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Investigating the extent of PFAS contamination in the Upper Danube Basin across environmental compartments

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Abstract

Background Per- and polyfluoroalkyl substances (PFAS) are emerging organic pollutants widely detected in environmental systems, posing risks to human health and the ecosystem. Despite increasing efforts to monitor PFAS in river systems, knowledge gaps remain regarding sources and emissions via different pathways. This study investigates PFAS contamination across multiple environmental compartments in the Upper Danube Basin, including surface water, groundwater, wastewater, landfill leachate, surface runoff, and atmospheric deposition. The primary objectives are to assess the extent of PFAS contamination, identify key emission sources and transport pathways, and evaluate associated risks in terms of the potential exceedance of current and proposed environmental regulatory thresholds in the European Union.

Results The findings reveal a widespread presence of PFAS, with PFOA, PFOS and short-chain compounds being predominant. The Alz River and Gendorf chemical park emerge as hotspots with far-reaching effects downstream, contributing significantly to diffuse legacy contamination of PFOA and being a significant source of two industrial PFOA substitutes, ADONA and GenX. Wastewater treatment plants, old municipal landfills, and sites with a history of fire-fighting foam application are identified as key pathways or sources of legacy pollution, exhibiting higher concentrations compared to the other matrices. Notably, no significant removal is observed when comparing influent and effluent samples from conventional WWTPs. The study further demonstrates that groundwater is vulnerable to contamination from point sources and to infiltration from rivers, with bank filtration proving largely ineffective in preventing PFAS contamination.

Conclusions The study underscores the necessity for source and pathway control measures to mitigate PFAS pollution, the implementation of advanced treatment technologies to safeguard drinking water and surface water quality, and targeted remediation for legacy soil and groundwater contamination. Additionally, strong use regulations should be explored to minimize ongoing emissions. The multi-compartment monitoring proves to be a crucial approach to understand the complexity of PFAS distribution at the catchment scale. Comparative analysis and risk assessment highlight challenging situations for water management, offering an indispensable basis for emission modeling as a next step for quantitative assessment of the relevance of different sources and pathways for surface water pollution.

Keywords Water pollution, Emerging contaminants, Catchment monitoring, Source identification, Watershed management, Water Framework Directive, Drinking Water Directive, Environmental Quality Standards

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Background

Per- and polyfluoroalkyl substances (PFAS) have gained increasing attention at the worldwide level in recent years, as a growing number of studies have revealed links between these synthetic chemicals and adverse effects on human health [97, 116]. Once produced, PFAS are distributed and accumulated in the environment, leading to human exposure through pathways such as drinking water, food, aerosols, and indoor dust [26, 107, 119, 123, 128, 135].

PFAS have been used in a wide range of industrial and household applications since the 1950 s due to their desirable properties such as chemical stability, hydrophobicity, oleophobicity, and the ability to lower surface tension [14, 41]. However, most PFAS are either environmentally and microbiologically non-degradable or ultimately transformed into terminal products that are still PFAS [23, 127]. Extensive studies have found positive associations between PFAS exposure and immunotoxic, neuro-developmental toxicity, thyroid and kidney disorders, hormonal effects, carcinogenic potency, infertility, and cancers [98, 111, 119].

PFAS can enter environmental media throughout their life cycle, resulting in a continuous exchange of an ever increasing amount of PFAS between the environmental compartments [5]. Surface waters, in particular, serve as conduits for the transport and accumulation of PFAS [103]. Understanding the fate and transport of PFAS through different routes to surface water is crucial for identifying emission sources and pathways, as well as developing effective management strategies to control pollution and protect public health [63].

Surface water contamination occurs through both the point source and diffuse pathways [63]. In rural and non-industrial catchments, diffuse inputs can be significant due to wet and dry atmospheric deposition [84, 99]. PFAS can sorb to particulate matter in aerosols, allowing atmospheric transport over long distances [35]. PFAS deposited on soils can reach groundwater and surface water during precipitation events, and PFAS have been widely detected in runoff water samples [22, 57, 133]. In addition, urban storm water can contain not only PFAS accumulated on sealed surfaces through atmospheric deposition, but also PFAS washed-out from various materials applied in the built environment [9]. Major pollution pathways or identifiable emission points include certain industrial facilities, wastewater treatment plants (WWTPs) and the use of sludge generated from PFAS-contaminated WWTPs, the application of aqueous film-forming foam (AFFF) for firefighting-related activities, and landfills [8, 16, 41, 85, 100]. Interactions between surface water and groundwater can transport PFAS from point sources to groundwater and contribute to further diffuse contamination [12, 49, 109]. In addition, the river itself can also diffusely affect groundwater quality [72].

Despite increasing efforts to document the contamination of PFAS in rivers, a systematic understanding of the relative contributions of different environmental pathways remains lacking. Multi-compartment monitoring can provide the necessary information basis for a more comprehensive understanding of PFAS sources, fate, and transport within aquatic systems [55].

Among the different environmental compartments, bank-filtrated water represents a critical but underexplored one. As a sustainable and cost-effective drinking water supply method, riverbank filtration is widely used across Europe, particularly in cities such as Berlin and Budapest [78, 86], as well as in developing regions [53, 106]. However, little is known about the levels of PFAS contamination and transport mechanisms within the water that flows through the river bank, raising concerns about its effectiveness in removing these persistent pollutants.

Similarly, while numerous studies have investigated PFAS contamination in wastewater in Europe, relatively few have systematically examined both the influent and effluent. Such investigations are essential to evaluate the removal efficiencies of PFAS and to understand the source of PFAS contamination from the profile of influent samples [61].

The Upper Danube Basin (UDB) presents an important case for understanding PFAS contamination on a large catchment scale. This region has been the focus of micropollutant monitoring [7, 73, 74], providing opportunities to integrate external data sets into a harmonized assessment of contamination profiles. However, previous studies have focused mainly on a limited subset of PFAS, such as PFOA, PFOS, and short-chain perfluoroalkyl acids (PFAA). Recent non-target and suspect screening studies have revealed a broader spectrum of PFAS in the Danube [88, 124], highlighting the need for expanded targeted analysis to enhance our understanding of their occurrence and distribution in the region.

Given the extensive presence of PFAS and their diverse pathways into aquatic systems [102, 103], regulatory efforts have been implemented to control their environmental impact. The Stockholm Convention on Persistent Organic Pollutants [117], the US National Primary Drinking Water Regulation [125], and the European Union (EU) Drinking Water Directive (DWD) [33] have established guidelines to limit PFAS pollution. More recently, within the EU, a draft version of Environmental Quality Standards (EQS) [30] has proposed updated regulatory limits for PFAS in surface and groundwater. Assessing PFAS contamination levels in the Danube in

the context of these evolving standards would provide valuable insights for water management.

To address knowledge gaps, a comprehensive monitoring campaign was conducted in the UDB, targeting 31 individual PFAS in multiple environmental compartments, including atmospheric deposition, surface water, groundwater, surface runoff, landfill leachate, and wastewater. Specific efforts were made to collect samples from the Danube and its bank-filtered water in two cities, as well as influent and effluent from the same WWTPs. Furthermore, additional external PFAS monitoring data from countries within the basin were integrated into a harmonized database [71], providing a basis for a more comprehensive assessment of PFAS concentrations and distribution.

By adopting a holistic approach to multi-compartment monitoring, this study provides the first comprehensive assessments of PFAS contamination in a large part of the Danube region. It offers insights into PFAS transport via different pathways, identifies key emission sources and contamination hotspots, evaluates the efficacy of traditional removal mechanisms, and assesses the risks of exceedance of current and proposed regulatory thresholds. These findings advance an integrated understanding of PFAS dynamics at the catchment level, and offer a transferable approach that can support micropollutant monitoring and management efforts in other catchments beyond the Danube.

Methods

Study area description

The Danube is Europe's second largest river, providing resources for numerous human activities along its course. This study focuses on the UDB, which spans approximately 186,059 km^2 and extends to Budapest, Hungary. The region is home to over 27.5 million inhabitants in five major countries: Germany, Austria, Czech Republic, Slovakia, and Hungary. Figure 1 illustrates the location of the UDB in relation to the entire Danube basin in a global context.

Sampling

A comprehensive monitoring campaign was conducted between 2021 and 2023 within the UDB, targeting various environmental compartments, including river water, groundwater, wastewater, landfill leachate, surface runoff and atmospheric deposition.

River water grab samples were collected under base flow conditions in nine main tributaries of the Danube. Along the Danube, Vienna and Budapest were selected as representative sites, where base flow samples and groundwater samples were taken bimonthly. Groundwater samples were collected from nearby bank-filtration sites, as bank filtration serves as primary and backup drinking water sources in Budapest [86] and Vienna [20], respectively. In addition, depending on the number of high-flow events and the feasibility of sampling on site, one to three high-flow samples were also collected at surface water sites. More details on sampling at bank-filtration sites and related analyzes are available in [93].

For wastewater, weekly composite samples were taken at seven municipal wastewater treatment plants and four industrial wastewater treatment plants, from both inflow and outflow points. At four legacy municipal landfills—remnants of former waste disposal practices no longer allowed under current EU regulations—samples of leachate or groundwater directly beneath the landfill were collected. Surface runoff samples from unsealed soil were collected during precipitation events from three sites representing agricultural, forest, and pasture land uses. Composite atmospheric bulk deposition samples were collected at three sites over three periods of 4 months.

All sampling activities followed the recommendations of multiple PFAS sampling guide documents [17, 81]. The samples were collected and stored in 1-l high-density polyethylene (HDPE) bottles. After collection, the samples were transported to the laboratory in 48 h under cooled conditions (0–10 ° C) and stored at 6 ° C upon arrival. Detailed information on sampling sites is available in the concentration database [71].

Chemical analysis and quality control

For quality control, at least one laboratory blank sample and one field blank sample was prepared for each environmental matrix. To prevent cross-contamination, all sampling materials and equipment have been thoroughly cleaned before use. The targeted analysis of these compounds was performance by liquid chromatography tandem mass spectrometry (LC–MS/MS), following EPA method 1633 [126]. The sample preparation included concentration steps using either automated inline solid-phase extraction (SPE) or manual SPE, depending on the sample matrix, to ensure the highest analytical accuracy. During laboratory processing, extracted internal standards were added during the SPE step to evaluate recovery rates, while non-extracted internal standards were included to establish the initial calibration and ensure the precision during LC–MS analysis.

For sample injection, a PAL RTC sampler was used. Separation was achieved using an Agilent 1290 Infinity II HPLC pump, coupled with a Sciex Qtrap 6500^+ mass spectrometer equipped with an electrospray ionization source (EIS). A Phenomenex Luna Omega 3 µm PS C18 (100 × 3.0 mm, 100 Å) analytical column was maintained at 40 ° C, with an injection volume of 40 µL. Furthermore, a Phenomenex Luna C18 (50 × 3 mm, 110 Å) delay

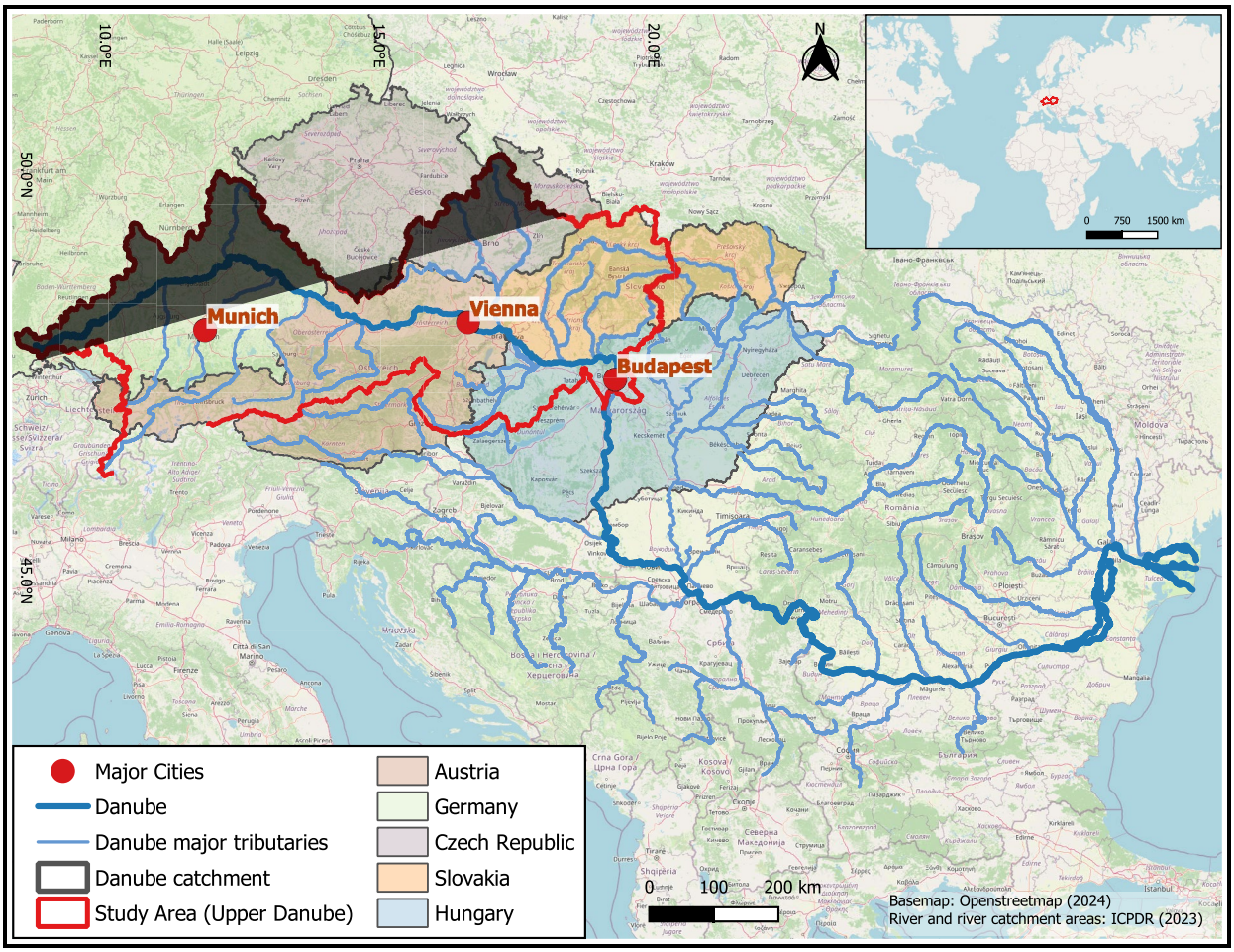

Fig. 1 Map of the study area—Upper Danube (red boundary), its relative position to the whole Danube Basin (black boundary) and in the world (small map upper right corner). Danube and its major tributaries are outlined in blue; administrative regions for major countries in the Upper Danube are shaded in different colors; major large cities in the study area are shown in red points and labeled with names

column was installed. Chromatographic separation was performed using a mobile binary gradient phase, and the gradient conditions are provided in Table s1. The ESI of the mass spectrometer operated in negative ion mode, using multiple reaction monitoring for the target components listed in Table 1. The limit of quantification (LOQ) for each substance was determined by direct injection, following the DIN 32645 guideline [25]. Detailed LOQ values are provided in Table s2.

The validity of the LC–MS/MS analysis results has been initially verified internally by the data management team. Questionable results have undergone repeated analysis before being stored in the designated PFAS database.

Additional data collection

Based on the monitoring results collected during our sampling campaign, we have further expanded the dataset by incorporating PFAS concentration data from other surveys, covering the study area as comprehensively as possible. Several monitoring campaigns have been conducted in the Danube region, such as the EU Project "DHm3c" [59] and the Joint Danube Survey 4 [52], which provide valuable data that enhanced the temporal resolution at some sampling sites, and extended spatial coverage beyond the scope of our own campaign. Furthermore, some national-level studies extensively focuses on specific environmental compartments, contributing substantial additional data, for example, groundwater measurements from the Austrian National Groundwater Monitoring Campaign [15] and wastewater measurements from Germany [92]. In addition, certain data are not publicly available but obtainable through direct requests to local environmental ministries. In general, these efforts have led to substantial increases in the volume of concentration data, improvement in spatial and temporal coverage, and increased reliability of the

Table 1 Overview of the PFAS compounds investigated in this study

Substance	CAS number	PFAS group	In DWD (2020)	In proposed EQS (2022)	RPF
PFBA	375-22-4	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	0.05
PFPeA	2706-90-3	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	0.03
PFHxA	307-24-4	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	0.01
PFHpA	375-85-9	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	0.505
PFOA	335-67-1	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	1
PFNA	375-95-1	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	10
PFDA	335-76-2	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	7
PFUdA	2058-94-8	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	4
PFDoDA	307-55-1	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	3
PFTrDA	72629-94-8	Perfluoroalkyl carboxylic acids (PFCA)	Yes	Yes	1.7
PFTeDA	376-06-7	Perfluoroalkyl carboxylic acids (PFCA)	No	Yes	0.3
PFBS	375-73-5	Perfluoroalkyl sulfonic acids (PFSA)	Yes	Yes	0.001
PFPeS	2706-91-4	Perfluoroalkyl sulfonic acids (PFSA)	Yes	Yes	0.3005
PFHxS	355-46-4	Perfluoroalkyl sulfonic acids (PFSA)	Yes	Yes	0.6
PFHpS	375-92-8	Perfluoroalkyl sulfonic acids (PFSA)	Yes	Yes	1.3
PFOS	1763-23-1	Perfluoroalkyl sulfonic acids (PFSA)	Yes	Yes	2
PFNS	68259-12-1	Perfluoroalkyl sulfonic acids (PFSA)	Yes	No	–
PFDS	335-77-3	Perfluoroalkyl sulfonic acids (PFSA)	Yes	Yes	2
GenX	13252-13-6	Per- and Polyfluoroether carboxylic acids (PFECA)	No	Yes	0.06
ADONA	919005-14-4	Per- and Polyfluoroether carboxylic acids (PFECA)	No	Yes	0.03
4:2 FTS	757124-72-4	Fluorotelomer sulfonic acids (FTS)	No	No	–
6:2 FTS	27619-97-2	Fluorotelomer sulfonic acids (FTS)	No	No	–
8:2 FTS	39108-34-4	Fluorotelomer sulfonic acids (FTS)	No	No	–
PFOSA	754-91-6	Perfluorooctane sulfonamides (FOSA)	No	No	–
N-MeFOSA	31506-32-8	Perfluorooctane sulfonamides (FOSA)	No	Yes	0.02
N-EtFOSA	4151-50-2	Perfluorooctane sulfonamides (FOSA)	No	No	–
N-MeFOSAA	2355-31-9	Perfluorooctane sulfonamidoacetic acids (FOSAA)	No	No	–
N-EtFOSAA	2991-50-6	Perfluorooctane sulfonamidoacetic acids (FOSAA)	No	No	–
9Cl-PF3ONS	73606-19-6	Ether sulfonic acids (ESA)	No	No	–
11Cl-PF3OUdS	763051-92-9	Ether sulfonic acids (ESA)	No	No	–
N-MeFOSE	24448-09-7	Perfluorooctane sulfonamide ethanols (FOSE)	No	No	–
N-EtFOSE	1691-99-2	Perfluorooctane sulfonamide ethanols (FOSE)	No	No	–

Columns are also given to indicate whether the compound has been included in the lists of calculating PFAS sum from the Drinking Water Directive (DWD, 2020) [33] and the proposed Environmental Quality Standards (EQS, 2022) [30]. For compounds included in the proposed EQS (2022), relative potency factors (RPFs) as PFOA-equivalents are given

Classifications of PFAS group is according to the EPA Method 1633 [126]

results, which helps provide a more complete picture of PFAS contamination patterns across the UDB.

To systematically manage and store the collected data, we have constructed a harmonized database [71], which is used to present the results in this study. This comprehensive database is publicly available and will provide support for future studies and analysis in the UDB. It not only includes essential measurements information, such as sample matrices, concentration values, units and LOQ, but also provides extensive metadata, such as sampling site coordinates, sampling type, sampling techniques, the laboratory conducting the chemical analysis, and analytical methods applied. Details on data sources, environmental matrices and the number of measurements included in the database are provided in Supplementary Material 2.

Statistical analysis

Concentration data collected from the database are first classified into different types based on environmental compartments and specific characteristics.

Data collected from the Danube tributaries are further classified to assess the impact of wastewater. The

average annual river discharge values (2015–2021) were calculated using data from official hydrological gauges. Similarly, the average annual discharge of treated municipal wastewater during the same period was obtained by aggregating data from the Urban Wastewater Treatment Directive (UWWTD) Waterbase [31] at the catchment level using QGIS software [104]. The proportion of municipal wastewater treatment effluent in river water at each sampling site was then calculated as the ratio of annual effluent discharge to annual river discharge. Based on these results, the tributary sites are classified into three groups, with the share of effluent in river water below 1%, between 1% and 3% and above 3%.

Although the database includes comprehensive PFAS measurements from Danube samples along the entire river stretch up to Budapest, considering the varying characteristics of Danube at different sections, a selective subset is employed for further analysis and visualizations. Specifically, only samples from Vienna and Budapest are included in this focused dataset. This approach excludes data from upstream of a known hotspot region (the Alz river) in the UDB, thereby minimizing potential confounding influences. Additionally, as both surface water and bank-filtered groundwater were sampled in parallel at Vienna and Budapest, this selection improves the comparability of results between compartments.

Groundwater data are categorized into three groups. Sampling points located within 5 km of areas where AFFF was potentially applied or near legacy municipal landfills are classified as potentially impacted by hotspot contamination, respectively. All other sampling points are classified as groundwater without known influences from hotspot.

PFAS occurrence is visualized using heatmaps, displaying detection frequencies across different sample types. Boxplots are employed to illustrate concentration distributions, where the box dimensions represent the interquartile range (IQR), spanning from the first to the third quartile. A line inside the box indicates the median value, while whiskers extend to the largest or smallest values within 1.5 times the IQR from the quartiles. Values beyond the whiskers are considered outliers and are shown as individual points [131].

For some PFAS concentration boxplots, the regression on order statistics (ROS) method is applied [67]. This semiparametric approach assumes a log-normal distribution for environmental concentration data and imputes censored values accordingly [47, 48]. It is important to note that these estimates are used solely for statistical analysis and do not represent true measured values. In addition, the variability and uncertainty of the estimated values may increase as the proportion of censored measurements increases. In this study, if the censored values exceed 80% or fewer than three values are detected above LOQ for a specific substance/type combination, a substitution method is applied, replacing measurements below the LOQ with half the LOQ value. Consequently, boxplots may display boxes based on varying half-LOQ values. If a single LOQ dominates the dataset, this may appear as a line at half its value, while "outliers" in the plot may represent either half-LOQ values from less common LOQs, or actual measurements above LOQ. Careful evaluation is necessary when interpreting these results, and it is recommended to always consider the accompanying information on the percentage of measurements above LOQ for each substance that given in the boxplots. Nevertheless, the combination of ROS and substitution methods is adopted as it ensures the most unbiased and robust way to estimate summary statistics.

Boxplots have also been used to visualize the levels of the PFAS sum parameters. The sums of the compounds of PFAS are calculated according to the EU Drinking Water Directive (DWD, 2020/2184) [33], which considers the sum of 20 PFAS, and the proposed Environmental Quality Standard Directive (EQS, 2022) [30], which considers the sum of 24 PFAS adjusted to PFOA equivalent toxicity levels, respectively. It is important to note that only 17 of the 20 PFAS listed in DWD (2020) and 20 of the 24 PFAS listed in the proposed EQS (2022) are within the scope of this study (Table 1), and not all samples contain measurements for all listed PFAS. To avoid excessive omissions, only samples that contain at least 10 of the substances appearing on both lists are included. Additionally, all values below LOQ are treated as zero, as required by regulations, although this does not imply the absence of non-quantifiable concentrations. To facilitate visualization on a logarithmic scale, values of the sum parameters equal to zero are adjusted to 0.0001 ng/l. This replacement represents the minimum potential true value, calculated as the product of the lowest LOQ and the lowest RPF among the PFAS compounds from the drafted EQS. Therefore, the estimates in the boxplots represent the minimum likelihood of exceeding the threshold levels.

Due to the proportion of censored data and the likelihood of non-normal distributions, nonparametric statistical tests are used to assess concentration differences between environmental compartments and sample types. The Wilcoxon signed rank test [130] is applied for pairwise comparisons, while the Kruskal–Wallis test [62] is used for multi-group comparisons. If intragroup differences are detected, Dunn's test [27] is performed for post hoc pairwise analysis. The significance level (p-value) for all statistical tests is set at 0.05.

All data analyses were performed with the statistical software R (v4.1.0)[105]. The following R packages were

used for data processing: the odbc package [50] for database import, the tidyverse collection [129] and the ggsci package [134] for data manipulation and visualization, the NADA package [66] for the implementation of the ROS method and the FSA package [94] for the Dunn test.

Results and discussion

PFAS occurrence

At least one PFAS compound listed in Table 1 is present in 60% of all samples (referred as 'sample-level detection' below). The PFCA and PFSA are the most frequently detected compound groups, with sample-level detections of 50% and 46%, respectively. This is followed by the FTS (11%) group. The detection rates for the remaining groups encompassed by this study are all below 10%. Among individual compounds, PFOA exhibits the highest sample-level detection rate (40%), while for PFOS the level is 33%. Except for these two long-chain compounds, short-chain compounds are predominant, comprising PFBA (38%), PFBS (37%), PFHxA (36%), PFPeA (29%), PFHpA (27%) and PFHxS (23%).

This observation is consistent with global findings [85, 90, 101], and can be attributed to the widespread distribution and application of these short-chain PFCA and PFSA compounds in the industrial and commercial activities. Furthermore, they are the degradation products of other PFAS precursor compounds, and are persistent in the environment. In contrast, the presence of the other substances is detected in less than 20% of the samples. Specifically, *N*-EtFOSAA and *N*-EtFOSE are not detected in any of the samples. As these two compounds have only limited fields of application and are reported without contemporary usage [41], it is possible that both substances are not present in the water environment of UDB.

However, the detection rates can vary significantly by environmental matrix, as shown in other cross-compartment studies from Europe [4] and the United States [46]. In our study, among all leachate and surface runoff samples, the rate with at least one PFAS being detected is 100%, followed by samples of wastewater (98%), surface water (83%), atmospheric deposition (73%) and groundwater (50%).

Figure 2 further illustrates the variability of dominant PFAS across different sample types. The heatmap presents measurement-level detection for each substance-type combination, which refers to the detection rate of measurements above LOQ for a specific compound, with numerical data provided in Supplementary Materials 3. For example, groundwater samples potentially impacted by AFFF applications or landfills have significantly higher detections of many PFAS compounds compared to groundwater sample without known source of contamination. This could be explained by the transfer of PFAS from contaminated lands to the groundwater [13, 19, 49].

To summarize, the results of PFAS occurrences demonstrate the widespread presence of PFAS contamination, with noticeable differences observed across environmental compartments. Furthermore, variations in detections across different types within the same compartments reveal the relationships between point-source emissions and contamination degrees, as surface water samples collected from hotspot regions or groundwater samples impacted by contaminated lands show clearly higher detections than others.

PFAS spatial distribution

Surface water

Figures 3 and 4 illustrate the concentration distributions of commonly detected PFAS in surface water samples. The analysis includes the Alz River, an indirect tributary of the Danube via the Inn, the main Danube at Vienna and Budapest, and other Danube tributaries, which are classified based on the proportion of treated wastewater discharges relative to their total annual river discharge.

The Alz River exhibits a distinct contamination pattern compared to other surface water groups, particularly for PFCAs and PFECAs. Not only the detections of these compounds in Alz are 100% or close to it, but also their concentrations are much higher, ranging from hundreds to even thousands of nanograms per liter. Dunn's tests confirm the observation (Table s3), revealing that for selected PFCAs concentrations in the Alz are significantly higher than all the other surface water groups. For PFECAs, the differences between the Alz and other tributary groups are significant, but not for the Danube. For PFSAs, Alz does not exhibit higher concentrations than the other groups. In contrast, the level of PFHxS is significantly lower in the Alz compared to other tributaries.

The Gendorf industrial park is a recognized contamination hotspot within the Alz catchment. This area hosts several facilities for the production of plastic and PFAS, some with a history of fluoropolymer production dating back to the 1960s [29]. Reports from the Bavarian State Office for the Environment indicate extensive contamination by PFOA in soils and groundwater over an area of approximately 230 km^2 near Gendorf [6, 13]. According to the local environmental authority [6], PFOA concentrations in the Alz River were reported at 5000–8000 ng/L in 2006, decreasing to below the LOQ of 20 ng/L by 2016. However, our results with samples collected from 2019 to 2023 show that PFOA concentrations in the Alz downstream range from 14 to 220 ng/L. This is similar to the findings of Joerss et al. [54], who measured PFOA levels at three sites downstream of Gendorf along the Alz in

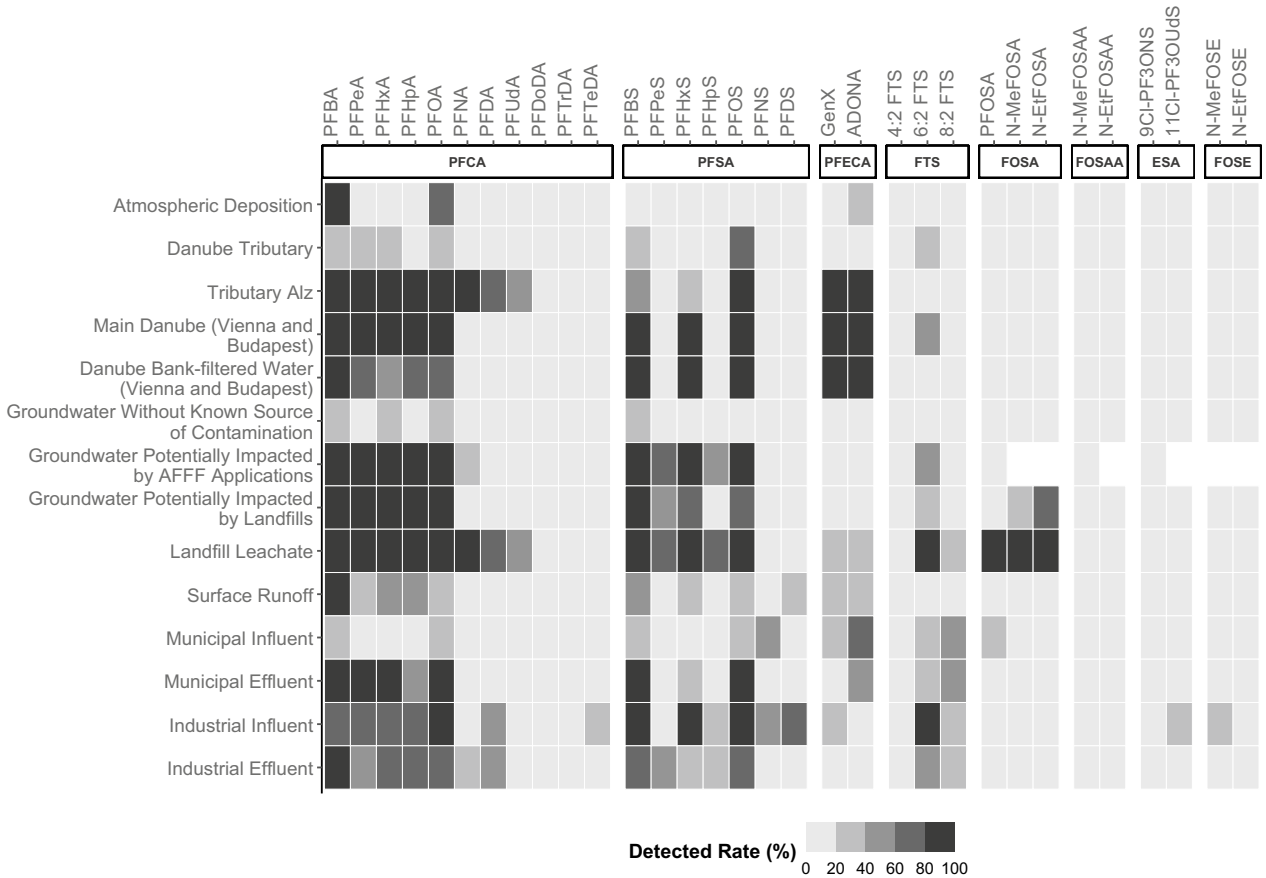

Fig. 2 Heatmap showing the measurement-level detection rates of each PFAS substance–sample type combinations analyzed in this study. The X-axis lists the substance name, while the Y-axis shows the sample type. Darker shades indicate higher detections, as shown by the gradient color bar from light-gray to black (0–100%). The LOQ values for each compound are provided in Table s2

2018, reporting concentrations from 20 ng/L to 180 ng/L. Although PFOA production at this site was phased out in 2008 [6], both our study and Joerss et al. [54] highlight the persistence of legacy PFOA emissions from contamination in the surrounding soil and groundwater.

For other compounds, our study observes similar levels of PFCA, PFSA and FTS compared to Joerss et al. [54] in the Alz. However, for GenX, our measured mean concentration (38 ng/L) is much lower than the previously reported 2600 ng/L. ADONA concentrations have decreased from a mean level of 2100 ng/L to 1501 ng/L, still remaining at high levels. As replacement compounds for PFOA, ADONA and GenX have been detected in surface waters in China, Europe, and North America [96]. It is of particular interest that within the UDB, the presence of these two compounds is found to be almost exclusively confined to the Alz and the Danube section downstream of Alz. This finding provides strong evidence that the Gendorf chemical park is a major source of these specific PFAS contaminants.

Previous studies on PFAS contamination in the Danube report average PFOS concentrations of 7 ng/L (2010) [73], 5.9 ng/L (2017) [74], and approximately 2.1 ng/L (2023) [7], while our study detects an average level of 1.8 ng/L. For PFOA, historical average concentrations in the Danube are 16.4 ng/L (2007) [79], 20 ng/L (2010) [73], 4.9 ng/L (2017)[74], and 2.8 ng/L (2023) [7], whereas our study finds an average level of 2.3 ng/L. In general, a decreasing trend is observed in PFOS and PFOA concentrations after their gradual phase-out and regulatory restrictions, consistent with observations in North America [102]. However, the persistence of legacy contamination remains an issue due to the prolonged use of PFOS-containing products, the degradation and transformation of precursor compounds [68, 89], and the long environmental residence time of long-chain PFAS [45]. Our findings related to the Gendorf site highlight how such factors continue to contribute to contamination in the Danube.

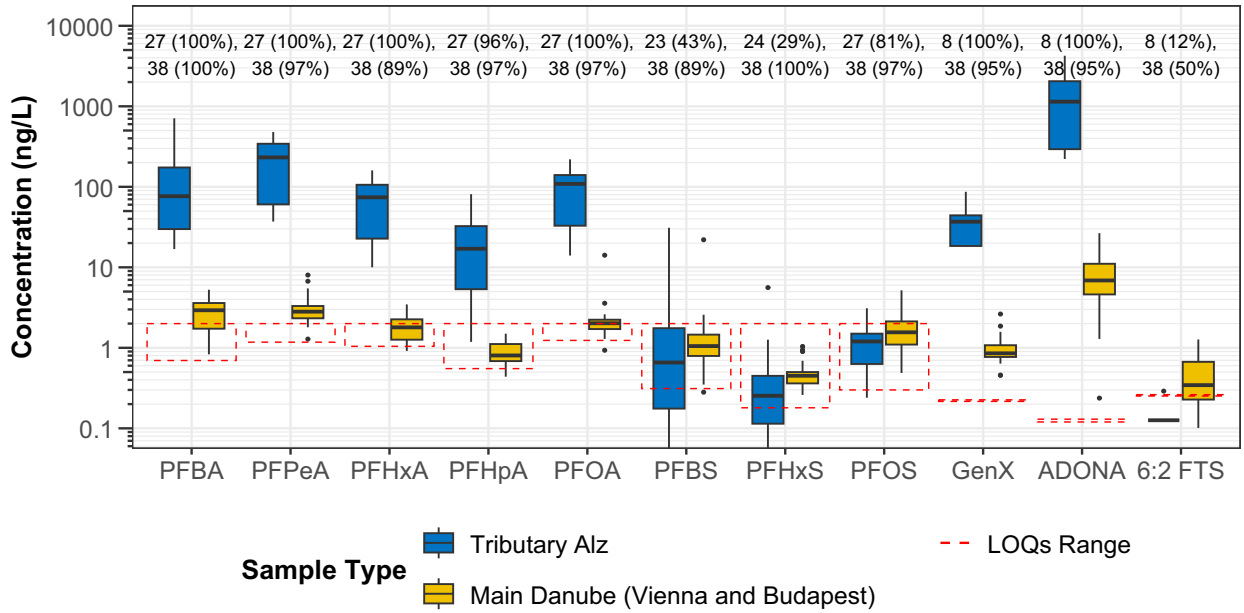

Fig. 3 PFAS concentrations on a logarithmic scale for samples from Danube mainstream (Vienna and Budapest) and river Alz. Box in red dashed outline represents the range of LOQ values among measurements; for different compounds, sample sizes and detection above the LOQ (%) of each type are listed on top of the graph, in a sequence of their appearance on the graph. Values below LOQ are semi-quantitative

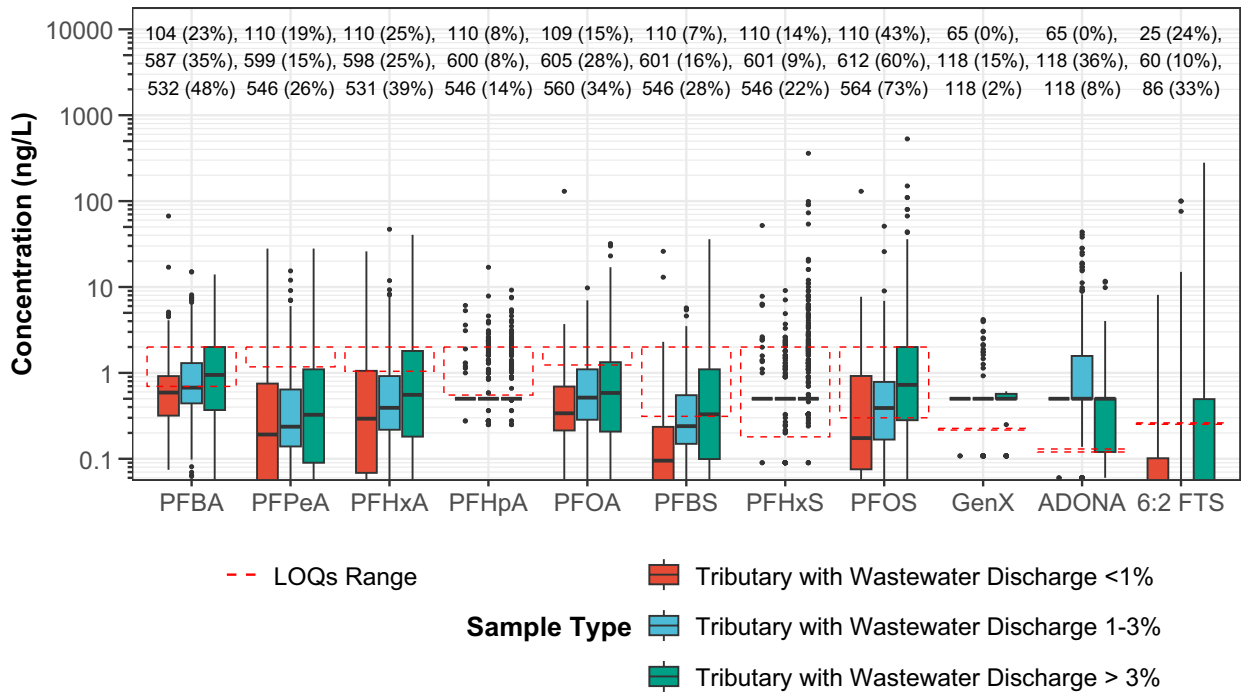

Fig. 4 PFAS concentrations on a logarithmic scale for samples from Danube tributaries classified into three groups according to the proportion of wastewater dilution. Box in red dashed outline represents the range of LOQ values among measurements. For different compounds, sample sizes and detection above the LOQ (%) of each type are listed on top of the graph, in a sequence of their appearance on the graph. Values below LOQ are semi-quantitative

For the Danube mainstream and its tributaries, most measured concentrations fall within a median range of 0.4 to 0.8 ng/L, with IQR typically between 0.1 and 2 ng/L. Dunn's tests (Table s4) show that, except for PFHxS, which is significantly higher in the tributary samples, the concentrations of the remaining ten compounds are significantly higher in the Danube at Vienna and Budapest. Higher levels of PFAS are often observed in tributaries influenced by WWTPs and industrial discharges [113, 118]. Consistent with these findings, our results indicate that within different groups of tributary samples, at least one significant intragroup difference is detected for PFCA and PFSA, suggesting that rivers with lower wastewater dilution exhibit generally higher PFAS concentrations. Although wastewater emissions alone cannot fully explain the observed PFAS levels in these tributaries, WWTPs remain relevant contributors to PFAS contamination in surface waters [58].

Overall, the analysis of surface water samples highlights significant PFAS contamination in the Alz River, particularly from the Gendorf industrial park, which contributes to point-source emissions of replacement compounds for PFOA and diffuse emissions of legacy PFOA. In addition, WWTPs play a key role in influencing surface water quality.

Groundwater

As illustrated in Fig. 5, the concentration distributions of the 12 most frequently detected PFAS compounds in groundwater samples are presented. In conjunction with the sampling of the Danube at Vienna and Budapest, groundwater samples were collected from bank-filtration sites and subjected to statistical analysis (Table s5). For selected PFCAs (with the exception of PFHpA), PFBS and ADONA, concentrations are found to be higher in the Danube. Interestingly, for PFPeS and PFHxS, the concentrations in the bank-filtered samples are significantly higher than the Danube, yet the possible mechanism or reasons need further exploration. Furthermore, in comparison with groundwater exhibiting no discernible source of contamination, the concentrations observed in the bank-filtered samples are found to be considerably elevated for all selected compounds with the exception of PFPeS and 6:2 FTS. Notably, ADONA and GenX are

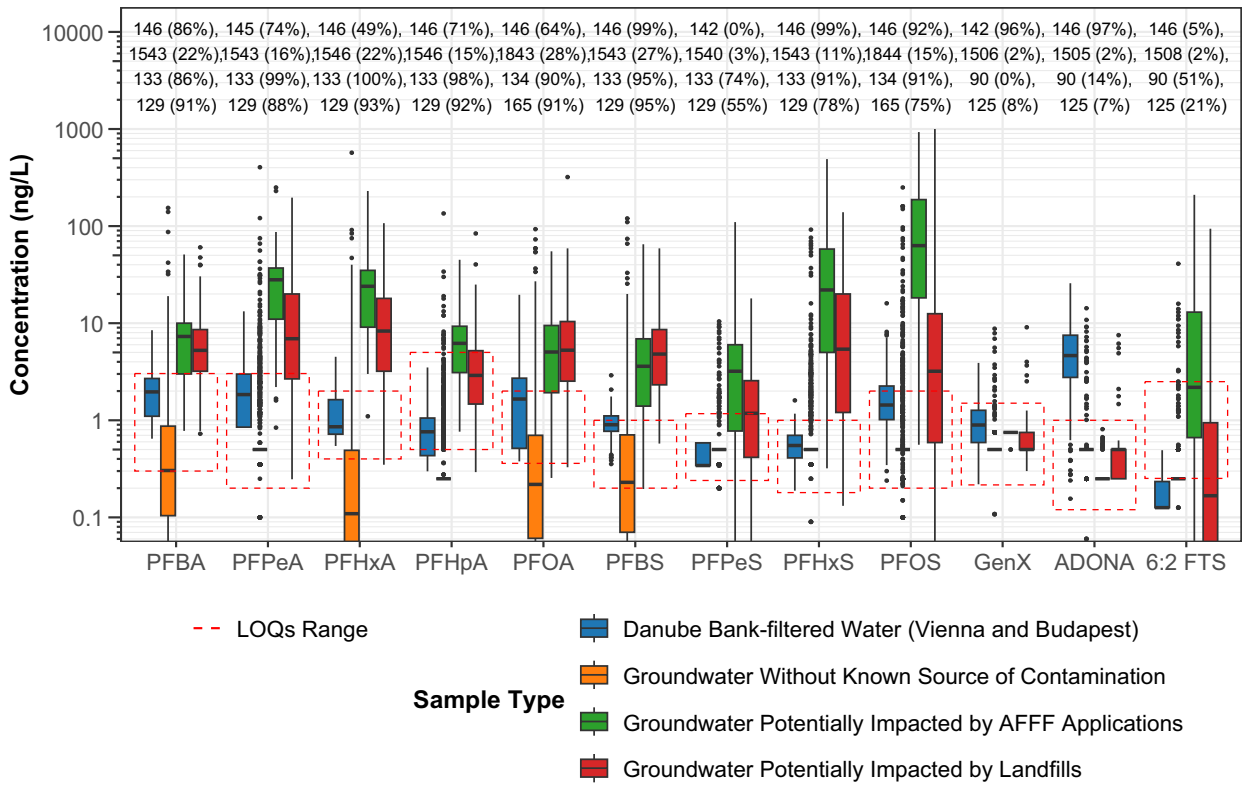

Fig. 5 PFAS concentrations on a logarithmic scale for samples from Danube bank-filtrated water, as well as groundwater samples with unknown and known source impacts. Box in red dashed outline represents the range of LOQ among measurements; for different compounds, sample sizes and detection above the LOQ (%) of each type are listed on top of the graph, in a sequence of their appearance on the graph. Values below LOQ are semi-quantitative

widely detected in the bank-filtrated samples but hardly found in any other groundwater sample groups. Previous studies have reported industrial influences on the contamination of groundwater with PFAS [10, 38, 39, 51]. Given the findings for surface water samples, the observation highlights the impacts from the Danube to its bank-filtration sites, which exhibit comparable contamination patterns. These patterns are likely originated from the same sources in the UDB, and the ADONA and GenX levels may be mainly attributed to discharges from the Gendorf chemical park.

Compared to the limited number of global studies, PFAS concentrations in Danube bank filtration samples are slightly lower, but remain within the same magnitude as those reported for the Ganges [112] and rivers in northern China [72]. These results emphasize the influence of riverbank infiltration on groundwater close to rivers. Despite being an effective natural treatment process for removing many micropollutant from surface water sources[76, 86], the two study sites have relatively short residence time [93]. Considering that hydrophilic organic contaminants can persist and migrate for decades under stable bio-geochemical conditions [3], the bank filtration mechanism may not sufficiently reduce contamination for many PFAS substances.

In groundwater samples without known sources of contamination, PFAS concentrations are generally low, with mean concentrations below 2.5 ng/L and a large proportion of measurements falling below 1 ng/L or LOQ. Compared to the groundwater dataset from a literature review [115], both the detection rates and concentrations in the UDB are lower than the global average.

On the other hand, groundwater samples with potentially known influences from landfills or AFFF applications display distinct contamination patterns, with detection rates ranging from 74% to 100% for selected PFCAs and PFSAs. This is further confirmed by the statistical analyses results shown in Table s6, where concentrations of PFCAs and PFSAs from these two groups are all significantly higher than the groundwater without known source of contamination. Similar observations have been reported in Europe and the USA [42, 70, 80].

Depending on the manufacturer and the production year, AFFF formulations have contained significant amounts of FTS, PFOS, and PFCAs [1]. In the case of 6:2 FTS, mostly known as a substitute for PFOS in fire-fighting foams [41], analysis reveals its presence in 51% and 21% of the groundwater samples potentially impacted by AFFF applications and landfills, respectively. Notably, the detection rate for the remaining two groups is less than 5%. Furthermore, the level of this substance in the group potentially impacted by AFFF applications is significantly higher than in the other groups, highlighting the strong associations between this specific compound and its usage in firefighting-related activities. In groundwater potentially impacted by landfill leachate, PFCAs and fluorotelomer carboxylic acids (FTCAs) are typically the dominant detected groups [108]. FTCAs can undergo degradation process that leads to the formation of compounds belonging to the group of FTS and eventually PFCA [75]. This process may provide a mechanistic explanation for the occurrence of 6:2 FTS in groundwater samples potentially impacted by landfills.

In contrast, both ADONA and GenX have been more closely associated with industrial sources [11, 96] and are detected in nearly all bank-filtered samples, but in less than 15% of the groundwater samples. This observation emphasizes again the close relationships between the Gendorf chemical park and sources of these two PFECA compounds in the UDB.

In general, our findings indicate the potential migration of PFAS from the river to riverbank groundwater, with the bank-filtration mechanism demonstrating limited effectiveness against the contamination. The results from the groundwater classified by potential impacts indicate that landfills and AFFF-application sites are significant sources of PFAS contamination in groundwater.

Wastewater

In Fig. 2, it can be seen that wastewater samples exhibit a unique composition profile of PFAS. Compared to other environmental compartments, wastewater contains a greater diversity of PFAS compounds with a detection rate exceeding 10%. Long-chain PFCAs and PFSAs are more frequently detected, as well as FTS and FOSA. This diversity may stem from PFAS being washed-out from consumer products [36, 60, 91], being emitted from industrial activities [21, 65, 132], and being released from landfill leachate treated in wastewater treatment plants [75, 122]. Furthermore, population density has been found to be positively correlated with PFAS levels in wastewater and groundwater affected by human waste [68, 114, 133]. Upon receiving discharges from various human and industrial activities, as well as landfill leachate [2], municipal WWTPs can be a significant PFAS contamination pathway [44].

Figures 6 and 7 illustrate the concentration distributions of 12 PFAS compounds with overall detection rates exceeding 20% in wastewater samples. It is important to note that the LOQs for influent and effluent are different. In municipal WWTPs, the detection rates of PFCAs and PFSAs are significantly higher in effluent than in influent, particularly for PFPeA, PFHxA, PFHpA and PFHxS, which have detection rates below 20% in influent. The results of the Wilcoxon and Dunn's test (Table s7) further indicate that the concentrations of PFNS and 6:2 FTS are

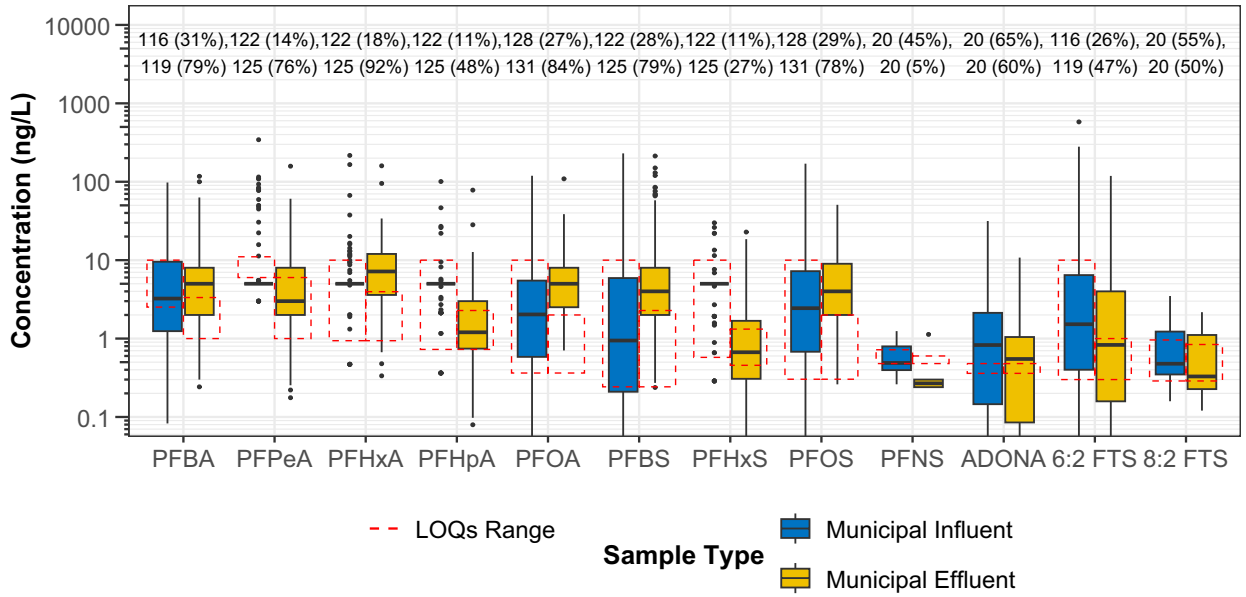

Fig. 6 PFAS concentrations on a logarithmic scale for samples from municipal wastewater treatment plants where both influent and effluent measurements are available. Box in red dashed outline represents the range of LOQ values among measurements; for different compounds, sample sizes and detection above the LOQ (%) of each type are listed on top of the graph, in a sequence of their appearance on the graph. Values below LOQ are semi-quantitative

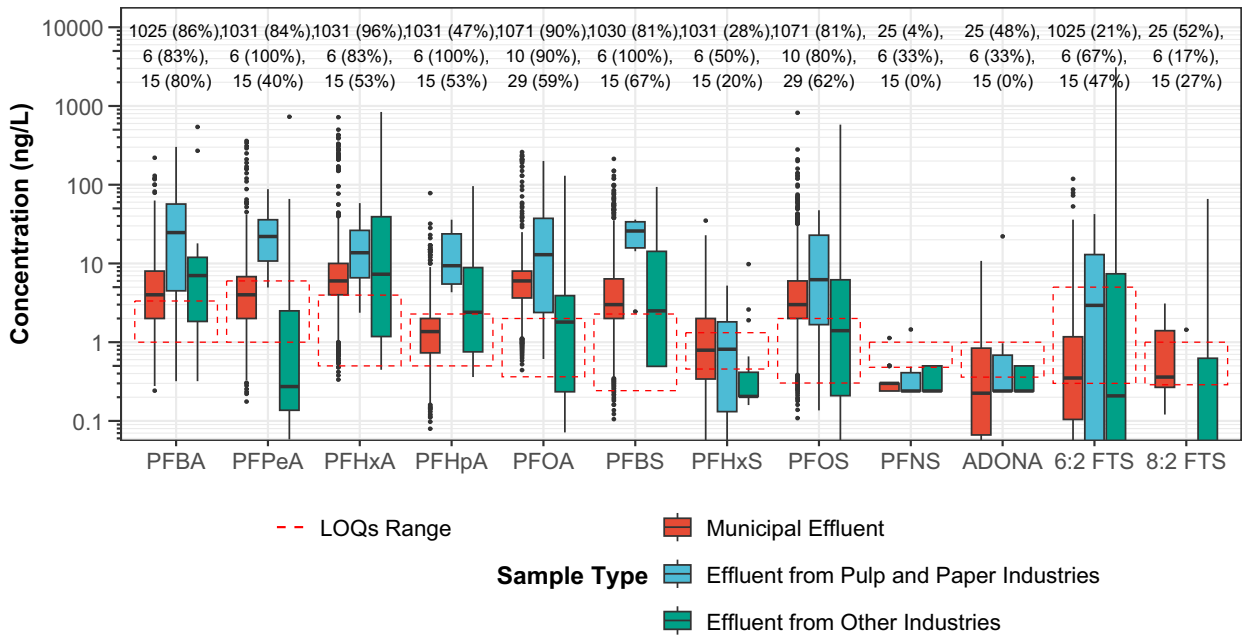

Fig. 7 PFAS concentrations on a logarithmic scale for all effluent samples from municipal or industrial treatment plants. Box in red dashed outline represents the range of LOQ values among measurements; for different compounds, sample sizes and detection above the LOQ (%) of each type are listed on top of the graph, in a sequence of their appearance on the graph. Since values below LOQ are semi-quantitative, the whole graph was cut at level of 0.1 ng/L for better visualization

significantly higher in the influent, while the concentrations of PFOA, PFBS, and PFOS are significantly higher in the effluent. This pattern may be attributed to precursor transformation processes occurring within WWTPs, where compounds such as FTS and FOSA degrade into PFOS, PFOA, and short-chain PFCAs [28, 56, 68, 89, 110]. Additionally, the reduction in long-chain PFAS concentrations may result from sorption to sludge [40, 43].

For selected compounds, mean concentrations range from 1 ng/L to 17 ng/L in the influent and from 0.95 ng/L to 17.6 ng/L in the effluent of municipal WWTPs. [4] characterize wastewater effluents in the Danube Basin and observe PFCAs and PFSAs at levels exceeding 20 ng/L, which aligns with our findings from the UDB. On a global scale, PFAS concentrations in the UDB are lower than those reported in Italy [83], Sweden [43], the United States [110], China [95] and Australia [37], but higher than those reported in New Zealand [68]. However, PFAS levels in influent and effluent samples vary depending on the presence of specific substances, and statistical analysis of PFAS sum parameters concentrations (Table s8) reveals that levels in municipal effluent are significantly higher than in influent. Aligning with findings from other studies [56, 68, 100, 121], the results highlight the ineffectiveness of the traditional wastewater treatment process in removing PFAS.

As indicated in the relevant literature, specific industrial activities have been identified as source of PFAS contamination [82, 120]. In order to investigate potential industry-related patterns, the effluent samples are categorized into three groups based on their sources: municipal WWTPs, pulp and paper industries, and other industries. Differences are observed to some extent, as indicated by the Dunn's test results (Table s9). In the context of 8:2 FTS, a stronger association is found with municipal WWTPs, exhibiting higher concentrations in municipal wastewater. For the other compounds including PFPeA, PFHpA, PFOA, PFBS and PFHxS, a general pattern is observed: concentrations in effluent samples sourced from the pulp and paper industries are highest, followed by municipal WWTPs, then other industries. A global review by [1] has suggested that the concentrations of PFAS in the paper industries are not significantly different from those in other industrial activities. However, our results indicate that the pulp and paper industries may be a significant source of PFAS contamination, as also reported in a few earlier studies [21, 65]. Nevertheless, considering the limited number of industrial wastewater measurements in the database, enhanced monitoring and data collection are needed to ensure more conclusive results.

In summary, the results highlight the contributions of various urban and industrial sources to PFAS contamination in wastewater. The transformation of precursors and the limited removal by traditional treatment technologies likely contribute to the different PFAS profiles observed between influent and effluent samples.

Other compartments

The landfill leachate samples exhibit unique PFAS profiles, characterized by high diversity and distinct distribution patterns (Fig. 2, Figure S1). The analysis reveals that for PFCA compounds with carbon chain length ranging from 4 to 11 (from PFBA to PFUdA), and PFSA compounds with carbon chain length ranging from four to eight (from PFBS to PFOS), the measurement-level detections are all above 50%. Furthermore, the investigation found that FOSA compounds are present in 100% of the landfill leachate samples. PFOSA, *N*-MeFOSA and *N*-EtFOSA have been detected at measurement-levels of 9%, 29% and 71% in groundwater samples potentially impacted by landfills, respectively, but have been detected in less than 5% of groundwater samples potentially impacted by AFFF applications, and even absent in groundwater samples without known source of contamination. Furthermore, they have been detected in 15% and 6% of municipal influent and effluent samples, respectively, but never in industrial influent and rarely in other sample types (<3%).

Given that some municipal WWTPs receive landfill leachate [46, 77], landfills could contribute to the increasing detection of FOSA in municipal wastewater. These findings suggest that landfills are a major source of FOSA emissions in the UDB. As FOSA compounds have been widely reported in landfill-related samples [18, 24, 43, 64, 69], future research could explore their potential as indicators of landfill-derived contamination.

Surface runoff from unsealed soils and atmospheric deposition samples exhibit relatively low PFAS contamination, with concentrations ranging from below the LOQ to a maximum of 23.1 ng/L and 11.7 ng/L, respectively (Figures S2,S3). PFBA has been detected in 100% samples from both matrices, representing the highest observed concentrations. However, the current dataset is insufficient to accurately quantify their contributions to diffuse emissions and further monitoring is needed.

Contamination level in the context of existing and proposed environmental standards in Europe

The EU WFD currently sets an EQS of 0.65 ng/L for PFOS in surface waters [32]. The analysis of the dataset reveals a widespread exceedance of this threshold among samples of the Alz River (74%) and the main stream of the Danube at Vienna and Budapest (97%). In the tributary dataset, exceedance rates are positively correlated with the proportion of treated effluent in the river.

Specifically, the proportion of samples exceeding the EQS has increased from 29% when effluent made up less than 1% of river discharge, to 30% when effluent contributions were between 1% and 3%, and further to 54% when effluent comprised more than 3% of river discharge. These observations suggest that the contamination of rivers are primarily attributed to the factors such as hotspot contamination and the amount of wastewater it receives. Although the exceedance of surface water EQS does not necessarily indicate the failure to meet water quality targets, since biota concentrations can be used alternatively to assess chemical status, it confirms a widespread occurrence with potentially significant implications for water quality management.

Rivers are often the aquatic system most affected by PFAS contamination [115]. Implementing consistent regulatory limits covering a broad spectrum of PFAS compounds is crucial for effective control of PFAS pollution and to protect surface and groundwater quality [116]. In this study, we calculate the minimum contamination potential based on the methodologies outlined in the EU DWD for drinking water [33] and in the proposed new EQS Directive for surface and groundwater [30]. Figure 8 illustrates the results, including compartments not covered by current and proposed thresholds for the sum parameters. It is important to note that the summed concentrations of PFAS are influenced by differences in the inclusion of the compound and the methodological change from the simple additive approach in DWD (2020) to the toxicology-based evaluation in the proposed EQS (2022), which accounts for differences in PFAS toxicity [115].

Notably, 100% of Alz River samples, as well as 98% and 90% of groundwater samples potentially impacted by AFFF applications and landfills, respectively, exceed both the DWD and the proposed EQS threshold levels. For the Danube and the Danube bank-filtrate water at Vienna and Budapest, 13% and 16% of the samples do not meet the DWD threshold. This proportion has increased significantly under the proposed EQS threshold, rising to 92% and 62%, respectively. The probability of not meeting the reference level has also increased, though to a lesser extent, for the tributary samples of the Danube (from 8% to 26%) and groundwater samples without known source of contamination (from 8% to 13%). A closer examination of the tributary samples with the highest sum values reveals that many of these were taken from locations near industrial sites, indicating contributions from potential local contamination sources.

Our findings emphasize the significant contribution of point sources to contamination, highlighting the need to identify hotspots and implement targeted water management strategies [87]. The results underscore the challenges of achieving water quality standards in the UDB, particularly if stricter EQS are adopted. Preventive measures, such as controlling PFAS at source, offer an effective approach to reducing PFAS pollution in surface waters. In parallel, effective groundwater remediation at contamination hotspots is crucial, especially in areas that rely on groundwater resources for drinking water supply.

Currently, there are no environmental standards that specifically regulate PFAS concentrations in wastewater. However, stricter surface water standards will still pose considerable challenges for WWTP operators, as WWTPs remain a significant pathway of PFAS contamination in rivers. Recent EU regulations require improvements in urban wastewater treatment by 2035 [34]. In order to meet the evolving regulatory requirements and ensure preparedness for future standards, it is recommended that PFAS removal capabilities be incorporated during the selection of advanced treatment technologies.

Furthermore, it is advised that future research incorporate non-targeted analytical and eco-toxicology approaches to comprehensively quantify total PFAS levels and their health impacts. This would facilitate a more accurate assessment of compliance with the total PFAS limits stipulated in the DWD, and help prevent underestimation of contamination by accounting for compounds beyond current regulatory targets.

Conclusion

Our findings underscore the significant role of point sources, such as legacy pollution from former AFFF-application areas and old municipal landfills, in PFAS emissions causing local groundwater pollution and also exerting a broader regional impact. WWTP effluents have been identified as relevant pathways for surface water pollution, as the effectiveness of traditional wastewater treatment processes is limited. Surface waters may also significantly affect groundwater bodies adjacent to rivers, as riverbank filtration mechanisms are also ineffective in mitigating PFAS contamination. Altogether, this presents a pressing challenge for water quality management. In particular, the chemical park at Gendorf emerges as a persistent contamination hotspot, as evidenced by the presence of ADONA, which appears to be almost exclusively linked to this site. With the primary manufacturer in Gendorf having announced its intention to stop PFAS production in 2022 and fully phase it out by 2025, follow-up studies could provide additional valuable insights into the persistence of legacy PFAS pollution. PFOA still being significantly

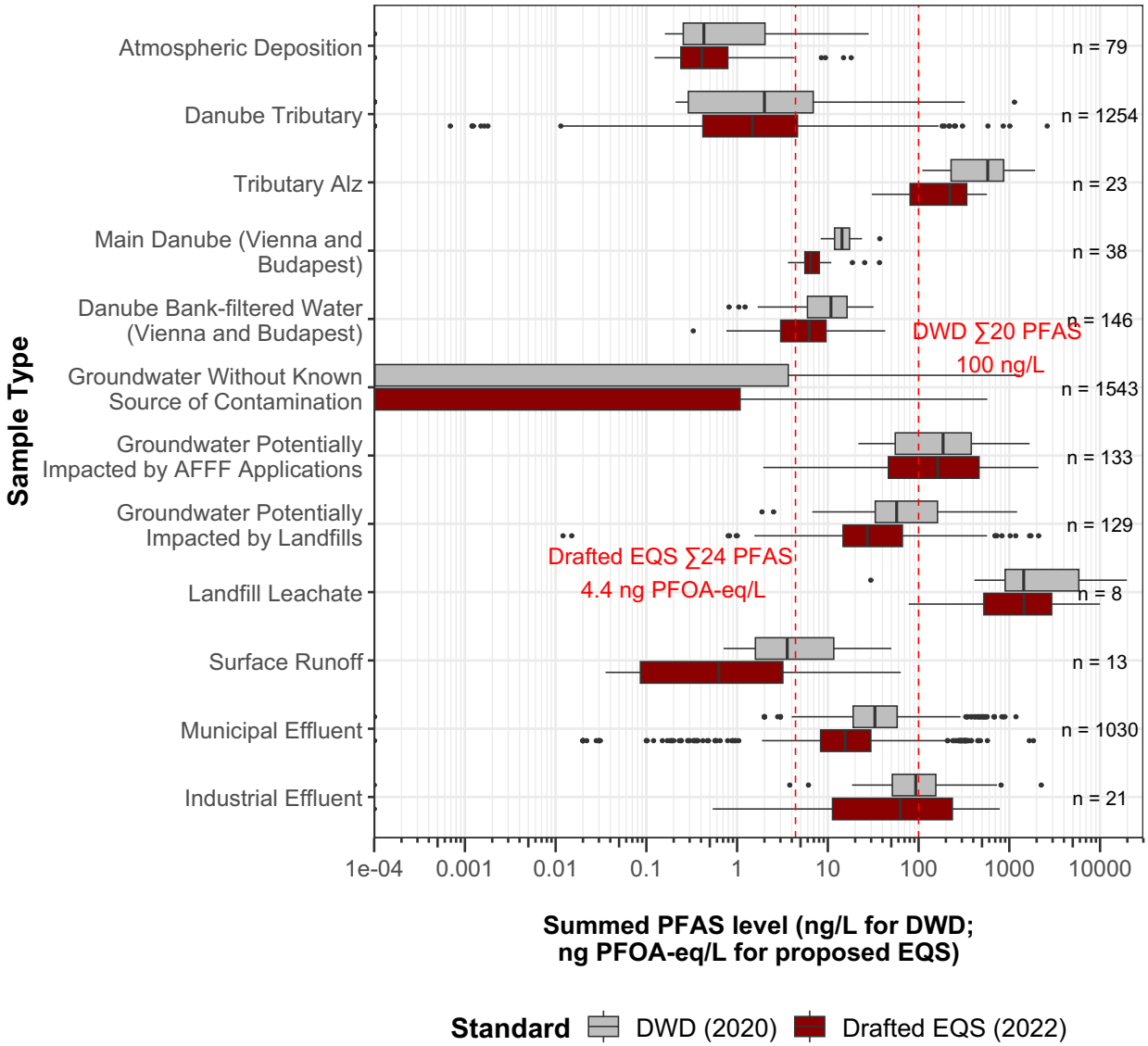

Fig. 8 Boxplot of summed PFAS concentrations in different sample types. Only samples with more than 10 different PFAS observations are selected for sum calculations. Red dashed lines showing the guided PFAS sum level in two standards: DWD (2020) with 100 ng/L for equal-weighted 20 PFAS, and drafted EQS (2022) with 4.4 ng PFOA-equivalent/L for 24 PFAS based on RPF. Sample sizes (n) are listed right of the boxplots. Black dots indicate values beyond 1.5 times of IQR. Measurements below LOQ were treated as zero, and samples with sum level of zero were further replaced as 0.0001 to be displayed on a logarithmic scale. This replacement represents the minimum potential true value, calculated as the product of the lowest LOQ and the lowest RPF among the PFAS compounds from the drafted EQS. Therefore, this graph only aims at showing the minimum contamination potential for different samples

discharged from the Gendorf region, despite the phase-out of its production in 2008, already shows the effect of legacy pollution from this area.

This study provides a comprehensive assessment of PFAS contamination in multiple environmental compartments, revealing variations in the occurrence and distribution of different PFAS compounds. By analyzing multiple compartments simultaneously, we contextualize their specific relevance, identify key contamination patterns, and establish a critical data foundation for future efforts to develop integrated emission models for PFAS on broader spatial and temporal scales. These insights

are particularly valuable for quantifying and comparing emissions through multiple pathways, especially diffuse emissions, which are often underrepresented in compartment-specific assessments.

The comparative analysis highlights key areas that require enhanced monitoring efforts and further reveals variability in risk levels between environmental compartments, providing crucial information to prioritize resource allocation to meet environmental quality targets. Although this study focuses on the UDB, PFAS contamination is a global concern. The insights gained on the distribution of PFAS in our study can contribute to a better understanding of the patterns of contamination, with implications for water management strategies in other river systems facing similar challenges.

Abbreviations

4:2 FTS	4:2 Fluorotelomer sulfonic acid
6:2 FTS	6:2 Fluorotelomer sulfonic acid
8:2 FTS	8:2 Fluorotelomer sulfonic acid
AFFF	Aqueous film-forming foam
ADONA	4,8-Dioxa-3H-perfluorononanoic acid
DWD	Drinking Water Directive
EU	European Union
EIS	Electrospray ionization source
EQS	Environmental Quality Standards
ESA	Ether sulfonic acids
FOSE	Perfluorooctane sulfonamide ethanols
FOSA	Perfluorooctane sulfonamides
FOSAA	Perfluorooctane sulfonamidoacetic acids
FTCA	Fluorotelomer carboxylic acids
FTS	Fluorotelomer sulfonic acids
GenX	Perfluoro-2-methyl-3-oxahexanoic acid
IQR	Interquartile range
LC–MS/MS	Liquid chromatography–tandem mass spectrometry
LOQ	Limit of quantification
N-EtFOSA	*N*-Ethylperfluorooctane sulfonamide
N-EtFOSAA	2-(*N*-Ethylperfluorooctanesulfonamido)acetic acid
N-EtFOSE	*N*-Ethyl-*N*-(2-hydroxyethyl)perfluorooctanesulfonamide
N-MeFOSA	*N*-Methylperfluorooctanesulfonamide
N-MeFOSAA	2-(*N*-Methylperfluorooctanesulfonamido)acetic acid
N-MeFOSE	*N*-Methyl-*N*-(2-hydroxyethyl)perfluorooctanesulfonamide
PFAA	Perfluoroalkyl acids
PFBA	Perfluorobutanoic acid
PFBS	Perfluorobutanesulfonic acid
PFCA	Perfluoroalkyl carboxylic acids
PFDA	Perfluorodecanoic acid
PFDS	Perfluorodecanesulfonic acid
PFHxA	Perfluorohexanoic acid
PFHxS	Perfluorohexanesulfonic acid
PFHpA	Perfluoroheptanoic acid
PFHpS	Perfluoroheptanesulfonic acid
PFOA	Perfluorooctanoic acid
PFNA	Perfluorononanoic acid
PFOS	Perfluorooctanesulfonic acid
PFPeA	Perfluoropentanoic acid
PFPeS	Perfluoropentanesulfonic acid
PFTrDA	Perfluorotridecanoic acid
PFTeDA	Perfluorotetradecanoic acid
PFUdA	Perfluoroundecanoic acid
PFOSA	Perfluorooctanesulfonamide
ROS	Regression on order statistics
SPE	Solid-phase extraction
UDB	Upper Danube Basin
WFD	Water Framework Directive
WWTP	Wastewater treatment plant

Supplementary Information

The online version contains supplementary material available at https://doi.org/10.1186/s12302-025-01141-6.

Supplementary material 1.

Supplementary material 2.

Supplementary material 3.

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Author contributions

M.L.: data curation, formal analysis, visualization, writing—original draft; E.S.: methodology, investigation, writing—review and editing; T.J.O.: investigation, resources; A.A.A.O.: investigation, resources, writing—review and editing; Z.NK.: resources; B.L.: resources; S.K.: validation, writing—review and editing; O.Z.: validation, writing—review and editing; J.K.: writing—review and editing; J.D.: conceptualization, methodology, validation, writing—review and editing, supervision, funding acquisition; M.Z.: conceptualization, methodology, validation, writing—review and editing, supervision, funding acquisition.

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Availability of data and materials

The dataset generated and analyzed during the current study is available in the repository *[Per- and Polyfluoroalkyl Substance (PFAS) Concentrations in the Upper Danube Catchment: Integrated data set from the H2020 Project PROMISCES—Case Study 2]*,https://doi.org/10.5281/zenodo.14027087[71]. The R code supporting the data analysis and computational environmental setup of the current study is available in the Gitlab project, [https://gitlab.tuwien.ac.at/meiqi.liu/promisces_cs2_monitoring].

Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Competing interests

The authors declare that they have no conflict of interest.

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