fluid flushing**		
General description of the remediation measure/technique In situ remediation measure of soil and groundwater contaminated with aqueous firefighting foam by site flushing. The process uses a non-Newtonian liquid based on xanthan and ethanol to extracted PFAS from groundwater and separate contaminants from the soil matrix.		
1. Fields of application		
1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFAS	Groundwater, Soil	Extraction/separation treatment
2. Implementation Duration		
The duration of the treatment can take several weeks or months depending on the contamination site. It takes approximately between 2 and 4 pore volumes of flushing solution to treat the soils.		
3. Risks		
The formulation of non-Newtonian liquid is based on xanthan and ethanol. The use of ethanol should be done with caution. Ethanol is biodegradable. Xanthan is not toxic.		
4. Innovation potential (vs classical technologies)		
Classic flushing solutions are made without non-Newtonian liquids. As a result, it is difficult to inject these solutions homogeneously into a heterogeneous medium. Shear thinning liquids (whose viscosity decreases as a function of shear stress) allow heterogeneous soils to be swept homogeneously. The flushing efficiency is therefore higher compared to classic flushing solutions.		
5. Remediation yield		
Polymer (xanthan) injection with solvent (ethanol) was performed on soils spiked with PFOA, PFBS, PFHxS, and PFOS. Remediation yields were 99 %, 98 %, 92 % and 90 % respectively for PFOA, PFBS, PFHxS, and PFOS with the addition of xanthan and ethanol (versus 82 %, 90 %, 70 %, 67 % respectively for PFOA, PFBS, PFHxS, and PFOS when flushing with water).		
6. Technology readiness level (TRL)		
TRL 6		
7. Energy Aspects		
Not available yet.		
8. Cost aspects (€/ton or €/m3)		
Not available yet.		
9. Environmental evaluation (if available: LCA, others)		
Not available yet.		

10. Flow schematic/process description



Non-Newtonian fluid injection process with inputs and outputs [44]

11. Solution owner and contacts

BRGM [44]

Colas Environnement [45]

Table A.9 — Factsheet for cold atmospheric plasma

Cold atmospheric plasma		
General description of the remediation measure/technique The cold atmospheric plasma treatment is a technology based on the production (in the water or immediately above the liquid) of electrical discharges capable of producing reactive species both in the liquid and gaseous phase. These highly reactive oxygen and nitrogen species (e.g. singlet oxygen, hydroxyl radicals, nitrite) can react with recalcitrant compounds (e.g. PFAS) and instigate their mineralization.		
1. Fields of application		
1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFOA, PFOS and PFPeA	Water	Destruction treatment
2. Implementation Duration		
12 months		
3. Risks		
Potential formation of toxic transformation products		
4. Innovation potential (vs classical technologies)		
The cold plasma process for treatment of wastewater/groundwater, particularly those containing PFAS, represents a groundbreaking and innovative research/technological approach on a global scale. The main innovation of cold plasma lies in the simultaneous action of both oxidative and reductive reactive species, and emission of UV radiation. This makes plasma unique for targeting pollutants like PFAS, compared to existing technologies (ozonation, photocatalysis, etc.), whose effectiveness is limited as the strong C-F bond cannot be broken by the action of only oxidative species such as ozone and hydroxyl radicals.		
5. Remediation yield		
After 30 minutes of treatment, the degradation of PFOA in ultrapure water was >99,9 % (plasma-air), 99 % (plasma-N2), 95 % (plasma-Ar), and 63 % (plasma-O2). PFOA degradation was equally effective across the studied range of initial concentrations (0,1 to 10 mg/L). Air was effective in degrading PFOA in ultrapure water and tap water, whereas argon was much more effective in degrading PFOA in tap water (> 99,9 % after 20 minutes).		
6. Technology readiness level (TRL)		
TRL 4		
7. Energy Aspects		
20 kWh/m^3 for PFOA destruction		
8. Cost aspects (€/ton or €/m^3)		
3 €/m^3 for PFOA destruction		
9. Environmental evaluation (if available: LCA, others)		
Not assessed yet		
10. Flow schematic/process description		
The technology involves placing electrodes above the water surface, allowing the reactive species generated by the plasma (vide infra) to diffuse into the water by passing through the plasma-water interface. In case of the bubbling method, plasma is produced inside bubbles that are injected into the solution. Here, the reactive species are formed inside the bubbles and readily disperse in water.		
11. Solution owner and contacts		
Foundation for Research and Technology Hellas (FORTH)		

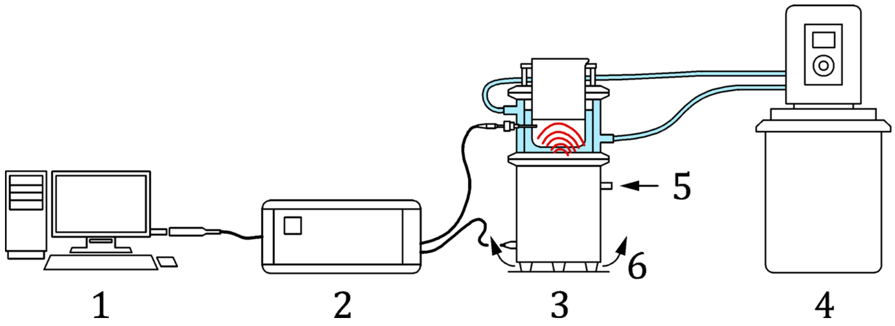
Table A.10 — Factsheet for Plasma

Plasma		
General description of the remediation measure/technique Compounds are destroyed by applying an electrical current to produce ions, highly-reactive short-lived radicals, and short-wave radiation from air and atmospheric oxygen.		
1. Fields of application		
1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFBA, PFOA, PFHxA, PFPeA, PFDA	Landfill leachate, water, sludge	Destruction treatment
2. Implementation Duration		
Still under assessment		
3. Risks		
Possible degradation of the compounds to more toxic by-products		
4. Innovation potential (vs classical technologies)		
Due to the presence of charged particles (electrons and ions), UV radiation, reactive particles (excited atoms, molecules and radicals), electromagnetic fields, and the temperature, plasma is a highly reactive and useful treatment for various applications. It is particularly interesting for highly concentrated liquid streams.		
5. Remediation yield		
Not yet available.		
6. Technology readiness level (TRL)		
TRL 4		
7. Energy Aspects		
Still under evaluation		
8. Cost aspects (€/ton or €/m3)		
Still under evaluation		
9. Environmental evaluation (if available: LCA, others)		
Not yet available		
10. Flow schematic/process description		
Treatment with Beta (plasma type) device in two configurations: 1) underwater mode 2) surface mode. Pilot investigation of a novel microwave plasma source, the argon plasma torch at 2,45 GHz, designed for wastewater treatment and the mitigation of chemical pollution, with a primary focus on removing PFAS.		
11. Solution owner and contacts		
Sofia University [47]		

Table A.11 — Factsheet for ultrasonic cavitation

Ultrasonic cavitation		
General description of the remediation measure/technique High power ultrasounds stimulate the formation and collapse of cavitation bubbles in a liquid medium. The energy released during the collapse can be used to break down chemical bonds.		
1. Fields of application		
1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFAS	Liquid media	Destruction treatment
2. Implementation Duration		
It requires 3 to 4 hours to almost completely degrade PFAS in 300 mL solution at 100 W in diluted media. No tests in continuous mode have been performed yet, but treatment time is expected to decrease by increasing the power density.		
3. Risks		
There are no risks to health or the environment through the use of ultrasound at the tested frequency value (20 to 500 kHz).		
4. Innovation potential (vs classical technologies)		
Ultrasonic cavitation is a chemical free degradation technology that can be combined with other oxidation techniques and can be implemented in industrial environments.		
5. Remediation yield		
97 % average PFAS degradation yield regardless of carbon chain length. Tested on a PFOS simulated aqueous solution model and on a PFAS mixture from groundwater from Spain: PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFPrS, PFBS, PFPeS, PFHxS, PFHpS, PFOS, PFNS, 6:2 FTSA, 8:2 FTSA, 10:2 FTSA, FBSA, FBSA, FHxSA, PFHxSAM, 6:2 FTAB, 6:2 FTSaAM.		
6. Technology readiness level (TRL)		
TRL 4 in PROMISCES [2], but available at TRL 9 for industrial applications.		
7. Energy Aspects		
412 kWh/m^{3} in diluted media and based on lab scale experiments.		
8. Cost aspects (€/ton or €/m^{3})		
76 €/m^{3} in diluted media and based on lab scale experiments (based on basic professional rate of 0,1845€/kWh).		
9. Environmental evaluation (if available: LCA, others)		
Not available		
10. Flow schematic / process description		
A liquid in contact with high power ultrasound will experience the cavitation phenomenon. Each cavitation bubble can be considered as a liquid-gas chemical reactor due to the high energy involved.		

The cavitation generated has the potential to break even highly energetic chemical bonds.



Key

1	Integrated monitoring
2	Generator
3	Reactor
4	Thermostat
5	Air in
6	Air out

Schematic of the integrated ultrasonication system [48]

11. Solution owner and contacts

SinapTec [48]

Table A.12 — Factsheet for Vermichar

Vermichar		
General description of the remediation measure/technique Vermichar, derived from vermicomposting agricultural waste with biochar, immobilizes PFAS in soils.		
1. Fields of application		
1.1 Target compounds	**1.2 Receptors/media**	**1.3 Solution category**
PFAS (tested: PFOA, PFOS)	Soil	Physical and biological treatment of PFAS, immobilisation
2. Implementation Duration		
Minimum 3 months		
3. Risks		
Potential transformation product formation: observed transformation of PFOS into 6:2 FTSA.		
4. Innovation potential (vs classical technologies)		
Agricultural waste is used to create biochar activated by earthworm activity. This technology reduces the generated agricultural waste, ensuring a circular economy approach as well as improving the agricultural soils through immobilization of pollutants like PFAS.		
5. Remediation yield		
Still under assessment		
6. Technology readiness level (TRL)		
TRL 3		
7. Energy Aspects		
Not assessed yet		
8. Cost aspects (€/ton or €/m3)		
Not assessed yet		
9. Environmental evaluation (if available: LCA, others)		
Not assessed yet		
10. Flow schematic/process description		
An illustrated process description can be found in reference [27].		
11. Solution owner and contacts		
Universidad de Castilla-La Mancha (UCLM) [49]		

A.2 Filled factsheets for solutions on monitoring

Table A.13 — Factsheet for NAM by CALUX panel for PMTs

Non-animal methods (NAM) by CALUX panel for PMTs		
1. Fields of application		
1.1 Target compounds	**1.2 Type of sample/matrices**	**1.3 Type of method/category**
— Cytotoxic compounds [such as TBT-, several aromatic phenols/phosphates- and benzotriazoles-derivatives] — Estrogenic compounds [such as estradiol-, several aromatic phenols/ phosphates-, benzotriazoles-and plastic additive-derivatives] — Dioxin-like compounds [such as dioxins, PCBs and PAHs] — Androgenic inhibiting compounds [such as many biocide, plastic additives and pharmaceuticals] — Early warning toxicants [such as nicardipine, aromatic phosphates and galaxolide] — All thyroid-hormone transport competing PFAS	Water/solid/sludge...	in lab/cell culture based *in vitro* testing (non-animal based)
2. General description of the technology		
CALUX bioassays (Chemical Activated Luciferase eXpression; BioDetection Systems BV, Amsterdam, the Netherlands) were applied for the analysis of all kinds of water samples. Sample preparation was performed following fully validated methods and standard operational procedures, which are described in detail in [24], [25]. Briefly, optimized solid-phase extraction (SPE) was applied to extract water samples. The enriched extract with a mixture of compounds was exposed to genetically modified cell lines. The cell lines utilized in CALUX® bioassays were incorporated with firefly luciferase gene, which is coupled with responsive elements (REs) such as reporter genes. The presence of specific compounds triggers the activation of such RE2 and consequently initiates the creation of luciferase, which emits light in the presence of an appropriate substrate. Under such a mechanism, the amount of light produced and measured by luminometer is proportional to the amount of ligand-specific receptor binding, which is benchmarked against the relevant reference compounds.		
Generic description of the method		
a) Non-animal and effect-based bioanalysis tools to measure concentration-response curves for developing relative potency factors (RPFs) b) Ultratrace bioanalysis to analyze the total sum of reference compounds-like compounds (e.g. estradiol-like compounds are mentioned in ISO 19040-3). Methods are based on analysis agonists and/or anti-agonists of the different toxic compound classes		

(e.g. ER agonistic CALUX measures estrogenic compounds such as phthalates, bisphenol A, many pesticides).

It is recommended to use a typical panel of such NAM: agonistic estrogenic (ERα), antiandrogenic (anti-AR), glucocorticoid (GR), xenobiotic metabolism (e.g., binding to peroxisome proliferator-activated receptor gamma (PPARγ)), polycyclic aromatic hydrocarbon activity (PAH), oxidative stress (Nrf2) and pregnane X receptor (PXR). The reference compounds for the 7 bioassays were 17ß-estradiol for ERα, flutamide for anti-AR, dexamethasone for GR, rosiglitazone for PPARγ, B[a]P for PAH, curcumine for Nrf2, and nicardipine for PXR.

4. Sensitivity/ Effect-based trigger value EBT [surface water]

- Cytotoxic Compounds by Cytotox CALUX : LOQ 0,3-0,7 and EBT below LOQ [in µg TBT-BEQ/L]
- Estrogenic Compounds by ERα CALUX (ISO 19040): LOQ 0,05-0,1 and EBT 0,1 [in ng estradiol-BEQ/L]
- Dioxin-like compounds by DR CALUX (ISO 24295): LOQ 0,002-0,003 and EBT 0,05 [in ng TCDD-BEQ/L]
- Androgenic inhibiting compounds by anti-AR CALUX (OECD TG 458): LOQ 2,0-4,0 and EBT 14 [ug Flutamide-BEQ/L]
- Early Warning toxicants by PXR CALUX: LOQ 5,0-10 and EBT 3 [in µg nicardipine-BEQ/L]

5. Cost aspects

Initial invest + cost/per sample:

- Cell-culture laboratory: 20 - 30 TEUR; Luminometer: 15-20 TEUR; Cell-lines: 2 500 to 6 000 TEUR/year/NAM.
- Cost per sample for reagents/materials (incl. water extraction): ca. 30-40 EUR/sample/NAM
- Cost per sample for bioanalysis: 100 to 200 EUR/sample/NAM
- (excl. extraction)

6. Technology readiness level (TRL)

- Routine analyses in the Netherlands
- The results are provided in µg reference compound-BEQ/L covering hundreds to thousands of PMTs
- ISO 19040 (ER CALUX) and ISO 24295 (DR CALUX) are available (TRL 8-9)
- Cytotox- and AR CALUX are not yet ISO standardized, but described in OECD guidelines (TG 458). (TRL 5-6)
- CALUX panel standardized by ECVAM JRC DB-Alm Method Nr. 197.
- Several publications (see references)

7. Warning about limitations/drawbacks

- Total measurements of known and unknown PMTs
- Selected single compounds testing not in focus of standard testing
- Capacity: 4 – 8 samples/NAM/week/operator

8. Duration/sample turn around time (TAT). Time from the lab to the report

Typical TAT: 7-10 working days

9. Hands on time: how many samples can be considered by 1 person

Hands on time (batch of 10 samples): 1-2 hour/sample

10. References

Alygizakis, 2023 [24]
Alygizakis, 2019 [50]
Choi, 2024 [51]
Houtman, 2020 [52]
Phan, 2021 [25]
Tue, 2023 [53]
Välitalo, 2017 [54]

11. Solution user

- Goethe University Frankfurt [55]
- German Environment Agency (Umweltbundesamt, UBA) – Section II 3.6 Toxicology of Drinking Water and Swimming Pool Water [56]

12. Solution owner

- BioDetection Systems (BDS) [68]

Table A.14 — Factsheet for PFAS CALUX

<table>
<tr><th colspan="3">PFAS CALUX</th></tr>
<tr><td colspan="3">1. Fields of application</td></tr>
<tr><td>1.1 Target compounds</td><td>1.2 Type of sample/matrices</td><td>1.3 Type of method/category</td></tr>
<tr><td>PFAS, Total PFAS
[PFOA-BEQ]</td><td>Water / sediment</td><td>in lab/cell culture based *in vitro* testing; in situ, online...</td></tr>
<tr><td colspan="3">2. General description of the technology</td></tr>
<tr><td colspan="3">The TTR-TRβ (PFAS) CALUX assay measures the replacement of the thyroid hormone thyroxine (T4) from its transport protein transthyretin (TTR) because of competition with compounds for TTR-binding sites. Different concentrations of a compound (sample) are mixed with a fixed concentration of T4 and TTR. After reaching equilibrium, the TTR-bound T4 is separated from the free T4. The T4 that remained bound to the TTR is quantified by the TRβ CALUX measured by luminometer. The amount of luciferase produced by the samples is related to known concentrations of reference compounds and the results are therefore expressed as reference compound equivalents.</td></tr>
<tr><td colspan="3">3. Generic description of the method</td></tr>
<tr><td colspan="3">a) Non-animal and effect-based bioanalysis tool to measure concentration-response curves for developing relative potency factors (RPFs)
b) Ultratrace bioanalysis to analyze total PFAS reported in PFOA-bio-equivalents.
Method is based on a dual-step bioassay with a binding competition part using T4- thyroid transport protein transthyretin (TTR) as step one and a TRβ-reporter cell-based readout as second step. PFAS potently bind to the TTR thereby competing with the natural hormone thyroxine (T4) which can lead to reduced thyroid hormone levels. Compounds that compete with T4 for its binding site on TTR, in fact replace T4 on the TTR protein. Therefore, when TRβ-reporter cells are exposed to media containing TTR-loaded with a T4-competitor, these compounds also enter the cell and can interfere with all other TH-binding proteins within the cell, which include (a) TH transporters, b) T4-converting enzymes such as deiodinases and, c) the thyroid hormone receptor protein [22].</td></tr>
<tr><td colspan="3">4. Sensitivity/range of concentration measured</td></tr>
<tr><td colspan="3">LOQ 0,1-0,2 µg PFOA-BEQ/L</td></tr>
<tr><td colspan="3">5. Cost aspects</td></tr>
<tr><td colspan="3">Initial invest + cost/per sample:
Cell-culture laboratory: 20 - 30 TEUR; Luminometer : 15-20 TEUR ; Cell-lines : 2 500 to 6 000 TEUR/year.
Cost per sample for reagents/materials (incl. water extraction): ca. 30-40 EUR/sample
Cost per sample analysis: 300 to 400 EUR/sample</td></tr>
<tr><td colspan="3">6. Technology readiness level (TRL)</td></tr>
<tr><td colspan="3">TRL 5-6
— RD approaches/ routine analyses in the Netherlands
— Not yet ISO standardized.
— TR CALUX standardized by EU JRC DB-Alm Method Nr. 197.
— Several publications (e.g. [22], [57])</td></tr>
</table>

7. Warning about limitations/drawbacks
— Limited high-throughput potential: 4 to 8 samples/week/operator — PFAS CALUX is covering hundreds to thousands of PFAS, from which more than hundred are similar in toxicity to PFOA/PFOS (Sosnowski et al. submitted to J. Hazard Materials).
8. Duration/sample turn around time (TAT). Time from the lab to the report
Typical TAT: 7-10 working days
9. Hands on time: how many samples can be considered by 1 person
Hands on time (batch of 10 samples): 1-2 hour/sample
10. References
Behnisch, 2021 [22] de Schepper, 2023 [57] Behnisch, 2022 [58] Sosnowska, Submitted [59]
11. Solution user
— Goethe University Frankfurt [55] — German Environment Agency (Umweltbundesamt, UBA) – Section II 3.6 Toxicology of Drinking Water and Swimming Pool Water [56]
12. Solution owner
— BioDetection Systems (BDS) [68]

Table A.15 — Factsheet for Surface Enhanced Raman Scattering (SERS)

Surface Enhanced Raman Scattering (SERS)		
1. Fields of application		
1.1 Target compounds	**1.2 Type of sample/matrices**	**1.3 Type of method/category**
PFAS (short and long chain)	Water /solid/human serum	In lab but could be further exploited for the development of on-line setups for on-site monitoring
2. General description of the technology		
Surface Enhanced Raman Scattering (SERS) technique has been widely implemented for the detection of different molecules being rapid and achieving very low detection limits; few or even single molecule detection is reported. Compared to existing methods, a SERS-based detection can provide a highly sensitive analysis within a few seconds, with a very-low operational cost. In addition, the method could be adjusted to on-site conditions by using a portable (micro)-Raman setup. These features lead to an advantageous alternative based on SERS technique for the detection of PFAS. The SERS-detect will contribute on both scientific and industrial level. The technique was optimized for a SERS based detection of PFAS at the lowest possible detection limit. SERS technique relies on the interactions between the analyte and the surface of noble metal nanoparticles (i.e. Ag or Au NPs in colloidal suspensions or even extended on solid substrates). A brief description of these methods is described as follows.		
3. Generic description of the method		
The additive assisted PFAS detection. For the accomplishment of the SERS signal, a certain amount of an additive (non-disclosed due to IPR reasons) is added in the SERS medium. In this strategy a specific additive that was alleged to promote the interaction between the PFAS and the noble metal nanoparticles was investigated in detail. Detailed parametric analysis, in terms of the amount of the additive, the retention time of the colloidal/additive/PFAS system towards the maximization of the signal, has been performed. The meticulous parametrization of the system (i.e. different amounts of the additive, retention time, mixing protocol, etc.) resulted in the lowest LOD (so far accomplished) at approximately 100 ppb. **The dye-PFAS ion-pairing detection.** In this strategy, the ability of the method introduced by the USA Environmental Protection Agency, EPA, to detect surfactants, using methylene blue, MB, which is identified as an ideal candidate for PFAS-MB ion pairing, was exploited. Ion-pairing extraction combined with detection methods (e.g. spectrophotometry) has been previously utilized for the quantification of different molecules including some PFAS. Ion-pairing reagents, such as dyes, are compounds that can form ion pairs with PFAS molecules, facilitating their extraction from an aqueous phase into an organic solvent phase (i.e. chloroform). In this context, the dyes-PFAS ion pairs are transferred into the organic phase, while the excess of the dye remains in the aquatic phase since it is insoluble in the organic phase. The EPA has developed a method using MB active substances (MBAS) for detecting surfactants in drinking water, surface water, and domestic and industrial wastewater. One of the advantages of the extraction procedure established by the EPA is the ability to selectively isolate the PFAS-dye ion pairs to the chloroform solution, whilst at the same time any other co-existing substances (not anionic surfactant) remain in the aqueous phase. This is very important since interference phenomena can be avoided. The method introduced by the US EPA detects PFAS anionic surfactants indirectly by adding the cationic dye MB. This process relies on ion pair formation, which is then extracted in chloroform. The method is extended by a simple additional step involving the dissociation of ion pairs in water. This		

approach firstly provides the critical flexibility to develop a generic detection of applying a single method across a wide range of both short and long chain PFAS, or even on total PFAS, while in parallel extending the possibility towards low detection limits. A SERS based analytical method was applied to both long-chain and short-chain PFAS with the achievement of very low detection limits down to 5 ppt (5 pg mL-1). The fact that this method is independent of the PFAS nature and could be applied generically to different PFAS, or even to total PFAS, while at the same time providing the possibility of very low detection limits - the SERS or of any other analytical method detection limit of the dye - is promising towards its potential use for wider exploitation.

Solid substrates are currently investigated towards the direct detection of PFAS. These substrates are based on Ag NPs combined with probe molecules that are capable of strongly interacting with PFAS. This work is in progress.

4. Sensitivity/range of concentration measured

The sensitivity range is within the 100 ppb - 5 ppt.

5. Cost aspects

The investment cost for an industry to adopt the SERS-detect approach can be around € 150.000 for the capital costs. The operational costs are anticipated to be low. Without proceeding to an official business plan, the costs per sample are estimated to be within the range 0,5-2,5 euros/sample, depending on the method followed.

6. Technology readiness level (TRL)

The proof of concept in the SERS method has been established in a lab scale environment for targeted analysis (TRL 4). The next steps include the detection in real wastewater samples to further establish the technology.

7. Warning about limitations / drawbacks

Investment cost

8. Duration/sample turn around time (TAT). Time from the lab to the report

The complete analysis time is approximately 5 min. (sample preparation and analysis)

9. Hands on time: how many samples can be considered by 1 person

Approximately 90-100 samples per day could be analyzed.

10. References

Zoi, 2024 [60]

11. Solution Owners & Contact

Foundation for Research and Technology, Hellas (FORTH) Institute of Chemical Engineering Sciences (ICE/HT) [46]

A.3 Filled factsheets for solutions on hazard and exposure assessment

Table A.16 — Factsheet for PFAS physicochemical predictions app

PFAS physicochemical predictions app (QSARlab)
1. Type of assessment
Assessment of physicochemical properties, to be used in hazard and exposure assessments
2. Type of methodology
In silico
3. Subtype of methodology
Qualitative Structure Property Relationship
4. Brief description of solution
This app allows the prediction of basic physicochemical properties for per-and polyfluoroalkyl substances (PFAS) compounds
5. Target substances
PFAS compounds
6. Target media
Not relevant
7. Type of input information
Molecular structure descriptors
8. Type of result
Physical/chemical properties of PFAS (Vapor Pressure, N-octanol water partition coefficient, Water Solubility, Bioconcentration Factor)
9. Applicability domain
PFAS compounds
10. Reference to EU-project/deliverable
PROMISCES deliverable D2.1 - Toolbox improved *in silico* models for identification of PMT properties [31]
11. Reference to tool/model/publication/…
Streamlit application: [61] Published articles: — BCF QSPR model: [62] — logKOW QSPR model: [63]
12. Contact
QSARLAB [64]

Table A.17 — Factsheet for MLR-QSAR models for predicting the binding score of PFAS to selected nuclear hormone receptors

MLR-QSAR models for predicting the binding score of PFAS to selected nuclear hormone receptors
1. Type of assessment
Hazard assessment
2. Type of methodology
In silico
3. Subtype of methodology
Multiple Linear Regression – Quantitative Structure – Activity Relationship (MLR – QSAR)
4. Brief description of solution
QSAR models to predict the binding score of PFAS to 12 Nuclear Hormone Receptors.
5. Target substances
PFAS
6. Target media
— 12 Nuclear Hormone Receptors, 4 with additional antagonist conformation; — Peroxisome Proliferator-Activated Receptors alpha, beta and gamma - PPAR a, b, and g, Thyroid Hormone Receptors alpha and beta - TR a and b; — Retinoid X receptor alpha - RXRα, Liver X receptor alpha - LXRα, Liver X receptor beta - LXRβ, Estrogen receptor alpha - ERα, Estrogen receptor alpha antagonist - anti-ERα, Estrogen receptor beta - ERβ, Estrogen receptor beta antagonist - anti-ERβ, Glucocorticoid receptor - GR, Glucocorticoid receptor antagonist - anti-GR, Androgen receptor - AR, Androgen receptor antagonist - anti-AR.
7. Type of input information
To model development: Binding score calculated using endocrine disruptome tool [26] and structure descriptors. To prediction: selected 2D descriptors of PFAS; easy to calculate structure features.
8. Type of result
Quantitative information about BS [kcal/mol]
9. Applicability domain
Type of AD assessment of model: Williams Plot (chemical space where the compounds are considered as similar to the training set (±3 standard deviations from the mean value (y-axis) and critical hat value-h* (x-axis), which depends on the number of compounds in the training set).) AD assessment for prediction: Developed models are dedicated for PFAS, each of them take into account the presence of fluorine atoms and size/branching of molecule. The AD assessment was conducted using the Insubria graph, where an area of application is defined by the minimum and maximum value of the estimated endpoint for the training set (y-axis) versus leverages (h*; x-axis)
10. Reference to EU-project/deliverable
PROMISCES, Deliverable 1.5 [31]
11. Reference to tool/model/publication/...
Models for PPARs and TRs: [65] Rest of models: manuscript under revision (submitted after revision in Chemosphere)
12. Contact
QSARLAB [64]

Table A.18 — Factsheet for integrated approach TTR-TRβ CALUX assay

Integrated *in silico* and *in vitro* approach TTR-TRβ PFAS
1. Type of assessment
Hazard assessment
2. Type of methodology
Hybrid *in vitro*/*in silico* approach
3. Subtype of methodology
Qualitative Structure Property Relationship and TTR-TRβ CALUX assay
4. Brief description of solution
A hybrid *in vitro*/*in silico* approach for screening PFAS in terms of their *in vitro* toxicity potency to disrupt the thyroid hormone transport. First, a set of 45 PFAS has been tested using the TTR-TRβ-CALUX bioassay. Based on this set a classification model was developed, distinguishing active and inactive PFAS. Next, compounds that were active during the experimental studies were used to develop two regression approaches (i.e. multiple linear regression MLR and a second approach aimed at identifying multiple valid QSAR models obtained as a function of different data splitting) to estimate the potency of interference with the T4-TTR binding.
5. Target substances
PFAS compounds
6. Target media
Thyroid hormones
7. Type of input information
Molecular structure descriptors
8. Type of result
The potency of PFAS interference with the T4-TTR binding.
9. Applicability domain
PFAS compounds
10. Reference to EU-project/deliverable
PROMISCES [2]
11. Reference to tool/model/publication/...
Draft in preparation
12. Contact
QSARLAB [64]

Table A.19 — Factsheet for aquatic toxicity prediction

Aquatic toxicity prediction
1. Type of assessment
Effect modelling
2. Type of methodology
AI-based *in silico* prediction of aquatic toxicity
3. Subtype of methodology
-
4. Brief description of solution
A uniform model has been developed for the prediction of aquatic toxicity of organic chemicals for various biotic species. This model is applicable for single PFAS structures. In addition, a tool is developed to integrate the model predictions into a Species Sensitivity Distribution (SSD) that is the basis for risk assessment in Europe.
5. Target substances
All single PFAS structures
6. Target media
Aquatic
7. Type of input information
SMILES of the chemical. On the basis of the SMILES code, the required input parameters of the model are calculated.
8. Type of result
Effect level (most notable: EC50 and NOEC) of single PFAS structures for various biota.
9. Applicability domain
In general terms the applicability domain includes all single PFAS structures. However, when a calculation is performed it is separately assessed whether the PFAS is indeed within the Applicability Domain.
10. Reference to EU-project/deliverable
PROMISCES – D1.2 [31]
11. Reference to tool/model/publication/…
M. Viljanen, 2023 [66]
12. Contact
RIVM [67]

Table A.20 — Factsheet for NAMs for *in vitro* toxicity testing of PMTs compounds and complex mixtures

Non-animal methods (NAMs) for *in vitro* toxicity testing of PMTs compounds and complex mixtures (such as water, soil and sediment)
1. Type of assessment
In vitro toxicity testing for PMTs
2. Type of methodology
Non-animal method (NAM) human cell based
3. Subtype of methodology
In vitro toxicity; CALUX NAM panel following ECVAM DB Alm Nr. 197 method; ISO 19040-3 (ER CALUX); ISO 24295 (DR CALUX); Bio-EQ analysis (ISO 23196)
4. Brief description of solution
Non-animal testing of PMTs resulting in *in vitro* relative potency factors (RPF) as well as analyzing total *in vitro* toxicity for cytotoxic-, estrogen-, anti-androgen, anti-obesity,- anti-PXR-, and thyroid hormone disruption-like compounds expressed in reference compound BEQ/L water
5. Target substances
— Cytotoxic (TBT-like)-, genotoxic (Actinomycin D-like)-, AhR (BaP-like)-, metabolic disrupting-via PPAR (obesity drugs-like)- early warning PXR (nicardipine-like); — endocrine disrupting (EAT)-like (e.g., Estradiol- and flutamide-like) chemicals; — All thyroid-hormone transport competing PFAS. (see in PROMISCES [2] tested PMT list [74])
6. Target media
Compounds, water, soil, sediments
7. Type of input information
Amount of compound (mg) or water (L) to be tested
8. Type of result
— PC50 value (all *in vitro* testing) or ng reference compound-BEQ/L (reference compounds such TBT, estradiol, BaP, nicardipine, flutamide and rosiglitazone) — PC80 value (PFAS compounds) or µg PFOA-EQ/L (complex matrix such as water, soil or sediment)
9. Applicability domain
Compound and/or Complex matrix testing (such as water, soil and/or sediment)
10. Reference to EU-project/deliverable
Many such as PROMISCES [2], DEMEAU, SafeCrew, TECHNEAU, SOLUTIONS, OneBlue.
11. Reference to tool/model/publication/…
Alygizakis, 2021, 2022 ; Pham, 2023, Behnisch, 2021 [22], 2022; de Schepper, 2023 [57]
12. Contact
BioDetection Systems (BDS) [68]

Table A.21 — Factsheet for 2/3D modelling train for reactive transport of PFAS in unsaturated and saturated zone

2/3D modelling train for reactive transport of PFAS in unsaturated and saturated zone

1. Type of assessment

Exposure assessment

2. Type of methodology

In silico

3. Subtype of methodology

Multi-phasic model or multi-compartment model

4. Brief description of solution

This model train simulates water flow and PFAS transport in 3D, providing spatial and temporal simulations of PFAS plumes in the soil-groundwater continuum (SGW). It integrates a 1D model for the unsaturated zone (UNZ) with 3D groundwater (GW) flow and transport models, effectively simulating water flow and solute transport across SGW.

Water flow is modelled using MODFLOW, with an improvement that simulates recharge through 1D-Hydrus. This direct coupling allows for more accurate PFAS transport simulations by considering capillary fringe effects. For solute transport, MT3DMS uses MODFLOW’s water flow output and incorporates an indirect coupling with 1D-Hydrus to simulate mass transfer from the unsaturated zone. Multiple 1D solute transport models can be used to account for spatial variation/heterogeneity.

The main physical, chemical, and biological processes controlling PFAS distribution between the solid, gas, and water phases in the unsaturated and saturated zones can be simulated. The model includes sorption and degradation processes and can model multi-component reactive transport. Non-linear and non-equilibrium sorption reactions can be applied to simulate PFAS sorption at soil-water interface (SWI) and air-water interfaces (AWI), including interactions between PFAS.

This model train is capable of simulating PFAS fate and transport helping to identify PFAS mobility processes, predict concentrations, and forecast contamination evolution under different conditions.

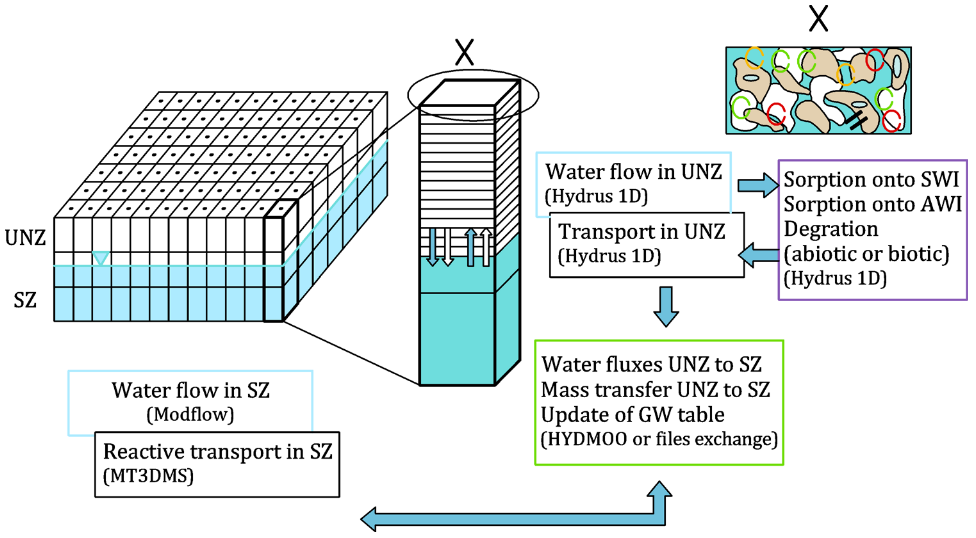


Diagram of models train simulating water flow and PFAS transport in 3D

5. Target substances

PFAS

6. Target media
Soil, unsaturated zone, aquifer and groundwater
7. Type of input information
Emission, PFAS molecular properties, soil, hydrogeological and meteoric characteristics
8. Type of result
Prediction of pollutant (PFAS) concentration in soils and water
9. Applicability domain
This model is suitable to simulate the transport of PFAS in soil-groundwater continuum to predict in any locations in space and time PFAS concentration from contaminated site to watershed scale.
10. Reference to EU-project/deliverable
PROMISCES D2.3 & D2.4 [31]
11. Reference to tool/model/publication/…
GitHub
12. Contact
BRGM, French Geological Survey (Orléans, France) [44]

Table A.22 — Factsheet for SimpleBox aquatic persistence dashboard

SimpleBox aquatic persistence dashboard
1. Type of assessment
Exposure assessment
2. Type of methodology
In silico
3. Subtype of methodology
Multi-compartment model
4. Brief description of solution
SimpleBox is a multimedia mass balance model, simulating the degradation and transport of substances as dynamic environmental fate processes occurring at regional, continental, and global scale systems. The Aquatic Persistence Dashboard in SimpleBox enables the user to evaluate the time that a substance remains in the water phase and hence its tendency to flow downstream and eventually reach the ocean.
5. Target substances
(v)P(v)M substances
6. Target media
Soil, ground and surface water
7. Type of input information
Phys/chem properties of substances
8. Type of result
Aquatic persistence, i.e. the time a substance resides in the aquatic phase
9. Applicability domain
(v)P(v)M substances
10. Reference to EU-project/deliverable
PROMISCES D2.6 [31]
11. Reference to tool/model/publication/...
Aquatic Persistence Module in Excel: [69] SimpleBox model, which will contain the module after March 31, 2025: [70]
12. Contact
RIVM, SimpleBox [71]

Table A.23 — Factsheet for HHEA model

Human Health Exposure Assessment (HHEA) model
1. Type of assessment
Exposure assessment
2. Type of methodology
Strategy for safe reuse
3. Subtype of methodology
Probabilistic model
4. Brief description of solution
A risk-based human health exposure assessment (HHEA) is a probabilistic tool for evaluating the risk posed to human health. It has been applied to evaluate 4 circular economy (CE) routes which result in a product – e.g. drinking water or lettuce, that can be consumed by humans.
5. Target substances
PFAS, industrial persistent, mobile and toxic (PMT) substances, substances for which health guideline or threshold values exist
6. Target media
Soil, sludge, water, lettuce
7. Type of input information
Concentrations and removal percentages for compounds before and after a particular treatment or dilution step in a treatment train
8. Type of result
Probabilistic distribution of substance concentrations; probabilistic distribution of reference quotients for substances
9. Applicability domain
Wherever enough literature or experimental concentrations exist for the compound of interest
10. Reference to EU-project/deliverable
PROMISCES D2.5 [31]
11. Reference to tool/model/publication/...
Model will be available by May 2025: [72]
12. Contact
Kompetenzzentrum Wasser Berlin[73]

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[2] PROMISCES. EU research project, online: https://promisces.eu/

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[4] SCENARIOS. EU research project, online: https://scenarios-project.eu/

[5] Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (CLP regulation), access: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A02008R1272-20241210

[6] https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:52020DC0667 COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS Chemicals Strategy for Sustainability Towards a Toxic-Free Environment

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