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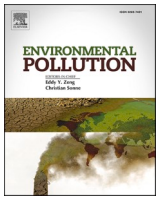

Modelling PFAS transport in Lake Ekoln: Implications for drinking water safety in the stockholm region☆

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ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) are found frequently in both groundwater and surface water sources across Sweden posing challenges to drinking water supply. Lake Ekoln is located south of Uppsala and is the basin of Lake Mälaren; Lake Mälaren is the third largest lake in Sweden and is the drinking water source for more than two million people. The aim of this study was to simulate the fate and transport of PFAS in Lake Ekoln during the period 2017–2020 using three-dimensional hydrodynamic modelling. The simulated water temperatures were in agreement with the observed water temperatures. The simulated PFAS concentrations were generally in agreement with the available measurements, but the lack of measurements made the comparison uncertain. The modelling results described the seasonal variations of PFAS in Lake Ekoln informing the operation of the drinking water treatment plants located downstream. The modelling results confirmed that the main inflow to the lake – the river Fyrisån – is the main source of PFAS to Lake Ekoln, highlighting the importance of mitigating this source in the context of ensuring safe drinking water supply in the Stockholm region. Regular monitoring of PFAS in the river Fyrisån is needed, and additional measurements in Lake Ekoln would facilitate further model development.

1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are a group of highly fluorinated industrially produced organic substances that have a strong and stable carbon and fluorine bond and are characterized by high persistence in the environment (Buck et al., 2011). Due to their unique physio-chemical properties, PFAS have been manufactured and used extensively in different industrial and commercial products (Prevedouros et al., 2006; Buck et al., 2011; Wang et al., 2017). Also, these substances do not degrade easily and are highly mobile in natural conditions and therefore have been found ubiquitously across the globe in air, water, soil, sediment and biota (Abunada et al., 2020). The structure of PFAS consists of a backbone of carbon chain, in which the hydrogen atom is replaced wholly or partially by fluorine atoms, and a functional group. Based on the number of carbon atoms present in the carbon chain, PFAS are described as a long-chain and short-chain PFAS (Buck et al., 2011; Wang et al., 2017). Long-chain PFAS are considered less reactive, more persistent and hydrophobic in nature compared to short-chain analogues (Li et al., 2020). Thus, long-chain PFAS tend to have a stronger sorption to surfaces and particles, and show a higher degree of bioaccumulation compared to shorter chain PFAS (Buck et al., 2011; Ng and Hungerbühler, 2014). Short-chain PFAS are mostly found in the aqueous phase and are more mobile compared to long-chain PFAS (Wang et al., 2015).

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PFAS can be found in the dissolved or particulate phase in water (Ahrens, 2011), and their fate and transport in aquatic environment are influenced by their physio-chemical properties and water characteristics such as dissolved organic carbon content (Phong Vo et al., 2020). Some PFAS, so called PFAS precursors, are able to transform in nature into persistent terminal PFAS products, which are chemically persistent (Environment Agency, 2021). Once released into the environment, PFAS can bioaccumulate in the food chain and be potentially toxic to animals and humans (Barry et al., 2013; Ankley et al., 2021; Podder et al., 2021). The major routes of PFAS exposure to humans include ingestion of food (fish and other products), drinking water, and inhalation of air and dust particles (D'Hollander et al., 2010). The body of literature on PFAS is rapidly expanding, and for further information the interested reader is referred to recent reviews on physicochemical properties (Leung et al., 2023), fate and transport in the water environment (Christensen et al., 2022), toxicity and human health risks (Ojo et al., 2021; Dickman and Aga, 2022). To address the issue of human exposure through drinking water and implement remediation, it is essential to analyse the sources and pathways, seasonal changes, and the processes affecting the spatio-temporal distribution of PFAS in the aquatic environment.

The spread of different pollutants in water sources can be investigated by modelling hydrodynamics and water quality (Li et al., 2017). Transport of PFAS as a conservative tracer was simulated in the Daling River in China (Li et al., 2017) and in the Kokemäenjoki River in Finland (Happonen et al., 2016) using one-dimensional hydrodynamic models. In the Danube River catchment, the fate and transport of PFAS were simulated using catchment-scale hydrological and water quality modelling (Lindim et al., 2015). Three-dimensional hydrodynamic models were used to study the spread of pollution from aqueous film forming foam, without accounting for the specific properties of PFAS, in coastal environments in Canada (Hodgkins et al., 2019), and in USA in Providence (Katz et al., 2022) and in Houston (Aly et al., 2020). Moreover, Miyake et al. (2014) simulated PFAS spread in the water and sediment in the Tokyo Bay, Japan, using a three-dimensional hydrodynamic model, which accounted for sedimentation, decomposition, adsorption and desorption in seawater, and resuspension from the sediment. Compared to rivers and coastal waters, there are fewer examples of PFAS modelling in lakes. A fugacity-based multimedia model was used for modelling fate, transport, and transformation of perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA) in freshwater lakes in China (Kong et al., 2018). This study highlighted model sensitivity to the Freundlich sorption to organic carbon, and the importance of including the process of bioaccumulation (Kong et al., 2018).

PFAS are found frequently in both groundwater and surface water sources across Sweden posing challenges to drinking water supply (Banzhaf et al., 2017; Gobelius et al., 2018). High concentration of PFAS was found in Lake Ekoln (Malnes et al., 2022), a northern basin of Lake Mälaren – the source of drinking water for more than two million people in Sweden. Understanding the fate and transport of PFAS within the lake as well as the contribution of different pollution sources is needed to assess design of drinking water treatment and remediation measures (Ekman and Ejhed, 2023). Among the detected PFAS in Lake Ekoln were PFOS and perfluoroalkyl hexane sulfonate (PFHxS) (Malnes et al., 2021). These two compounds make up a large percentage of the total measured PFAS concentrations in the study area in groundwater (Sörengård et al., 2022), surface water (Gago-Ferrero et al., 2017; Malnes et al., 2021; Sörengård et al., 2022), and wastewater (Gago-Ferrero et al., 2017), emphasizing the importance of PFOS and PFHxS when estimating mass fluxes at this site. In the European Union, both PFOS and PFHxS are included in the POPs Regulation (EU) No 2019/1021.

The aim of this study was to simulate the fate and transport of PFOS and PFHxS in Lake Ekoln during the period 2017–2020 using three-dimensional hydrodynamic modelling. The specific objectives were to i) assess the effect of seasonal circulation pattern in the lake on the spatio-temporal distribution of PFAS; ii) evaluate how much of the observed PFAS concentrations in the lake that can be explained by the fluxes from the known pollution sources; and iii) identify the data needs for further development of the modelling approach.

2. Methods

2.1. Study area

Lake Ekoln is located south of Uppsala (see map in Fig. S1) and is the northern most basin of Lake Mälaren; Lake Mälaren is the third largest lake in Sweden and is used to supply drinking water to more than two million people. Lake Ekoln has a surface area of 52 km^2 and volume of 0.639 km^3, with a mean depth of 12 m and a maximum depth of 42 m. The major inflows to Lake Ekoln are the rivers Fyrisån, Örsundaån, Sävaån, and Hågaån, and a minor inflow through the Uppsala esker, which together account for 95% of the inflow into the lake, while 5% come from other diffuse inflow sources (Lindqvist, 2019). Fyrisån and Örsundaån are the two major rivers that account for 11% of total inflow into Lake Mälaren (Persson et al., 2012). Lake Ekoln has only one outflow in Erikssund located in the southern part of the lake, and the theoretical water retention time in the lake is about one year. The catchment area of Lake Ekoln has a land use pattern consisting of around 62% forest areas, 30% agricultural areas, and 2% urban areas, including the city of Uppsala, with soil types of post glacial clay and moraine soils (Goedkoop et al., 2011; Persson et al., 2012). Lake Ekoln is a dimictic lake; mixing of water is observed during spring and autumn, while during summer and winter, the water temperature shows gradients resulting in stratification preventing mixing of water (Lindqvist, 2019).

Various anthropogenic activities affect the water quality in the lake, including the water resource recovery facility (WRRF) Kungsängsverket that discharges its effluent into the river Fyrisån, and pollution from urban and agricultural areas (Goedkoop et al., 2011). Several environmental pollutants like PFAS, mercury (Hg), polybrominated diphenyl ethers (PBDEs) have been detected in Lake Ekoln, and the chemical status of water is considered critical (VISS, 2024). Since PFAS were detected in drinking water in Uppsala in 2012 upstream of Lake Ekoln, many studies were conducted to investigate PFAS in the study area. PFAS were detected in the Uppsala esker (Gyllenhammar et al., 2015; Sörengård et al., 2022), in Lake Ekoln (Malnes et al., 2021), in the river Fyrisån (Ahrens et al., 2014; Norström et al., 2015; Gago-Ferrero et al., 2017; Malnes et al., 2021; Sörengård et al., 2022), in effluent from Kungsängsverket WRRF (Gobelius et al., 2023; monthly monitoring by the municipal company Uppsala Vatten), at the site of Ärna air base (Johansson and Helldén, 2015), the firefighting site Viktoria (Johansson and Helldén, 2015; Sörengård et al., 2022), and the landfill site Hovgården (Bonnet, 2017). In addition, an average concentration of PFOS was 0.1 ng/L (47 samples collected during Dec 2017–Nov 2021) in precipitation in Uppsala (SMHI, 2024a). Other potential sources of PFAS include on-site wastewater treatment facilities (there are approx. 7000 in Uppsala Municipality), industrial sites Librobäck and Fyrislund, and sludge and leachates from other landfills in the study area (Hansson and Josefsson, 2021).

2.2. Hydrodynamic model

The spread of PFAS in Lake Ekoln was simulated using MIKE 3 FM three-dimensional hydrodynamic model coupled with ECO Lab module for water quality (MIKE Powered by DHI). MIKE 3 FM was developed to simulate three-dimensional hydrodynamic processes in water environments, e.g., tidal processes, stratified flows, entrainment and mixing of plumes and jets (DHI, 2024). The model solves the three-dimensional incompressible Reynolds-averaged Navier-Stokes equations, while assuming the hypothesis of Boussinesq for Reynolds stresses and a vertical hydrostatic pressure. The model consists of continuity equation and momentum equations, and it is closed by a turbulent closure scheme.

The model equations are spatially discretized in conserved form using a finite volume method. The equations are integrated in time using a semi-implicit scheme. The vertical convective and diffusion terms are discretized using an implicit scheme, while the horizontal terms are discretized using an explicit scheme (DHI, 2024).

The original set-up of the model for Lake Ekoln was constructed by Tyréns AB, and further refined by Lindqvist (2019), followed by Ekman (2021), Hansson and Josefsson (2021), and Prajapati (2022). The model accounts for heat exchange with the atmosphere, density-driven circulation in lake, the effect of wind, precipitation and evaporation, and the inflows into the lake. In the water quality module, advection and dispersion of PFAS were simulated as a passive tracer. The eddy viscosity was calculated in the horizontal direction using the Smagorinsky formulation, and in the vertical direction using the two-equation turbulence model. The modelling domain was approximated by a flexible mesh consisting of prismatic elements of varying size over the domain. In the horizonal plane, the length of the side of the triangles varied between approximately 60 m and 320 m. In the vertical direction, the modelling domain was approximated by 1 sigma-layer on the surface followed by 41 z-layers of 1 m thickness. The number of nodes in the mesh was 2152 and the number of elements was 3500.

Inflows that were included in the model were the tributaries Fyrisån, Örsundaån, Sävaån, Hågaån (modelled discharge and water temperature data from SMHI Vattenwebb (2024), resolution 1 day), discharges from Kungsängsverket WRRF (measured discharge and water temperature data from Uppsala Vatten, resolution 1 day), and the Uppsala esker (assumed constant inflow of 0.05 m^3/s and water temperature of 8 °C). The outflow from the lake was specified using the water level in Lake Mälaren (data from SMHI (2024b), resolution 1 day), and the boundary condition for the water temperature at the outflow was described as zero gradient.

The meteorological data included wind speed and direction, air temperature, and relative humidity (data from Uppsala University, CELSIUS (2024), station Geocentrum, resolution 10 min), as well as cloudiness (data from SMHI (2024c), station Uppsala airport, resolution 1 day) and precipitation on the lake surface (data from SMHI (2024c), station Uppsala Aut, resolution 1 day). Ice cover on the lake was described in terms of ice thickness of 0.1 m during the periods when the lake was covered (data from SMHI (2024b), for Mälaren Skarven, resolution 1 day).

As initial conditions, the average water elevation for Lake Mälaren was used (data from SMHI (2024b)). Water density was simulated as a function of water temperature, and the initial conditions for water temperature were described using the vertical profile measured on 20 Feb 2017 (data for 26 depths at station Vreta Udd in Lake Ekoln, data from Miljödata-MVM (2024)). Initial conditions in terms of velocity were defined as a state of rest.

The model was calibrated by Lindqvist (2019) using vertical profiles of water temperature measured in the lake in 2018 with good results (NSE = 0.96 and RMSE = 1.05 °C); this was achieved by adjusting parameterisation of the heat exchange with the atmosphere. In the current study, the same parameterisation was used, and the model performance was further validated using the water temperature data measured during the simulated period 2017–2020. The vertical water temperature profiles were measured on 6 occasions per year, generally with 1 m vertical resolution (station Vreta Udd in Lake Ekoln, data from Miljödata-MVM (2024)).

2.3. PFAS data and simulated scenarios

From previous studies, the river Fyrisån and Kungsängsverket WRRF were identified as two important sources of PFAS to the lake. In this study, the period 2017–2020 was simulated using hydrodynamic modelling. At Kungsängsverket WRRF, the PFAS concentrations in the effluent were monitored monthly during 2015–2021 (data from Uppsala Vatten). However, in Fyrisån, PFOS and PFHxS concentrations during 2017–2020 were measured only on seven occasions (Bonnet 2017, Malnes et al., 2021, Nygren et al., 2021; see Table S1 and Fig. S2 in Supporting Information (SI)). On the other hand, during 2013–2015, PFOS and PFHxS were measured in Fyrisån on 21 occasions (Norström et al., 2015; Gago-Ferrero et al., 2017; Nguyen et al., 2017; Tröger et al., 2018; Nguyen et al., 2022; Sörengård et al., 2022; see Table S1 and Fig. S2 in SI). The PFAS concentrations in Fyrisån were measured at a location close to the mouth of the river, i.e., downstream Kungsängsverket WRRF. Thus, to account for these two sources separately, the load from Fyrisån needed to be specified in the model without the contribution from Kungsängsverket WRRF (see Table S2 in SI).

To encompass the uncertainties associated with describing the load from Fyrisån in the model, two scenarios were formulated (Table 1). In Scenario A, the load from Fyrisån was described as the median load calculated over the period 2013–2020 (using all available measurements in Fyrisån), minus the median load from Kungsängsverket WRRF calculated over the period 2015–2021 (using all available measurements for Kungsängsverket WRRF). In Scenario B, the load from Fyrisån was described as the median load calculated over the period 2017–2020 (using only seven measurements for PFOS and PFHxS), minus the median load from Kungsängsverket WRRF calculated over the period 2017–2021. In both scenarios, the selected period for Kungsängsverket WRRF included the year 2021, in order to increase the certainty of the estimate. The median loads were calculated by first multiplying each measured concentration with the corresponding discharge, and then calculating the median of these values. The discharge of Fyrisån for each measurement date was specified using modelling data from SMHI Vattenwebb (2024). The discharge at Kungsängsverket WRRF was provided by Uppsala Vatten.

While the input of PFAS from Fyrisån was specified as a constant load in the model, as necessitated by the lack of data on PFAS concentrations during the simulated period 2017–2020 (Table S1 and Fig. S2 in SI), as described above, the input from Kungsängsverket WRRF varied over time. As the concentrations at Kungsängsverket WRRF were measured monthly, these were assumed to be representative for each month, while the discharge data had daily resolution (data from Uppsala Vatten).

PFAS can also enter the lake with groundwater. Based on communication with Uppsala Vatten, the inflow from the esker into the lake was assumed to be 0.05 m^3/s, and the concentrations of PFOS and PFHxS were assumed to be 14.6 ng/L and 53.6 ng/L, respectively (average of the three measurements in 2019–2020 at location Ultuna källa, Uppsala Vatten). Thus, average loads originating from the groundwater were 0.730 μg/s and 2.68 μg/s for PFOS and PFHxS, respectively.

The tributary Örsundaån was assumed to carry negligible concentrations of PFOS and PFHxS based on the data reported in Malnes et al., (2021). However, there were no measurements for the tributaries Hagaån and Sävaån. Thus, the contributions of these tributaries were not

Table 1
Assumptions in Scenarios A and B to account for uncertainties regarding the PFAS load from Fyrisån.

	PFOS load (μg/s)	PFHxS load (μg/s)
Scenario A		
Fyrisån total[a]	47.6	42.0
Kungsängsverket WRRF[b]	8.16	4.27
Fyrisån only[c]	39.4	37.8
Scenario B		
Fyrisån total[d]	25.7	27.2
Kungsängsverket WRRF[e]	8.28	3.74
Fyrisån only[c]	17.4	23.4

[a] Median 2013–2020 (n = 28).
[b] Median 2015–2021 (monthly).
[c] "Fyrisån only" was calculated as "Fyrisån total" minus "Kungsängsverket WRRF".
[d] Median 2017–2020 (n = 7).
[e] Median 2017–2021 (monthly).

included in the model.

Assuming the total precipitation on the lake surface during 2017–2020 was 3001 mm (data from SMHI (2024c), station Uppsala Aut, resolution 1 day), the lake surface area of 52.1 km^2, and the concentration of PFOS in precipitation of 0.1 ng/L (SMHI, 2024a), the total load of PFOS into the lake with precipitation during this period was calculated to be 15.6 g, which corresponds to 0.12 μg/s. This load can be considered negligible in comparison to the loads from Fyrisån and Kungsängsverket WRRF (Table 1) and thus was not included in the model.

The initial conditions in the lake were described using the concentrations of PFOS and PFHxS measured in Lake Ekoln (location Vreta Udd) on 20 Feb 2017. As the concentrations were measured at three depths, linear interpolation was used to describe the concentration gradient in the water column. The concentrations were 1.2 ng/L, 1.5 ng/L, and 1.4 ng/L for PFOS, and 1.1 ng/L, 1.6 ng/L, and 1.6 ng/L for PFHxS, at the depths 0.5 m, 15 m, and 30 m, respectively (data from Fyrisån's Water Conservation Organisation).

The PFOS and PFHxS spread in the lake was simulated as that of a conservative tracer, i.e., without taking into account such processes as decay, sedimentation, and bioaccumulation (Ahrens et al., 2009; Ahrens et al., 2010).

The modelling results were compared with the observed concentrations of PFOS and PFHxS in Lake Ekoln at location Vreta Udd. The observed concentrations were reported for 2017–2018 on eight occasions at three depths (0.5 m, 15 m, 30 m) by Fyrisån's Water Conservation Organisation and on four occasions in 2019–2020 at two depths (0.5 m and 30 m) by Malnes et al. (2021).

3. Results and discussion

3.1. Seasonal changes in Lake Ekoln

The hydrodynamic conditions and the spread of PFAS in Lake Ekoln were simulated for the years 2017–2020, and the simulated water temperatures were in agreement with the observed water temperatures (Fig. 1). The model performance was assessed based on 591 pairs of observed and simulated values for water temperature with good results:

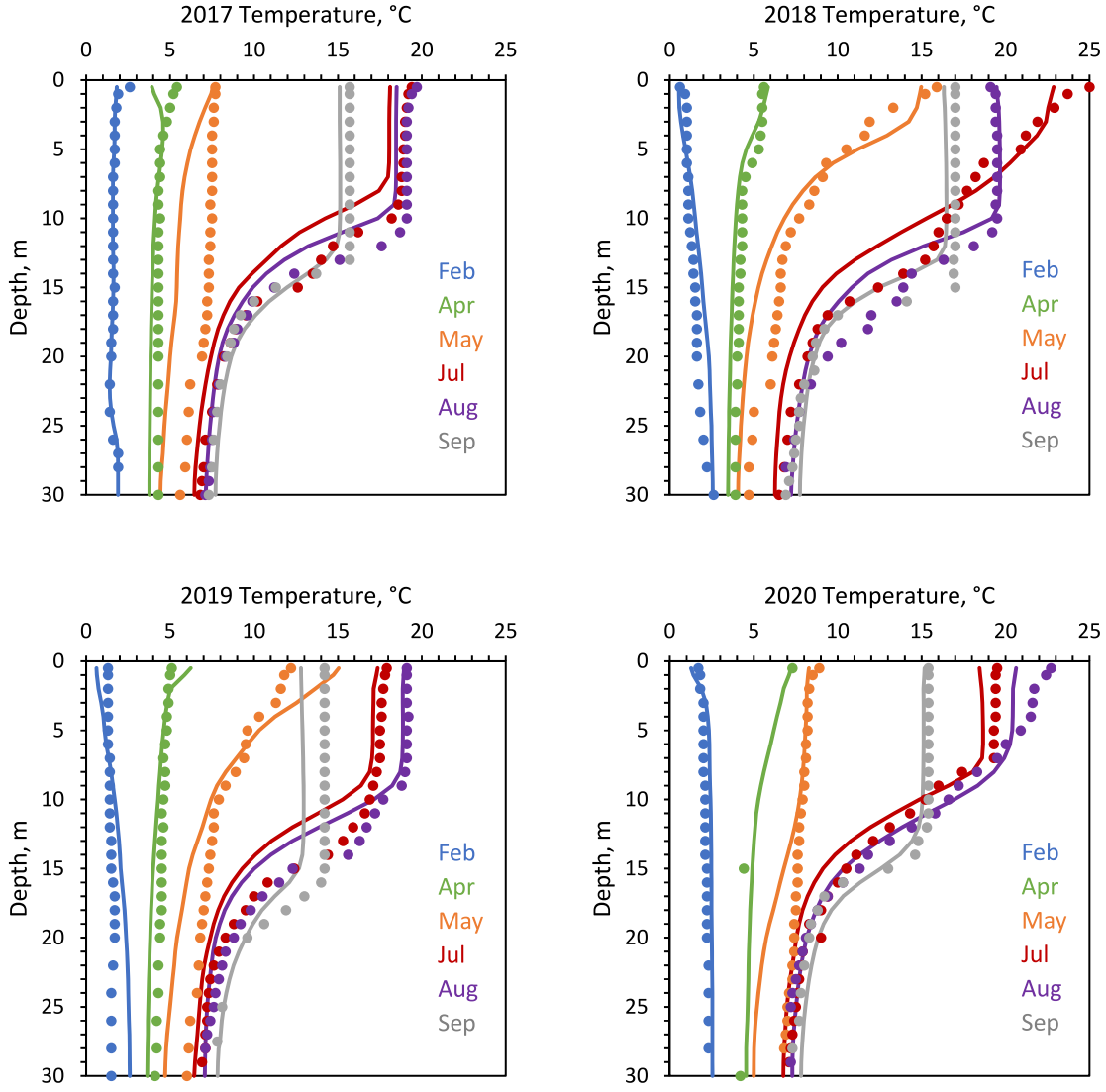

Fig. 1. Simulated (continuous) and observed (dots) water temperature in Lake Ekoln at the location Vreta Udd in the years 2017, 2018, 2019, 2020. The colours indicate the timing: blue – February, green – April, orange – May, red – July, purple – August, grey – September. Each year, the measurements were performed once in each of these months, but on different dates. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Nash-Sutcliffe efficiency of 0.96 and root mean square error of 1.18 °C. A clear temperature and thus density stratification and mixing pattern were observed in the lake (Fig. 1, Fig. S3 in SI).

By comparing the simulated PFAS concentrations at the different depths, we can see periods of mixed and of stratified conditions (Fig. S3 in SI). During spring, the water mixing usually occurred in April (see years 2017, 2018 and 2019), while in 2020, the spring mixing occurred already in January, and the mixed conditions lasted for more than three months (Fig. S3 in SI). During autumn, the water mixing occurred in October in all simulated years. During the periods of summer stratification, the PFAS concentrations were lower at the deeper levels in the lake (Fig. S3 in SI). During the inverse stratification in spring, episodically, the opposite was the case, i.e., the PFAS concentrations were lower at the surface than at the deeper levels (Fig. S3 in SI). Although the PFAS load in the model was constant over time, the water flow variations in the river Fyrisån had an impact on the simulated PFAS concentrations in the lake, particularly in the surface layer during the periods of high flows in Jan 2018, Apr 2018, Mar 2019, and Dec 2020, when the concentrations decreased (Fig. S3 in SI). The model may be used in the future to simulate the effect of changes in runoff and temperature on stratification and eventually the distribution of pollutants in the lake.

3.2. Simulated PFOS and PFHxS concentrations in Lake Ekoln

The simulated concentrations in Scenario A were higher than in Scenario B by a factor of on average 1.5 for PFOS and 1.4 for PFHxS (calculated over 0.5 m, 15 m, and 30 m depths; Table S3 in SI). As explained in Methods, Scenarios A and B differed in terms of the assumptions regarding the load from Fyrisån. Scenario A was based on 28 measurements, but of these, 21 were conducted outside of the simulated period (Table 1). Scenario B was based on the measurements conducted during the simulated period, but only seven measurements were available (Table 1), thus, making the assumptions less reliable than in Scenario A.

The simulated concentrations in Lake Ekoln at location Vreta Udd in the surface layer were higher and had a larger range, i.e., 0.41–5.1 ng/L for PFOS and 0.4–3.1 ng/L for PFHxS, comparing to 15 m and 30 m depths (Figs. 2 and 3, Table S3 in SI). The observed concentrations at the same location showed the largest range at the 30 m depth, i.e., 0.8–4.5 ng/L for PFOS and 0.3–3.6 ng/L for PFHxS (Figs. 2 and 3, Table S3 in SI). Calculated over time for the different depths, the mean simulated concentrations at Vreta Udd agreed with the mean observed values (Table S3 in SI), with the maximum difference in mean concentrations of 1.0 ng/L for PFOS (Scenario B, the model underestimated the concentration at 30 m) and of 0.8 ng/L for PFHxS (Scenario B, the model underestimated the concentration at 15 m). The RMSE for the entire dataset (32pairs of simulated and observed concentrations) was 0.95 and 1.13 ng/L for PFOS and 0.91 and 0.96 ng/L for PFHxS, for Scenarios A and B respectively, showing better agreement for Scenario A. The agreement was the best for the 15 m depth, where the RMSE was 0.63 ng/L for PFOS and 0.67 ng/L for PFHxS in Scenario A (based on 8 pairs of simulated and observed concentrations, Table S3). The RMSE was the highest for the 30 m depth (1.20 ng/L for PFOS and 1.10 ng/L for PFHxS in Scenario A, based on 12 pairs of concentrations, Table S3), indicating

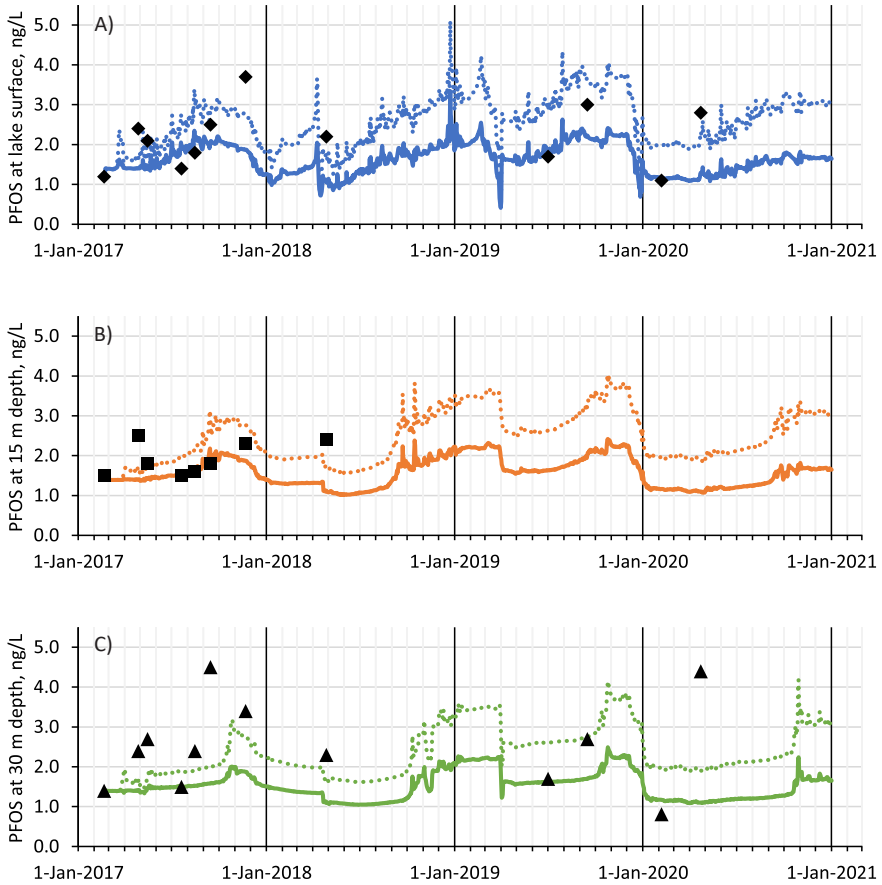

Fig. 2. Simulated (lines) and observed (symbols) PFOS concentrations in Lake Ekoln at location Vreta Udd at A) lake surface, B) 15 m depth, C) 30 m depth. Scenarios A and B, which differ in terms of assumed PFOS load from Fyrisån, are shown with dotted and continuous lines respectively. The observed concentrations were reported for 2017–2018 at three depths (surface, 15 m, 30 m) by Fyrisån's Water Conservation Organisation and for 2019–2020 at two depths (surface and 30 m) by Malnes et al. (2021).

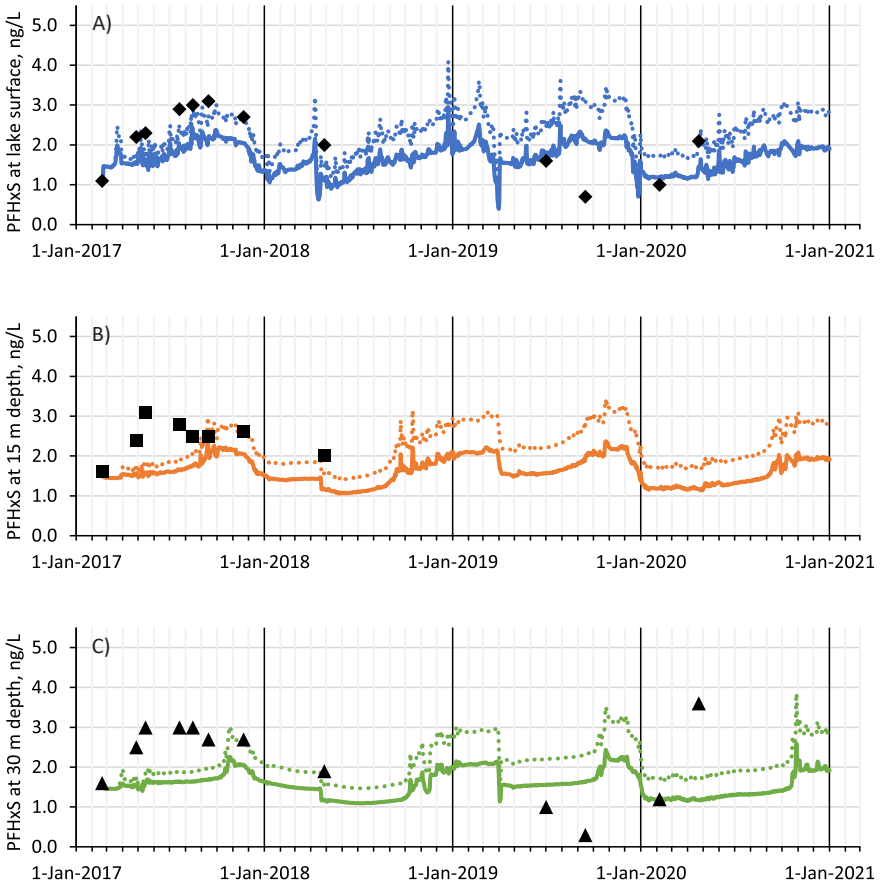

Fig. 3. Simulated (lines) and observed (symbols) PFHxS concentrations in Lake Ekoln at location Vreta Udd at A) lake surface, B) 15 m depth, C) 30 m depth. Scenarios A and B, which differ in terms of assumed PFHxS load from Fyrisån, are shown with dotted and continuous lines respectively. The observed concentrations were reported for 2017–2018 at three depths (surface, 15 m, 30 m) by Fyrisån's Water Conservation Organisation and for 2019–2020 at two depths (surface and 30 m) by Malnes et al. (2021).

the model performed better at the surface and the 15 m depth.

The concentrations were also calculated for the outflow from Lake Ekoln for the years 2019–2020 (Fig. S4 in SI). The simulated concentrations at the outflow were 1.8–3.5 ng/L of PFOS and 1.7–3.0 ng/L of PFHxS in Scenario A, and 1.0–2.1 ng/L of PFOS and 1.1–2.0 ng/L of PFHxS in Scenario B (Fig. S4 in SI); however, these estimations should be interpreted with caution in the context of modelling uncertainties. In future studies, measurements of PFAS concentrations at the outflow from the lake need to be performed, to validate the model output, and most importantly to understand the magnitude and the temporal variations of the PFAS load on the downstream drinking water source – the eastern part of Lake Mälaren.

3.3. Contribution of different sources to PFOS and PFHxS concentrations in Lake Ekoln

In the beginning of the simulation, the initial conditions regarding PFOS and PFHxS concentrations in the lake were specified based on measurements. As the theoretical water retention time in the lake is about one year, over the simulated years 2017–2020, the concentrations stemming from the specified initial conditions are decreasing (Fig. 4). Therefore, the contributions from the different sources to the total simulated concentration at Vreta Udd were calculated for the year 2020, when the impact of the initial conditions was the lowest (Table S4 in SI). In both scenarios, Fyrisån was the dominating source (Fig. 4 and Table S4 in SI): in Scenario A, the mean contribution of Fyrisån to the total simulated concentration was 77–79% for PFOS and 82–83% for PFHxS, while in Scenario B, it was 60–62% for PFOS and 74–75% for PFHxS. The mean contribution of Kungsängsverket WRRF was 18–19 % for PFOS and 9–10% for PFHxS in Scenario A, while in Scenario B, it was 33–34% for PFOS and 14% for PFHxS (Table S4 in SI).

The local water company in Uppsala is currently planning to implement quaternary treatment of wastewater for removal of organic pollutants. It is expected that this will decrease the load of all PFAS from Kungsängsverket WRRF substantially (>75%). Based on the modelling results (Fig. 4, Table S4 in SI), this will however have limited effect on PFAS concentrations in the lake. Model simulations indicate that a 75% reduction in the load from Kungsängsverket WRRF will decrease the concentrations in the lake by 14–26% for PFOS and by 8–11% for PFHxS (the range stems from the two simulated scenarios).

The results of both Scenarios A and B demonstrated that, by all estimates, Fyrisån (without Kungsängsverket WRRF) is the dominating source of PFOS and PFHxS into Lake Ekoln (Fig. 4, Table S4 in SI). Scenario A is more reliable as it is based on more measurements of concentrations in Fyrisån compared to Scenario B, but these were conducted mainly outside of the simulated period and are older (2013–2015), while Scenario B is based on very few more recent measurements. In this study, a constant load from Fyrisån was assumed, as the available data were insufficient to describe the variations over time. However, based on monthly PFAS measurements conducted between

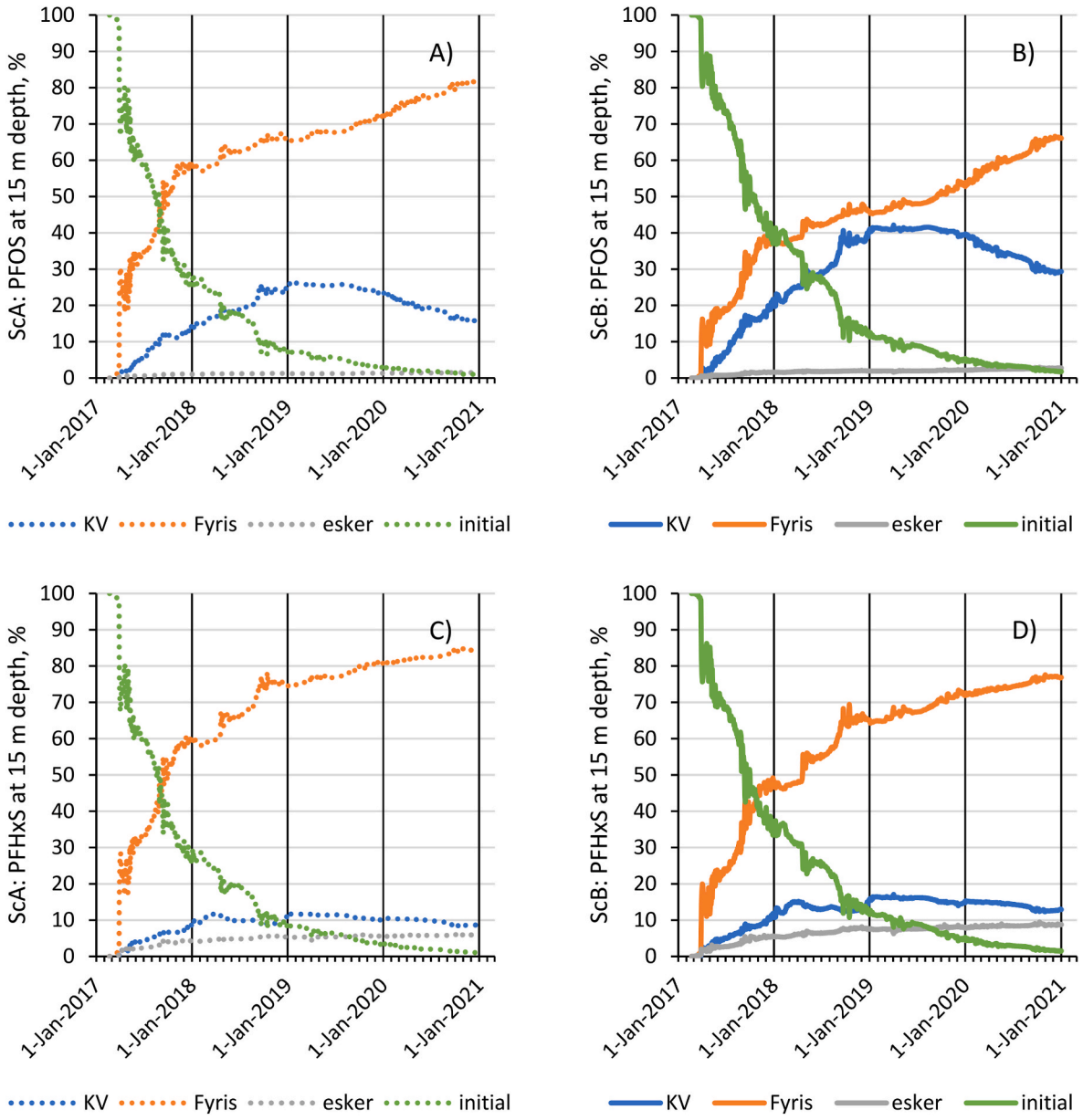

Fig. 4. Simulated contribution (percentages) from the different sources (Kungsängsverket WRRF – KV, Fyrisån – Fyris, esker, and initial conditions – initial) to the concentrations of PFOS (A, B) and PFHxS (C, D) in Lake Ekoln at location Vreta Udd at 15 m depth. Scenario A (ScA) is shown by dotted lines (A, C) and scenario B (ScB) is shown by continuous lines (B, D).

March 2013 and April 2014, Nguyen et al. (2022) showed that the load from Fyrisån exhibits clear seasonal variations (Fig. S2). This highlights the importance of regularly monitoring the concentrations in Fyrisån, as it is the dominating source (Nguyen et al., 2017).

Nguyen et al. (2022), Sörengård et al. (2022), and Nygren et al. (2021) reported measurements of PFAS along the river Fyrisån in 2013/2014, 2014, and 2020, respectively. All three studies emphasised the impact of Ärna air base and of Kungsängsverket WRRF. Sörengård et al. (2022) also mentioned the impact of two other firefighting training sites on PFAS concentrations in the river. Moreover, in a recent report (Öckerman et al., 2024), the municipality of Uppsala stated that, based on current knowledge, the PFAS in Fyrisån primarily originates from the firefighting foam used in the past at training sites, including Ärna air base.

Although the lack of measurements in the lake made the comparison of observed and simulated concentrations uncertain, there are indications that the PFAS sources included in the model do not fully explain the total observed concentrations in the lake (Figs. 2 and 3, Table S3 in SI), especially since none of the removal processes of PFAS were accounted for in the model. This points to potential underestimation of the sources included in the model and/or existence of other PFAS sources polluting the lake. These sources could be on-site wastewater treatment systems, as was previously observed in Fyrisån and Lake Ekoln area (Gago-Ferrero et al., 2017).

In Görväln, which is a bay of Lake Mälaren located downstream of Lake Ekoln, PFOS and PFHxS were measured in sediments in concentrations up to 7.81 ng/g dry weight and 0.24 ng/g dry weight, respectively (NIRAS Sweden AB, 2019), while in water, the concentrations of 3.10 ng/L and 1.65 ng/L were reported, respectively (Filipovic et al., 2018). These concentrations suggest that Log Kd values in Görväln can be up to 3.4 and 2.2, and Log Koc values up to 4.8 and 3.5 (assuming the organic content of 0.041 g/g in sediments in Görväln (Sahlin et al.,

2018)), for PFOS and PFHxS, respectively. These estimations suggest that sediments of Lake Mälaren may act as a sink of PFOS and PFHxS; this was not accounted for in this study. However, other studies have shown that under certain conditions, desorption of PFAS from lake sediments can occur (Reif et al., 2022). The model can be further developed in the future to better account for the environmental processes affecting the fate of PFAS, and the model can be further extended to include other parts of Lake Mälaren, beyond Lake Ekoln.

Moreover, in the future, the model can be used to study more/other PFAS compounds. Based on the available measured data for the studied period 2017–2020, the contributions of PFOS, PFHxS, PFOA, and perfluorononaoate (PFNA) to PFAS 4 (sum of these compounds) concentrations were 51 %, 25 %, 16 %, and 8 % in the effluent of Kungsängsverket WRRF (based on 47 observations), 40 %, 42 %, 17 %, and 2 % at the mouth of the river Fyrisån (based on 7 observations), and 38 %, 36 %, 15 %, and 11 % in Lake Ekoln at location Vreta Udd (based on 32 observations), respectively. For the purpose of these calculations, the concentrations below the detection limit were replaced with half of the detection limit. Although the simulated compounds PFOS and PFHxS constitute 74–82% of PFAS 4 in the studied area, future studies should consider including more PFAS compounds.

This study contributes to the growing body of scientific literature on three-dimensional hydrodynamic modelling of PFAS pollution in the water sources (Miyake et al., 2014; Hodgkins et al., 2019; Aly et al., 2020; Katz et al., 2022; Zhang et al., 2024) and further underscores the benefits of this modelling approach.

3.4. Implications for the drinking water supply

In Sweden, two new limit values for PFAS in drinking water will be implemented from January 2026 (LIVSFS 2022:12): PFAS 4 of 4 ng/L and PFAS 21 (sum of 21 PFAS) of 100 ng/L. Many drinking water producers in Sweden are affected by these new limit values (Lindfeldt et al., 2021), particularly the limit value for PFAS 4, which is very close to background levels at some places in Sweden (Gobelius et al., 2018) and in parts of the world also close to the concentration in precipitation (Cousins et al., 2022). The spread of PFAS in the environment, coupled with their persistent, bioaccumulative, and toxic properties, not only imposes a significant ecological cost, but also presents a substantial economic burden for society (Goldenman et al., 2019). Treating PFAS at a drinking water treatment plant is an ineffective, costly, and short-term end-of-pipe way of dealing with PFAS (Brunn et al., 2023; Franke et al., 2021). Franke et al. (2021) showed how cost of treatment and concentration are related in a nonlinear fashion. In the Uppsala area, drinking water treatment cost doubled due to the presence of PFAS in the source water (Lagerstedt, 2024). Therefore, it is critical to identify PFAS-hotspots and take measures at the source to treat PFAS, preventing it from spreading further in the environment and polluting drinking water resources.

Levels of PFAS 4 in the eastern part of Lake Mälaren, which provides more than two million people with drinking water, are around the upcoming limit value (Ekman and Ejhed, 2023). Therefore, it is important to identify critical hotspots affecting Lake Mälaren and treat PFAS upstream of the drinking water treatment plants. The river Fyrisån was pointed out as one of the major inflows of PFAS affecting the PFAS concentration in the eastern Mälaren based on mass-flow calculations (Ekman and Ejhed, 2023). The PFAS modelling presented in this study highlights what sources contribute the most to the concentration in Lake Ekoln and thus further implicates the sources that affect the eastern Mälaren. The results are in line with mass-flow calculations by Ekman and Ejhed (2023) showing that Fyrisån is the major contributor of PFAS to Lake Ekoln. Earlier, Nygren et al. (2021) showed that the main source of PFAS in Fyrisån is Ärna air base because of the use of aqueous film forming foam containing PFAS at their firefighting training site. The three large drinking water treatment plants, supplying the greater Stockholm area, are located downstream from Lake Ekoln and thus need to take preventive actions, which are estimated to create an extra cost of several million Swedish kronor per year. Given that the leakage of PFAS from the pollution in the north of Uppsala could potentially go on for several decades, the absence of mitigation is a socioeconomic challenge. In 2018, a comprehensive statement was published by a group of renowned experts describing which measures may be taken to address PFAS (Ritscher et al., 2018), that could serve as a first step.

Understanding how pollution, including PFAS, is distributed in the environment is needed for source tracking and prioritising mitigation measures. In case of Lake Mälaren, some efforts were made to use widely available digital tools for operational management and long-term decision making, e.g., modelling the spread of petroleum products and microbial pollution. Modelling of PFAS spread presented in this study constitutes another step in this direction. Modelling concentrations in a lake with a comparably long turnover time allows partly to compensate for the lack of high-resolution PFAS measurements. Moreover, since modelling provides a quantitative assessment of the contribution of different sources, it makes it possible to attribute the required cost for treatment to the polluter upstream. This is especially interesting in the context of the Uppsala case, as the responsibility of who should cover the additional costs of drinking water treatment are currently disputed. Modelling can also be used to estimate the lag time of lake water concentration after remediate action has been taken. For example, given the limit value for PFAS 4, it can now be calculated what minimum remediate action would need to be taken to keep lake water concentration below 4 ng/L throughout the year.

4. Conclusions

- The modelling results confirmed that the river Fyrisån is the main source of PFAS into Lake Ekoln. For the year 2020, the simulated contributions to the total concentrations in Lake Ekoln were on average: 19–33 % from Kungsängsverket WRRF and 61–78 % from the river Fyrisån for PFOS; and 9.6–14 % from Kungsängsverket WRRF and 75–83 % from the river Fyrisån for PFHxS (the ranges stem from the two simulated scenarios). This points to the importance of mitigating this PFAS source in the context of ensuring safe drinking water supply in the Stockholm region.
- The modelling results describe the seasonal variations of PFAS in Lake Ekoln, informing the operation of the drinking water treatment plants located downstream. The simulated average concentrations over the year 2020 at the outflow from Lake Ekoln were 1.2–2.1 ng/L for PFOS and 1.3–1.9 ng/L for PFHxS (the ranges stem from the two simulated scenarios).
- The study provides an approach to assess the quantitative effects of mitigation measures.
- Regular monitoring of PFAS in the river Fyrisån is needed to better quantify its contribution, map seasonal changes in PFAS load, and to assess the long-term trends and outcomes of future mitigation measures.
- More measurements of PFAS concentrations in Lake Ekoln, particularly in the lake outlet and in sediments, would facilitate further model development as well as understanding of the impact on the drinking water source downstream.

CRediT authorship contribution statement

Ekaterina Sokolova: Writing – original draft, Supervision, Project administration, Funding acquisition, Formal analysis, Conceptualization. **Prajwol Prajapati:** Writing – original draft, Methodology, Formal analysis. **Frida Ekman:** Writing – review & editing, Methodology, Formal analysis, Conceptualization. **Namika Maharjan:** Formal analysis. **Sandra Lindqvist:** Methodology, Formal analysis. **Johan Kjellin:** Writing – review & editing. **Anna Karlsson:** Writing – review & editing, Methodology. **Mia Bondelind:** Writing – review & editing, Supervision, Funding acquisition. **Lutz Ahrens:** Writing – review & editing. **Stephan Köhler:** Writing – review & editing, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envpol.2024.125581.

Data availability

Data will be made available on request.

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