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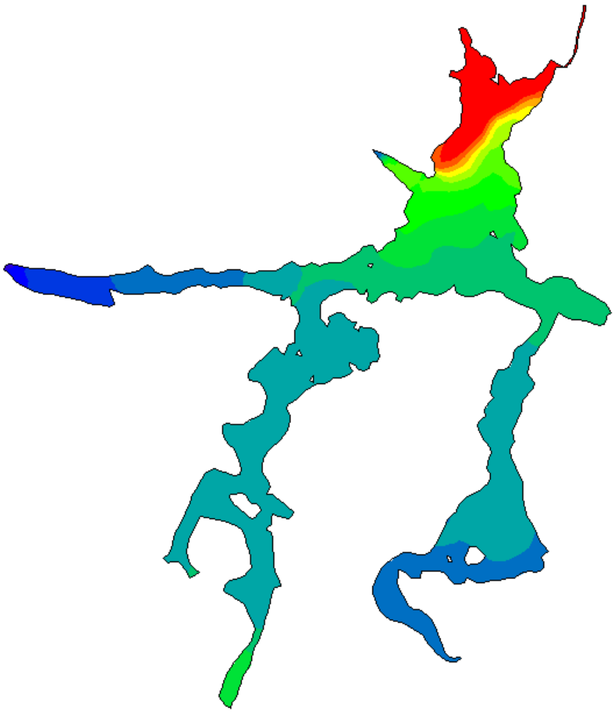

Hydrodynamic modelling of current and future spread of PFOS in Lake Ekoln

Impacts of Climate Change and Socioeconomic Development

Master’s thesis in Infrastructure and Environmental Engineering

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Cover:
Modelled horizontal distribution of PFOS in Lake Ekoln in July 2017
Department of Architecture and Civil Engineering

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ABSTRACT

The spread of Per- and polyfluoroalkyl substances (PFAS) is a global issue since it has been detected in aquatic environments all around the world and may have adverse effects on human health. The major exposure pathway for humans is drinking water. High levels of PFOS, one of the most harmful PFAS, have been detected in Lake Ekoln - a sub basin to Mälaren, and its surrounding environment. The aim of this study was to analyse current and future spread of PFOS in Lake Ekoln. Sources to PFOS in the area, and processes affecting fate and transport of PFOS were investigated. Hydrodynamic modelling in MIKE 3FM was applied to simulate the current spread of PFOS in the lake, but also to investigate future conditions in regards to climate change and socioeconomic development. Future scenarios were set up for 2050 where climate change was described by Representative Concentration Pathways (RCPs) and socioeconomic development by Shared Socioeconomic Pathways (SSPs). Major sources of PFOS in Lake Ekoln are firefighting training sites where firefighting foam containing PFOS historically have been used, and the Wastewater Treatment Plant (WWTP) Kungsängsverket. Fyrisån receives water from both of these sources and is considered to be the major pathway for PFOS entering Lake Ekoln. Other possible sources are landfills, industrial activities and On-site Wastewater Treatment Systems (OWTS), and other pathways are Uppsalaåsen, precipitation and other rivers. Processes affecting the fate and transport of PFOS are sedimentation and bioaccumulation, however, these were not included in the modelling. Climate change will not affect the situation with PFOS remarkably until 2050 while socioeconomic development will have a larger impact; the concentration of PFOS is assumed to decrease, however the extent of the decrease varies a lot between the different SSPs. Considering the possibilities to use Lake Ekoln as drinking water source in regard to PFOS, the quality is good and will remain so in 2050, according to the current regulations. However, other kinds of PFAS could be as harmful as PFOS why research regarding the spread of PFAS in the area needs to proceed.

Key words: climate change, drinking water, hydrodynamic modelling, MIKE 3 FM, PFAS, PFOS, RCP, socioeconomic development, SSP, water quality

Hydrodynamisk Modellering av Nuvarande och Framtida Spridning av PFOS i Ekoln
Påverkan av Klimatförändringar och Socioekonomisk Utveckling

Examensarbete inom mastersprogrammet Infrastruktur och Miljöteknik

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SAMMANFATTNING

Spridningen av Poly- och perfluorerade alkylsubstanser (PFAS) är ett globalt problem sedan de har upptäckts i vattenmiljöer i hela världen och kan ha negativ effekt på människors hälsa. Den största exponeringsvägen för människor är dricksvatten. Höga halter av PFOS, en av de mest skadliga typerna av PFAS, har upptäckts i Ekoln - en del av Mälaren, och dess omgivande miljö. Syftet med den här studien var att analysera den aktuella och framtida spridningen av PFOS i Ekoln. Källor till PFOS i området, och processer som påverkar spridningen av PFOS undersöktes. Hydrodynamisk modellering i MIKE 3FM användes för att simulera aktuell spridning av PFOS i sjön, men också för att undersöka framtida förhållanden med avseende på klimatförändringar och socioekonomisk utveckling. Framtida scenarier sattes upp för år 2050 där klimatförändring beskrevs av Representative Concentration Pathways (RCPs) och socioekonomisk utveckling av Shared Socioeconomic Pathways (SSPs). Stora källor till PFOS i Ekoln är brandövningsplatser där brandskum som innehåller PFOS har använts, och avloppsreningsverket Kungsängsverket. Fyrisån tar emot vatten från båda dessa källor och antas vara den största transportvägen för PFOS som når Ekoln. Andra möjliga källor är deponier, industriell aktivitet, och mindre avloppsreningssystem, och andra transportvägar är Uppsalaåsen, regn och andra floder. Processer som påverkar spridningen av PFOS är sedimentation och bioackumulation, dock inkluderades dessa inte i modelleringen. Klimatförändringar kommer inte påverka situationen med PFOS anmärkningsvärt fram till 2050 medan socioekonomisk utveckling kommer ha större påverkan; koncentrationen av PFOS antas minska, dock olika mycket i de olika SSP-scenarierna. Med hänsyn till situationen med PFOS är vattenkvalitén tillräcklig för att använda Ekoln som dricksvattentäkt, och kommer kvarstå år 2050, enligt nuvarande föreskrifter. Dock kan andra typer av PFAS vara lika farliga som PFOS varför forskning på spridningen av PFAS i området bör fortsätta.

Nyckelord: dricksvatten, hydrodynamisk modellering, klimatförändringar, MIKE 3 FM, PFAS, PFOS, RCP, socioekonomisk utveckling, SSP, vattenkvalité

Contents

Preface

This master thesis was carried out at Chalmers University of Technology, Sweden. The thesis was conducted within the research project "ClimAQua – Modelling climate change impacts on microbial risks for safe and sustainable drinking water system" (grant number: 2017-01413), funded by Formas – the Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning. Supervisors were Ekaterina Sokolova, Associate Professor in Water System Modelling, and Mia Bondelind, Senior Lecturer, both at the Water Environment Technology division at Chalmers University of Technology. We would like to thank both Ekaterina and Mia for being very supportive throughout our project, and providing us with valuable feedback, knowledge and ideas during our work.

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We would also like to thank Frida Ekman, who laid the foundation for our work through her master thesis. Frida was a great help for us in the start-up of our work, provided us with inspiration, knowledge and data for the modelling.

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Göteborg May 2021

Amanda Hansson

Elin Josefsson

1 Introduction

Accessible and clean water is a basic precondition for all living organisms on earth, and thus a fundamental part of human health and a sustainable development (UNDP, 2020). According to the UN General Assembly, everyone has the right to safe and sufficient water for domestic and personal use at an affordable price (WHO, 2019). However, both the quantity and quality of the global water system is under pressure (Brack et al., 2017). The quality of water is impacted by contaminants related to anthropogenic activities, such as consumption, overexploitation, and dumping of toxic material. The use of chemical substances might pose a risk for human health through discharge and spreading in water sources, and thus reach humans through e.g., drinking water.

Per- and polyfluoroalkyl substances (PFAS) is a collective name for a group of highly fluorinated chemicals that are industrially produced, where PFOS is one of the most known and widely spread (Kemikalieinspektionen, 2021a). PFAS are used in products in order to repel water, oil, and dust, such as apparel, paper- and packaging products, cookware, and beauty products. It is also highly present in some fire-fighting foams. Some of the chemicals have been found to have adverse effects on human health where cancer and impaired immune system are two examples (Sunderland et al., 2019). The occurrence of PFAS is highly connected to urban activity and the chemicals can enter aqueous environments from e.g. wastewater treatment plants (WWTP), landfill leachate, atmospheric deposition and surface runoff (Ahrens et al., 2011). PFAS have properties that make them very persistent which mean that they remain in the environment for a very long time, and can be spread long distances (Kemikalieinspektionen, 2021b). The chemicals have been found in many water sources, and for humans, a major exposure pathway is drinking water (Sunderland et al., 2019).

It is important to look at the condition today, but it is also of high importance to ensure access to safe and sufficient water in the future. Since the future may bring different conditions than today, investigation of what impact it will have on the water quality and supply is needed. Two major changes that are predicted for the future are climate change and socio-economic development (IPCC, 2014; Riahi et al., 2017). Climate change is foreseen to impact humans and ecosystems in terms of e.g. rising air temperature, more frequent events with heat waves and extreme precipitation, warming ocean, and rising sea levels (IPCC, 2014). These changes will disrupt the hydrological cycle and impact the quality and quantity of water sources. Regarding socio economic development, major drivers are population growth, urbanisation, and economic activity where questions that must be considered are resource availability, technology development, and lifestyle changes (Riahi et al., 2017). This development may impact the use of chemical substances, and how and to what extent these are emitted to the environment.

Lake Ekoln is a sub basin to Mälaren, Sweden's third largest lake and the largest drinking water source in Sweden, serving over two million people (Mälarens Vattenvårdsförbund, n.d.). High levels of PFAS have been detected in Lake Ekoln and its surrounding environment, why further research and studies are necessary to ensure the quality of the water and the possibility to proceed using Mälaren as a drinking water source. A previous study made of PFAS in Lake Ekoln identified some possible sources to PFAS in the area but concluded that more sources than was identified in the study are contributing to spreading PFAS in the lake, and the situation needs to be investigated further (Ekman, 2021). How future conditions, such as climate change and socio-economic development, will impact the situation with PFAS in the area of Lake Ekoln is also important to investigate, to be able to take action before it causes too much damage.

1.1 Aim and objectives

The aim of this study was to analyse current and future spread of PFOS in Lake Ekoln. The objectives were to:

- Identify sources of, and pathways for, PFOS into Lake Ekoln
- Identify processes affecting the fate and transport of PFOS in Lake Ekoln
- Formulate scenarios to describe future climate and socioeconomic conditions affecting spread of PFOS
- Apply hydrodynamic modelling to simulate the fate and transport of PFOS in Lake Ekoln for the current situation and the formulated future scenarios

1.2 Scope and limitations

The literature review in this study included research regarding PFAS in general, but the only PFAS that was included in the modelling was PFOS. The study was limited to investigate the current and future spread of PFOS in Lake Ekoln, but no further analysis of the effect on human health and ecosystems were made. The focus was either not on investigating measures or purification techniques to reduce the amount of PFOS in the area. The study was based on existing data and information regarding PFOS in Lake Ekoln, no sampling was made. The study was also limited to focus on the hydrodynamics in the lake without any hydrological modelling of the surroundings and contamination of surrounding land and groundwater will not be evaluated in depth. Lastly, due to heavy simulations, the future conditions will be represented by, and limited to, some few chosen scenarios.

2 Literature review

2.1 Per- and polyflouralkyl substances (PFAS)

Per- and polyflouralkyl substances (PFAS) is a collective name for a group of highly fluorinated chemicals that since 1950 have been widely used in the industry and commercial trade (Buck et al., 2011). Several of the chemicals have been detected around the globe in water, wildlife and humans and they are found to have adverse effects on the environment and health (Ahrens et al., 2010; Sunderland et al., 2019; Naturvårdsverket, 2021a). Baabish et. Al (2021) presents a study that indicates that location of point sources, such as production and use, and the surrounding environment have a large impact on the local concentration of PFAS. But since the use of PFAS is spread worldwide and the dispersion of the substances is effective, the issue with PFAS is global and studies and research regarding it is a current subject (Ahrens et al., 2010; Sánchez-Soberón et al., 2020; Schrenk et al., 2020; EPA, 2021).

2.1.1 Structure and properties

There are more than 4,000 different substances that are registered as PFAS, and the common denominator is the backbone of aliphatic carbon where the hydrogen atoms have been replaced by fluorine (Rahman et al., 2014; Miaz et al., 2020). If the hydrogen atoms are completely replaced, the substance has the prefix per and if they are partly replaced the prefix is poly. Since the C-F bond is extremely strong, these perfluoroalkyl moieties (CnF2n+1) in PFAS make the substances very chemical- and thermal stable (Buck et al., 2011). This persistent property makes PFAS useful in many ways since they can resist tough conditions, such as high temperatures, but are negative looking from an environmental perspective since they are hard to degrade and therefore accumulate in ground, water and biota, and can be transported long distances (Kemikalieinspektionen, 2021b). The general structure of PFAS has one part that is hydrophobic and one that is hydrophilic, which makes them very surfactant and thus also water and lipid repellent (Al Amin et al., 2020). The water-solubility varies among the different PFAS and decreases with the length of the backbone (Kemikalieinspektionen, 2021b). In general, the solubility is high among all PFAS which increases the distances these substances can get transported. It is also common that a functional group is connected to the backbone, such as a sulfonate- or carboxyl group, which give them different properties (Conder et al., 2008). PFAS are often named as "long-chained" or "short-chained" where the chain refers to the backbone, and the length of this chain affects the properties of the specific PFAS (Ahrens & Bundschuh, 2014). PFAS with n>8 are classified as long-chained and the longer the chain, the lower the reactiveness, which means that they are less probable to degrade and are more prone to bioaccumulation (Al Amin et al., 2020; Buck et al., 2011; Rahman et al., 2014). It has been found that some short-chained PFAS, that may be seen as less harmful, can degrade to the more persistent long-chained ones with time (Ahrens & Bundschuh, 2014).

One long-chained PFAS that has received attention worldwide is PFOS (Wang et al., 2017). PFOS have been detected in different types of areas in the whole world (Giesy & Kannan, 2001). Giesy & Kannan (2001) presents samples collected from both urbanised and less urbanised areas, the samples from the urbanised areas had higher concentrations of PFOS, but the substance was also detected in the samples from less urbanised areas which confirms its ease to get transported. As mentioned, long-chained

PFAS have been found to have bioaccumulative properties which is confirmed regarding PFOS in the study by Giesy & Kannan (2001).

2.1.2 Use and sources

The chemical- and thermal stability of PFAS together with their repellence to water and lipids, makes them very useful. PFAS are commonly used, or in some cases *have* been commonly used, in products in order to repel water, oil, and dust such as apparels, paper- and packaging products, cookware, and fire-fighting foams (Naturvårdsverket, 2020). The occurrence of PFAS is highly connected to urban activity, and patterns that present that higher concentration of PFAS comes with higher population density have been identified (Ahrens et al., 2011).

PFAS are released into the environment during all stages of their life cycle - the production, supply chain, product use, and disposal of industrial and consumer products, and the sources can be identified as point or diffuse sources (Ahrens & Bundschuh, 2014). Wastewater treatment plants (WWTP), landfills, and application of products containing PFAS in a concentrated area (e.g., firefighting foams) are examples of point sources and examples of diffuse sources are runoff from contaminated ground and atmospheric deposition. Water containing PFAS that enter WWTPs can come from industries, households, and landfill leachate, and WWTP that manage water from industries contain more PFAS than those that only handle domestic water (Xiao et al., 2012). According to Xiao (2012), PFAS in WWTPs are of great concern since PFAS have been found not to be removed in wastewater treatment. Products that contain PFAS and end up at landfills contribute to the risk of spreading of PFAS in the environment through the leachate water via WWTP or via surface runoff (Busch et al., 2010). In firefighting foams, or in other words aqueous film forming foams (AFFFs), PFAS is one of the main components (Sunderland et al., 2019). This has resulted in discoveries of increased PFAS concentrations in areas connected to airports and military bases due to firefighting training activities that have occurred there. Among all PFAS, PFOS is the substance that has been used the most in firefighting foams, historically, and is therefore highly present in the environment today (Kemikalieinspektionen & Livsmedelsverket, 2013). The diffuse sources are harder to get track on but possible sources of PFAS detected in the air are manufacturing of PFAS and landfills (Ahrens & Bundschuh, 2014). PFAS in runoff water can come from contaminated land or streets where PFAS are present due to e.g., debris from products containing PFAS.

2.1.3 Dispersion

It is a challenge to track how PFAS spread in the environment due to different site-specific conditions and since different PFAS with different properties may behave differently in the environment (Kemikalieinspektionen, 2021a). However, identified dispersion routes are via ground, groundwater, stormwater and surface runoff, and the air.

How much PFAS that stays in the soil depends on the type of PFAS and the properties of the soil. In general, long-chained PFAS tend to bind more easily to the soil and it has been found that the substances can stay in the ground for a very long time (Kemikalieinspektionen, 2021a). PFAS in the ground can further reach the groundwater through infiltration of precipitation, irrigation, and flooding (Kemikalieinspektionen, 2021a). Groundwater is an important pathway for PFAS that can transport PFAS very far, therefore, it is of high importance to have knowledge about the hydrogeological conditions in a contaminated area. Parameters that affect the spread through groundwater are e.g., the hydraulic conductivity of the soil and the slope of the terrain. PFAS can enter surface water through runoff from contaminated ground, via groundwater, via emissions from point sources (such as those mentioned in the previous chapter), and via atmospheric deposition (Kemikalieinspektionen, 2021a). PFAS in surface water can also imply spread of PFAS to sediment where the length of the chain of the PFAS, grain size of the sediment, and organic carbon in the sediment are important parameters. The air is a possible pathway for PFAS and volatile PFAS have been detected at very far distances from the possible original source (Ahrens & Bundschuh, 2014). The volatile PFAS can further enter the aquatic environment through e.g. precipitation.

2.1.4 Processes affecting PFAS

As mentioned, PFAS are very resistant and are not easily affected by external conditions and processes. However, two processes that are commonly mentioned when talking about PFAS in aquatic environments are sedimentation and bioaccumulation, though there are many parameters that impact to what extent the processes are present, such as type of PFAS, what kind of biota that may take up the PFAS, and the content of organic matter in the water (Conder et al., 2008; Sánchez-Soberón et al., 2020).

PFAS can occur both in the particulate and dissolved phase where the relation between the phases depends on different environmental conditions (Ahrens et al., 2011). Since it is only the particulate PFAS that has the potential to settle, the partitioning behaviour of PFAS between the dissolved phase and suspended particles is essential to include when investigating the transport and fate of PFAS, but there is a lack of information regarding it (Ahrens et al., 2010). However, Ahrens et al., (2011), concluded that the characteristics of the sediment have great impact of the sorption capacity, e.g., higher content of particulate organic carbon has been correlated with higher concentration of PFAS detected in the sediment, and also the density of the sediment affects the sorption. This implies that sedimentation of PFAS can vary much between different places. It is also found that the physiochemical properties of PFAS affect the behaviour, where long-chained PFAS tend to bind stronger to particles and short-chained ones are exclusively detected in dissolved phase (Ahrens et al., 2010). Among all PFAS, PFOS is proven to be one that has the highest affinity for particles (Ahrens et al., 2010). Further, in the study by Ahrens et al. (2010), who investigated distribution of PFAS in water, sediment and on suspended particles in Tokyo Bay, it was found that in that specific case, the particulate fraction of PFOS in relation to the dissolved was 32 %. Figure 2.1 below illustrates the partitioning behaviour between dissolved and particulate PFOS, and storage in sediment, in an aquatic environment.

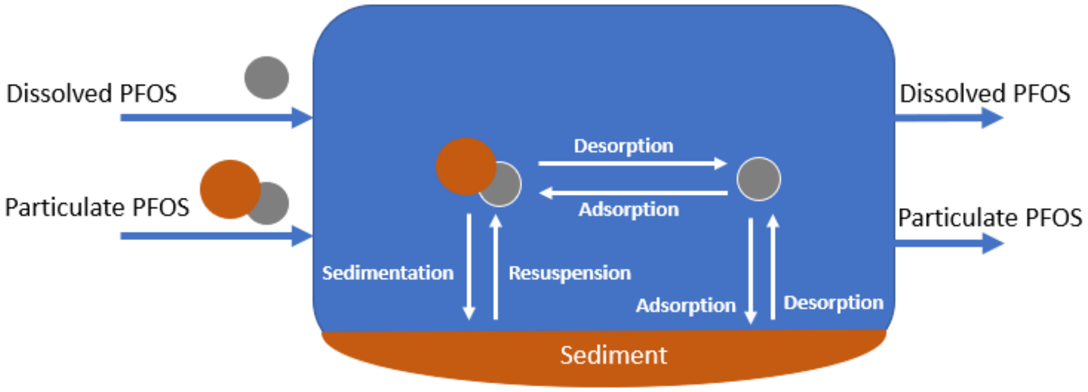

Figure 2.1 Conceptual model describing the partitioning behaviour between dissolved and particulate PFOS and storage in sediment, in an aquatic environment.

The fact that storage of PFOS in sediment could be of relevance is concluded in several studies (Kong et al., 2018; Sánchez-Soberón et al., 2020). Kong et al. (2018) stated that the water itself proved not to be a big sink for PFOS, since it was either transported to sediment or removed via outflows, and degradation of PFOS was negligible in both water and sediment. Sánchez-Soberón et al. (2020) developed a mass balance model to simulate the long-term distribution and concentration of PFOS and PFOA, which is another PFAS that has received a lot of attention, in water and sediment and tested the model in San Francisco bay. The results showed that due to phase out of the substances, the concentration in water had after approximately 50 years decreased to 96 % of the initial concentration for PFOA and 99 % for PFOS. However, considering sediments, the time before reaching stable state concentrations was around 50 years for PFOA and 500 years for PFOS. The parameter leading to the longer time for the decline of PFOS was believed to be the longer sediment half-life of PFOS.

The bioaccumulative potential have been found to vary depending on the structure of the substances where long-chained PFAS have higher potential than the short-chained ones, and those with sulfonyl functional group are more bioaccumulative than those with carboxylic functional group for the same chain length (Conder et al., 2008). Many studies have been made regarding detected PFAS in fish, and the most commonly detected substance is PFOS (Livsmedelsverket, 2021a; Stockholms Stad n.d.; Berger et al., 2009). According to Van der Oost et al. (2003), contaminants like PFOS can enter the fish via direct uptake from water through gills or skin, via uptake of suspended solids containing PFOS, and via ingestion of contaminated food. Detected levels of PFAS in higher trophic level bioa, such as polar bears and predatory birds, indicates that also biomagnification is an actual process, which mean that PFAS with low bioaccumulative potential still can bring adverse effects onwards (Conder et al., 2008).

Possible sources to PFAS, dispersion pathways, and processes affecting the concentration of PFAS in an aquatic environment are presented in Figure 2.2 below.

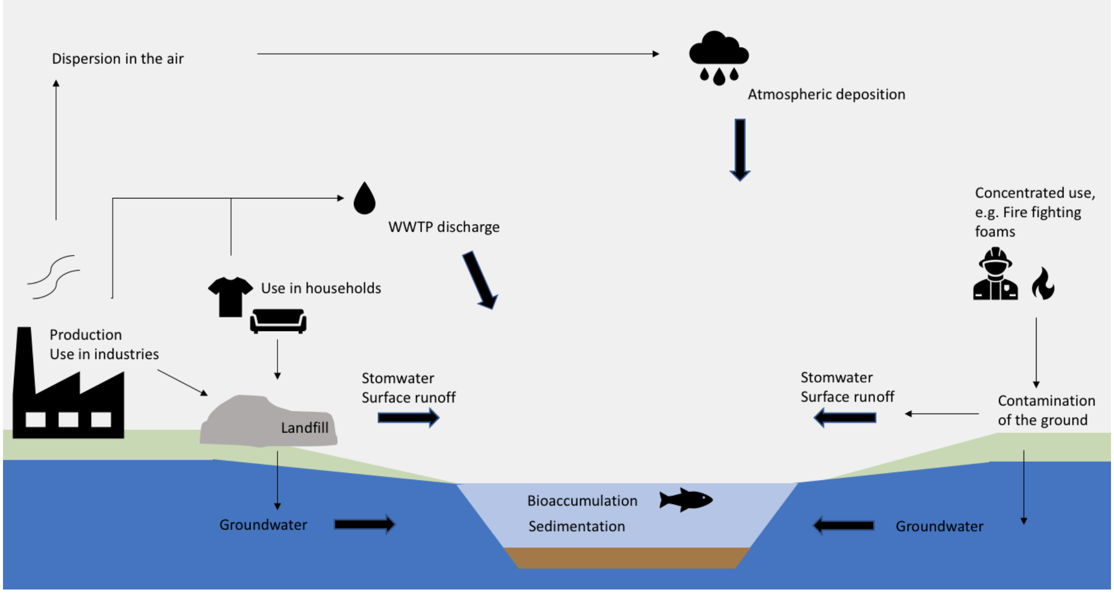

Figure 2.2 Sources, dispersion pathways, and processes affecting the concentration of PFAS in an aquatic environment.

2.1.5 Exposure and human health effects

Several studies have presented detection of PFAS in the human body (Lu et al., 2021; Pérez et al., 2013; Johnson et al., 2021). Even though the amount of PFAS humans normally intake does not cause acute health effects, the persistent properties may imply that the substances are stored in the body for a long time, which can be harmful in the long run (Livsmedelsverket, 2021b; Lu et al., 2021; Schrenk et al., 2020). Associations have been made between human exposure to PFAS and adverse effects on both the immune system and cancer (Sunderland et al., 2019).

The main pathways for human exposure to PFAS are via intake of drinking water and food contaminated with PFAS, use of products containing PFAS, and inhalation of dust indoors (Sunderland et al., 2019). Svenskt Vatten (2020) mentions in an article that Naturskyddsföreningen states that the major amount of PFAS humans have in the body have entered via inhalation and food, and that 20% comes from drinking water. Studies have also shown that a major pathway for small babies is via breast milk (FOI, 2013). Due to the bioaccumulation potential among some PFAS, its concentration can increase in the food chain (Sunderland et al., 2019). Since high concentrations of PFOS have been detected in fish, it is not recommended to eat fish from water courses contaminated with PFAS (Sunderland et al., 2019; Livsmedelsverket, 2021a).

2.1.6 Regulations of PFAS

To avoid adverse human health effects, the European Food Safety Authority (EFSA) has developed a limit value of PFAS (EFSA, 2021). The value refers to the intake of four main substances of PFAS; PFOA, PFOS, PFNA and PFHxS, and is set to a tolerable weekly intake (TWI) of 4.4 nanograms per kilogram body weight. This value was updated in September 2020 and is much stricter than the previous one, which implies higher demands on the food market (EFSA, 2021). Several of the recommendations Sweden has adopted are based on guidelines from EFSA. However, EFSA has not developed any limit regarding drinking water, but The Swedish National Food Administration has developed guidelines for drinking water producers (Svenskt Vatten, 2020). They recommend that if the concentration of PFAS in the drinking water exceeds 90 ng/l, drinking water producers should act, and if the values exceed 900 ng/l you should not drink the water or eat food that has been in contact with it (Livsmedelsverket, 2021a). In addition to the drinking water guidelines, the European Commission has in connection to the EU Water Framework Directive, decided on limit values for PFOS, for inland waters to be classified with good chemical status (2013/39/EU). The average yearly limit value for fresh water was set to 0.65 ng/l.

In December 2020, the EU also determined to implement benchmarks regarding PFAS in a new drinking water directive. The directive will apply to all member states of the EU and is a minimum directive, but all states can set up even stricter legislation. The directive will be introduced in the national drinking water regulations before 12th of January 2023 (Livsmedelsverket, 2021a). Also, the EU is focusing on exploring and developing precautionary approaches on how to manage PFAS (EEA, 2019).

Both PFOS and PFOA are classified as Persistent Organic Pollutants (POPs) in the Stockholm Convention, which is a global work that lists organic pollutants that need to be managed through implementation plans and regulations (Kemikalieinspektionen, 2021b). In 2008, the use of PFOS and substances that may degrade to PFOS were prohibited in the EU and in 2020 also PFOA was prohibited (Livsmedelsverket, 2021b). Other types of PFAS have replaced PFOS and PFOA, though it is uncertain whether these substances have a negative impact on human health and the environment as well.

There are countries outside Europe that still do not have any restrictions regarding PFAS at all, which is a critical issue since PFAS can be transported far distances (Ipen, 2019). Another issue is the lack of efficient treatment techniques. The water treatment techniques that are used on a large scale today are not efficient in removing PFAS, and lack of knowledge makes it hard to implement new ones in the treatment plants (Franke et al., 2017). Franke (2017) discusses that Granular Activated Carbon (GAC) is a technique that can treat the water from PFAS, but to make this technique efficient enough, the filters need to be changed often which is not sustainable and speaks for the fact that other techniques need to be developed.

2.2 Climate change and Representative Concentration Pathways

It is clear that human actions have a great impact on the climate system, and mainly due to anthropogenic activities, the climate has changed and is changing in a critical way (IPCC, 2014). Greenhouse gas (GHG) emissions are the main driver to a warmer climate, and the population growth and economic development that have occurred in the last decades have implied a significant increase in these emissions. Climate change has had an impact on, and is projected to impact, humans and ecosystems in terms of e.g., rising temperatures, more frequent events with heat waves and extreme precipitation, rising sea levels, demographic disruption, and infectious diseases (McMichael et al., 2006). In several regions, these changes affect the hydrological systems and the quality and quantity of water (IPCC, 2014). For example, heavy precipitation events lead to more runoff water which can be a problem itself, but it can also transport more contaminants from the ground to water sources, heat waves can lead to increased water demand and also water quality problems due to e.g. algal blooms. (IPCC, 2007).

IPCC (2014) have identified the key drivers to the anthropogenic GHG emissions as population size, economic activity, lifestyle, energy use, land use patterns, technology, and climate policy, and these factors are investigated to make projections for the future. In the work with the future climate, IPCC has adopted scenarios regarding different pathways for emissions and atmospheric concentrations of GHG, air pollutant emissions, and land use (IPCC, 2014). The scenarios are mentioned as Representative Concentration Pathways (RCPs), and the projected scenarios are RCP2.6, RCP4.5, RCP6.0 and RCP8.5, where the numbers represent the projected level of solar radiative forcing in W/m^2 by 2100. The different scenarios include, e.g., conceivable lifestyles, land use changes, and extent of climate policies. In Table 2.1, some of the characteristics of each scenario are presented, where RCP2.6 is the most environmentally sustainable one and RCP8.5 the least sustainable (SMHI, 2020a).

Table 2.1 Characteristics of each of the RCPs (SMHI, 2020a).

RCP 2.6	More stringent climate policy than today The energy intensity is low The use of oil will be less The population in the world is 9 billion The size of pasture area will remain the same as today Production of biofuels will lead to larger agriculture areas 40 % less emissions of methane Same level of CO_2 emissions as today, culminate year 2020 and negative year 2100 The content of CO_2 in the atmosphere culminates 2050
RCP 4.5	The climate policy is strict The energy intensity is lower than today Extensive forestry programs will be developed Smaller agriculture areas are needed due to changed consumption patterns and larger harvests World population slightly below 9 billion The emissions of CO_2 culminate in 2040
RCP 6	The dependency on fossil fuels will be large Lower energy intensity compared with RCP8.5 Greater areas of arable land, smaller pasture areas World population slightly below 10 billion The emissions of methane are stabilized The emissions of CO_2 culminate in the year 2060, when it is 75% higher than today. However, the level will decrease to 25% higher than today
RCP 8.5	The emission of CO_2 are three times larger than it is today Larger methane emissions World population will be 12 billion. Hence, pasture and cultivation areas will exploit The technology will continue to focus on energy efficiency, but the development will be slow The dependency on fossil fuels will be large The energy intensity will be high The climate policy will remain as it is today

2.3 Socioeconomic development and Shared Socioeconomic Pathways

Besides climate change, socioeconomic development is an important factor when assessing future changes in water quality and quantity (Bartosova et al., 2019). Major drivers to socioeconomic development are urbanisation, population growth, and economic activity (Riahi et al., 2017). Urbanisation is a main issue when talking about the hydrological cycle. It leads to an increased amount of impervious surfaces, which affect the natural water cycle and may have a negative impact on both surface and groundwater (Li et al., 2018). Removal of vegetation and introduction of impervious surfaces result in decreased infiltration and increased surface run-off, and thus a higher risk for floods. Further, the global water use is increasing, and several studies have concluded that this is largely because of population growth in developing countries and increases in gross domestic product (GDP) (Graham et al., 2018; Alcamo et al., 2007). With uncertainties in projections for future population and GDP, the future water demand and availability of clean water remains uncertain and an important topic.

To assess socioeconomic development and its implications on the future, five different scenarios called Shared Socioeconomic Pathways (SSPs) have been established (Riahi et al., 2017). The SSPs are developed by the climate research community with the aim to describe possible major changes in the society, likely to occur before 2100, which in the future may lead to different challenges for adaptation to, and mitigation of climate change. More specifically, SSPs describe alternative changes regarding economic, demographic, technological, social, and environmental factors (O'Neill et al., 2017). The SSPs are based on different narratives describing alternative pathways, which are Sustainability, Regional Rivalry, Inequality, Fossil-fueled Development, and Middle of the Road Development. Each of the SSPs are assumed to have different impacts on the water sector. Several studies have investigated the effect on demand and availability of water under different SSPs, and further incorporated assumptions within the SSP framework (Graham et al., 2018).

The outcomes of the SSPs describe how social development results in making adaptation to, or mitigation of, climate change harder or easier (O'Neill et al., 2017). Outcomes for each of the established SSP are presented in Figure 2.3. Sustainability (SSP1) describes a future where challenges to adaptation and mitigation of climate change are both low, while Regional Rivalry (SSP3) in contrast, leads to high challenges. Inequality (SSP4) combines high challenges for adaptation and low for mitigation, while Fossil-fueled Development (SSP5) implies the opposite. Lastly, Middle of the Road (SSP2), is a central case which describes a world with intermediate challenges for both adaptation and mitigation.

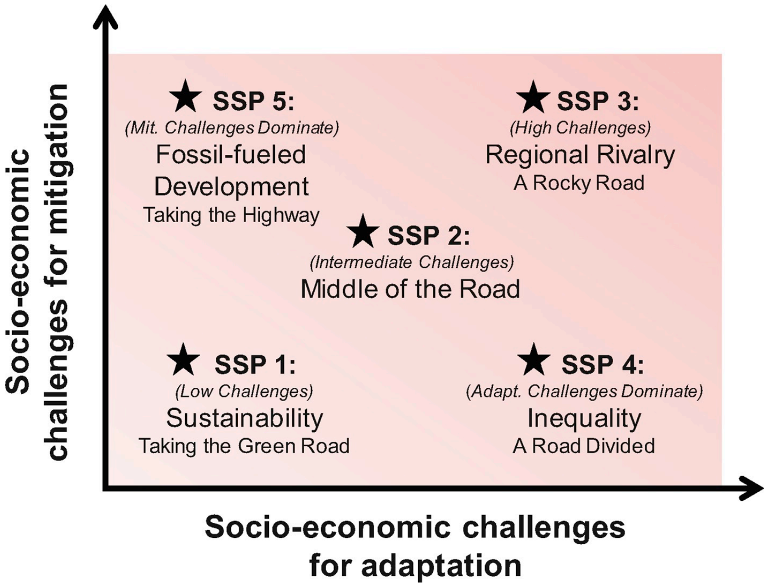

Figure 2.3 The five SSPs representing different combinations of challenges to adaptation and to mitigation of climate change (O'Neill et al., 2017).

SSP1 means that the world shifts gradually but steadily towards a more sustainable path, prioritising achieving sustainability goals, and reducing inequality both across and within countries (O'Neill et al., 2017). The major driver for this shift is the increasing evidence and awareness of the social, cultural, and economic costs that inequality and environmental degradation implies. Middle of the Road (SSP2) describes a future where economic, social and technology trends do not change much from historical patterns (Riahi et al., 2017). The national and international institutions work toward achieving sustainable development goals. However, the awareness of the environmental consequences when using natural resources is moderate, and the cooperation between institutions is relatively weak, leading to a slow progress towards a sustainable future. Regional Rivalry (SSP3) describes a nationalistic future, concerned about security and competitiveness, where countries focus on securing food and energy within their own regions at the expense of a broader global development (O'Neill et al., 2017). Inequality (SSP4) represents a world where the gap widens between the rich and the poor, and power becomes concentrated to a relatively small business and political elite (O'Neill et al., 2017). Environmental policies mainly focus on local issues around areas of middle and high income regions, while little attention is paid to global environmental concerns. Lastly, Fossil-fuelled Development (SSP5) is a world with rapid economic growth and urbanisation, development of human capital and technological innovations (Kriegler et al., 2017). However, the push for economic and social development is coupled with continued exploitation of fossil fuels and there is little effort to avoid global environmental concerns such as climate change.

In this project, SSP1 and SSP5 were combined with RCP4.5 and RCP8.5 respectively, when simulating future scenarios. Table 2.2 below presents a summary of some underlying assumptions for these two pathways.

Table 2.2 Underlying assumptions for SSP1 and SSP5 (O'Neill et al., 2017).

SSP1	The world shifts steadily towards a more sustainable path Emphasis on economic growth will shift to put more value in human well-being and a sustainable future Management of both the local environment and the global concerns improves Educational and health investments lead to a relatively low population Inequalities are reduced both within countries and globally Consumption is focused on low material growth, and low resource and energy intensity Urbanisation will be rapid in many developing regions of the world, but in a sustainable way Air and water pollution is likely to be low and results in enhanced protection of vulnerable ecosystems
SSP5	Faith is placed in innovation, competitive markets and participatory societies to achieve technological progress and development of human capital Rapid economic growth is combined with resource intensive production and consumption patterns Environmental consciousness exists on the local scale, and is focused on end-of-pipe engineering solutions for local environmental problems Lack of global environmental concern is coupled with high energy intensity and a strong reliance on fossil fuels The global population peaks and declines in the 21st century All regions of the world reach high levels of urbanisation

2.4 Previous modelling of PFAS

Modelling fate and transport of PFAS and characterising the hydrogeological properties that influence PFAS is a relatively undeveloped science, compared to for example modelling of contaminants such as petroleum hydrocarbons and chlorinated solvents, which is well-studied (Naidu et al., 2020). The modelling of PFAS is complicated by several factors, including the diversity and lack of data regarding the physicochemical properties, the low concentrations of concern, the potential for transformation, and PFAS affinity for phase interfaces (Naidu et al., 2020). This makes it difficult to establish reliable models that will predict the transport and fate of PFAS and how the composition and concentration will change with distance and contaminant age.

There are several studies that cover the modelling of transport and fate of PFAS in groundwater, including remediation techniques, mainly focused on Granular Activated Carbon (GAC) adsorption (Liu et al., 2019; Xiao et al., 2017). Further, there are studies on the distribution of PFAS in oceans and nearshore environments. Ademollo et al., (2021) used generalised linear models to predict seasonal variations in PFAS concentrations in seawater in Kongsfjorden, Norway, and Li et al., (2017) used the one-dimensional hydrodynamic model MIKE 11 to predict transport of PFOS and PFOA in the Daling River to the Bohai Sea in China. There are also studies that model the distribution of PFAS through several compartments, for example, Su et al., (2018a) used modelling to estimate the spatial distribution of PFOA to air, vegetation, freshwater, coastal water, soil and sediment in the Bohai Rim region of China.

Concerning PFAS in lakes, less is done. This view is shared by Kong et al., (2018), who states that models for specific lake environments are lacking and concludes that there is a knowledge gap when it comes to modelling PFAS in lakes. Kong et al., (2018) used a fugacity-based multimedia model to characterize the fate, transport, and transformation of PFOA and PFOS in a freshwater lake in China. The transformation and transport processes of PFOS and PFOA were defined as atmospheric outflow advection, water inflow/outflow advection, air-water/air-soil/water-sediment interface processes including diffusion, wet and dry deposition, sedimentation, resuspension, fish bioaccumulation, and lastly degradation in each of the compartments. Although Kong et al. (2018) mention several uncertainties and factors that could be improved the model simulates an overall behaviour of PFAS in the lake, and comparison with field data confirms the reliability of the model predictions. In the sensitivity analysis of the model, it was found that the nonlinear Freundlich sorption to organic carbon has a critical role and contributes to a significant part of the uncertainty in modelling predictions of PFOA and PFOS in aquatic systems. The importance of PFAS sorption to organic carbon when modelling fate and transport is also stated by several other studies (Ahrens et al., 2010; Higgins & Luthy, 2006). Further, Kong et al. (2018) concludes that including food-web bioaccumulation is a vital step towards better understanding of the fate of PFAS in lake environments. However, due to lack of relevant parameters regarding accumulation in biota, this was not included in their model. Lastly, the water itself was concluded to not be a sink for PFOS and PFOA, the contaminants were either transported away via outflows or to sediment, and degradation of PFOS was negligible in all compartments, while degradation of PFOA was highest in soil and sediment.

To our best knowledge, there is not much done regarding modelling the impact of climate change and socioeconomic development on PFAS distribution, and no studies are found that cover modelling future changes based on SSPs and RCP. However, some studies have investigated the impact of specific climate change parameters, for example, Mahinroosta et al., (2021) used a numerical model to predict PFOS migration in a contaminated site due to precipitation and evapotranspiration over 100 years. Another relevant study conducted by Su et al., (2018b), investigates potential future effects of changes in climate and emissions on the distribution, and fate of PFAS in different compartments on a regional level in China. Although there are no studies found on using RCP and SSP for modelling of PFAS, the combination of RCP and SSP is frequently used when studying future changes in other water quality parameters. Islam et al., (2018) used the hydrodynamic model MIKE 21 FM coupled with the water quality model ECO Lab to study future changes in microbial water quality by setting up scenarios combining different RCPs and SSPs. Other examples using the combination of RCP and SSP are studies of future nutrient load, eutrophication, suspended solids and heavy metals in water environments (Bartosova et al., 2019; Borris et al., 2016)

2.5 Modelling in MIKE 3 FM

Mike 3 FM is a 3-dimensional hydrodynamic modelling tool developed by the Danish Hydraulic Institute (DHI). It is typically used to simulate hydrodynamic phenomena in lakes, estuaries, coastal areas and seas (DHI, 2017a). Within MIKE 3 FM there are two different built-in models, a "Flow Model" and a "Wave model" which aims to simulate either flows or waves. In this project, the flow model will be used. The model area is divided into a grid, called a mesh, both in vertical and horizontal direction, where calculations are made in each element for each time step. The term "FM" stands for "Flexible Mesh" and means that the resolution of the mesh can be adjusted and vary over the domain depending on which detail level different parts require.

MIKE 3 FM consists of different modules, where one is the hydrodynamic module, which is always included. The hydrodynamic module simulates water levels and flows and provides the basis for the other modules (DHI, 2017b). The module is a numerical modelling system, taking bathymetry, density variations, external forcings such as meteorology and other hydrographic factors into account. It solves the three-dimensional incompressible Reynolds averaged Navier-Stokes's equations, while assuming the hypothesis of Boussinesq for Reynolds stresses and a vertical hydrostatic pressure (Soudi et al., 2019).

Different modules concerning transport mechanisms and water quality can be added to the hydrodynamic model, where the ECO Lab module, Mud Transport and Particle Tracking modules are some examples. In this project, the ECO Lab module will be used. ECO Lab is a generic tool to set up aquatic ecosystems in order to simulate for example eutrophication, heavy metals, ecology and water quality (DHI, 2017c). ECO Lab describes processes and interactions between ecosystems and chemical state variables and shows concentrations and distribution of the variables. This is done based on biological, chemical, physical transport, sedimentation, and resuspension processes. The state variables and associated processes are chosen, defined, and created by the user in a template. State variables can for example be nutrients, organic matter or as in the case of this project, PFOS. The processes describe the rate of change for each state variable and are formulated as a set of differential equations. In ECO Lab, the processes are divided in two categories, *transformation* and *settling*. Transformation is used to describe processes that transform the variable without any exchange with other elements, this could for example be degradation processes. Settling is a process that transports state variables downwards in the water column. Calculations of settling processes are therefore dependent on calculations and information from neighbouring elements. In order to integrate physical transport mechanisms based on advection and dispersion, the ECO Lab module is coupled to the Advection-Dispersion module of the DHI hydrodynamic flow modules.

3 Methodology

This section starts with a description of the study area and a presentation of research made regarding PFOS in the area. Further, the modelling set up and simulated scenarios and motives for these are described. As mentioned earlier, the only PFAS that was included in the modelling in this study is PFOS. The focus is also on PFOS in the following section regarding sources to PFAS in the study area. Motivations to study PFOS are that it is one of the most studied PFAS, which speaks for more available data, and that it occurs frequently in the environment (Prevedouros et al., 2006). In some measurements made in the area, several PFAS are combined in one measurement, and in all of these, PFOS is included, which made it possible to compare different measurements with each other and compare the modelled values with measured. Additionally, in some other kinds of measurements, e.g. PFAS in fish and PFAS in sediment, PFOS is the only PFAS that have been detected. PFOS is included in the group of four PFAS that EFSA has used to set their guideline values and is also classified as a POP in the Stockholm convention, which declares that it is relevant to study (Kemikalieinspektionen, 2021a). The fact that PFOS is prohibited in the EU also implies opportunities to analyse and discuss the effect of restrictions and regulations (Livsmedelsverket, 2021b).

3.1 Study area

Lake Ekoln is one of the subbasins to Mälaren, located in the most northern part of the lake, south of Uppsala city. South of Ekoln, in the subbasin Görväln, Norrvatten has a drinking water treatment plant. Norrvatten is the fourth largest drinking water producer in Sweden and water from Ekoln accounts for a major part of the water they are receiving (Norrvatten, n.d.; Ekvall et al., 2016). The fact that Mälaren is the largest drinking water source in Sweden and provides around two million people with drinking water makes Lake Ekoln an important water source to maintain in good condition (Edlund et al., 2018).

Lake Ekoln has an area of 22 km^2 and a maximum depth of 42 m (Sahlberg & Gustavsson, n.d.). Four rivers flow into the lake: Fyrisån, Örsundaån, Sävaån, and Hågaån, these account for 95% of the total inflow to the lake. The remaining 5% comes from diffuse sources where the esker Uppsalaåsen, located in the eastern part of the lake, counts for a part of that. Fyrisån and Örsundaån are the major rivers and account for as much as 11% of the total flow into Mälaren (Persson et al., 2012). Table 3.1 presents the average inflow to Ekoln from each river and the assumed inflow from Uppsalaåsen, together with the share for each inflow.

Table 3.1 Average water inflow during the period 2017-2018 for the inflows to Lake Ekoln and calculated share of the total flow.

Inflow	**Flow [m^3/s]**	**Share [%]**
Fyrisån[1]	11.05	65.7
Örsundaån[1]	3.89	23.1
Sävaån[1]	1.19	7.1
Hågaån[1]	0.65	3.9
Uppsalaåsen[2]	0.05	0.3

[1] (SMHI, n.d.-b)
[2] (P. McCleaf, personal communication, 1 March, 2021)

The location of the outflow is in Erikssund, in the southern part, where the water flows to the rest of Mälaren. The retention time of the water in the lake is assumed to be around 1.2 years (Ekman, 2021). In Figure 3.1 the locations of the inflows and outflow are presented. The figure also presents the location of the WWTP Kungsängsverket and the sampling station Vreta Udd. Kungsängsverket discharges into Fyrisån and is considered to be a source of PFAS in Ekoln and Vreta Udd is the location where measurements of PFAS have been made in the lake.

Figure 3.1 Locations of inflows and the outflow of Lake Ekoln, and location of WWTP Kungsängsverket and sampling station Vreta Udd.

The dominating land uses in the catchment area of Ekoln is forestry and agriculture, but several urban areas are also connected to the lake where Uppsala city is the major one (Persson et al., 2012). The urban activities around the lake affect the quality of it, and according to VISS (n.d.-a) the chemical status is critical since several environmental toxins have been detected, where mercury (Hg), polybrominated diphenyl ethers (PBDEs), and PFASs are some of them.

Ekoln is a dimictic lake, which means that the water is mixing twice in a year (Lindqvist, 2019). The mixing happens when the temperature of the water is the same in the whole vertical profile, which is during autumn and spring in Ekoln. The fact that the water is mixed during some parts of the year and stratified other parts, means that the water is of different quality during the seasons. The mixing is vital to oxygenate the water in the bottom part of the lake.

3.2 PFAS in Lake Ekoln and the surrounding area

In previous studies, sampling of PFAS was conducted at Vreta Udd - the sampling station in the middle of Ekoln, in the larger inflows Fyrisån and Örsundaån, in groundwater wells in Uppsalaåsen and at the outflow from Kungsängsverket. In addition, different studies have included sampling of soil, sediment, and surface and groundwater in connection to possible sources of PFAS in the study area. Several measurements indicate that there are high concentrations of PFAS within the area and that the situation needs to be put attention to.

Further, PFOS have been detected in perch in the subbasin Görväln, south of Ekoln (Stockholms Stad, n.d.). In the latest sampling, which was made in 2016, the concentration of PFOS in the perch was 9.4 µg/kg. Biota in lakes and coastal water should not have a concentration higher than 9.1 µg /kg, to be a water course classified with good chemical status (European Parliament and Council directives 2013/39/EU). Since Lake Ekoln does not meet the values for good chemical status, partly due to PFOS, it is assumed that the fish in Ekoln are prone to be carriers of PFOS as well.

In 2013, a study was done of 44 different rivers in Sweden and out of these, Fyrisån was found to be the fourth most contaminated regarding PFAS, with a concentration of approximately 30 ng/l (∑PFAS 13) (Ahrens et al., 2014). Another example when high concentrations of PFAS were detected in the area was in 2012, when sampling was made in groundwater wells in Uppsala´s drinking water source, Uppsalaåsen (Uppsala Vatten och Avfall, n.d.-d). The substances of most concern were PFHxS and PFOS (Gyllenhammar et al., 2015). The drinking water producer then took acute measures to limit the human exposure via drinking water and took the affected wells out of operation. New treatment technology with activated carbon was installed in the drinking water plant to remove PFAS, and in April 2015, the wells were put back into operation (Uppsala Vatten och Avfall, n.d.-d).

Table 3.2 presents a summary of sampling of interest within the area, and Figure 3.2 below presents the locations of the sampling together with the formation of Uppsalaåsen. The measurements of groundwater are taken at different wells within the sampling location, explaining the large range between min and max values, since the different wells can be affected to varying degrees. The same holds for the soil samples, while for surface water, wastewater/leachate and sediment the samples at each location are taken at the same point. In Fyrisån, samples are also taken at different locations along the river, these are not presented in Table 3.2, but investigated in the chapter *Mass flow of PFOS.*

Table 3.2 Summary of measured PFOS of interest within the area of Lake Ekoln.

Location	**Time**	**No. of samples**	**PFOS Min/Average /Max**	**Reference**
Surface water [ng/l]				
Fyrisån outlet	2014 - 2020	10	<0.48/6.5/17	(Malnes, et al., 2021; Fyrisåns Vattenvårdsförbund, 2020; Gago-Ferrero et al., 2017)
Örsundaån outlet	2019 - 2020	2	<0.3	(Malnes, et al., 2021)
Sävjaån Outlet	2020	4	7.4/15.5/22	(Fyrisåns Vattenvårdsförbund, 2020)
Vreta Udd	2017 - 2018 2019 - 2020	8[1] 3[2]	1.2/1.9/4.5 0.81/2.2/4.4	(SLU, 2020) (Malnes, et al., 2021)
Viktoria pond	2014	1	1292	(Bergström, 2014)
Groundwater [ng/l]				
Uppsala-Ärna	2013-2014	4	5/10004/ 28000	(Johansson & Helldén, 2015)
Viktoria	2014	12	<1.13/1451/ 15000	(Bergström, 2014; Bjerking AB, 2014)
Hovgården	2017	10	52[4]	(Bonnet, 2017)
Jumkilsåsen	2013-2014	17	34/1414/ 11000	(Bergström, 2014; Johansson & Helldén, 2015)
Uppsalaåsen[5]	2012-2014	103	47[4]	(Gyllenhammar, 2015)
Leachate/wastewater [ng/l]				
Kungsängsverket	2017-2018	Monthly	<10/21.6/55	(Uppsala Vatten och Avfall AB, n.d-a)
Ärna pumping station	2013	1	19000	(Johansson & Helldén, 2015)
Hovgården	2017	14	95[4]	(Bonnet, 2017)
Sediment [µg/kg dry sediment]				
Vreta Udd	2017	1	2.09[3]	Tjensvoll (2018)
Soil [µg/kg dry sediment]				

Uppsala-Ärna	2014	7	<10/31/94	(Johansson & Helldén, 2015)
Viktoria	2014	4	1.6/172/486	(Bergström, 2014)

[1] Samples taken at eight different times, but each time at three different depths (0.5 m, 15 m and 30 m).

[2] Samples taken at three different times, but each time at two different depths (0.5 m and 30 m).

[3] Concentration in sediment at depth 0-2 cm. Appendix A presents the vertical distribution of PFOS in sediment, with measurements at different depths.

[4] Value for each sample not available, the number presents the average.

[5] Samples taken in drinking water production wells, Stadsträdgården and Kronåsen.

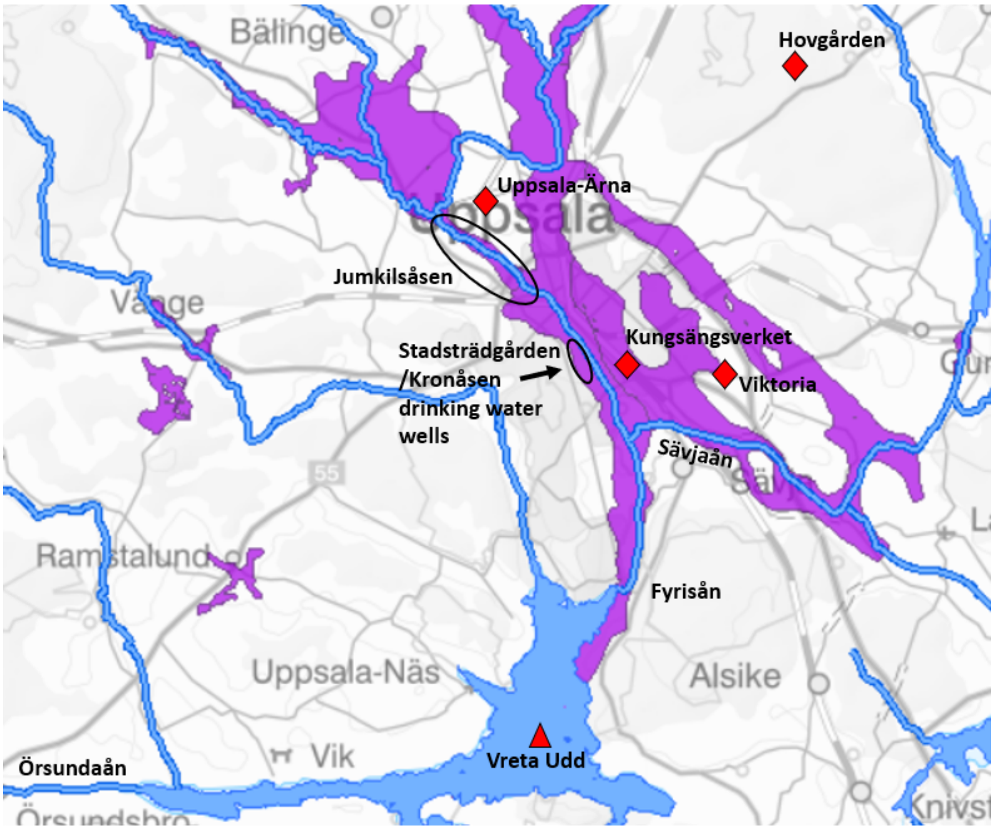

Figure 3.2 Locations where PFOS has been sampled. The red squares represent locations that can be considered as point sources to PFOS, and the red triangle present the location of the sampling station Vreta Udd. The formation of Uppsalaåsen is presented in purple (VISS, n.d.-b).

In order to assess future spread of PFOS into lake Ekoln, potential sources and pathways for PFOS in the area were investigated. Since Fyrisån and Uppsalaåsen are the only inflows where PFOS has been measured and detected, the focus was mainly to identify the sources of this contamination. Fyrisån is also the major inflow to the lake (Table 3.1), meaning that high concentrations of PFOS there will have a significant impact on the level of PFOS in Lake Ekoln. However, other possible sources and pathways for PFAS entering Lake Ekoln were also briefly investigated.

3.2.1 Point sources

Four different point sources where PFOS have been sampled in high concentrations were identified. These were Uppsala-Ärna airport, Viktoria firefighting site, the landfill

Hovgården and the WWTP Kungsängsverket (Table 3.2; Figure 3.2). All of these are considered as sources to PFAS in Fyrisån, and all except Kungsängsverket also contribute to PFAS in groundwater in Uppsalaåsen.

Uppsala-Ärna airport is probably one of the main sources of PFAS in Uppsalaåsen (Bergström, 2014). At the airport, firefighting training with firefighting foam containing PFAS took place between 1985 and 2005, after 2005 the foam was replaced with PFAS free foam. Sampling of groundwater at the site has presented concentrations of PFOS as high as 28 000 ng/l (Johansson & Helldén, 2015). Several studies indicate that there is a link where PFAS from the airport spreads via Jumkilsåsen to the groundwater reservoir in the central parts of Uppsalaåsen (Bergström, 2014; Johansson & Helldén, 2015). This is supported by the high measured concentrations in Jumkilsåsen (Table 3.2). In addition to the groundwater contamination from the airport, Fyrisån receives stormwater runoff from the site. Sampling of surface water in Fyrisån indicates that there is a supply of PFAS to the river along the section where it passes the airport (Johansson & Helldén, 2015). Lastly, wastewater is transported from Ärna to Kungsängsverket, and a concentration of 19 000 ng PFOS/l has been detected at a pumping station at Ärna (Table 3.2; Johansson & Helldén, 2015). The water at the pumping station originates for instance from a rock chamber where firefighting foam containing PFOS historically has been used and wells within the area where there is a risk that firefighting foam has been discharged on some occasions (Johansson & Helldén, 2015). Since PFOS has surfactant properties, it is possible that the substance has been adsorbed to the walls of the wastewater pipes and will be released from the pipes during a long period ahead.

At Viktoria firefighting site, training with firefighting foam took place roughly two times a year between 1990 and 2002. However, after 1996, the type of foam was changed but there are conflicting opinions whether the new foam was PFAS free or just contained less PFAS (Johansson & Helldén, 2015). Sampling presents high concentrations of PFAS in groundwater at the site, where PFOS was one of the most common substances with a highest measured concentration of 15 000 ng/l (Johansson & Helldén, 2015). The groundwater flow direction from the site is assumed to be southwest, which is supported by the fact that high levels of PFAS are detected in groundwater wells southwest of the Viktoria site (Johansson & Helldén, 2015). This means that it is possible that PFAS could spread to the southern parts of Uppsalaåsen, and thus there is a risk that PFAS from Viktoria reach Ekoln. In addition to the groundwater contamination, there is a sedimentation pond at the Viktoria site, where extinguish water from the firefighting training was collected. The water in the pond discharges into Sävjaån which downstream connects to Fyrisån. Bergström (2014) conducted sampling of water in the pond, and the concentration of PFOS was 1292 ng/l (Table 3.2).

In the WWTP Kungsängsverket, the level of PFAS is measured in the effluent regularly every month. The average concentration of PFOS is 21.6 ng/l based on monthly measured data from 2017 and 2018 (Uppsala Vatten och Avfall AB, n.d.-a). The average outflow during the same time period is 0.6 m^3/s. A major part of the wastewater reaching Kungsängsverket originates from households, and another significant part is industrial wastewater. As mentioned, some PFOS at Kungsängsverket also comes from Ärna. However, the average flow from the pumping station at Ärna, where high concentrations of PFOS have been measured is only 0.4 l/s (Johansson & Helldén, 2015), which is less than a thousandth of the average discharge from Kungsängsverket (600 l/s). This indicates that only a small part of the PFOS reaching Kungsängsverket originates from Ärna and the major part is most probably from industrial and domestic wastewater.

Hovgården landfill is located approximately 12 km north east of Uppsala city. Sampling was made at the site in 2017 and presented high concentrations of PFAS both in landfill leachate and in groundwater (Bonnet, 2017). There is a treatment facility for sludge and leachate water at the site, the effluent enters a small stream that further downstream discharges into Sävjaån and then Fyrisån. Bonnet (2017) performed sampling in those streams as well and conducted mass flow estimations in order to evaluate the impact from Hovgården on the surrounding environment. These estimations showed that there must be other larger sources contributing to PFAS in Fyrisån and Sävjaån, and that the effect from Hovgården is small. Regarding groundwater contamination at Hovgården there are no investigations made on further spread in the environment. However, since PFAS are extremely persistent and can be transported long distances, there is a risk of further spread in the groundwater system.

3.2.2 Diffuse and other potential sources

Atmospheric deposition could, as mentioned in the literature review, be a diffuse source of PFAS. Measured concentrations in precipitation are available at a station in Uppsala, with an average concentration of PFOS of 0.15 ng/l during 2017 (Fredricsson et al., 2017). PFOS can via precipitation enter Ekoln directly at the surface or indirectly via groundwater, stormwater runoff or surface waters.

Other possible sources are on-site wastewater treatment systems (OWTS). In Uppsala Municipality, there are roughly 7000 OWTS, and there are previous studies that have concluded OWTS to be a diffuse source of PFAS (Svensk Avloppsrening, n.d.; Gros et al., 2017). Gros et al., (2017) performed sampling of wastewater from 12 OWTS in the vicinity of Stockholm and Umeå and analysed 26 different kinds of PFAS. The results were compared with measurements in effluent of different European and U.S. WWTP and found to be in the same order of magnitude. However, since the treatment techniques and surrounding hydrogeological properties among the OWTS vary, the potential to spread PFAS in the environment is difficult to evaluate.

Industrial activities can also be a source of PFAS. There are two larger industrial areas around Uppsala city; Fyrislund and Librobäck. These areas have not been investigated in depth, and to what extent PFAS is used in the different industrial activities is not known. Johansson & Helldén (2015) investigated some industries within the area that have either used or are suspected of having used PFAS; Bärby fire station, S:t Eriks Betong, Sveflour AB, Gamla brandstationen, Uppsala former cement foundry, the Academic Hospital's helicopter plate, Kap former fire training site, GE Health Care and Habia teknofluor AB. However, according to Johansson & Helldén (2015), the investigation of these possible sources is lacking in information, and for most of the objects, no soil or groundwater sampling of PFAS has been carried out at all.

In addition to Hovgården there are more than 100 closed landfills in Uppsala Municipality (Uppsala kommun, 2014). The knowledge about these landfills is currently low but depending on the content in the landfills and the hydrogeological properties, it can be a risk that they contribute to spreading of PFAS in the environment.

Lastly, Naturvårdsverket (2021b) has collected and compiled a risk assessment of specific sites, on national level in Sweden, where firefighting foam containing PFAS has been used between 1998 and 2015. This includes firefighting training sites as well as specific sites where PFAS has been handled, and firefighting in case of accidental fires. In addition to these already mentioned sources, Naturvårdsverket (2021b) has listed three accidental fires which could have caused possible risk for spread of PFAS to Fyrisån, either via groundwater or surface water. However, the impact on the recipient is classified as small for all three of them.

3.2.3 Mass flow of PFOS

In order to assess the impact from each source, mass flow estimations of PFOS were conducted. The mass flows were calculated at five different locations: Fyrisån, Sävjaån, the outflow from Kungsängsverket, at the interface between Uppsalaåsen and Lake Ekoln, and also the mass flow from precipitation. Since no measurements of PFOS were available in Örsundaån, Hågaån and Sävaån, these could not be included in the calculations. To our best knowledge, there are no large sources contributing to PFOS in those rivers, however, they can be affected by smaller and diffuse sources, such as those described in the previous chapter *Diffuse and other potential sources.*

The calculations in Fyrisån and Sävjaån were based on sampling of PFOS made by Fyrisåns Vattenvårdsförbund (2020) on four occasions between the 15th of June 2020 and the 14th of September 2020. The locations at each sampling occasion were; upstream and downstream Ärna, upstream and downstream Kungsängsverket, the outlet of Fyrisån and in Sävjaån just before the outlet to Fyrisån. The measured concentration at each location was multiplied by the water flow the same day. The flow was daily modelled data from SMHI (SMHI, n.d.-b). Since SMHI only has modelled flow data in specific points, the points considered most representative for the sampling location were selected. Lastly, the average mass flow of the four sampling occasions of PFOS at each location was calculated.

In Kungsängsverket, the measured PFOS is done in monthly collection samples, which means that the value can be seen as an average for the whole month, not as a concentration for a specific day. The mass flow from Kungsängsverket was based on the average concentration in the outflow between January 2019 and August 2020, and the average water flow during the same period. In Uppsalaåsen, the calculations were based on a flow of 0.05 m^3/s, and the average concentration of PFOS in groundwater, 5 ng/l, where there is contact with surface water in Lake Ekoln (P. McCleaf, personal communication, 29 March, 2021). For precipitation, the average precipitation per day in mm, in 2017-2018, was multiplied by the surface area of Lake Ekoln, in order to get the average volume of precipitation reaching the lake each day. This was then multiplied by the average concentration of PFOS in precipitation (0.15 ng/l). The result of these mass flow estimations is presented in Figure 3.3 below. The figure also presents the location of the point sources and the formation of Uppsalaåsen.

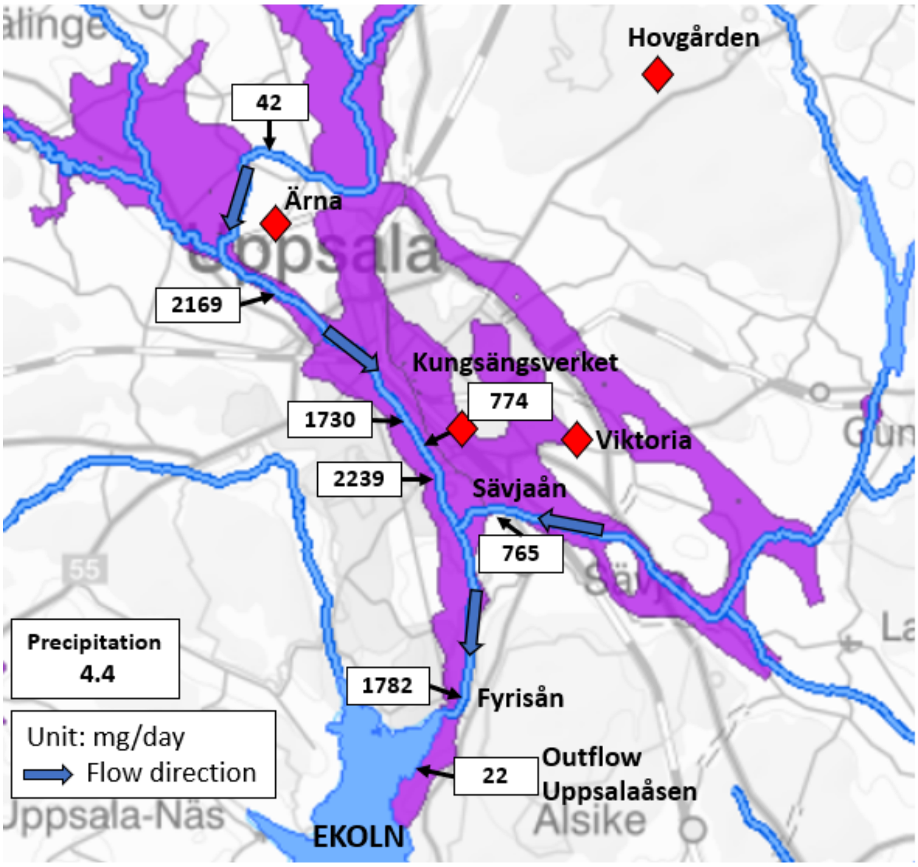

Figure 3.3 *Mass flow of PFOS in Fyrisån and Sävjaån, the outflow from Kungsängsverket, precipitation and the outflow from Uppsalaåsen, together with location of Kungsängsverket, Uppsala-Ärna airport, Viktoria firefighting site and Hovgården landfill. The esker Uppsalaåsen is presented in purple (VISS, n.d.-b).*

According to the mass flow estimations, Fyrisån is the major contributor to PFOS in Lake Ekoln, among the investigated inflows. The contribution from Uppsalaåsen and precipitation is almost negligible in comparison.

The mass flow calculations show that there is a great supply of PFOS along the section where Fyrisån passes Ärna (Figure 3.3), where the mass flow increases a lot. This is in line with what Johansson & Helldén (2015) stated. At the section after Ärna and before Kungsängsverket, there is a decrease in mass flow. Between the points before and after Kungsängsverket there is an increase again with approximately 500 mg/day. This is a bit lower than the calculated mass flow of PFOS in the outflow from Kungsängsverket (774 mg/day). However, the mass flow in Kungsängsverket is calculated based on average concentration and water flow during a longer period. which probably affects the result. Between the points after Kungsängsverket and the outlet of Fyrisån, there is a decrease in mass flow, despite the fact that also Sävjaån discharges into Fyrisån at this section. The sum of the mass flow after Kungsängsverket and Sävjaån is 3004 mg/day compared to 1782 mg/day at the outlet of Fyrisån. The fact that the mass flow of PFOS decreases along some sections indicates that there may be processes affecting PFOS in the river. The measured concentrations of PFOS are only in the dissolved phase, and as explained in the literature review, some PFAS tend to adsorb to particles, and thus the mass flow in the dissolved phase will decrease.

Overall, it is important to be aware of the uncertainties in these estimations. The points in Fyrisån and Sävjaån represent sampling of PFOS only on four occasions during summer 2020, while for Kungsängsverket, Uppsalaåsen, and precipitation, the mass flow was calculated based on average values during a longer period, meaning that those may not be representative for the same period as the measurements in Fyrisån and Sävjaån. Other factors that may influence the mass flow are uncertainties in the analysis results of PFOS and in the modelled flow data from SMHI. Also, since the water is in constant movement in the rivers, the concentration when taking a sample can differ even if it is during the same day.

3.3 Modelling

The software package MIKE 3 FM, coupled with the ECO Lab Module, was used for the modelling, and an already existing model developed by Tyréns AB was used and interpreted to fit the project. Different scenarios were further set up and simulated to represent the current and future situation.

3.3.1 Previous modelling of lake Ekoln

The model used in this project was a MIKE 3 Flow Model FM developed by Tyréns AB (2018). Tyrén's primary intention with the model was to simulate how the flow from Fyrisån, containing water from Kungsängsverket, spreads in Lake Ekoln in order to investigate an appropriate location for a raw water intake. The model has then been used and elaborated by others in different studies.

The aim of one of these studies was to simulate and analyse the water mixing pattern for future scenarios based on climate change (Lindqvist, 2019). Lindqvist calibrated and adapted the model to simulate temperature profiles for the lake and also to simulate a whole year, instead of only three months which Tyréns used it for, to cover seasonal changes. Parameters in the hydrodynamic module were calibrated for 2018.

In a study by Ekman (2021), an ECO Lab module was added in the model with the aim to simulate water quality in terms of concentration of Natural Organic Matter (NOM) and PFAS. The simulation time was increased to 1.2 years in order to cover the retention time for the lake. Ekman (2021) only included Kungsängsverket and precipitation as sources to PFAS due to limited data from other sources and time constraints. The results from the study presented that the total simulated concentration of PFAS accounted for approximately 40% of the total observed concentration of PFAS in the lake, and that the contribution from precipitation was negligible. The conclusion of the study was that there must exist other major sources to PFAS in the area, and that Fyrisån is considered an important source to include in future studies. Ekman did not include processes within the lake that can impact the fate and transport of PFAS, which she thinks would be interesting to look more into. The study also discusses the lack of measurements of PFAS in the area, and that these are required to be able to perform appropriate analysis in the future.

Both Lindqvist (2019) and Ekman (2021) have with their studies laid the foundation for this study in the way they have developed the model. Results from the study by Ekman gave a good understanding of what is relevant to focus on when it comes to the sources, spread, and distribution of PFAS in Lake Ekoln.

3.3.2 Setting up the model

The model was firstly set up for a base scenario in order to simulate the current situation regarding spread of PFOS in Lake Ekoln. After that, input parameters affected by climate change and socioeconomic development were adjusted in the model, to simulate the future scenarios. The future scenarios are described more in detail in section 3.4.

The first step in the set-up of the model was to specify the domain. The model area was discretized using a flexible mesh, meaning that the grid size varies over the domain. The mesh used was developed by Lindqvist (2019) in order to shorten the computational time, compared to the original mesh developed by Tyréns AB. Lindqvist (2019) created a coarser horizontal resolution of the mesh, while keeping the more detailed vertical resolution. Since this project aims to simulate more than one year, and Tyréns AB only simulated 3 months, Lindqvist's (2019) coarser mesh with shorter computational time was considered more appropriate. The mesh and bathymetry are presented in Figure 3.4. In vertical direction, the mesh is divided into 41 layers, one meter each. The number of nodes in the mesh is 1758 and the number of elements is 2570.

The set-up of the model is then divided in two parts, the hydrodynamic module and the ECO Lab module. As mentioned, Lindqvist (2019) already calibrated the parameters for the hydrodynamic module for 2018, therefore, the same settings were used when setting up the hydrodynamic module in this project. The ECO Lab module was then added to simulate the spread of PFOS.

One factor that was changed compared to Lindqvist was the simulated time period. The time period chosen for the base scenario in this project was 2017-02-20 to 2018-05-04. The motivation to simulate this period was that it is the period with the most available measurements of PFOS in Lake Ekoln, which could be used to compare the simulated results with, and it covers the water retention time of 1.2 years. Measurements during this time exist at three different depths (0.5, 15, and 30 meter), at 8 different times. This time period is similar to what Ekman (2021) simulated (2017-02-20 to 2018-09-15), and one thing she mentions regarding the time period is that 2018 was a year with higher water levels and discharges than an average year, which is important to consider.

3.3.2.1 Hydrodynamic module

The hydrodynamic module is driven by input data for inflows, meteorological data, water level at the outflow, and initial conditions for Ekoln regarding water elevation and temperature. The inflows considered in the model are those mentioned previously; Fyrisån, Örsundaån, Hågaån, Sävaån and the esker Uppsalaåsen, and the outflow is located in Erikssund. In addition, Kungsängsverket is added separately as an inflow since it is considered as a point source of PFOS. Figure 3.4 presents the modelled area, inflows and outflow, mesh and bathymetry.

The equations in the model were set to the numerical solution of shallow water equations, Coriolis forcing was set as varying in domain, and horizontal and vertical eddy viscosities were modelled using the Smagorinsky and k-epsilon formulations, respectively. The water temperature was simulated based on heat exchange between the atmosphere and the lake, and the density of the water was simulated as a function of temperature to describe the seasonal stratification of the lake. As mentioned, Lindqvist (2019) calibrated the model to simulate mixing patterns in the lake, when doing this, the parameters for heat exchange were adjusted. The adjusted parameters were coefficients for heating, cooling, and light extinction, resulting in values of 0.0011, 0.002 and 1 m^{-1}, respectively. The coefficients for heating and cooling are included in the sensible heat flow, and light extinction describes how the sunlight decreases with depth in the lake.

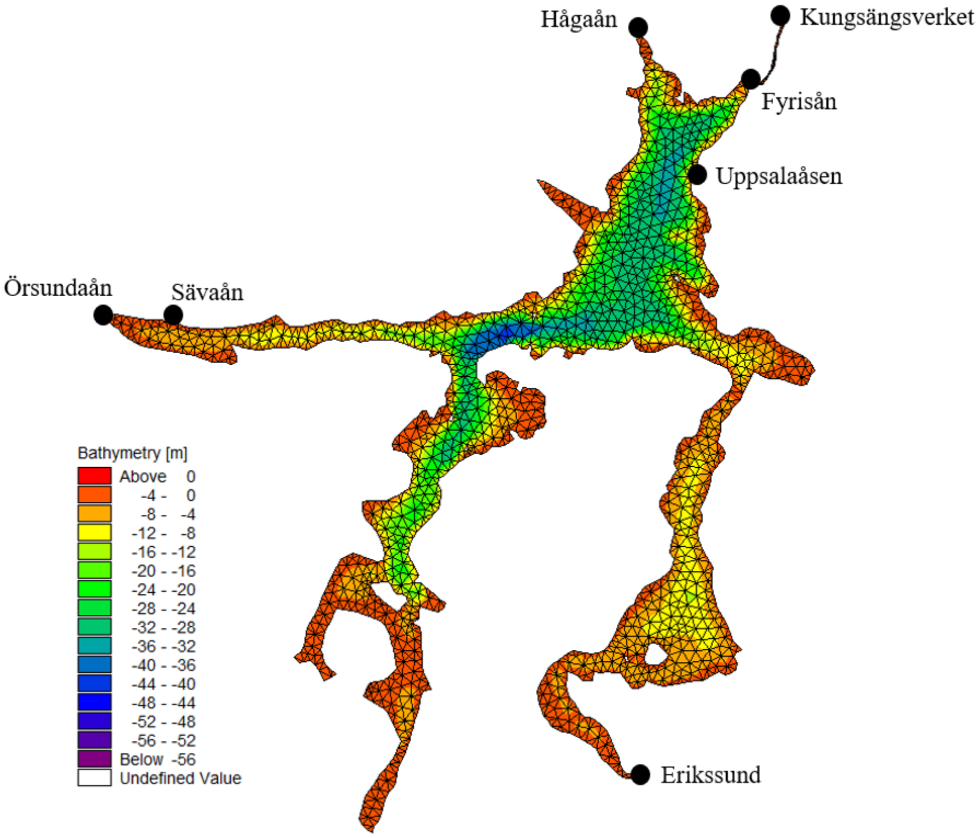

Figure 3.4 Map of the modelled area, mesh, bathymetry, inflows and outflow.

Data for discharge and water temperature for the rivers and Kungsängsverket was included in the model as time series. There was no available measured discharge and temperature data from the rivers, instead modelled values from SMHI were used for all rivers (SMHI, n.d. -b). For Kungsängsverket, measured data was available and retrieved from Uppsala Vatten och Avfall AB via Ekman (2021). The discharge from Uppsalaåsen was set to a constant value of 0.05 m^3/s and temperature to a constant value of 8 °C, based on personal contact with Uppsala Vatten och Avfall AB (P. McCleaf, personal communication, 1 March, 2021). At the outflow, the boundary condition was set to water level varying in time, and the values used were the water level of Mälaren, retrieved from SMHI (n.d. -b).

The meteorological data included wind speed, wind direction, air temperature, relative humidity, clearness coefficient and precipitation. Precipitation represents only the precipitation entering the lake directly and does not include run-off from the surrounding area. The meteorological data was downloaded observations from SMHI, and all data except for the clearness was gathered from the station Uppsala Aut, in the centre of Uppsala. Clearness was observed at Uppsala airport. All meteorological data was set to varying in time and constant in domain, and included in the model as time series. In addition, ice coverage was included as input data, with a specified ice thickness of a constant value of 0.1 m for those days the lake was covered with ice. No data was available for the number of days with ice coverage for Lake Ekoln, instead ice coverage data from Skarven was used. Skarven is another subbasin of Mälaren, located approximately 13 kilometers south-east of Ekoln and was covered with ice between 2017-01-04 and 2017-03-27, and between 2018-01-10 and 2018-04-18 (SMHI, n.d. - c).

The initial conditions of the lake included water level and temperature. The initial water level was set as the value retrieved when subtracting the average water level of Mälaren between 2017-2020 from the water level of Mälaren on the starting date of the simulation, 2017-02-20. The initial temperature in Ekoln was based on measurements at 26 different depths at Vreta Udd at the simulation starting date, and the vertical variation was assumed to represent the whole lake, i.e. no horizontal variation. All data used as input in the hydrodynamic module is summarized in Table 3.3 below.

Table 3.3 Input data for the hydrodynamic module.

	Parameter	**Resolution**	**Location**	**Source**
Meteorology	Wind speed	1 h	Uppsala Aut	SMHI[1]
	Wind direction	1 h	Uppsala Aut	SMHI[1]
	Relative humidity	1 h	Uppsala Aut	SMHI[1]
	Air temperature	1 h	Uppsala Aut	SMHI[1]
	Clearness	1 h	Uppsala airport	SMHI[1]
	Precipitation	24 h	Uppsala Aut	SMHI[1]
Discharge	Fyrisån	24 h	Outlet	SMHI[2]
	Örsundaån	24 h	Outlet	SMHI[2]
	Hågaån	24 h	Outlet	SMHI[2]
	Sävaån	24 h	Outlet	SMHI[2]
	Uppsalaåsen	Constant	Interface Ekoln-Uppsalaåsen	McCleaf[3]
	Kungsängsverket	24 h	Outlet	UVA[4]
Water temperature	Ekoln	6 times/year	Vreta Udd	SLU[5]
	Fyrisån	24 h	Outlet	SMHI[2]
	Örsundaån	24 h	Outlet	SMHI[2]
	Hågaån	24 h	Outlet	SMHI[2]
	Sävaån	24 h	Outlet	SMHI[2]
	Kungsängsverket	24 h	Outlet	UVA[6]
Other	Ice coverage	24 h	Mälaren Skarven	SMHI[7]
	Water level Erikssund	24 h	Mälaren	SMHI[2]

[1](SMHI, n.d.-a)
[2](SMHI, n.d.-b)
[3](Philip McCleaf, personal communication, 1 March, 2021)
[4](Uppsala Vatten och Avfall AB, n.d.-b)
[5](SLU, n.d.)
[6](Uppsala Vatten och Avfall AB, n.d.-c)
[7](SMHI, n.d.-c)

3.3.2.2 Water quality module - ECO Lab

In the ECO Lab module, the input data regarding PFOS was added. This information was added into the calculated flows from the hydrodynamic module in order to simulate how PFOS spreads. All available measurements of PFOS in Lake Ekoln and the inflows were limited to the dissolved phase, and thus it was only the dissolved PFOS that was included in the modelling. As mentioned in the literature review, two processes that are considered to affect the fate of PFAS are sedimentation of particulate PFAS and bioaccumulation of PFAS in fish. Initially, the possibilities to include these processes in the model were investigated, however, the lack of previous studies and information regarding it, and time constraint, made it difficult to construct reliable processes in the model. However, PFOS has been detected in perch in the subbasin Görväln and PFOS is proven to be one of the PFAS with highest affinity for particles, thus, both bioaccumulation and sedimentation could be important processes to include in the modelling. The possible effects of exclusion of the processes is further analysed in the *Discussion*.

The added sources of PFOS into the model were Kungsängsverket, Fyrisån, Uppsalaåsen, and precipitation. In Örsundaån, PFAS was also measured at two times, however the concentration of PFOS was below the detection limit, therefore Örsundaån was not included as a source of PFOS in the model (Malnes et al., 2021). In Hågaån and Sävaån, there were no measurements available, and thus these rivers were not included as sources of PFOS. The flow from Hågaån and Sävaån are also significantly lower than from Örsundaån and Fyrisån, and no literature indicating that these rivers should be large contributors of PFOS to Ekoln was found. In the outflow, Erikssund, no data for PFOS exist, therefore the concentration was set to zero gradient, i.e. the same concentration as the lake.

The data for Kungsängsverket and Fyrisån was included in the model as daily time series, while for Uppsalaåsen and precipitation, the concentration of PFOS was set to a constant value. Important to be aware of is that measurements in the outlet of Fyrisån also include PFOS originating from Kungsängsverket. For the outlet of Fyrisån the measured data was sporadic, and no measured data was available during the simulated period (2017-02-20 to 2018-05-04), but values from other time periods were used to approximate the concentration. In Kungsängsverket, measurements of PFOS are made monthly, which means that the data is of significantly better quality than the data from Fyrisån, therefore Kungsängsverket was added as a separate source. The measurements in Kungsängsverket are made as monthly collection samples, which means that the values can be seen as an average for the whole month, and the concentrations in the model were therefore added as the same for every day in each month. The concentration from Uppsalaåsen was set to 5 ng/l, based on the average concentration of PFOS where there is contact between Ekoln and groundwater in Uppsalaåsen, according to Uppsala Vatten och Avfall AB (P. McCleaf, personal communication, 29 March, 2021). In precipitation, the concentration of PFOS was set to 0.15 ng/l, based on an average of measured values in 2017 at an observation station just outside Uppsala (Fredricsson et al., 2017).

In order to assess the concentration in Fyrisån, the PFOS originating from Kungsängsverket needed to be subtracted. This was done by calculating the mass flow of PFOS from both Kungsängsverket and Fyrisån, and then subtracting the mass flow from Kungsängsverket from Fyrisån. In Fyrisån, four measurements of PFOS were available in 2014-2015, one in 2019, and five during 2020. Four of the measurements were made during the summer months, four during autumn, and two during spring. The measurements were multiplied by the water flow in Fyrisån the same day in order to get the mass flow of PFOS. Since the measurements were few and not during the simulated period, the data was considered insufficient to assume different mass flow of PFOS depending on water flow or season. Therefore the average mass flow from Fyrisån was calculated and then subtracted by the average mass flow from Kungsängsverket. The average mass flow from Fyrisån was 29.61 µg/s, and from Kungsängsverket 10.754 µg/s, leading to an average mass flow from Fyrisån without the contribution from Kungsängsverket of 18.856 µg/s. The obtained value was then divided by the water flow each day during the simulated period, in order to create a time series for the concentration of PFOS in Fyrisån. This means that the mass flow from Fyrisån was constant, but the concentration, which is added in the model, varied depending on the flow.

The initial conditions for PFOS in Lake Ekoln, were based on measurements at three depths (0.5, 15 and 30 meter) for the starting date of the simulation, 2017-02-20. The measured values were linearly interpolated and assumed to represent the vertical variation in the whole lake, i.e. no horizontal variations. Table 3.4 presents the data used for modelling of PFOS.

Table 3.4 Data used for modelling PFOS for the period February 2017 to May 2018.

Location	**Resolution**	**Depth [m]**	**Source**
Ekoln Vreta Udd	8 times	0.5, 15, 30	(SLU, 2020)
Fyrisån outlet	10 times (2014-2015 and 2019-2020)	-	(Malnes, et al., 2021; Fyrisåns Vattenvårdsförbund, 2020; Gago-Ferrero et al., 2017)
Kungsängsverket	Monthly	-	(Uppsala Vatten och Avfall AB, n.d-a)
Uppsalaåsen	Constant value	-	(P. McCleaf, personal communication, 29 March, 2021)
Precipitation	Constant value	-	(Fredricsson et al., 2017)

Dispersion of PFOS was described using the scaled eddy viscosity formulation with a constant value of 1 for horizontal and 0.01 for vertical dispersion. Furthermore, two outputs were added, one of the type 3D volume series, which records the concentration of PFOS in the entire domain for each time step. The other output was a 3D point series, presenting the concentration of PFOS at Vreta Udd at three depths (0.5, 15, and 30 meter) as a function of time. The point series was used to compare with the measured values at Vreta Udd. The time step of the calculations was set to 10 minutes and the output was stored every sixth time step, meaning every hour.

3.4 Modelled scenarios

Scenarios were set up to study the changes of PFOS with regards to different outcomes of climate change and socioeconomic development until 2050. One base scenario was set up to represent the current situation, and further scenarios were set up to represent possible outcomes for the future. When setting up the scenarios, RCPs were used to represent climate change projections and SSPs to represent socioeconomic development. Except from the base scenario, four scenarios were modelled; two scenarios which include only climate change predictions and two scenarios which include both climate change and parameters related to socioeconomic development (Table 3.5). The motivation to first simulate scenarios with only climate change was to evaluate the effect of that aspect separately, and adding socioeconomic development made it possible to evaluate which changes have the largest impact.

Table 3.5. The five different simulated scenarios.

Description	**RCP and SSP**	**Year**
Base scenario	-	2017-2018
Climate change	RCP4.5	~2050
Climate change	RCP8.5	~2050
Climate change and socioeconomic development	RCP4.5 + SSP1	~2050
Climate change and socioeconomic development	RCP8.5 + SSP5	~2050

In this study RCP4.5 and RCP8.5 were chosen to represent scenarios related to climate change, with the motivation that these two scenarios cover a large span of outcomes. In fact, modelling RCP2.6 instead of RCP4.5 would present an even larger span, but RCP2.6 requires rapid reduction of CO_2 emissions and implementation of very stringent policies soon, which is assumed not to be realistic. Much focus in previous research has been put on RCP4.5 and RCP8.5 which has led to more existing and available data for these scenarios (Sjökvist et. al., 2015).

In the scenarios where parameters representing socioeconomic development are included, RCP4.5 was combined with SSP1 and RCP8.5 with SSP5. First, the motivation to choose SSP1 and SSP5 for socioeconomic development was that these two pathways provide a wide span, with one more sustainable scenario and one with continued reliance on fossil fuels and little effort to avoid global environmental concerns. Further, the combination of SSP1 and RCP4.5 has been used in previous studies and is assumed to be a reasonable combination, both presenting a sustainability focus and limited climate change (Iqbal et al., 2019; Samuelsson & Östberg, 2020). The scenario of SSP1 is also assumed to likely occur in Sweden, taking the country's signing of the Paris agreement and the United Nations Sustainable Development goals into consideration (Regeringskansliet, n.d.-a; Regeringskansliet, n.d.-b; United Nations, n.d.-a; United Nations, n.d.-b). The combination of SSP5 and RCP8.5 was chosen since SSP5 is the scenario closest to the emission pathway of RCP8.5, and thus the only scenario that reaches the level of solar radiative forcing that is projected for RCP8.5. (Riahi et al., 2017). SSP3 could also be motivated to combine with RCP8.5 considering the emission level, however, SSP3 describes a society that is resurgent, has regional conflicts and cares most about regional issues, which is considered not to be that descriptive for Sweden (O'Neill et al., 2017).

All future scenarios were simulated for the year 2050. The motivation to study particular 2050 was that it was found to be a time horizon commonly used in climate change projections (Sjökvist et al., 2015; Stensen et al., 2017). However, the parameters related to climate change will not differ that much between RCP4.5 and RCP8.5 until 2050, according to Sjökvist et al. (2015) the major divergent trends will occur in the second half of the century. This knowledge could be a motivation to simulate for a year beyond 2050, e.g. 2100 which also is commonly used in climate change projections, to analyse the differences between RCP4.5 and 8.5. However, the uncertainties in the assumptions regarding socioeconomic development increase with time, and therefore 2050 was chosen in this study.

3.4.1 Climate change projections in the area of Lake Ekoln

In 2014, SMHI was commissioned by the Swedish government to make a climate study of Sweden based on the RCP scenarios that were adopted by IPCC in 2013 (Sjökvist et al., 2015). International climate data was collected and processed in order to analyse changes on a local level in Sweden. SMHI has presented results of projected changes in e.g. temperature, precipitation, and water flows for each county in Sweden, with projections until 2100 for RCP4.5 and RCP8.5.

The report by Sjökvist et al. (2015) presents projections for the county of Uppsala, where Lake Ekoln is located. A summary of some of the projections for the area reads as follows. By 2100 the air temperature may have increased with 3 degrees Celsius according to RCP4.5 and 5 degrees to RCP8.5, the vegetation period will be longer, and the number of warm days will increase. The yearly precipitation may increase by 20-30% where the largest increase will occur during winter and spring. The average yearly flows in the watercourses will increase by 10%, though it may decrease during spring and summer but increase during autumn and winter. Also, the typical yearly shape of the flows will change; the spring-peak will be less distinct, the flows during winter will increase, and the period of low flows will be longer. However, Sjökvist et al. (2015) also mention the many uncertainties and assumptions included in the climate models, which are important to be aware of.

3.4.1.1 Model changes due to climate change

The parameters that were adjusted in the model due to climate change are air temperature, precipitation, water flow in the rivers, and ice coverage of the lake. The flow from Uppsalaåsen was assumed to not change in the future. This is a simplification, since in reality changes in climate may affect the water level in the esker and thus the water flow between the esker and Lake Ekoln, however, to what extent climate change will impact this is difficult to evaluate. It is uncertain how the relative humidity, wind, solar radiation, and cloudiness will change in the future (SMHI, 2019; SMHI, 2020b), and therefore the change of these parameters has not been taken into consideration in this study, which is an exclusion that has been motivated in a similar study before (Samuelsson & Östberg, 2020). Expected land rise and rise of sea level may bring changes to the water level in the future, however, this was not taken into consideration in this study since the reconstruction of Slussen in Stockholm probably will make it possible to regulate this (Andréasson et al., 2011). This assumption was made by Lindqvist (2019) as well, who made a study regarding future hydrodynamic conditions in lake Ekoln.

The change in air temperature, which was taken into account in the future simulations, is considered the most important parameter to include when simulating the changes in water temperature of the lake (Stensen et al., 2017). The temperatures in the inflowing rivers may be a bit higher in the future due to increased air temperature, however this was not changed in the model and is assumed to not have any major effect on the temperature in the lake when considering the whole simulation period. Further, the initial temperature profile was not changed from the base scenario. The change in initial temperature is assumed to be relatively small and the simulation period is assumed to be long enough to make the water temperature adjust to the air temperature, which makes the initial temperature profile less important to change.

Air temperature and precipitation

The changes in air temperature and precipitation were estimated based on projections made by SMHI regarding how these parameters will change in different parts of Sweden, for each season, for the different RCP-scenarios developed by IPCC (SMHI, 2021). The climate data from SMHI are derived from one regional model which is driven by nine different global models. The fact that only one regional model was used is an uncertainty factor to be aware of. The changes are presented as a change in degrees for the air temperature and as a change in percentage for the precipitation, for every year from the reference period, which is between 1961 and 1990, until 2100. These data were downloaded from SMHIs webpage as excel data (SMHI, 2021). How the specific values regarding air temperature and precipitation, presented in Table 3.6, were derived from the excel data is described in Appendix B.

Flow

Values of how the flow in the rivers will change were estimated from diagrams presented in a report made regarding climate change related to RCP-scenarios, in the county of Uppsala (Sjökvist et. al., 2015). The report is directed by SMHI and presents the climate today and predictions for the future, based on observations and climate models where international modelling data have been processed and downscaled to use on a regional level. The expected changes in the flow in Fyrisån and Örsundaån, presented in Table 3.6, were estimated from diagrams for the year 2050 for each season. Reading values from diagrams introduces uncertainties, but since the projections are less detailed overall, these values were not evaluated in depth. Figure 3.5 presents the diagrams that were used regarding the flow in Fyrisån, and similar diagrams were used for Örsundaån, which can be seen in Appendix C. Sjökvist et al. (2015) does not present any predictions for the flow in Hågaån and Sävaån. However, Lindqvist (2019) discussed that since Hågaån and Fyrisån are located in the same catchment area and Sävaån in the same as Örsundaån the same change for those respectively can be assumed.

Worth to notice is that even though the precipitation is predicted to increase for all seasons in the future, it does not mean the flow automatically will increase (Lindqvist et al., 2019). A warmer climate will bring longer vegetation periods and increase evaporation which explains why the flow is predicted to decrease during spring and summer.

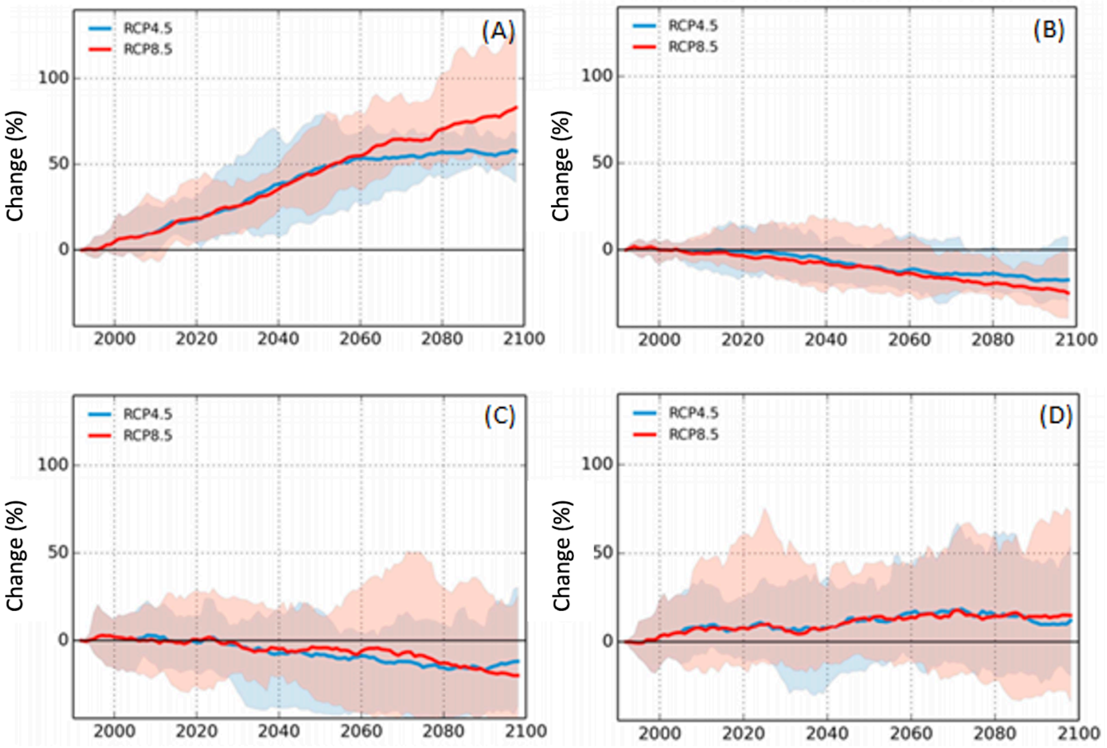

Figure 3.5 Change in average flow in Fyrisån during (A) winter, (B) spring, (C) summer, and (D) autumn for RCP4.5 and RCP8.5 (Sjökvist et al., 2015).

Ice coverage

Values regarding how climate change is predicted to affect the ice coverage of Mälaren are presented in a report written by SMHI (Stensen et al., 2017). In the report, Mälaren is divided in an eastern and a western part where values for the eastern part were chosen in this study in regard to the location of Lake Ekoln. The report presents the change in the number of days the lake will be covered with ice, from the reference period, which is 1997-2015, until 2032-2050. In this study it was assumed to be the same change between 2017-2018 and 2050 as presented in the report by Stensen et al., (2017), and the specific days that were removed were chosen so that the icing started later, and the ice released earlier. In RCP4.5, the lake was assumed to be covered with ice between 18/1 - 13/3 and 24/1 - 4/4 for the first and second simulated winter respectively, in the same way the ice coverage for RCP8.5 was assumed to be between 17/1 - 13/3 and 23/1 - 4/4 for each winter, respectively.

Table 3.6 presents a summary of the parameters that were used in this study to reflect how the climate will change in the area around Lake Ekoln, for the scenarios RCP4.5 and RCP8.5, respectively. Where winter refers to December - February, spring is March - May, summer is June - August and autumn is September - November.

Table 3.6 Parameters that are projected to change due to climate change in Uppsala county, for climate scenarios RCP4.5 and RCP8.5 in 2050.

Season	**RCP4.5**	**RCP8.5**
Air temperature [°C][1]		
Winter	+1.26	+1.75
Spring	+1.11	+1.3
Summer	+0.54	+0.96
Autumn	+0.7	+0.99
Precipitation [%][1]		
Winter	+ 3.95	+10.61
Spring	+6.89	+8.38
Summer	+6.69	+7.32
Autumn	+4.92	+5.19
Water flow from Fyrisån and Hågaån [%][2]		
Winter	+49	+46
Spring	-10	-10
Summer	-9	-5
Autumn	+13	+13
Water flow from Örsundaån and Sävaån [%][2]		
Winter	+40	+40
Spring	-11	-10
Summer	-10	-5
Autumn	+10	+10
Ice coverage [number of days/year with ice][3]		
	-28	-27

[1](SMHI, 2021; Appendix B)
[2](Sjökvist et. al., 2015)
[3](Stensen et. al., 2017)

3.4.2 Socioeconomic projections in the area of Lake Ekoln

Factors related to socioeconomic development that were considered to affect the situation with PFOS in Lake Ekoln are development of soil remediation and water treatment techniques, restrictions and regulations, and urbanisation. However, the direction and consequences of the development were assumed to differ between SSP1 and SSP5. It is important to be aware of the uncertainty factors related to the several assumptions made related to socioeconomic development.

Contaminated ground and remediation techniques

Since PFOS is very resistant and attaches to particles, soil that has been exposed to high concentration of PFOS can cause contamination of the surrounding environment over a long period of time and will need a long time before the PFOS concentration reaches background levels. A study made by Norström et al., (2015), who investigated the levels of PFOS in a lake near Arlanda airport, concludes that if no remediation of the contaminated site takes place, it will proceed to emit PFOS but the concentration of PFOS in the lake will decrease by approximately 45% until 2050 due to leaching of the soil over time. Today, remediation techniques of soil contaminated with PFAS is an emerging science. A variety of remediation technologies have been tested in laboratory scale, some in pilot-studies and some have been tested in field (Mahinroosta & Senevirathna, 2020). However, each of the emerging techniques currently tested in the field has its disadvantages and limitations, and long-term efficiency is yet to be investigated. Heavily contaminated areas that have been identified around Ekoln are mainly Uppsala-Ärna airport, Viktoria fire-fighting facility, but also some landfills, both old and active ones, which are suspected to emit PFOS.

Since SSP1 is a scenario where people are concerned about a sustainable future and the local environment, along with rapid technological development, the remediation technologies for PFAS were expected to continue to improve in this scenario. For SSP5, rapid technological development was also expected, but with less concern about the environment, and technical solutions are mainly focused on end-of-pipe solutions. Therefore it was assumed that not much effort will be put on remediation of contaminated soil in SSP5, focus will rather be on for example removing PFOS in drinking water treatment plants (DWTP).

Treatment techniques in wastewater treatment plants

Today, Kungsängsverket does not treat the water from PFAS (Malnes et al., 2021). However, several technologies for removing PFAS are available, but the problem lies in scaling up these technologies and making them efficient and sustainable (Militao et al., 2021). Much focus is put on research in finding usable techniques today (Franke, 2017; EPA, n.d.), and according to Ahrens (L. Ahréns, personal communication, 2 March, 2021), it is in the coming decades possible to develop techniques that remove 100% of PFAS in wastewater treatment plants.

Since SSP1 represents a society that puts much value on environmental sustainability and human health, an assumption was made that proper and efficient treatment techniques for WWTP will be developed until 2050 that are able to treat the water in Kungsängsverket from PFOS before it reaches Ekoln. SSP5 represents a scenario with rapid technology development which speaks for new treatment techniques. However, as mentioned before, focus is put on end-of-pipe solutions and therefore it was assumed that the treatment will be in DWTP instead of in WWTP.

Restrictions and regulations

In the EU there are restrictions regarding the use and production of PFOS and more are planned to be implemented (EEA, 2019). Although, there are countries outside Europe that still do not have any restrictions regarding PFAS at all (Ipen, 2019). Despite the distance, PFOS produced in countries outside the EU can enter the environment in Sweden, partly via atmospheric deposition due to the persistence properties of PFAS, but also via products containing PFOS which are imported from these countries.

SSP1 is a scenario where the management of both local and global concerns regarding the environment improves and where the water and air pollution will be low. Therefore an assumption was made that restrictions of PFOS will be spread worldwide and that all production of PFOS and products containing PFOS will be banned. SSP5 was assumed to not bring any harder restrictions than those in place today since it is hard to see any motive for that. The scenario focuses on economic growth and intensive production and consumption patterns. This in combination with the many uses of PFOS in products will probably not reduce the production or use of it.

Urbanisation

According to Region Uppsala (2019), the population in the county of Uppsala will increase by 107,400 persons between 2019 and 2050. This urbanisation will lead to increased consumption in the area which in turn could lead to increased load of PFOS entering Kungsängsverket if the use of PFOS continues as today. According to Uppsala Vatten och Avfall (Anna Maria Sundin, personal communication, 29 March 2021) the water flow from Kungsängsverket will be 27 Mm^3/year 2050, which is around 50 % higher compared to 2017.

Urbanisation is also expected to increase the impermeable areas, which could lead to more PFOS in Ekoln due to more runoff water entering the lake, which is a pathway for contaminants (Guo et al., 2020). However, the influence of increased impermeable areas was not included in this study due to lack of data regarding the concentration of PFOS in stormwater. Major assumptions regarding how the extent of impermeable areas will change in the study area were also required which make the load of PFOS from this source very uncertain. The combination of increased impermeable areas due to urbanisation and more precipitation due to climate change will probably lead to greater volumes of stormwater. If stormwater is a major pathway to PFOS in Ekoln, this could lead to increased levels of PFOS in the lake, but if the stormwater does not contain much PFOS, the greater volume of stormwater will rather lead to dilution of PFOS. The exclusion of this aspect in this study is important to be aware of.

SSP1 implies urbanisation in developing areas but not that much in developed areas. Uppsala was not assumed to be a developing area, which speaks for less urbanisation here. SSP5 on the other hand speaks for high levels of urbanisation in all regions of the world.

3.4.2.1 Model changes due to socioeconomic development

Due to projected socioeconomic development, the concentrations of PFOS entering Ekoln from the sources Uppsalaåsen, Kungsängsverket, Fyrisån and precipitation, and the initial concentration of PFOS in the lake, were adjusted. The changes in the concentrations in the model, and motivation, are presented in Table 3.7. The discussion behind the motives is presented in the sections below Table 3.7.

Table 3.7 Change in concentration of PFOS due to socioeconomic development from the base scenario until 2050 for SSP1 and SSP5.

	Motives	SSP1	SSP5
Uppsalaåsen	Soil remediation Natural reduction	- 80 %	- 45 %
Kungsängsverket[1]	Treatment techniques in WWTP Restrictions and regulations Urbanisation	-100 %	+ 50 %
Fyrisån[2]	Soil remediation Natural reduction Urbanisation	- 80 %	- 40 %
Precipitation[2]	Restrictions and regulations	- 90 %	-
Initial in Ekoln	Summary of all motives	- 90 %	- 10 %

[1] Increase of flow from Kungsängsverket due to expected urbanisation is represented by increased concentration of PFOS instead. Explained in more detail in the section "Kungsängsverket" below.

[2] The flow from Fyrisån and the amount of precipitation are assumed to increase due to climate change until 2050 in both SSP1 and SSP5.

Uppsalaåsen

Soil remediation of the area around Ärna airport and Viktoria fire-fighting site and other heavily contaminated sites will lead to a major reduction of PFOS entering Ekoln via Uppsalaåsen. The remediation of these places was assumed to be effective and remediate the soil from close to 100% of PFOS (Mahinroosta & Senevirathna, 2020). However, since it was assumed to be unrealistic to identify all areas with contaminated soil that affect the groundwater, the concentration of PFOS from Uppsalaåsen was reduced by 80 % in SSP1. In SSP5 only the natural reduction was assumed to contribute to a reduction of the concentration of PFOS from Uppsalaåsen. Therefore the value presented in the report by Norström et al. (2015) was used to represent the reduction, which was 45 %.

Kungsängsverket

Factors that were assumed to affect PFOS from Kungsängsverket are urbanisation, improved treatment techniques, and restrictions. In both SSP1 and SSP5 urbanisation was expected to bring an increment of the flow from Kungsängsverket according to Uppsala Vatten och Avfall, mentioned earlier. To get a value of the increment from the base scenario until 2050, the measured flow for 2017 was compared with the projected flow for 2050, 27 Mm^3/year (Anna Maria Sundin, personal communication, 29 March 2021). The comparison presented that the flow will increase by 52 %. Due to time constraints and longer simulation time required for running changes in the hydrodynamic module, the change due to urbanisation was considered to be represented by a change in concentration of PFOS instead of the flow, since it leads to the same mass flow of PFOS. 52 % was rounded to 50 % in the modelling, hence, the concentration of PFOS from Kungsängsverket was multiplied with 1.5 in SSP5. In SSP1, this aspect will not affect the PFOS entering Ekoln from Kungsängsverket since the scenario was assumed to bring treatment techniques that treat 100 % of PFOS in Kungsängsverket, and also it was assumed that there will be restrictions that prohibit

WWTP to emit PFAS (L. Ahréns, personal communication, 2 March, 2021). The reduction in the concentration of PFOS was therefore set to 100 % in SSP1.

The fact that the urbanisation was represented by increased concentration instead of increased flow implied a lower flow from Kungsängsverket in the model compared to projected flow, but since the flow from Kungsängsverket is low in relation to the flow from the rivers it was assumed not to affect the modelling results that much. To exemplify, the average flow in Fyrisån 2017-2018 was 11.05 m^3/s, compared to 0.6 m^3/s in Kungsängsverket during the same period.

Parts of the water that Kungsängsverket receives comes from Ärna airport, where the ground is contaminated with PFOS. Remediation techniques of the ground, assumed in SSP1, and natural reduction in both SSP1 and SSP5 could lead to less PFOS in the water from Ärna airport in 2050 compared with today. But since the proportion of the water that Kungsängsverket receives from Ärna is relatively small, as mentioned previously in the report, the impact on the total concentration of PFOS entering Ekoln was assumed to be negligible.

Fyrisån

Soil remediation, natural reduction, and urbanisation are factors that were taken into consideration regarding PFOS in Fyrisån. In SSP1, effective soil remediation of Ärna airport and Viktoria firefighting site, was assumed to bring a major reduction of the PFOS concentration in Fyrisån due to less PFOS transported with runoff water (Mahinroosta & Senevirathna, 2020). However, it is unrealistic to assume that 100 % of the contaminated soil is treated, thus, a reduction of 80 % was used in SSP1.

In SSP5 no remediation of the contaminated areas was assumed to be likely, however it was assumed that the contaminated soil will be leached out with time, with a reduction of 45 % until 2050 (Norström et al., 2015). Increased urbanisation may lead to increased use of products containing PFOS which could cause a greater risk of release of the substance to the environment. After considering both a possible increase of PFOS entering Fyrisån with stormwater due to urbanisation and the natural leaching of PFOS in the ground, a reduction of PFOS in Fyrisån was in SSP5 assumed to be 40 %. As mentioned in the section regarding urbanisation, greater volume of stormwater could also lead to dilution, but here a “worst case” scenario was assumed.

Precipitation

Due to the assumption that hard restrictions regarding PFOS will be implemented in the whole world in SSP1, the PFOS entering Ekoln via precipitation was assumed to be close to zero (EEA, 2019). Taking into consideration that it may be hard to control to what extent the restrictions are followed in the whole world, and the uncertainty regarding how long time PFOS can be preserved in the atmosphere, it seemed too bold to assume a reduction of 100 %, why 90 % was assumed. In SSP5, the situation with restrictions was assumed to be the same as today and therefore the concentration of PFOS entering Ekoln via precipitation was assumed not to change from the base scenario until 2050. However, due to the expected increase in precipitation, there will be a slight increase in the total amount of PFOS reaching Ekoln via precipitation.

Initial PFOS in Ekoln

The change in the concentration of PFOS in the included sources Uppsalaåsen, Kungsängsverket, Fyrisån, and precipitation were summarised in order to assume the change of the initial concentration of PFOS in the lake. In SSP1, all of the sources were assumed to lead to a decrease of PFOS concentration. The extent of the decrease ranged between 80 % and 100 % in the sources, thus, a reduction of 90 % was assumed for the initial concentration. Regarding the change of the initial concentration in SSP5 it is more complex due to major differences between the concentration in the sources where Kungsängverket leads to an increase and the other to a decrease. Since Fyrisån is the major source to Ekoln, the value of the reduction from Fyrisån was weighted higher than the values for the other sources. However, the increase in Kungsängsverket, which also is assumed to be a major source, needs to be considered. Considering all sources, the reduction in SSP5 was assumed to be 10 % of the initial concentration of PFOS in the base scenario.

4 Results

4.1 Base scenario

Observed and simulated PFOS

The concentration of PFOS in the lake varied during the year, where the pattern was different for different depths, as can be seen in Figure 4.3 which presents the concentration at Vreta Udd. The figure also presents observed concentrations of PFOS at Vreta Udd, and the flow in Fyrisån.

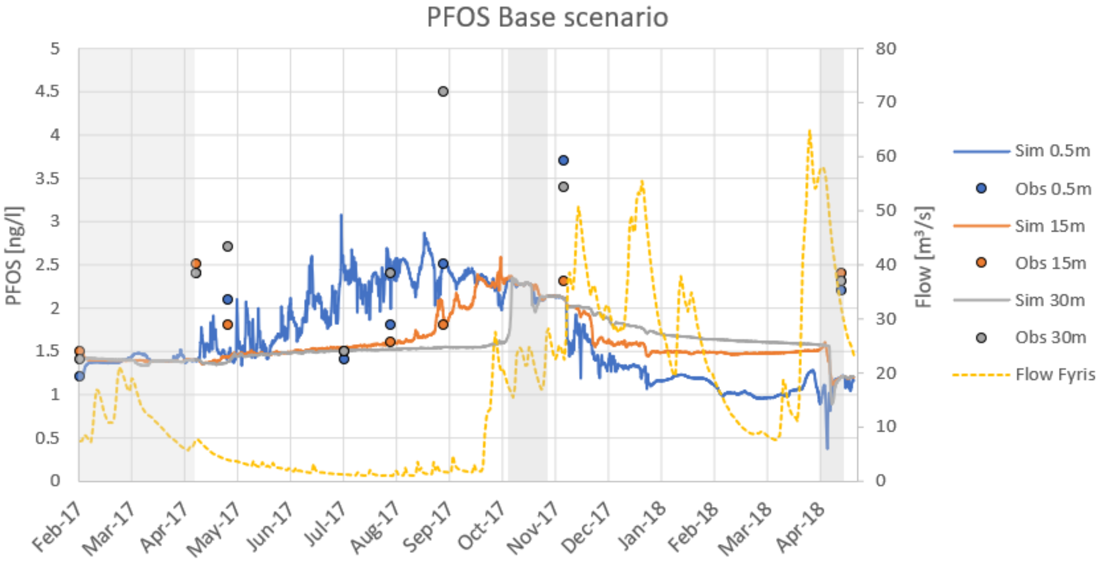

Figure 4.3 Simulated and observed PFOS concentration at three different depths (0.5 m, 15 m and 30 m) at Vreta Udd, for the base scenario. The grey areas represent periods when the water temperature is homogeneous in the lake and mixing takes place. The dashed yellow line represents the water flow in Fyrisån for the base scenario, presented on a secondary y-axis to the right. The vertical lines represent the 20th of each month. When only two dots are visible for the observed measurements, the values for the different depths overlap.

The general trend for the simulated values, for all depths, was that the concentration of PFOS increased until around september to november 2017 and then started to decrease. The increase of the concentration at 0.5 meters depth started and had its peak earlier, than the increase at 15 and 30 meters depths. The increase for the 15 meters depth started and had its peak a bit earlier than at 30 meters depth. When the concentration started to decrease, the slope was flatter for the simulation at 30 meter than closer to the surface. And at the end of the simulation, from December 2017 to April 2018, the concentration of PFOS was higher at larger depths. When mixing took place, around April both years, and November 2017, the concentrations were similar at the different depths, for both simulated and observed values.

Regarding the vertical trend of the simulated values, the highest concentration was closer to the surface in the beginning of the simulation while in the end, the highest concentration was closer to the bottom. There was no clear vertical trend of the observed values during the investigated time period. The measurements varied regarding whether the highest concentration has been detected closer to the surface or closer to the bottom of the lake.

A comparison of the observed and the simulated values shows that they were in the same order of magnitude. However, some of the observed values differed from the simulated ones, where many of the observed values were higher than the simulated, in September 2017 this difference was very large.

Horizontal distribution of PFOS

The horizontal distribution of PFOS at the surface in Lake Ekoln varies during the year, as can be seen in Figure 4.1, where the simulated distribution in July, October, and January is presented.

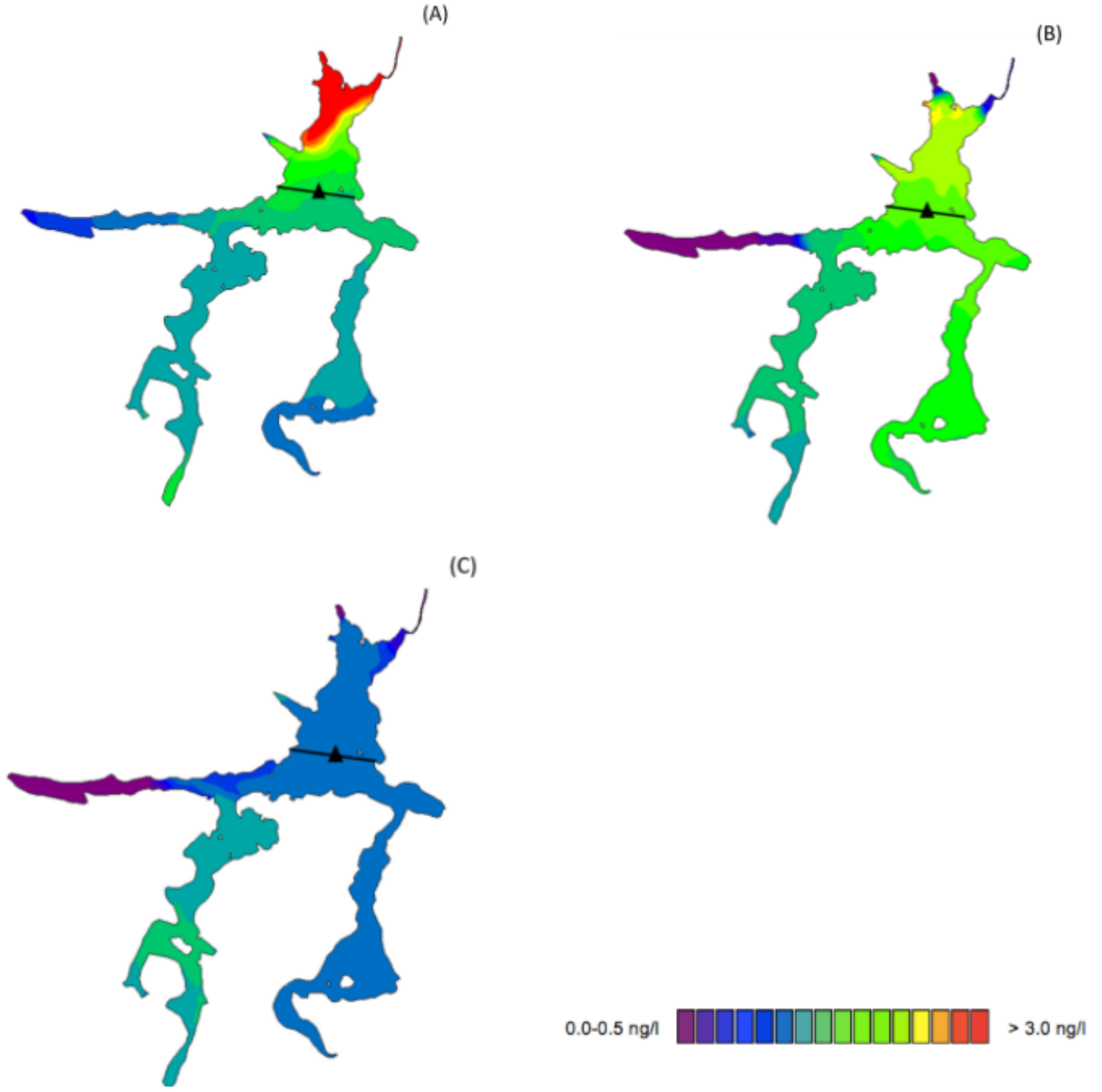

Figure 4.1 Horizontal simulated distribution of PFOS at the surface in Ekoln on 15 July 2017 at 04:00 (A), 28 October 2017 at 04:00 (B), and 2 January 2018 at 04:00 (C). The black line presents the location of the vertical profiles in Figure 4.2, and the black triangle the approximate location of Vreta Udd.

In July 2017 (Figure 4.1A) the concentration of PFOS was high in the northern part of the lake, where the outlet of Kungsängsverket and Fyrisån was located. The concentration was lower in the western part of the lake, where the outlets of Örsundaån and Sävaån were located, and in the south-west bay, while the concentration increased towards the south. In October 2017 (Figure 4.1B), the overall concentration was lower than in July 2017. Here the highest concentration was in the middle of the lake and towards the outlet of the lake, Erikssund. The concentration was lowest in the area close to the outlet of Örsundaån and Sävaån. In January 2018 (Figure 4.1C), the concentration was lower than in both July 2017 and October 2017. The lowest concentration was still in connection to the outlets of Örsundaån and Sävaån. A major difference between these three months was the flow. The flow was very low in July 2017, increased by a factor of approximately 18 in October 2017 compared to July, and in January 2018 the flow was double as high as in October (Appendix D, Figure D3).

Vertical distribution of PFOS

The simulated vertical distribution of PFOS changes between different months during the year, as presented in Figure 4.2.

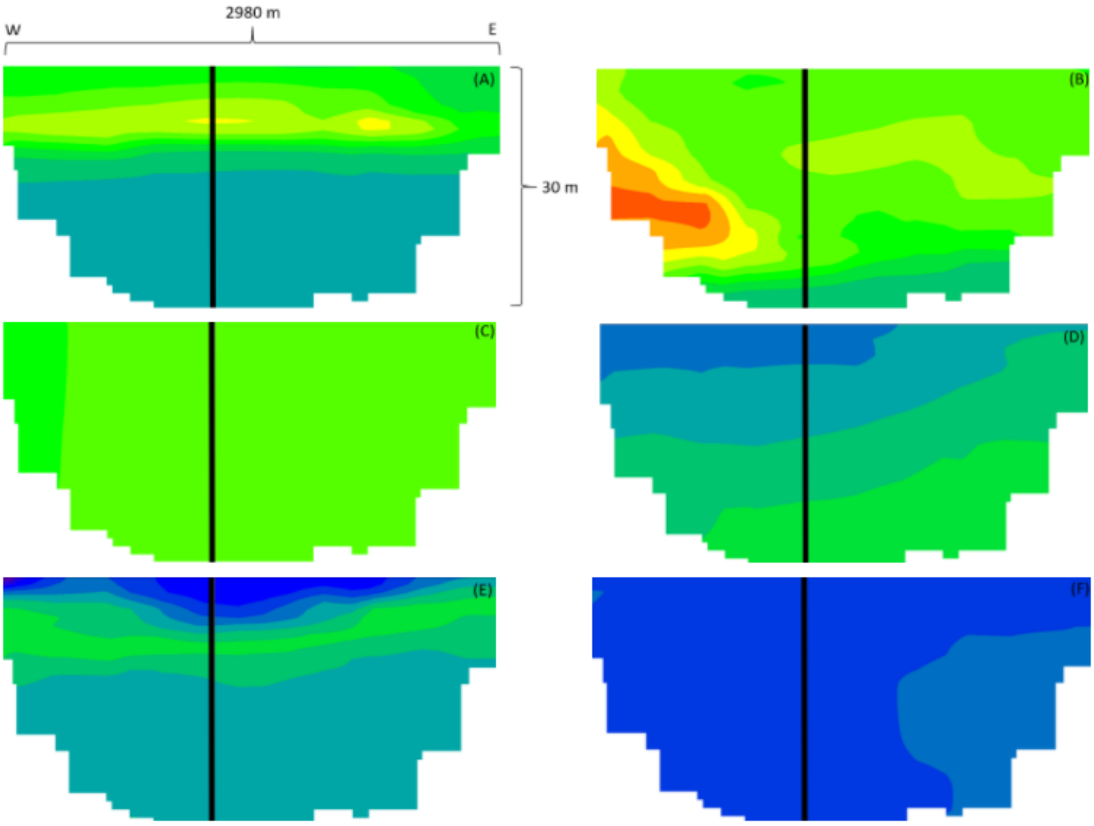

Figure 4.2 Vertical profiles of PFOS concentration in 15 July 2017 at 04:00 (A), 15 October 2017 at 04:00 (B), 15 November 2017 at 04:00 (C), 15 December 2017 at 04:00 (D), 15 April 2018 at 04:00 (E), and 4 May 2018 at 00:00 (F). The black line presents the location of Vreta Udd. The colour palette in Figure 4.1 describes the range in concentration PFOS.

In July (Figure 4.2A) the water was stratified in the lake, with the highest concentration close to the surface, in October (Figure 4.2B), one can see that the concentration started to even out and in November (Figure 4.2C) the concentration of PFOS was the same in the whole vertical profile. In December (Figure 4.2D) the water was stratified again, but this time with the lowest concentration close to the surface. In April (Figure 4.2E), the water was still stratified, but with a more distinct stratification closer to the surface and in May (Figure 4.2F), the concentration was the same in the whole vertical profile. This series indicates that mixing of the water occurred in November 2017 and May 2018, which is probably typical for all years.

4.2 Simulated PFOS concentration - all scenarios

Climate change and socioeconomic development affected the concentration of PFOS in Lake Ekoln to different extent, as can be seen in Figure 4.4 which presents the concentration of PFOS at Vreta Udd for the base, and future scenarios, at different depths. It was clear that the RCPs had little effect on the concentration of PFOS in the lake in comparison to the SSPs. Further, SSP1 implied much lower concentration of PFOS than SSP5. The low concentration in SSP1 is explained by the sustainability focus in this scenario, bringing measures and strict regulations to reduce the amount of PFOS that is spread in the environment.

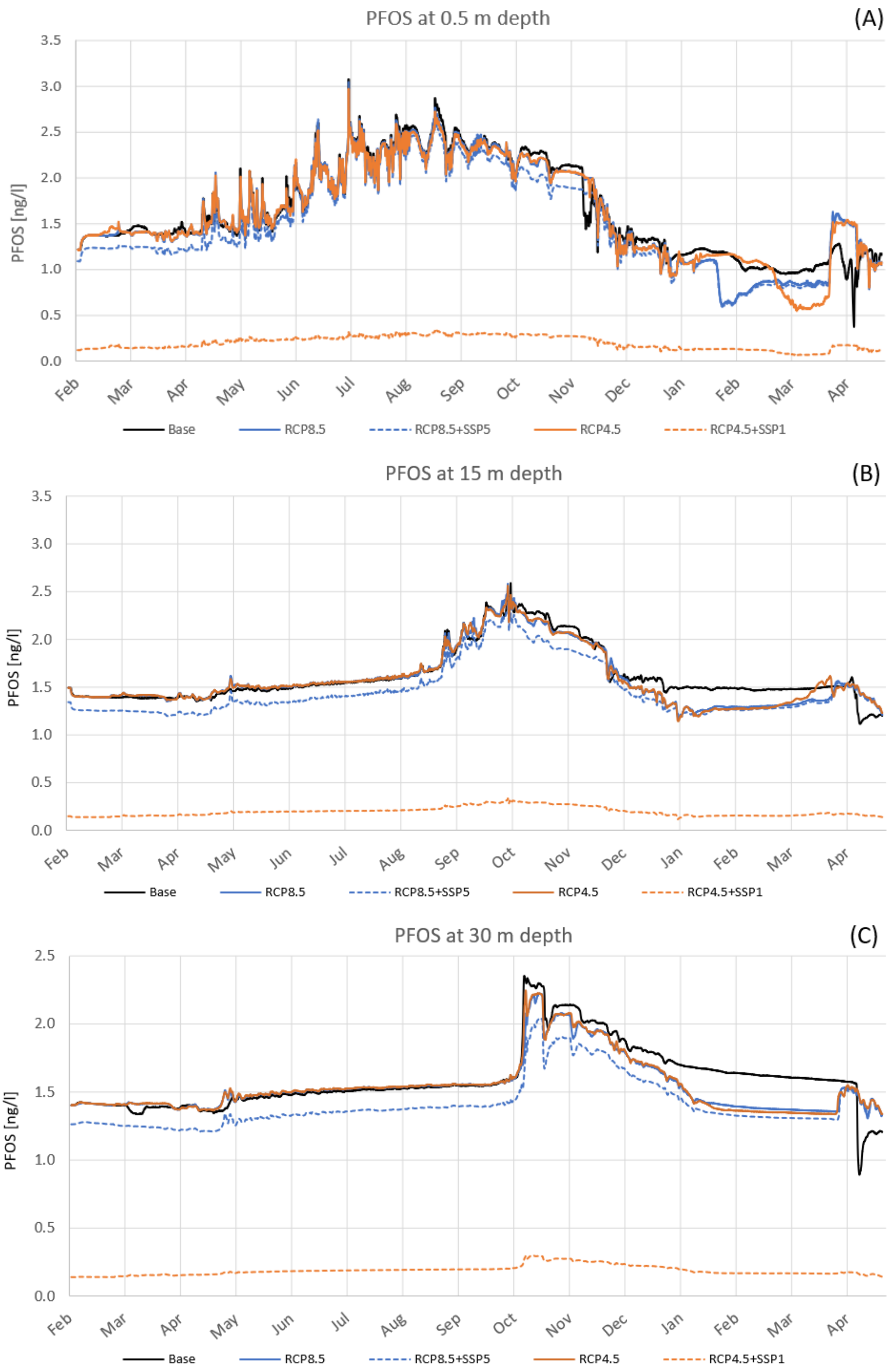

Figure 4.4 PFOS concentration at Vreta Udd at 0.5 m (A), 15 m (B) and 30 m (C) depth, for all 5 scenarios: base, RCP8.5, RCP8.5+SSP5, RCP4.5, RCP4.5+SSP1. The vertical lines in the graphs represent the 20th of each month. The base scenario is in 2017-2018, while the other scenarios are the same months but around 2050.

When the base scenario was compared with RCP4.5 and RCP8.5, the concentration and spreading pattern of PFOS was in general very similar for all three scenarios. In the first half of the simulation period, the variations of PFOS concentration were almost the same, but in the second half some differences were visible. For all three depths, the concentration decreased a bit more for RCP4.5 and 8.5 in comparison to the base scenario. At 0.5 meters depth there was a significant drop in PFOS concentration in the beginning of February the second year for RCP8.5, while for RCP4.5 a similar drop could be seen in the beginning of March. At 15 meters depth, the decrease compared to the base scenario started earlier, around the end of December, for both RCP4.5 and RCP8.5. At 30 meters depth, the concentration in both RCPs was lower than in the base scenario from October, and the difference increased even more from December where the slope in the RCPs was steeper than in the base scenario. In the end of the simulation, for all depths, there was a significant drop in PFOS concentration for the base scenario, while for RCP4.5 and 8.5 at the same time, the concentration first increased a bit followed by a slight decrease at all three depths.

RCP8.5+SSP5 followed the same pattern as RCP8.5 but with a lower initial concentration, however towards the end of the simulation, the concentration was almost the same for these two, which held for all three depths. Also, worth mentioning is that RCP4.5+SSP1 followed the same pattern as RCP4.5, however this was not clear in Figure 4.4 since the concentration in RCP4.5+SSP1 was much lower than in all the other scenarios.

4.3 PFOS from different sources

The origin of PFOS in Lake Ekoln was divided between different sources: Fyrisån, Kungsängsverket, Uppsalaåsen, and precipitation, and the contribution to the total concentration from each source varied during the simulation and in the different scenarios (Figure 4.5). The initial concentration of PFOS dissipated during the simulation, which clearly affected the total concentration of PFOS, which was the sum of the remaining part of the initial concentration and the contribution from the inflows. The results for 0.5 meters and 30 meters depth were similar to the ones at 15 meters for each scenario (Appendix F).

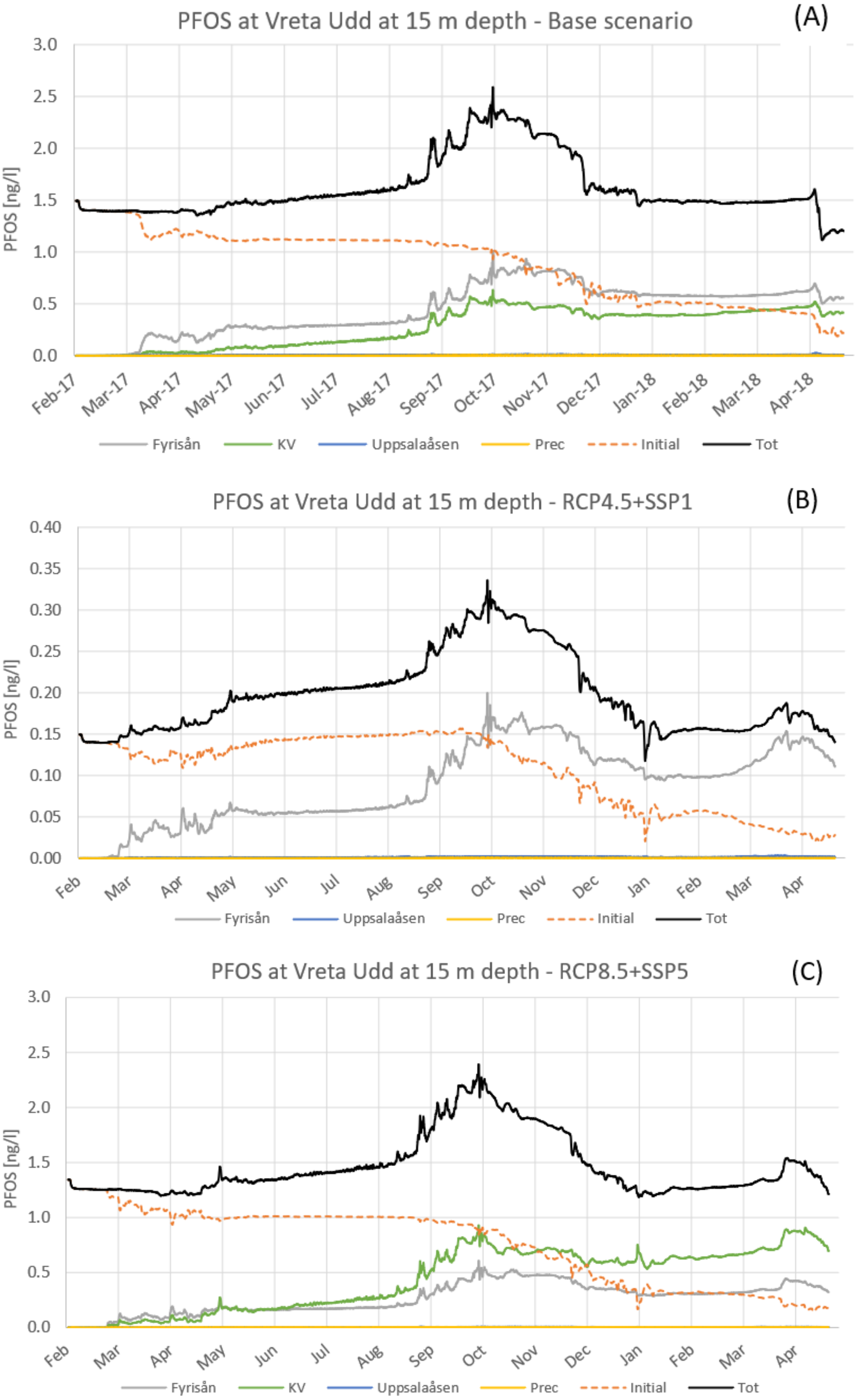

Figure 4.5 *Total PFOS concentration and concentration separated in terms of origin, Fyrisån, Kungsängsverket (KV), Uppsalaåsen, precipitation (Prec), and the dissipation of the initial concentration (initial), at 15 m depth at Vreta Udd, for the base scenario (A), RCP4.5+SSP1 (B), and RCP8.5+SSP5 (C). Note that the y-axis in RCP4.5+SSP1 (B), is of different range since the concentration in this scenario is significantly lower.*

For all scenarios it was clear that the contribution from the esker Uppsalaåsen and precipitation was negligible in comparison to Fyrisån and Kungsängsverket (Figure 4.5). In the base scenario, Fyrisån was the largest contributor to PFOS in lake Ekoln, followed by Kungsängsverket. In RCP4.5+SSP1, the contribution from Kungsängsverket was zero, since the wastewater was considered to be 100 % purified from PFOS, and thus the PFOS in this scenario originated almost exclusively from Fyrisån. On the other hand, in RCP8.5+SSP5, Kungsängsverket was the largest contributor of PFOS. This was since urbanisation brought a larger amount of wastewater in the WWTP and thus more PFOS. At the same time, a natural reduction of PFOS leaching out from the contaminated sites to Fyrisån was assumed.

As mentioned, the dotted lines present the dissipation of the initial concentration in the lake. The initial values were represented by the measured concentration at the starting date of the simulation for the base scenario. For the future scenarios, the initial concentration was changed according to Table 9. For all three scenarios in Figure 4.5, the PFOS concentration originating from the initial concentration was relatively high in the first half of the simulation, and then started to decrease. The decrease started around the beginning of October. At approximately the same time the contribution from Fyrisån and Kungsängsverket increased. This also coincided with a major increase in water flow in the inflows (Figure 4.4; Appendix D, Figure D3-4). In the end of the simulation, the initial concentration was not completely dissipated, indicating that not all water in the lake was exchanged during the simulation.

4.3.1 Mass flow of PFOS

In the section *Mass flow of PFOS* in the Methodology*,* the mass flow of PFOS in the base scenario from different sources was calculated and presented. In order to get an understanding of the importance of each source in the future, the mass flow of PFOS was also calculated for the future scenarios, and the calculations were made at the same points as in the base scenario and in the same way. The concentrations and flows for the future scenarios were changed according to Table 3.6 and Table 3.7. The flow and concentration in Sävjaån were assumed to change in the same way as Fyrisån, while the concentration at Ärna was assumed to change in the same way as Uppsalaåsen, and the flow from Uppsalaåsen was assumed to not change. Table 4.1 presents the results of the mass flow from the outlet of Fyrisån, Uppsalaåsen and precipitation. The results showed that Fyrisån by far was the largest contributor to PFOS in Lake Ekoln for all scenarios, and the contribution from Uppsalaåsen and precipitation was almost negligible in comparison. This was also the case for the simulation results (Figure 4.5).

Table 4.1 Mass flow of PFOS from Fyrisån, Uppsalaåsen and precipitation [mg/day].

	Fyrisån Outlet	**Uppsalaåsen**	**Precipitation**
Base scenario	1782	22	4.4
RCP4.5	1661	22	4.7
RCP8.5	1726	22	4.8
RCP4.5+SSP1	332	4.3	0
RCP8.5+SSP5	1035	12	4.8

The mass flow of PFOS from the different sources along Fyrisån is presented in Figure 4.6 below. Observe that in these results, Kungsängsverket was considered as a contributor to PFOS in Fyrisån, while in the modelling Kungsängsverket was added as a separate source. From Ärna, the mass flow was calculated as the increment in mass flow of PFOS in Fyrisån along the section where the river passes Ärna, while for Kungsängsverket and Sävjaån the mass flow is presented as the average in the outlets. Identified sources to PFOS in Sävjaån are Hovgården landfill and Viktoria firefighting site. Observe that the sum of the mass flow from the three sources (Ärna, Sävjaån and Kungsängsverket) was larger than the mass flow in the outlet of Fyrisån (the black line in Figure 4.6), meaning that PFOS dissipated in Fyrisån. This could be an indicator that there are processes affecting PFOS in the river.

The mass flow of PFOS from the different sources along Fyrisån is presented in Figure 4.6 below. Observe that in these results, Kungsängsverket is considered as a contributor to PFOS in Fyrisån, while in the modelling Kungsängsverket is added as a separate source. From Ärna, the mass flow was calculated as the increment in mass flow of PFOS in Fyrisån along the section where the river passes Ärna, while for Kungsängsverket and Sävjaån the mass flow is presented as the average in the outlets. Identified sources to PFOS in Sävjaån are Hovgården landfill and Viktoria firefighting site.

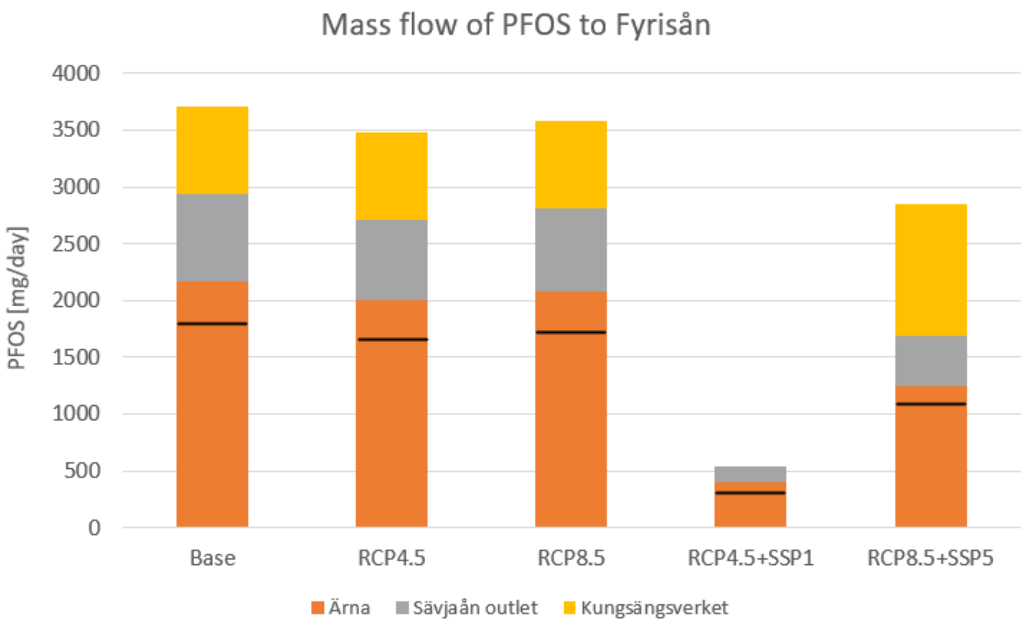

Figure 4.6 Mass flow of PFOS from Ärna, Sävjaån and Kungsängsverket to Fyrisån. From Ärna and Sävjaån the mass flow is presented as the average based on sampling of PFOS on four occasions between 15th of June and 14th of September 2020. The mass flow from Kungsängsverket is the average based on monthly collection samples of PFOS between January 2019 and August 2020. The horizontal black lines represent the mass flow in the outlet of Fyrisån, calculated in the same way as Ärna and Sävjaån.

For the base scenario, RCP4.5 and RCP8.5, the difference in mass flow only depended on changing water flows and as can be seen in Figure 4.6, the difference between the mass flow of PFOS in these scenarios was very small. For these three scenarios, Ärna was the largest contributor to PFOS in Fyrisån, followed by Kungsängsverket and Sävjaån. When the SSPs were added, major changes were visible. For both scenarios including SSP there was a decrease in mass flow of PFOS. In RCP8.5+SSP5 the contribution from Ärna and Sävjaån decreased, while the contribution from Kungsängsverket increased, leading to Kungsängsverket being in the same order of magnitude as Ärna. In RCP4.5+SSP1 the mass flow of PFOS was significantly lower than for the other scenarios. This was because the contribution from Kungsängsverket was zero, and there was a large decrease in the contribution from both Ärna and Sävjaån.

The results in Figure 4.6 can give an indication of the importance and magnitude of each of the identified sources, but it is important to be aware of the uncertainties. The sampling occasions in Fyrisån were few and the variations in mass flow of PFOS were large (Table 4.2). The mass flow in the outlet of Fyrisån ranged between 70 and 4121 mg/day, in Sävjaån the range was between 250 and 2034 mg/day, and from Ärna the mass flow ranged between 958 and 4738 mg/day (Table 4.2), for the four sampling occasions made by Fyrisåns Vattenvårdsförbund (2020). In Kungsängsverket the mass flow ranged between 399 and 1294 mg/day, between January 2019 and August 2020, the mass flow for each month was presented in Appendix G.

Table 4.2 Mass flow of PFOS [mg/day] for the current situation, from Fyrisån, Ärna and Sävjaån on different days. The mass flow is based on observed concentrations of PFOS by Fyrisåns Vattenvårdsförbund (2020) and modelled water flow from SMHI (n.d. -b) the same day.

Date	**Fyrisån Outlet**	**Sävjaån outlet**	**Ärna**
2020-06-15	70	665	1427
2020-07-13	4121	2033	4738
2020-08-17	2203	250	958
2020-09-14	733	111	1382
Average	1782	765	2127

5 Discussion

5.1 Analysis of current spread of PFOS

The general trend of the simulated PFOS concentration at Vreta Udd is that the concentration increases until autumn 2017, and then decreases. One major reason for the increase in the first half of the simulation and the decrease in the second half is probably due to the dissipation of the initial concentration, which starts to decrease significantly around the beginning of October, as shown in Figure 4.5. The relatively stable concentration originating from the initial concentration in the first half of the simulation followed by the decrease starting in October can be explained by changes in water flow from the inflows. During the first half, from February to October, the water flow in all rivers is relatively low, while during the second half it is significantly higher (Figure 4.3, Appendix D). The low water flow during a relatively long period in the beginning may lead to low exchange of water in the lake, meaning that not much PFOS leaves the lake. When the water flow increases in the second half of the simulation, more water leaves the lake and thus more of the initial PFOS in the model leaves as well. Among the inflowing rivers, it is only Fyrisån that contributes with PFOS. The increased flows in the other rivers, do only contribute with more water to the lake, which means that the concentration of PFOS in the lake does not increase at the same rate as the inflow of water, which implies dilution. This can also be seen in Figure 4.1 where the high flows in October 2017 and January 2018 could be a reason for lower concentration of PFOS in the whole horizontal extent of the lake compared to higher concentration, especially in the northern part of the lake, in July 2017. Also notice that the concentration in the bay, where the outlet of Örsundaån and Sävaån are located, is very low, indicating that the high flow in these rivers in both October 2017 and January 2018 limit the spread of PFOS to this part of the lake, and instead the water from these rivers contributes to dilute the PFOS concentration in the lake.

Looking at the different depths, the simulated concentration of PFOS starts and has its peaks at different times (Figure 4.3). One reason why the increase of the concentration starts earlier at 0.5 meters depth than at larger depths is probably the seasonal stratification of the lake. PFOS enter the lake close to the surface in the model, and when the lake is stratified not much PFOS spreads to the deeper parts. In the same way, the reason why the increase of the concentration starts earlier at 15 meters depth than at 30 meters could be because the water temperature at 15 meter coincides with the temperature of the surface water earlier which implies spreading of PFOS down to this depth. At 30 meters, there is a significant increase in PFOS concentration at the end of October, which coincides with when the water temperature is the same in the whole lake and mixing takes place (Appendix E). Interesting to notice is that the simulated concentration as well as the observed is similar for all depths when mixing takes place, indicating that mixing affects the distribution of PFOS in the lake. One thing worth noticing is that in the end of the simulation, there is a significant drop in simulated PFOS concentration at all depths. The drop occurs right after the start of the mixing period and some days after the melting of the ice in 2018. At the same time there is the highest peak in the water flow for the base scenario (Figure 4.4; Appendix D, Figure D3-4). The reason behind the drop in PFOS concentration could be a combination of the melting of the ice, the mixing, and the peak in water flow.

When analysing concentration of PFOS in the base scenario (Figure 4.3), and comparing observed values with simulated, one can see that the concentrations are in the same order of magnitude. However, the influence of the initial concentration is large, mainly in the first half of the simulation which makes it difficult to evaluate whether the included sources in the model can make up for the observed concentration alone. In the second half of the simulation, the initial concentration decreases, but a limiting factor during this period is the few observations of PFOS. Further, the general trend for the simulated concentration in the lake is similar to the observed concentration, with increased concentration in the first half of the simulation followed by a decrease.

Despite that the simulation presents concentrations in the same order of magnitude as the observed, there are variations in the observed concentrations that are not captured by the model. Already in April-May 2017 there is an increase in the observed concentrations that is not visible in the simulation (Figure 4.3), which indicates that the supply of PFOS during this period is too low in the model. This may be due to the fact that the mass flow of PFOS from Fyrisån was constant and does not capture variations that occur in reality. It could also be due to run off from diffuse sources or contribution of PFOS from the other rivers. During the period from July to November 2017, there are four measurements where the model captures the concentration at 15 meters depth very well, while at 0.5 meters and 30 meters the variations in concentration are much larger and not captured as well as at 15 meters. Since the lake is stratified from approximately the beginning of May to the end of October (Appendix E), and the water entering the lake enters relatively close to the surface, the great increase in observed PFOS concentration mainly at 30 meters depth in September was quite surprising. This indicates that despite the stratification, PFOS spread to larger depths. It could also be due to sedimentation and resuspension of particulate PFOS, and desorption from the particles, which are not included in the model. The depth at Vreta Udd is approximately 30 meters, and a possibility is that resuspension and desorption from both particles and directly from the sediment could cause larger concentrations of PFOS close to the bottom. Another reason that PFOS spread to larger depths could be that the water in the inflowing rivers is of higher salinity than the water in the lake, and thus it has a higher density and spreads to larger depths. The effect that salinity has on the density of the water is not captured in the model, since density is only set as a function of temperature. A factor which is clearly connected to salinity is conductivity, and according to data from SLU (n.d.) the average conductivity between July and September 2017 in the outlet of Fyrisån is 55.3 mS/m, compared to a conductivity of 41.6 mS/m at Vreta Udd the same period. Further, in a study by Doverfelt (2013) it was concluded that the conductivity in Fyrisån decreases during spring flood and increases when the water flow is low, and that the conductivity increases along the section where wastewater is discharged from Kungsängsverket. This indicates that the effects of salinity may have a larger influence on the density of the water when the flow is low, which it clearly is between May and September 2017 (Figure 4.3).

One of the objectives in this project was to identify the pathways for PFOS into Lake Ekoln. Based on earlier studies and sampling done of PFOS it was found that PFOS enters Ekoln via Fyrisån, Uppsalaåsen, and precipitation. Sampling of PFOS has also been done in Örsundaån on two occasions, but the concentration of PFOS was below the detection limit. Whether PFOS enters Ekoln via Sävaån and Hågaån is not fully investigated, and to our best knowledge, no sampling of PFOS has been done in these rivers. The four inflowing rivers account for 95 % of the total water flow to the lake, and the remaining 5 % comes from diffuse flows where Uppsalaåsen accounts for a part of that. Other diffuse flows could be stormwater runoff and diffuse groundwater flows, which possibly could contribute with PFOS to the lake. However, Fyrisån alone stands for approximately 65 % of the total water flow into lake Ekoln (Table 3.1), meaning that the amount of PFOS in Fyrisån is of great importance for the conditions in Lake Ekoln. Both the simulation results (Figure 4.5) and the mass flow calculations (Table 4.1) presents that Fyrisån is the major pathway for PFOS entering Lake Ekoln while the contribution from Uppsalaåsen and precipitation is negligible. In a previous study regarding PFAS in Ekoln, only Kungsängsverket and precipitation were included as sources which resulted in much lower simulated concentration than observed (Ekman, 2021). Since this study, which also included Fyrisån and Uppsalaåsen, resulted in simulated concentrations in the same order of magnitude as observed, it can together with the knowledge that the contribution from Uppsalaåsen is negligible, confirm that Fyrisån has a large impact on the PFOS concentration in Lake Ekoln.

As mentioned previously in the report, identified sources to the PFOS contamination of Fyrisån are Kungsängsverket, Ärna firefighting training site and Sävjaån which contributes with PFOS from Viktoria firefighting training site and Hovgården landfill. In the modelling, Kungsängsverket was added as a separate source and is thus not included in the PFOS from Fyrisån. What can be seen in Figure 4.5A is that for the base scenario, Kungsängsverket is an important source discharging PFOS to Lake Ekoln, but the contribution from Fyrisån excluding Kungsängsverket is larger. Towards the end of the simulation, most of the initial concentration has dissipated, which makes it even more interesting to analyse the contribution from the sources and compare the simulated concentration with observed. When looking at the last date when observed concentration of PFOS is available at Vreta Udd (2018-04-27), the simulated contribution of PFOS originating from Fyrisån and Kungsängsverket makes up for 24 and 18 % of the observed concentration, respectively, considering the average concentration at all depths. The inserted initial concentration in the model at this date makes up for 10 %, and probably consists of a large share both from Kungsängsverket and Fyrisån. The fact that the total simulated concentration is lower than the observed in the end of the simulation, could be an indicator that the inflow of PFOS is too low in the model. However, since there is only one observation to compare with towards the end of the simulation, it is difficult to draw any reliable conclusions based on this.

Since measurements of PFOS at Kungsängsverket are done monthly, the contribution of PFOS to Lake Ekoln in the model is considered relatively reliable. For Fyrisån, the measurements of PFOS are sporadic, making the simulated PFOS from Fyrisån much more uncertain. Meaning that the additional PFOS between the total simulated and the observed may be a contribution from Fyrisån, but it is also possible that it originates from other unidentified sources. Diffuse sources that have been identified in this study to potentially emit PFOS, but are not clearly included in the modelling, are OWTS, industrial activities, and landfills. Some part of the PFOS from these sources is probably included in the PFOS entering Ekoln via Fyrisån and Uppsalaåsen, but some parts enter the lake via runoff from other locations or via the other rivers, which are not included in the model.

Based on the mass flow of PFOS, Ärna is the largest contributor to PFOS in Fyrisån in the base scenario followed by Kungsängsverket and Sävjaån (Figure 4.6). However, there are uncertainties in the mass flow calculations, confirmed by the large range in mass flow of PFOS for each of the sampling occasions done by Fyrisåns Vattenvårdsförbund (2020) (Table 4.2). Meaning that the magnitude of each source may not be that accurate. For example, at the sampling done the 15th of June 2020, the mass flow in the outlet of Fyrisån was 70 mg/day compared to 665 mg/day in Sävjaån and 1427 mg/day from Ärna. Since Ärna and the outlet of Sävjaån is located upstream the outlet of Fyrisån, the highest mass flow should rather be at the outlet of Fyrisån. The variations whether the highest mass flow is in the outlet of Fyrisån or not, could indicate that there are processes affecting PFOS in the river, for example, adsorption to particles could lead to a decreased mass flow, since the sampled PFOS only is the dissolved phase. Other factors that could influence the mass flow are uncertainties in the analysis results regarding PFOS and in the modelled flow data from SMHI. In addition, since the water in the rivers is in constant movement, the concentration when taking a sample can differ even if it is during the same day.

Even though the uncertainties are many, primarily regarding the modelling of PFOS entering from Fyrisån and in the mass flow calculations, it can be concluded that Fyrisån is a large contributor to PFOS in lake Ekoln, and Kungsängsverket stands for a relatively large share of that. The fact that Kungsängsverket is an important source was also concluded by Ekman (2021), and according to Xiao et al. (2012) PFOS in WWTP are in general of great concern since it is not removed in conventional wastewater treatment. In addition, Ärna is most likely an important source spreading PFOS to Lake Ekoln. This is in line with what Johansson & Helldén (2015) concluded from sampling done in their study, that there is a supply of PFOS to Fyrisån along the section where it passes Ärna. Based on the sampling done by Fyrisåns Vattenvårdsförbund (2020) and the mass flow calculations, Sävjaån contributes with a significant part of the PFOS entering Lake Ekoln via Fyrisån. According to Bonnet (2017), the spread of PFOS from Hovgården landfill to Sävjaån is relatively small, and therefore the major part of the PFOS in Sävjaån is assumed to originate from Viktoria firefighting training site. The fact that PFOS from Viktoria spread to Sävjaån was confirmed by Bergström (2014) who performed sampling of PFOS at the site.

5.2 Projected future spread of PFOS

Evaluation of how climate change and socioeconomic development affect the concentration of PFOS in Ekoln needs to be done with caution due to uncertainties in the parameters describing the future scenarios.

A comparison of the base scenario and the climate scenarios, RCP4.5 and RCP8.5, without the addition of socioeconomic scenarios indicate that the predicted consequences of climate change will not affect the concentration of PFOS in Ekoln that much (Figure 4.4). As mentioned in the result in chapter 4.2 it is not until the second part of the simulation a difference between the base scenario and the RCP-scenarios is visible, where the general pattern for all depths is that the base scenario results in slightly higher concentrations than the RCP-scenarios. An explanation to why no differences are visible in the beginning could be that the initial concentration was not changed in the RCP scenarios and the model needs time to adjust to the hydrodynamics. However, one discussion why the concentration is lower in the RCP-scenarios than in the base scenario towards the end of the simulation could be that the water flow during the winter (Dec-Feb) is much higher in the RCP-scenarios. The higher water flow could imply dilution to a greater extent during winter and early spring. Since the simulation ends in May the second year, it is difficult to evaluate the differences in the summer months. However, since the general seasonal trend for the future is that the water flow will be lower than today during spring and summer, it may lead to higher concentrations of PFOS in the RCP-scenarios than in the base scenario during these seasons. The limited simulation period is a weakness in this study.

RCP4.5 and RCP8.5 result in very similar concentrations during the year, except from the concentration at 0.5 and 15 meters depth in a period at the end of the simulation, where the drop respectively peak in concentration occurs at different times. Since the climate parameters in RCP4.5 and RCP8.5 are very similar and the mixing period occurs around the same days (Appendix E), it is hard to find a clear explanation for this difference. However, since climate change is predicted to change even more further in the future, beyond 2050, one can expect that simulation of a scenario by then, would present results with larger impacts from the climate change (Sjökvist et. al., 2015). Major differences between RCP4.5 and RCP8.5 are also expected beyond 2050. One thing to have in mind is that PFOS entering Ekoln via runoff, from other areas than those that lead water to Fyrisån, is not included in the model, and since precipitation is predicted to increase in RCP4.5 and RCP8.5, compared to the base scenario, PFOS entering Ekoln via runoff is assumed to increase. This could imply that the simulated concentration of PFOS in the future scenarios is lower than it will be in reality. On the other hand, it could be that the PFOS concentration in runoff in general is very low, and in that case an increase in runoff may lead to dilution of PFOS in the lake.

When looking at the origin of PFOS for future scenarios one can see that the climate scenarios RCP4.5 and RCP8.5 does not have a large impact neither on the total mass flow of PFOS from Fyrisån nor the contribution from each source (Figure 4.6). For the climate scenarios, it is only the changes in water flow in Fyrisån that impacts the mass flow and during summer 2050 only a slight decrease in water flow is expected. Larger differences would be visible if the mass flow was calculated during winter 2050 when the water flow is expected to be almost 50 % higher than 2017-2018 (Table 3.6), or further in the future, beyond 2050, when greater differences are expected for all seasons. However, important to be aware of is that the calculated future mass flow for the climate scenarios does not consider possible changes in PFOS concentration that may come with changed water flow. Decreased water flow may imply a higher concentration of PFOS since dilution is less. On the other hand, a decreased water flow means less stormwater runoff and thus less PFOS will reach the river. Also, important to mention is that the mass flow from Kungsängsverket does not change in the climate scenarios since the water flow at the outlet is assumed to not change due to climate change.

Changes related to the SSP-scenarios, in this study, have an obvious effect on the concentration of PFOS since the parameters that are adjusted in the model are simply the concentration of PFOS from the different sources. The results were quite predicted regarding that SSP1 decreases the concentration of PFOS a lot and that SSP5 brings a minor reduction.

SSP1 is a positive scenario from an environmental perspective, leading to a cleaner aquatic environment. This is confirmed by the results in Figure 4.4, where the concentration of PFOS in RCP4.5+SSP1 is significantly lower than for the other scenarios. Currently much focus is put on finding suitable techniques to remove all kinds of PFAS in WWTPs (Franke, 2017; EPA, n.d.). According to Ahrens (L. Ahréns, personal communication, 2 March, 2021), it is in the coming decades possible to develop techniques that remove 100 % of PFAS in water treatment plants, why the contribution from Kungsängsverket is zero in SSP1, as seen in Figure 4.5B and 4.6. This means that PFOS discharged from Kungsängsverket may not be a problem in the future, if Sweden follows the pathway of SSP1. Instead it will be PFOS leaching out from the contaminated sites that need to be put attention to. However, PFOS leaching out from contaminated sites is also expected to decrease significantly in SSP1 (Figure

4.6), since there are emerging technologies regarding remediation of soil contaminated with PFOS which probably has the potential to manage this (Mahinroosta & Senevirathna, 2020). When aiming for a scenario like SSP1, it is also important to consider the conceivable negative effects of the implemented measures. Major remediation of contaminated areas is costly and requires access to areas where there may be existing buildings or infrastructure. It also means development of treatment techniques, which requires this to be prioritised before other research areas. Since PFOS has been used, and is used, in many products, restrictions that ban all production and use of PFOS require a substitute for PFOS, and thus it is important to investigate negative effects of the possible substitutes.

If you compare RCP8.5 with RCP8.5+SSP5 in Figure 4.4, one can see that the effect of SSP5 is small. SSP5 leads to an increased load of PFOS discharged from Kungsängsverket because of population growth and urbanisation, while the prohibition of PFOS in the EU will lead to a natural reduction of PFOS leaching out from the contaminated sites. This is visible in the mass flow of PFOS (Figure 4.6), where the contribution from Kungsängsverket has increased while the contribution from Ärna and Sävjaån has decreased, leading to the contribution from Kungsängsverket being in the same order of magnitude as the contribution from Ärna. However, important to mention is that the mass flow represents the situation for a few specific observations. When looking at the simulation results, Kungsängsverket contributes with more PFOS than the other sources along Fyrisån together (Figure 4.5). The fact that the PFOS concentration is still high in Kungsängsverket even though the use and production of the substance has been prohibited in the EU since 2008, is a bit surprising. However, possible causes could be that products produced before 2008 are still in use and releasing PFOS (e.g. cookware), and imported products from other parts of the world where PFOS is not prohibited. This means that the regulations in place today, and which are assumed to remain in SSP5 until 2050, are not enough to limit the spread of PFOS to Lake Ekoln. Even though PFOS is used in parts of the world outside the EU today, the assumption in SSP5 that it will continue like that until 2050 is quite conservative. A more realistic assumption could be that the production and use of PFOS will decrease to some extent also outside the EU, leading to less consumption of PFOS per person in 2050, in the area of Ekoln, and thus the effect of population growth will not be that significant.

Based on the mentioned drawbacks of SSP1 and SSP5, both of them may be unrealistic. Maybe a scenario "in between" is something more reasonable to expect. This should be a scenario that has enough restrictions and regulations to assure clean and safe water in Ekoln, but at the same time is sustainable from an economic perspective.

5.3 The performance of the model

The model was not calibrated or validated in this study. However, the hydrodynamics of the model were calibrated for 2018 by Lindqvist (2019). The calibration was successful, and the adjustments improved the model's performance in simulating vertical temperature profiles. Further Lindqvist (2019) conducted statistical validation of the model for both 1989 and 2018 and concluded that the model performed better for 2018, where the validation resulted in a clear correlation between measured and simulated vertical temperature profiles. A comparison of the measured and simulated vertical temperature profiles at Vreta Udd, from this study, also indicates that the performance of the model is good, considering the hydrodynamics (Appendix H, Figure

H1). However, the study by Lindqvist (2019) also concluded that the model did have some issues in simulating the heating and cooling in different times of the year, and also in simulating the depth of the epilimnion. One thing that indicates that the model in this study captures the mixing of the lake relatively well is that the observed concentrations of PFOS were approximately the same at all depths when mixing took place in the simulation results (Figure 4.3). Both Lindqvist (2019) and Ekman (2021) discuss the fact that the wind data used in the model are measured at a location that may not represent the wind conditions in the area of Lake Ekoln, which can be an explanation to the differences between measured and simulated water temperature. The deviation in the temperature could affect the motions in the water in the lake which hence could cause that the simulations do not capture the distribution of PFOS in the lake completely in line with reality. However, if there would have been processes included in the model that are dependent on the temperature, it would have been more important to analyse consequences of the deviation.

5.4 Water quality according to regulations

As discussed, none of the future scenarios analysed in this study bring an increase of PFOS in Ekoln. However, when discussing the conditions for drinking water, it is important to include all kinds of PFAS that are present in the lake. The recommended value of PFAS that drinking water producers in Sweden have to relate to, regarding when to act, is presented as a summarized value of the concentration of 11 different PFAS, where PFOS is included (Livsmedelsverket, 2021a). Measured values of these specific PFAS are available from Vreta Udd in 2019 and 2020, where the maximum value is 10 ng/l. The recommended value for drinking water producers to act is 90 ng/l which is much higher than the measured values at Vreta Udd. This indicates that the situation today does not mean a risk of using Ekoln as a drinking water source, and if the future trend for all PFAS will follow the same trend as presented for PFOS in this study it will not be a risk. However, the trend for all PFAS is not assumed to follow the one for PFOS since several of them are still in use, also research regarding them is lacking, which means the effects are still uncertain. This means that research regarding PFAS has to proceed and be followed up. Further, when comparing the results with the European benchmark for inland waters to be classified with good chemical status (0.65 ng/l), all scenarios except for RCP4.5+SSP1 exceed the benchmark, signifying that more research is needed (Europaparlamentets och rådets direktiv 2013/39/EU).

5.5 Uncertainties and simplifications

When analysing the simulated values, it is important to be aware that the concentration of PFOS coming from Fyrisån are processed from observations outside the simulation period. Due to few measurements and the fact that there is no clear seasonal trend in the available data, a constant average mass flow of PFOS coming from Fyrisån was used in the modelling. Even though a varying flow was used to derive the concentrations, it is an uncertainty factor that the concentration from Fyrisån is processed from a constant mass flow, since it implies that the model does not capture variations in incoming PFOS that occur in reality. Since the measurements are few also at Vreta udd, this is a limiting factor when comparing simulated values with measurements. Measurements are made on four occasions at Vreta Udd outside the simulation period; from 2019 and 2020 and these range between 0.81 and 4.4. This span covers the measured values at Vreta Udd during the simulation period, 2017 and 2018, which range between 1.2 and 4.5 ng/l, meaning that the order of magnitude of the observed values in the results are supported by other measurements. However, the lack of measurements of PFOS to compare with the simulated values remains to be a limiting factor when evaluating the results. Important to mention is also that most of the results in this study, and thus the discussion in this report, refer to Vreta Udd, since this is the only location with measured values of PFOS. It would have been interesting to also have measurements of PFOS in other parts of the lake, in order to better evaluate the spread within the lake. Worth mentioning is also that there are uncertainties related to the measurements of PFOS. As an example; for the measurements of PFOS in the outlet of Fyrisån 2014-2015, the recovery was 78% (Gago-Ferrero et al., 2017). Even if the recovery is in the acceptable range for the method of the measurement (>50% and <150%), the accuracy of the measurements is important to be aware of when analysing the results (Sörengård et al., 2019).

The values used to represent the SSP-scenarios include a lot of uncertainties, they are derived from assumptions summarised from literature from different sources which do not have the purpose to describe SSP-scenarios. Regarding the values describing RCP scenarios, the data are retrieved from literature with the purpose of describing these scenarios. However, regarding the values used in this study, of how precipitation and temperature will change in the future, there are uncertainties related to that only one regional climate model was used. According to Petter Lind from SMHI (Personal communication, 16 March, 2021), it is preferable to use results from several climate models to take uncertainties related to the modelling into account. There is data available from more models, e.g. from a project called EURO-CORDEX. However, this requires that you can handle the data format NetCDF, which was not the case in this study. Due to the effort, and time, that was assumed to be required for this, more climate data was not prioritised. The values used in this study for predicted change of air temperature are lower than values that can be derived from diagrams in a report by Sjökvist et. al. (2015). However, the changes in temperature until 2050, presented in table 3.6, is quite small and did not affect the situation with PFOS in this study that much. If a modelled scenario would be beyond 2050 when the changes are expected to be larger and differ more between the RCP scenarios, it would be more important to include climate data from several sources. The parameter regarding climate change that can be assumed to have the major effect in this study is the water flow, which will increase by approximately 50 % during winter for both RCP scenarios in 2050, while the change during the other seasons is less (Table 3.6). The values of change in water flow, used in this study, is as mentioned earlier in the report, obtained from reading diagrams, which is an uncertainty factor (Sjökvist et. al., 2015). However, the report with the diagrams has been used, with the same purpose as in this study, in previous studies (Lindqvist et al., 2019; Uppsala Kommun, 2018).

A sensitivity analysis of the parameters used to describe the scenarios would make it possible to discuss potential consequences of uncertainties in the data. The impact of uncertainties in the parameters used to describe the socioeconomic scenarios is easier to understand since it is either a decrease or increase of concentration of PFOS from the sources. How changes in the parameters describing climate change affect the results is harder to understand without further analysis. A sensitivity analysis in terms of changing e.g. air temperature or precipitation and evaluating the consequences would provide an indication of how important the uncertainties are to include in the evaluation of the results. However, due to time constraints it was not done in this study. The conclusion that socioeconomic development has larger impact on the contamination level in aquatic environments than climate change has, is drawn also in previous studies (Islam et al., 2018; Samuelsson & Östberg, 2020).

One simplification in this study is that only PFOS in the dissolved phase is investigated, not the total amount of PFOS. As discussed previously in the report, PFOS is also found attached to particles, in aquatic environments, which means that there is probably higher total concentration of PFOS in the lake than presented in the results of this study. However, the available measurements of PFOS are only in the dissolved phase, except for some measurements in sediment, which limited the analysis. The fact that only PFOS in the dissolved phase was investigated made it difficult to include the identified processes; sedimentation and bioaccumulation in fish. The difficulties to modelling processes affecting PFOS is also concluded by Naidu et al. (2020), who states that lack of data regarding physicochemical properties and PFOS affinity for phase interfaces complicates the modelling. Not including sedimentation could have implied that the simulated concentration of PFOS is too high, since some part of the PFOS entering the lake in the dissolved phase, in reality attaches to particles and settles (Kong et al., 2018; Ahrens et al., 2011). On the other hand, some part of the PFOS entering the lake in the particulate phase, which is not included in the model, could desorb and increase the concentration of PFOS in the dissolved phase. And further, resuspension of the sediment brings more particles in the water from where PFOS can desorb and increase the concentration of dissolved phase as well. Not including bioaccumulation could have implied that the simulated concentrations are higher than in reality, since some part is taken up by fishes (Berger et al., 2009; Stockholms Stad, n.d.). In a previous study by Kong et al. (2018) it was concluded that including bioaccumulation in fish when modelling PFOS is an important step to better understand the fate of PFOS in aquatic environments. Although, just as in this study, Kong et al. (2018) did not include bioaccumulation due to lack of relevant parameters regarding uptake in biota. However, it would have been even more important to focus on this if the study included investigation of the human health effects and risks related to eating fish from Lake Ekoln. The fact that sedimentation of particulate PFOS is present in Lake Ekoln was confirmed by sampling of PFOS in sediment done by Tjensvoll (2018), and since PFOS have been detected in fish from Görväln, close to Ekoln, bioaccumulation probably occurs in the lake (Stockholms Stad, n.d.). However, it is difficult to evaluate how much and in which direction the simplification of not including these processes affects the results regarding spread of dissolved PFOS.

5.6 Suggestions for future research

As mentioned briefly, simulations for scenarios further in the future would be interesting since climate change is predicted to bring more significant changes in precipitation, temperature and water flow, and thus probably have a larger impact on the spread of PFOS. Further, a longer simulation period, than in this study (1.2 years), would make it easier to see potential seasonal patterns in the results. Since the influence of the initial PFOS was large in the first half of the simulation, it was difficult to draw any reliable conclusions whether the PFOS in the inflows in the model were representative of reality. In the second half of the simulation, the initial concentration of PFOS influences less, but in that period the lack of measurements limits the discussion. A longer simulation period would remove the effect of the initial concentration, and thus give a better understanding of the performance of the model regarding inflow and spread of PFOS. However, constraining factors are the computational time and the limited observations of PFOS to compare the simulation results with.

In order to improve the modelling of PFOS in lake Ekoln in the future, more measurements of PFOS are required both in the inflows and in the lake, to be able to identify all sources and to evaluate the model performance regarding spread of PFAS. More continuous measurements in Fyrisån would make it possible to describe variations in inflowing PFOS that probably occur in reality. Also, measurements in the other rivers; Örsundaån, Sävaån and Hågaån would improve the knowledge regarding pathways and sources of PFAS to lake Ekoln. Further, measurements of particulate PFAS are recommended, in order to include sedimentation and also bioaccumulation and evaluate the effect of those processes.

The modelling in this study was limited to include only PFOS. In future modelling it would be interesting to investigate other kinds of PFAS, to analyse different behaviour of the substances. To analyse different behaviour of different PFAS it is also required to include processes affecting the fate and transport of PFAS. Since PFOS is a long chained PFAS, it could be interesting to analyse a short chained since these are known to have other properties e.g. considering adsorption to particles. One short chained PFAS that could be of interest is PFHxS since it is one of those that contribute the most to human exposure of PFAS, it has been detected in high concentrations in fish, and is planned to be included in the Stockholm convention in 2022 (Livsmedelsverket, 2021b; Norström et al., 2015; Kemikalieinspektionen 2021c).

This study has improved the knowledge regarding which sources are important considering the spread of PFOS in Lake Ekoln. The results can be used as a basis for further investigations regarding where to implement measures in order to reduce the spread of PFOS in the future.

6 Conclusion

This study has investigated the spread of PFOS in the area of Lake Ekoln. Pathways, sources, and processes affecting the spread of PFOS have been identified. The current and future spread considering climate change and socioeconomic development have been analysed.

- Fyrisån is the major pathway for PFOS entering Lake Ekoln, while the contribution from Uppsalaåsen and precipitation is almost negligible. Whether PFOS enters Ekoln via Örsundaån, Sävaån and Hågaån is not fully investigated.
- The major sources of PFOS are Kungsängsverket, Ärna airport and the Viktoria firefighting site. Other possible sources in the area are OWTS, landfills and industrial activities, which can enter the lake via the rivers, surface runoff or groundwater.
- Processes that affect the fate and transport of PFOS are sedimentation and bioaccumulation. However, these processes were not included in the modelling in this study due to time constraints and limited knowledge regarding PFOS in the particulate phase and uptake in biota.
- Climate change predicted until 2050 are assumed to not affect the situation with PFOS in Lake Ekoln much. Socioeconomic development is expected to affect more, where a scenario in line with SSP5 results in a minor decrease of PFOS, while in a scenario like SSP1, the decrease is significantly larger. Urbanisation may increase the emission of PFOS if the consumption continues as today. Remediation at the contaminated sites and developed treatment techniques to remove PFOS in Kungsängsverket are assumed to be important measures to reduce the emission from the sources.

According to the current regulations of PFAS in drinking water, there is no risk in using the water in Lake Ekoln as drinking water today and since none of the future scenarios in this study bring an increase of PFOS, this indicates that there will be no risk in the future either. However, there are uncertainties in the modelling that could possibly lead to an underestimation of PFOS concentration, which is important to be aware of. Further, the trend for all PFAS is not assumed to follow the same trend as PFOS, since some are still in use, while the use of PFOS has been restricted in the EU since 2008. In addition, the EU is working on new benchmarks regarding PFAS in drinking water and the requirements in the future may be stricter. This means that research regarding the spread of PFAS in Lake Ekoln needs to proceed.

7 References

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Appendix A

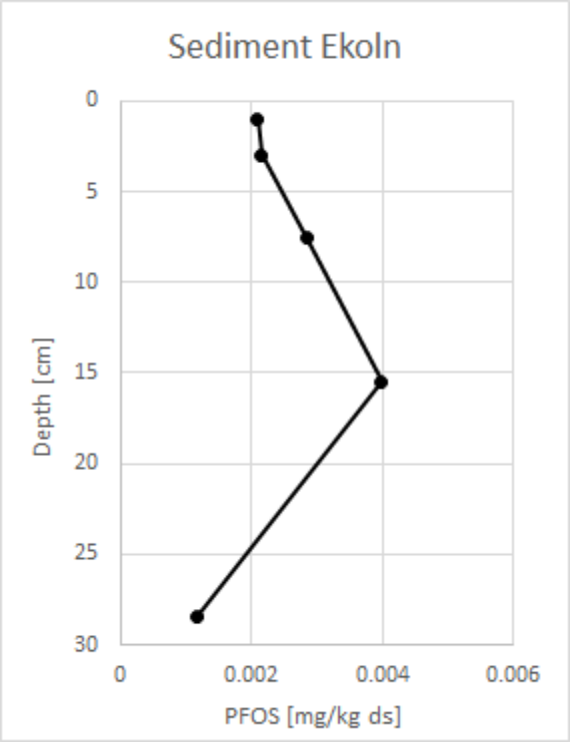
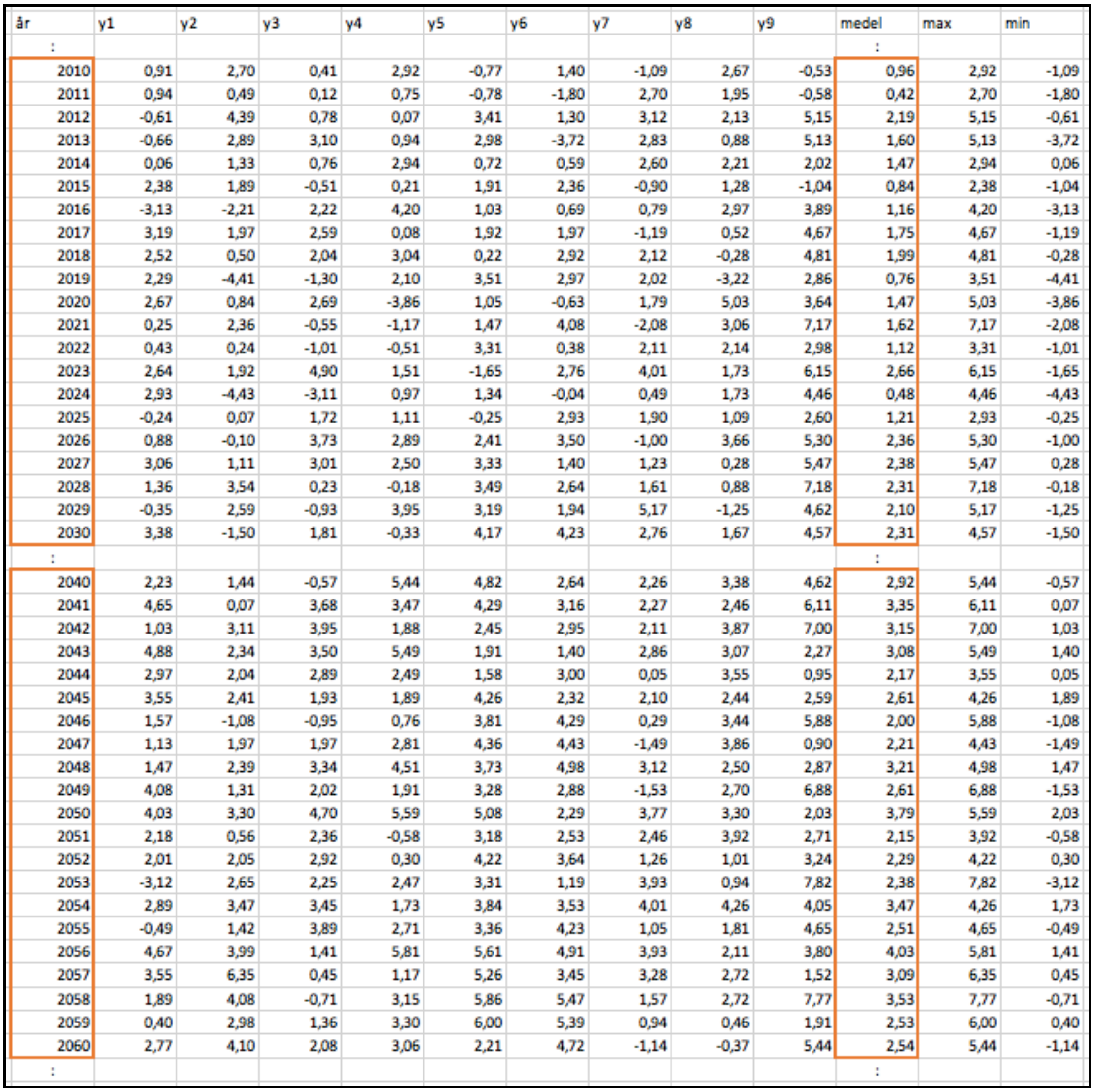


Figure A1 *Variation of PFOS concentration with depth in sediment in Lake Ekoln, based on measurements by Tjensvoll (2018). One measurement is taken at depth 40-43 cm; however the concentration was below detection limit, and therefore not included in the figure.*

Appendix B

The values used for the prediction of how the air temperature and precipitation will change until 2050, presented in Table 3.6 in the report, was derived from climate research made by SMHI (SMHI, 2021). On the website which the reference refers to, there are excel documents of climate data available to download where you can choose county, season, climate index, and RCP-scenario. The excel documents present changes from the reference period, 1961-1990, until each year up to 2100.

An explanation of how the value for the change in air temperature during winter, for RCP4.5, was derived is presented here. The other values in Table 3.6 in the report were derived in the same way, and all excel data was downloaded from the same webpage (SMHI, 2021). In Figure B1, parts of the excel document regarding change in air temperature in the County of Uppsala, during winter, for RCP4.5, is presented.



år	y1	y2	y3	y4	y5	y6	y7	y8	y9	medel	max	min
:										:		
2010	0,91	2,70	0,41	2,92	-0,77	1,40	-1,09	2,67	-0,53	0,96	2,92	-1,09
2011	0,94	0,49	0,12	0,75	-0,78	-1,80	2,70	1,95	-0,58	0,42	2,70	-1,80
2012	-0,61	4,39	0,78	0,07	3,41	1,30	3,12	2,13	5,15	2,19	5,15	-0,61
2013	-0,66	2,89	3,10	0,94	2,98	-3,72	2,83	0,88	5,13	1,60	5,13	-3,72
2014	0,06	1,33	0,76	2,94	0,72	0,59	2,60	2,21	2,02	1,47	2,94	0,06
2015	2,38	1,89	-0,51	0,21	1,91	2,36	-0,90	1,28	-1,04	0,84	2,38	-1,04
2016	-3,13	-2,21	2,22	4,20	1,03	0,69	0,79	2,97	3,89	1,16	4,20	-3,13
2017	3,19	1,97	2,59	0,08	1,92	1,97	-1,19	0,52	4,67	1,75	4,67	-1,19
2018	2,52	0,50	2,04	3,04	0,22	2,92	2,12	-0,28	4,81	1,99	4,81	-0,28
2019	2,29	-4,41	-1,30	2,10	3,51	2,97	2,02	-3,22	2,86	0,76	3,51	-4,41
2020	2,67	0,84	2,69	-3,86	1,05	-0,63	1,79	5,03	3,64	1,47	5,03	-3,86
2021	0,25	2,36	-0,55	-1,17	1,47	4,08	-2,08	3,06	7,17	1,62	7,17	-2,08
2022	0,43	0,24	-1,01	-0,51	3,31	0,38	2,11	2,14	2,98	1,12	3,31	-1,01
2023	2,64	1,92	4,90	1,51	-1,65	2,76	4,01	1,73	6,15	2,66	6,15	-1,65
2024	2,93	-4,43	-3,11	0,97	1,34	-0,04	0,49	1,73	4,46	0,48	4,46	-4,43
2025	-0,24	0,07	1,72	1,11	-0,25	2,93	1,90	1,09	2,60	1,21	2,93	-0,25
2026	0,88	-0,10	3,73	2,89	2,41	3,50	-1,00	3,66	5,30	2,36	5,30	-1,00
2027	3,06	1,11	3,01	2,50	3,33	1,40	1,23	0,28	5,47	2,38	5,47	0,28
2028	1,36	3,54	0,23	-0,18	3,49	2,64	1,61	0,88	7,18	2,31	7,18	-0,18
2029	-0,35	2,59	-0,93	3,95	3,19	1,94	5,17	-1,25	4,62	2,10	5,17	-1,25
2030	3,38	-1,50	1,81	-0,33	4,17	4,23	2,76	1,67	4,57	2,31	4,57	-1,50
:										:		
2040	2,23	1,44	-0,57	5,44	4,82	2,64	2,26	3,38	4,62	2,92	5,44	-0,57
2041	4,65	0,07	3,68	3,47	4,29	3,16	2,27	2,46	6,11	3,35	6,11	0,07
2042	1,03	3,11	3,95	1,88	2,45	2,95	2,11	3,87	7,00	3,15	7,00	1,03
2043	4,88	2,34	3,50	5,49	1,91	1,40	2,86	3,07	2,27	3,08	5,49	1,40
2044	2,97	2,04	2,89	2,49	1,58	3,00	0,05	3,55	0,95	2,17	3,55	0,05
2045	3,55	2,41	1,93	1,89	4,26	2,32	2,10	2,44	2,59	2,61	4,26	1,89
2046	1,57	-1,08	-0,95	0,76	3,81	4,29	0,29	3,44	5,88	2,00	5,88	-1,08
2047	1,13	1,97	1,97	2,81	4,36	4,43	-1,49	3,86	0,90	2,21	4,43	-1,49
2048	1,47	2,39	3,34	4,51	3,73	4,98	3,12	2,50	2,87	3,21	4,98	1,47
2049	4,08	1,31	2,02	1,91	3,28	2,88	-1,53	2,70	6,88	2,61	6,88	-1,53
2050	4,03	3,30	4,70	5,59	5,08	2,29	3,77	3,30	2,03	3,79	5,59	2,03
2051	2,18	0,56	2,36	-0,58	3,18	2,53	2,46	3,92	2,71	2,15	3,92	-0,58
2052	2,01	2,05	2,92	0,30	4,22	3,64	1,26	1,01	3,24	2,29	4,22	0,30
2053	-3,12	2,65	2,25	2,47	3,31	1,19	3,93	0,94	7,82	2,38	7,82	-3,12
2054	2,89	3,47	3,45	1,73	3,84	3,53	4,01	4,26	4,05	3,47	4,26	1,73
2055	-0,49	1,42	3,89	2,71	3,36	4,23	1,05	1,81	4,65	2,51	4,65	-0,49
2056	4,67	3,99	1,41	5,81	5,61	4,91	3,93	2,11	3,80	4,03	5,81	1,41
2057	3,55	6,35	0,45	1,17	5,26	3,45	3,28	2,72	1,52	3,09	6,35	0,45
2058	1,89	4,08	-0,71	3,15	5,86	5,47	1,57	2,72	7,77	3,53	7,77	-0,71
2059	0,40	2,98	1,36	3,30	6,00	5,39	0,94	0,46	1,91	2,53	6,00	0,40
2060	2,77	4,10	2,08	3,06	2,21	4,72	-1,14	-0,37	5,44	2,54	5,44	-1,14
:										:		

Figure B1 Change in air temperature from the reference period (1961-1990), until 2010-2030, and 2040-2060, during winter, for RCP4.5, in the County of Uppsala. The values are presented as changes in degrees Celsius.

To get the projected changes only between the base scenario, 2017-2018, and the future scenarios, 2050, the change predicted to occur between the reference period and the base scenario was subtracted from the change predicted between the reference period and 2050. Since the values in the modelled data fluctuate much from one year to another, the average value between 2010-2030 was used for the base scenario and the average value between 2040-2060 was used for the future scenario. The different columns in the excel documents, with title y1-y9, present retrieved results from the regional model using values from the nine different global climate models. In this study the average value between those was used, presented in the column with title "medel", which is marked in Figure B1. The values describe change in degree Celsius [℃].

Average value 2010-2030: 1.58 ℃
Average value 2040-2060: 2.84 ℃
Predicted change between base scenario and future scenario: 2.84-1.58 = 1.26 ℃

Appendix C

Diagrams that were used in the projections of how the flow will change in Örsundaån until 2050 for RCP4.5 and RCP8.5. These diagrams were also used for the change of flow in Sävaån which is motivated in the report.

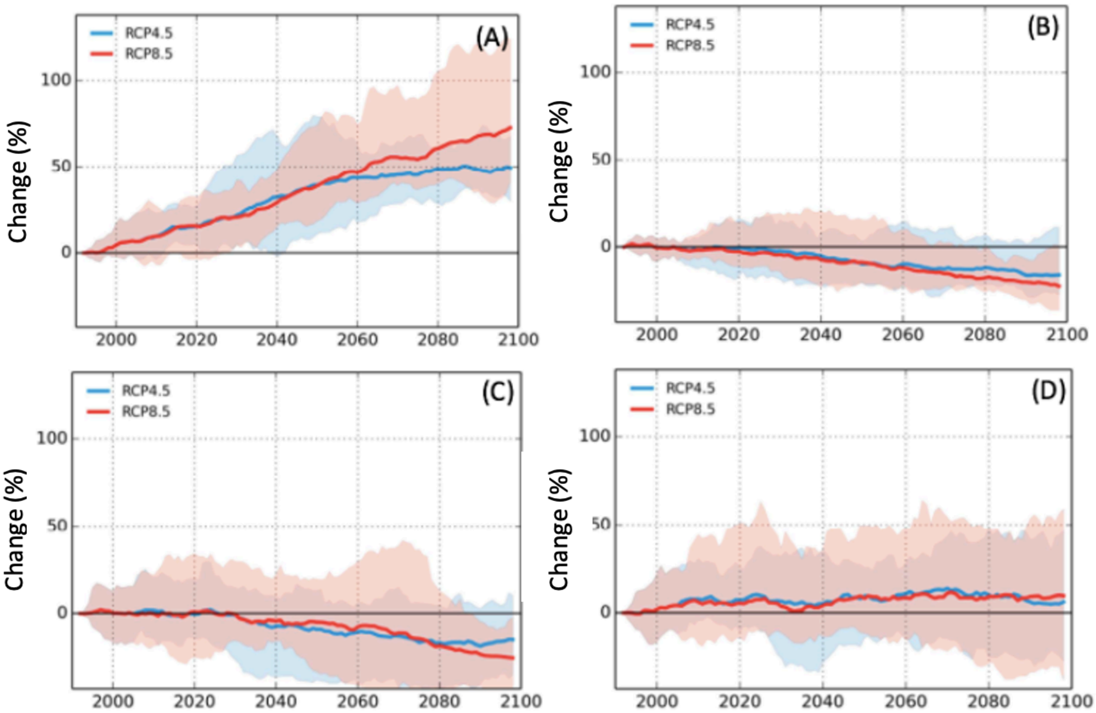


Figure C1 *Change in average flow in Örsundaån during winter (A), spring (B), summer (C), and autumn (D) for RCP4.5 and RCP8.5 (Sjökvist et al., 2015).*

Appendix D

Differences in precipitation, temperature and flow data for the base scenario and the future scenarios RCP4.5 and 8.5 is presented in Figure D1-4. Precipitation and water flow for the future scenarios is calculated by adding the change in percentage for each season to the time series for the base scenario, while air temperature is calculated by adding the change in degrees [ºC] for each season. The general trend for precipitation and temperature is that it will increase for the future scenarios, and the increment is larger for RCP8.5 compared to RCP4.5. The water flow will increase during autumn and winter, while it will decrease during spring and summer for the future scenarios. The greatest difference compared to the base scenario is the flow during winter, which will increase almost 50 % for the future scenarios.

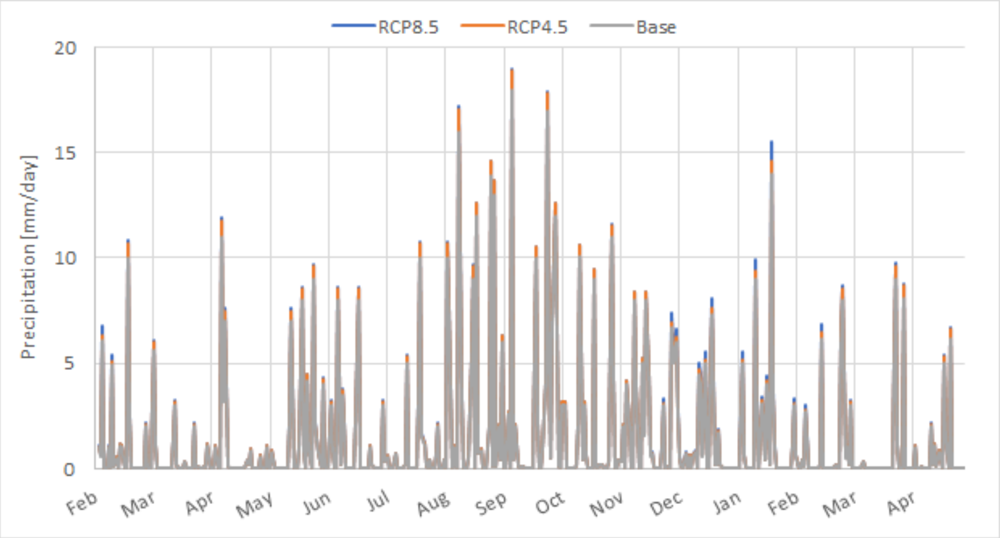


Figure D1 Variations in precipitation for the base scenario 2017-2018 (grey), and the future scenarios RCP4.5 (orange) and RCP8.5 (blue) at year 2050.

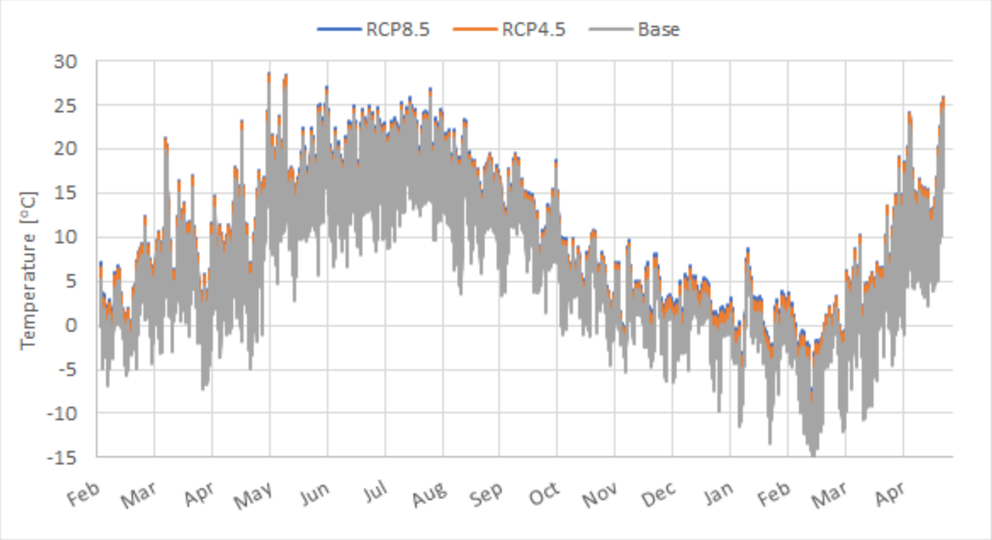


Figure D2 Variations in air temperature for the base scenario 2017-2018 (grey), and the future scenarios RCP4.5 (orange) and RCP8.5 (blue) at year 2050.

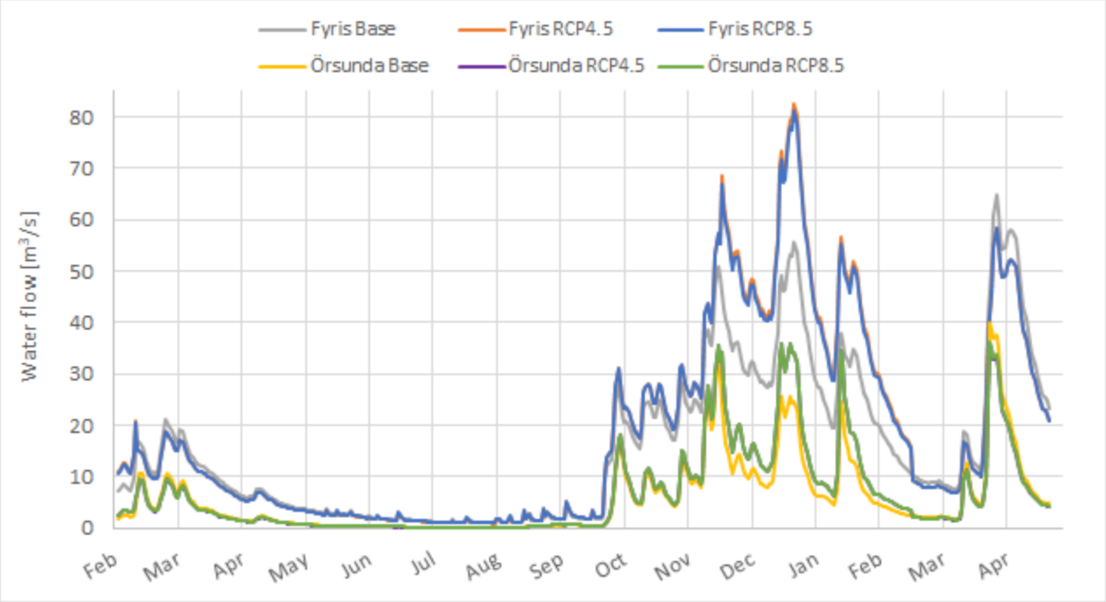


Figure D3 *Variations in flow for Fyrisån and Örsundaån for the base scenario 2017-2018 and the future scenarios RCP4.5 and RCP8.5 at the year 2050. RCP4.5 is almost not visible since the flow is very similar to RCP8.5.*

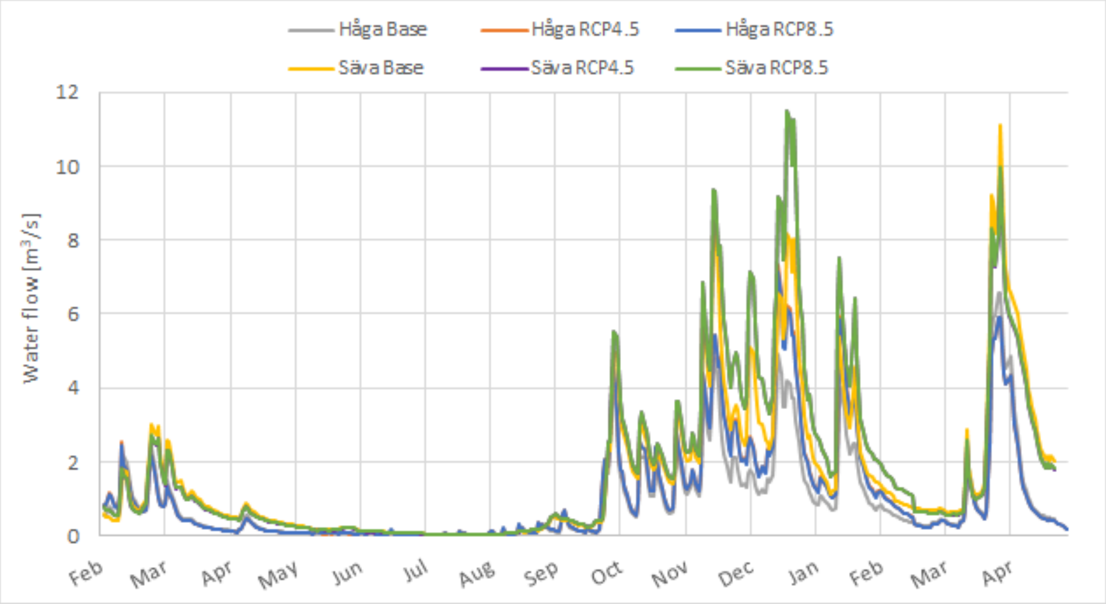


Figure D4 *Variations in flow for Hågaån and Sävaån for the base scenario 2017-2018 and the future scenarios RCP4.5 and RCP8.5 at the year 2050. RCP4.5 is almost not visible since the flow is very similar to RCP8.5. Also, note that the y-axis is of different scale than Figure D3.*

Appendix E

Figure E1 presents the simulated water temperatures at different depths. The grey areas represent the period when mixing of the lake takes place. The black rectangles in (B) and (C) represent the mixing periods of the base scenario and are presented to visualize the changing in mixing pattern between the base scenario and the RCPs. The most distinct differences between the base scenario and the future scenarios is that the mixing period in the beginning of the simulation is longer in the base scenario, and the mixing period in the end of the simulation starts earlier in RCP4.5 and 8.5 compared to the base scenario. The mixing in the autumn (October-November), is a little shorter in the base scenario compared to the future scenarios. The mixing in RCP4.5 and RCP8.5 is very similar to each other

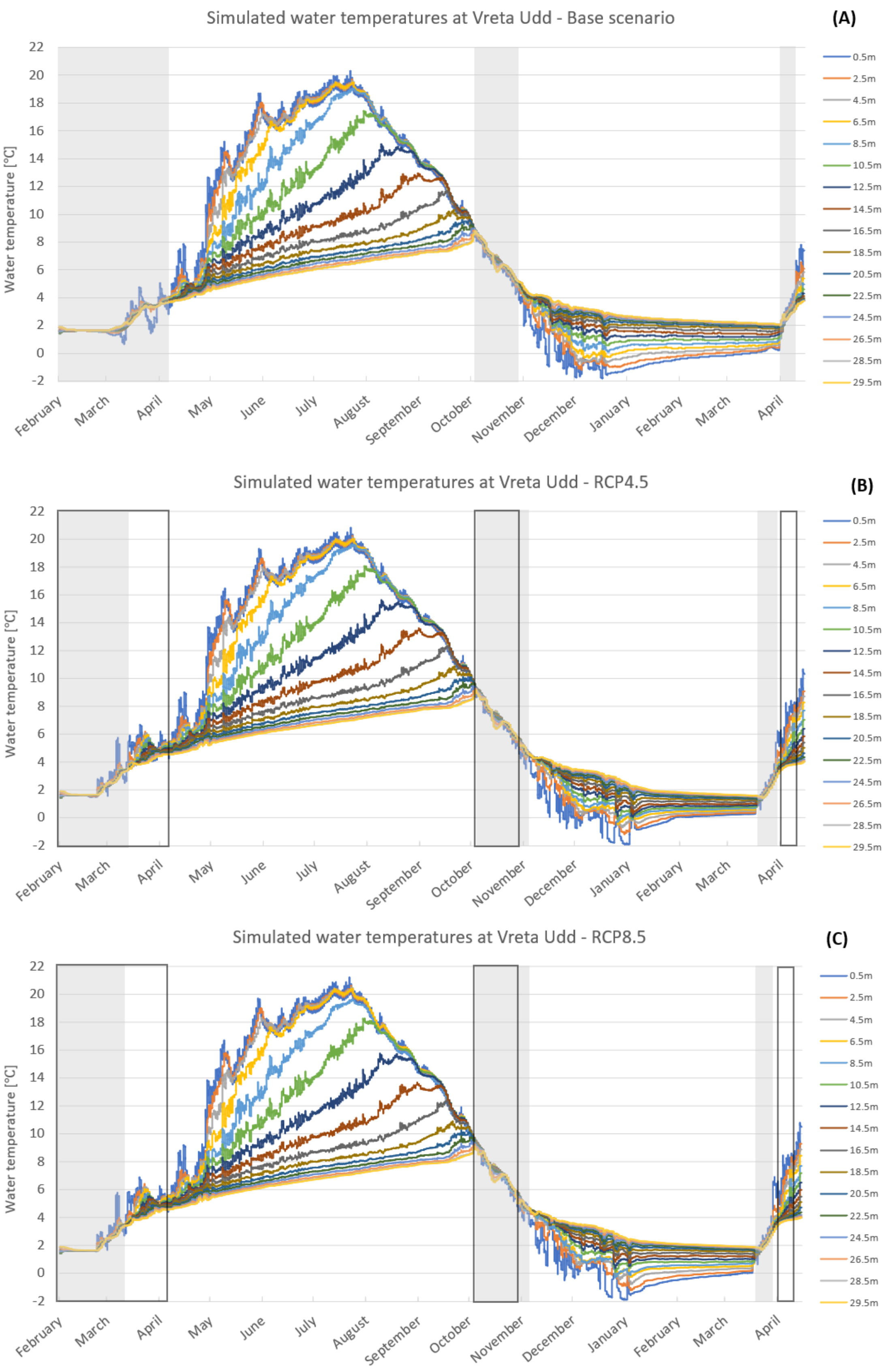


Figure E1 *Simulated water temperatures at different depths for the base scenario (A), RCP4.5 (B) and RCP8.5 (C). The grey areas represent the periods when mixing takes place.*

Appendix F

Figure F1-3 presents the total concentration of PFOS together with the concentration separated in terms of origin at 0.5 and 30 meters depth for the base scenario (Figure F1), RCP4.5+SSP1 (Figure F2) and RCP8.5+SSP5 (Figure F3).

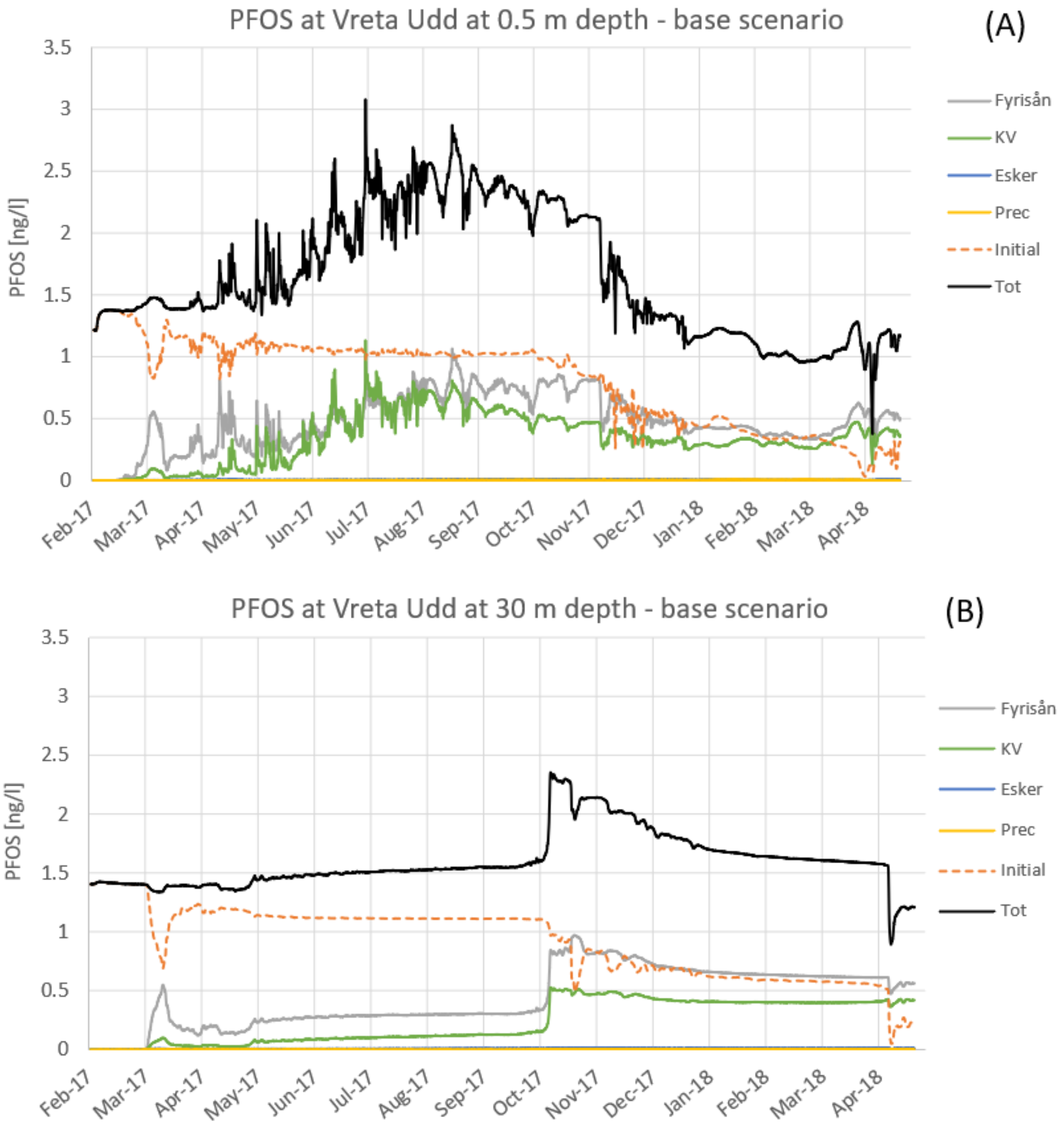
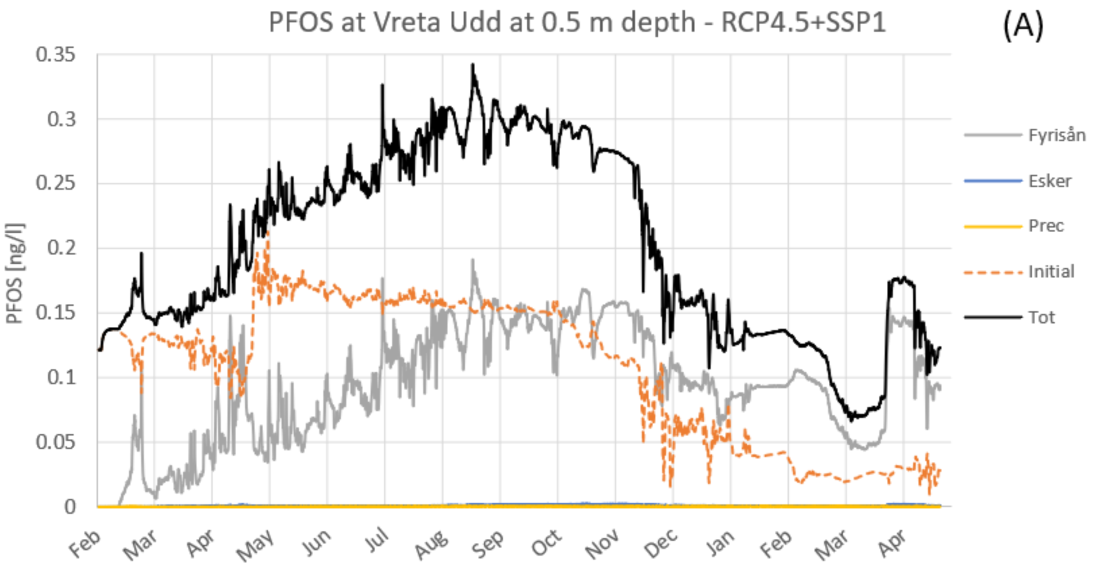


Figure F1 Total PFOS concentration and concentration separated in terms of origin at 0.5 m (A) and 30 m (B) depth for the base scenario.



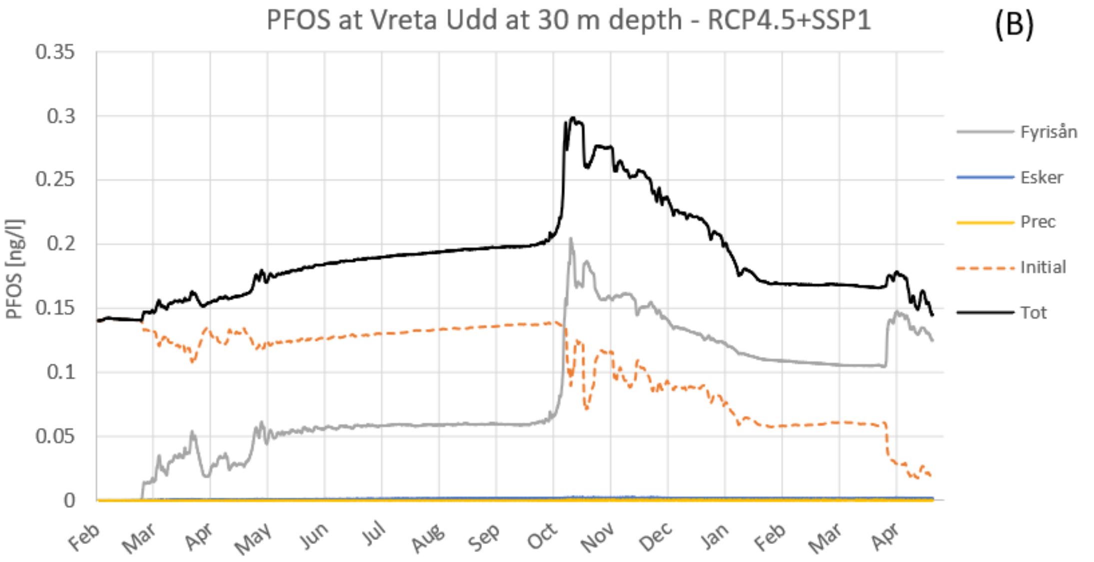


Figure F2 Total PFOS concentration and concentration separated in terms of origin at 0.5 m (A) and 30 m (B) depth for scenario RCP4.5+SSP1.

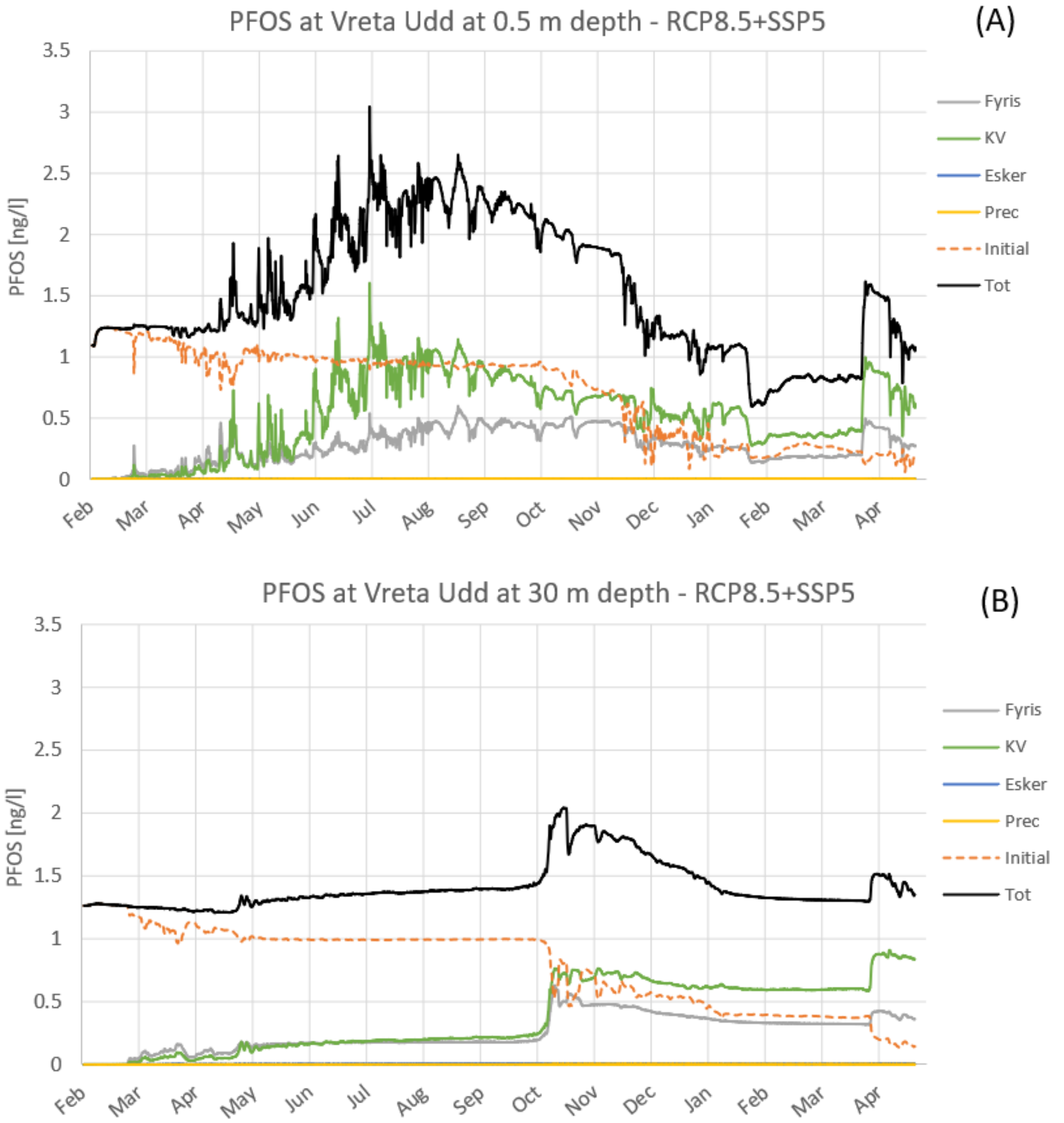


Figure F3 Total PFOS concentration and concentration separated in terms of origin at 0.5 m (A) and 30 m (B) depth for scenario RCP8.5+SSP5.

Appendix G

Table G1 *Mass flow of PFOS [mg/day] from Kungsängsverket, between January 2019 and August 2020. The mass flow is based on average concentrations and water flow for each month. In July 2019, sampling of PFOS is missing.*

Month	Mass flow [mg/day]
January 2019	968
February 2019	813
March 2019	1294
April 2019	927
May 2019	1285
June 2019	1163
July 2019	-
August 2019	755
September 2019	681
October 2019	1132
November 2019	668
December 2019	992
January 2020	609
February 2020	520
March 2020	704
April 2020	433
May 2020	481
June 2020	443
July 2020	399
August 2020	431

Appendix H

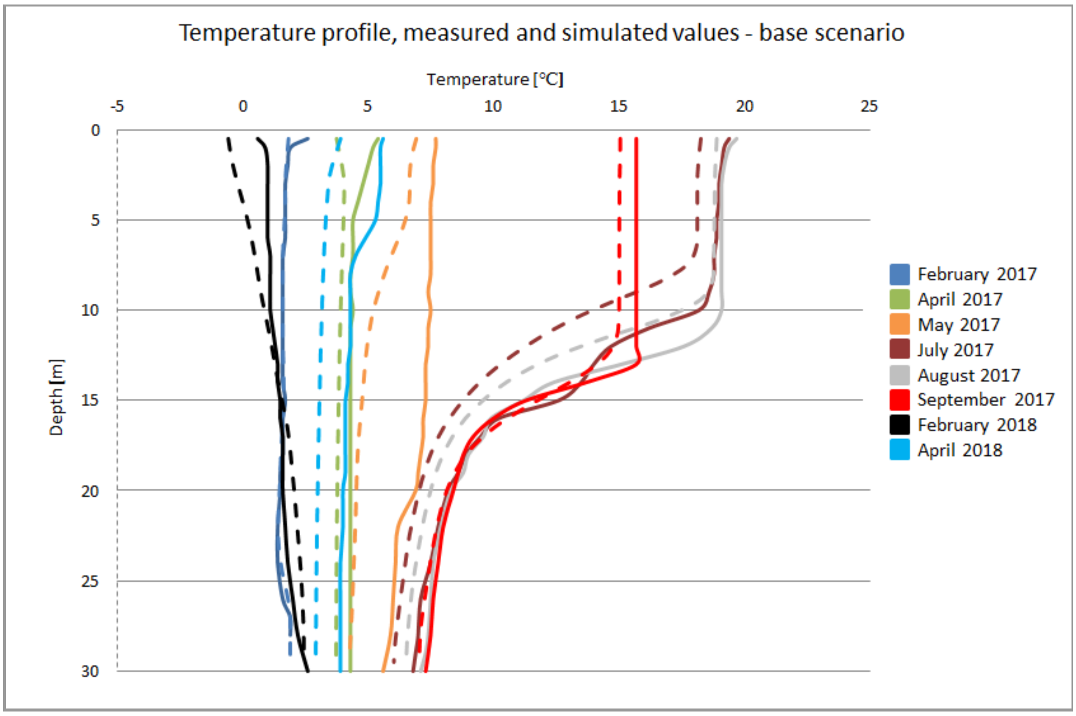


Figure H1 *Temperature profile of measured values (solid lines) and simulated values (dashed lines) for the base scenario.*

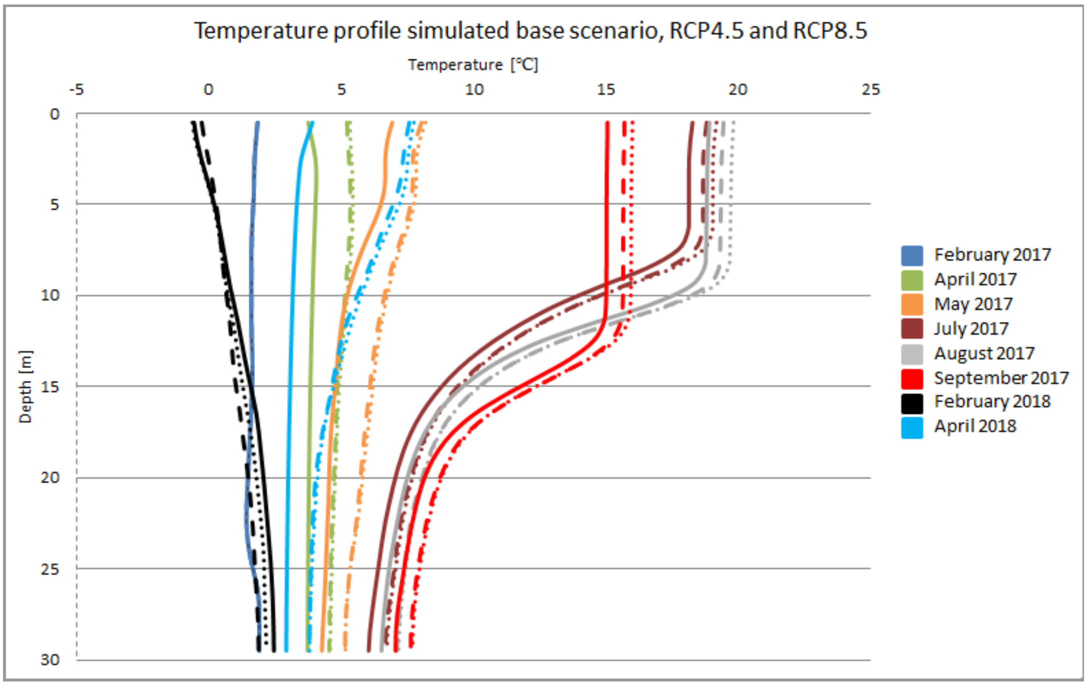


Figure H2 *Simulated temperature profile of base scenario (solid lines), RCP4.5 (dashed lines), and RCP8.5 (dotted lines).*

Overall, the temperature differs more closer to the surface than closer to the bottom, during the year. In most of the months, the simulated values are a bit lower than the measured ones. In February 2017, the measured and simulated values are very similar, and in February 2018 the simulated values are lower than the measured in the upper part of the lake but higher closer to the bottom. Observe that there are major differences between the temperature in the upper part of the lake and the lower part in July, August and September, than in the other months. All values in Figure H2 are simulated values, for the base scenario and the climate scenarios RCP4.5 and RCP8.5. The general pattern is that the climate scenarios result in slightly higher temperatures than the base scenario in the vertical profile of the lake, however February 2017 does not result in any noticeable differences and in February 2018, the RCP8.5 results in higher temperatures than in the base- and RCP4.5 scenario close to the surface, and RCP4.5 and RCP8.5 results in lower temperatures than in the base scenario closer to the bottom. Notice that the largest differences between the base- and the climate scenarios appear close to the surface in April 2018, and in the middle of the vertical profile in May and July 2017.

DEPARTMENT OF ARCITECHTURE AND CIVIL ENGINEERING

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