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Swedish University of Agricultural Sciences

Faculty of Natural Resources and
Agricultural Sciences

Removal of poly- and perfluoroalkyl substances from water using the BDD electrode.

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Removal of poly- and perfluoroalkyl substances from water using the BDD electrode

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Abstract

Poly- and perfluoroalkyl substances (PFASs) have been used for a wide range of purposes due to their unique properties. Unfortunately, these compounds have been associated with several adverse health effects and high persistence in the environment, therefore, creating a need for their elimination from the environment. In this study, electrochemical oxidation using boron-doped diamond electrodes (BDD) was tested for its treatment efficiency of 12 PFAS. Three different water types were used that is: Millipore, dissolved organic carbon (DOC) and membrane reject water. Both Millipore and DOC water were spiked and tested with three different current densities that is: 0.95 mA cm^{-2} , 4.8 mA cm^{-2} and 12 mA cm^{-2} . Quality assurance tests on the electrode revealed that the electrode was consistently efficient throughout the study and that pH change influenced PFAS removal. In this study, 12 mA cm^{-2} proved to be the most efficient tested current density achieving $> 80\%$ removal for PFASs except perfluorohexane carboxylate (PFHxA) (79%) and perfluorobutane carboxylate (PFBS) (34%) after two hours. At all current densities used, perfluoropentane carboxylate (PFPeA), a compound that was not spiked, was observed to have been formed in different quantities. In majority of the trials, PFAS removal was dependent on perfluorocarbon chain length and was found to increase with increase in perfluorocarbon chain length. The effect of water type on PFAS removal was dependent on the PFAS type. For example, while PFBS removal was enhanced in DOC water, for most of the compounds it was decreased. PFAS removal from membrane reject water was greater than that from DOC water except for PFHxA. In this study, short chained carboxylates had lower removals. This could be due to the treatment pathway undertaken by the BDD. This study examines factors that should be examined to transfer the treatment from a laboratory scale to water treatment plants. Further studies may examine wider ranges of water types as well as provide an account of all the products produced during water treatment.

Keywords: PFAS, drinking water, membrane reject water, advanced oxidation processes, electrochemical treatment and BDD electrodes.

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Abbreviations

AFFF	Aqueous film forming foams
AOPs	Advanced oxidation processes
BDD	Boron doped diamond
DOC	Dissolved organic carbon
DOM	Dissolved organic matter
FASAs	Perfluorinated sulphonamides
FOSA	Perfluorooctane sulphonamide
GAC	Granular activated carbon
PFAAs	Perfluoroalkyl acids
PFAS	Poly and perfluoroalkyl substances
PFBA	Perfluorobutane carboxylate
PFBS	Perfluorobutyric sulfonic acid
PFCAs	Perfluoroalkyl carboxylic acids
PFDA	Perfluorodecane carboxylate
PFHpA	Perfluoroheptane carboxylate
PFHxA	Perfluorohexane carboxylate
PFHxS	Perfluorohexane sulfonic acid
PFNA	Perfluorononane carboxylate
PFOA	Perfluorooctane carboxylate
PFOS	Perfluorooctane sulfonic acid
PFPeA	Perfluoropentane carboxylate
PFSAs	Perfluoroalkyl sulfonic acids
PFUnDA	Perfluoroundecanoic acid
TDI	Tolerable daily intake
PFHxDA	Perfluorohexadecanoic acid
PFDoDA	Perfluorododecanoic acid
PFTeDA	Perfluorotetradecanoic acid

Et-FOSA	n- Ethyl perfluorooctylsulfonamide
6:2 FTSA	6:2 Fluorotelomer sulfonic acid
8:2 FTSA	8:2 Fluorotelomer sulfonic acid

1 Introduction

Poly- and perfluoroalkyl substances (PFASs) have in the recent years gained a lot of attention due to their persistence in the environment, toxicity to humans and other living organisms and their ability to bioaccumulate (Ahrens & Bundschuh, 2014). Humans are commonly exposed PFASs through their diet and drinking water (Fromme *et al.*, 2009). It has been proven that water i.e. wastewater (Ahrens *et al.*, 2009), landfill leachate (Hamid *et al.*, 2018), surface runoff (Zhao *et al.*, 2013) are sources and/or modes of transport these contaminants.

Conventional water treatment like coagulation, aeration, chemical oxidation etc have been proved to be insufficient at removing PFASs during drinking water production (Appleman *et al.*, 2014; Rahman *et al.*, 2014; Boiteux *et al.*, 2017). Granular activated carbon (GAC) is most commonly used in water treatment for removal of chemical contaminants like PFASs from water (Appleman *et al.*, 2014). However, several studies have proven that the treatment does not efficiently remove shorter chained PFASs. PFAS removal using GAC was reduced in the presence of dissolved organic carbon (DOC) in the treated water (Rahman *et al.*, 2014; Kothawala *et al.*, 2017). The use of high pressure membranes is one of the most promising methods in water treatment (Rahman *et al.*, 2014). However, the method produces a water residue (membrane reject water) with high PFAS concentration, ions and a variety of other compounds. This presents challenges in the deposition of this water (Khan *et al.*, 2009).

Electrochemical oxidation methods are another promising method, particularly the use of boron-doped diamond (BDD) electrodes (Urriaga *et al.*, 2015; Merino *et al.*, 2016). BDD electrodes have several advantageous characteristics over other electrodes that may enable them to be combined with other water treatment methods (Anglada *et al.*, 2009). Several studies have been performed to test the BDD performance with only a few PFASs like perfluorobutane carboxylate (PFBA) perfluorohexane carboxylate (PFHxA) and perfluorooctane carboxylate (PFOA), and

perfluorooctane sulfonate (PFOS) (Carter & Farrell, 2008; Liao & Farrell, 2009; Ochiai *et al.*, 2011; Urtiaga *et al.*, 2015; Schaefer *et al.*, 2017; Soriano *et al.*, 2017). Only a few studies have examined the performance of the BDD in the removal of wide range PFASs and the effect of dissolved organic matter (DOM) which is done in this study.

1.1 Objectives and hypotheses

The goal of this study was to evaluate the performance of water treatment using BDD electrodes and the effect of DOC on the removal efficiency of PFASs. To achieve this goal, the following specific research objectives had to be fulfilled:

- Assess the influence of different applied currents on treatment efficiency.
- Assess the influence of different water types (i.e. Millipore water, DOC water and membrane reject water) on the treatment efficiency.
- Determine the energy consumption of the treatment.

The following hypotheses were tested.

- The removal efficiency of PFASs is dependent on the used current density.
- The removal efficiency of individual PFASs is dependent on their perfluorocarbon chain length and functional group.
- The water type can influence the removal efficiency of PFASs.
- Water type and current density have an impact on the energy efficiency.

1.2 Delimitations

Despite the presence of a wide variety of unwanted compounds in drinking water, this study is only conducted for selected PFASs. The spiked water in this study contained varied PFAS concentrations which are not in the same composition as untreated water. The trials carried out in this study were not replicated due to time limitations. This study can therefore only indicate trends and affects the certainty in which conclusions are drawn. Additionally, a range of current densities was tested. Hence, no conclusions for the efficiency of the treatment outside this range can be drawn.

2 Background

2.1 What are PFASs?

PFASs are omnipresent substances that have been highly utilized for their special properties. They can be found in waterproofing agents and lubricants, paints, paper, textiles, carpets, non-stick cookware, electronics and electrics, ski waxes, leather and firefighting agents (Paul *et al.*, 2009; Herzke *et al.*, 2012; Kotthoff *et al.*, 2015).

PFASs are a subset of a large group of fluorinated substances composed of an aliphatic chain with at least one or more hydrogen (H) replaced by a fluorine atom (F). The poly- and perfluoroalkyl moiety is $C_nF_{2n+1}-R$, where n is the number of carbons and R is the functional group (Buck *et al.*, 2011). The presence of F in the PFAS structure, makes PFASs special compounds over hydrocarbons (C_nH_{2n+2}) (Krafft & Riess, 2015).

F possesses 9 electrons and protons. In combination with its small size, F results to be the most electronegative element. This makes the C-F bond the strongest bond in organic chemistry and their C-C are exceptionally strong due to the influence of fluorine (Krafft & Riess, 2015).

PFASs possess a hydrophobic tail and a hydrophilic head (Ahrens, 2011). The hydrophobic nature of PFASs increases with an increase in chain length (Rahman *et al.*, 2014). Krafft & Riess (2015) reported a decrease in water solubility by 0.78 log units for each CF_2 increase in chain length. On the other hand, their solubility is highly influenced by the presence of a charged functional group. For example, perfluoroalkyl sulfonic acids (PFSAs) and perfluoroalkyl carboxylic acids (PFCAs) are more water soluble than perfluorinated sulphonamides (FASAs) because they carry a charged functional group contrary to the later (Ahrens, 2011). Because of these

properties, PFASs tend to coat surfaces and form films making them exceptional protective barriers, repelling dirt, fat, water and microorganisms (Krafft & Riess, 2015). This ability to repel substances has been used in the treatment of carpets, paper and packaging to repel dirt, grease and oil (Paul *et al.*, 2009). Their ability to form films has been used in metal plating, firefighting and other applications (Krafft & Riess, 2015).

PFASs lower the surface tension of water from 72 to 15 mN m⁻¹ which is better than the respective non- fluorinated analogues. As a result, they serve as good surfactants: spreading, emulsifying and adsorbing easily on solid or liquid particles. This makes them good ingredients for detergents (Krafft & Riess, 2015).

PFASs are also highly stable. This is evidenced by their high thermostability and kinetic inertness. Both properties are not only due to the bond strength but also due to the large size of the F atoms compared to the H atoms. These large F atoms provide a compact repellent shield that protects the molecule against chemical attack. PFASs are resistant to heat, strong acids, bases, oxidising and reducing agents. For this reasons, PFAS have been used in cookware and other harsh environments (Krafft & Riess, 2015).

Other characteristics PFASs possess include their ability to lower friction, facilitate levelling, provide lubrication and readily adsorb on solids and modulate wetting properties. They also have outstanding dielectric, piezoelectric, pyroelectric and optical properties (Krafft & Riess, 2015).

2.2 PFAS nomenclature

The terminologies used in this thesis to classify PFASs were suggested by- Buck *et al.* (2011).

PFASs can have complete (per) or partial (poly) substitution of H by F in the aliphatic chain. However, the H substitution does not include that in the functional group (Buck *et al.*, 2011: OECD, 2018). Polyfluoroalkyl substances are commonly precursors of perfluoroalkyl substances. Examples of polyfluoroalkyl substances include 6:2 and 8:2 fluorotelomer sulfonic acid (6:2 FTSA and 8:2 FTSA, respectively).

Linear vs branched: Depending on the production process both branched and linear PFAS isomers are created (Buck *et al.*, 2011). In compounds where some C atoms are bonded to more than 2 Cs, a branch is formed and thus termed as the branched

isomers. A mixture of both linear and branched isomers affects their physicochemical properties and thus their distribution in the environment.

Depending on the functional group. PFASs can be acids: perfluoroalkyl acids (PFAAs), which is also the most common group (Buck *et al.*, 2011). This is because PFAAs are widely used in a variety of industrial and consumer applications due to their unique properties (Buck *et al.*, 2011). This family includes perfluoroalkyl carboxylic, sulfonic, sulfinic, phosphonic and phosphinic acids. However, this study focused on the perfluoroalkyl carboxylic acids (PFCAs) and perfluoroalkyl sulfonic acids (PFSAs). The functional group on PFCAs is -COOH and -SO₃H on PFSAs. One of the most commonly used PFCAs being PFOA, whose ammonium salt has been used to manufacture fluorosurfactants (Buck *et al.*, 2011). On the other hand, perfluorooctane sulfonic acid (PFOS) and perfluorohexane sulfonic acid (PFHxS) are common PFSAs (Buck *et al.*, 2011) due to numerous industrial and commercial applications. Since most of these compounds are frequently detected in the environment, especially in water, a lot of research is focused on these compounds (Buck *et al.*, 2011) In order to reduce the levels of PFOA, PFOS and PFHxS, short chained PFAAs (perfluorobutyric acid, PFBA and perfluorobutyric sulfonic acid, PFBS), have been used replaced them. However, both PFBS and PFBA have been reported to have significantly increased in both water and air. This might be due to the new regulations that are aimed at phasing out long chained PFASs (Buck *et al.*, 2011). Please note that most PFAAs will appear in their deprotonated (ionic) form at environmentally relevant pH ranges and thus PFAAs will be referred to as acids and carboxylates or sulphonates interchangeably in this report.

Long chain vs short chain. PFASs occur with varying length of chain. This, in turn, affects their properties. PFCAs with 8 or more carbon atoms are referred to as long chained while PFSAs with 6 or more carbons are referred to as long chained PFASs. The difference in the definitions for long chained PFCAs and PFSAs is due to the greater tendency of the PFSAs with the same number of carbons as PFCAs to bioaccumulate more than PFCAs. Other PFASs other than PFCAs and PFSAs can be termed as long chained if perfluoroalkyl chain is 7 or more carbons (Buck *et al.*, 2011; OECD, 2018).

Table 1. Example of different PFASs and groups with the focus on those investigated in this study.

Grouping	Compound	Number of C
Precursors	6:2 FTSA	8
	8:2 FTSA	10
	FOSA	10
PFCAs	PFPeA	5
	PFH _x A	6
	PFHpA	7
	PFOA	8
	PFNA	9
	PFDA	10
	PFDoDA	12
	PFTeDA	14
PFSAAs	PFH _x DA	16
	PFBS	4
	PFH _x S	6
	PFOS	8

2.3 Toxicity and regulation

The major route of exposure of PFASs to humans is through the diet, while drinking water is the second major route of exposure (Fromme *et al.*, 2009).

Several types of cancer have been connected to PFAS exposure. For example, Barry *et al.* (2013) discovered a positive correlation between PFOA exposure through drinking water and incidence of kidney and testicular cancer among humans. Exposure to PFBS and PFH_xS, PFOS, PFBA, PFOA and 6:2 FTSA were associated with haemoglobin reduction, immunotoxicity, reduced serum cholesterol, obesity and kidney toxicity in humans respectively (Borg *et al.*, 2013).

The persistent, toxic and bioaccumulative nature of PFASs has led to the development of several regulations to control PFAS use and consumption. In the EU regulations to reduce PFOS and PFOA were developed in collaboration with the research community, industry and advocacy groups (OECD, 2017). The overall guidelines on tolerable daily intake (TDI) of 1500 ng per kg body weight per day for PFOA

and PFOS respectively were established (European Food Safety Authority (EFSA), 2008). In Sweden, the National Food Agency recommends that a sum of the concentration PFASs should not exceed 90 ngL^{-1} in drinking water. These PFASs include; 6:2 FTSA, PFBS, PFHxS, PFOS, PFBA, perfluoropentanoic acid (PFPeA), PFHxA, perfluoroheptanoic acid (PFHpA), PFOA, perfluorononanoic acid (PFNA) and perfluorodecanoic acid (PFDA) (Ankarberg & Lindberg, 2016)

2.4 Sources and transport in the aquatic environment

PFASs have been in existence since 1949 and have been used in a wide range of industrial processes (3M, 1999). Although there is a wide variety of PFASs in existence, PFOS and PFOA are the most detected PFASs in drinking water (Rahman *et al.*, 2014) and wastewater (Arvaniti & Stasinakis, 2015). Other compounds like PFBA, PFPeA, PFHpA, PFNA, PFUnDA (perfluoroundecanoic acid), PFHxS and FOSA (fluorotelomer octane sulfonic acid) have also been detected in drinking water (Ahrens, 2011; Rahman *et al.*, 2014). In a comprehensive review by Hamid *et al.* (2018), PFASs with <7 Cs were the most abundant in landfill leachate which could be due to the change in legislation or high mobility of these PFASs. The concentration and type of PFASs dominating in a water region are dependent on the distance from the pollution source, type of the pollution source as well as the type of waterbody (Boiteux *et al.*, 2017). For example, in sites impacted by PFAS containing aqueous film forming foams (AFFF), higher prevalences of PFOA and PFHxA are reported to have reported and surface waters will have higher prevalences of PFBA (Guelfo & Adamson, 2018).

PFASs are either directly or indirectly emitted into water environments. Direct emission of these PFASs is when they leaked during their use or manufacturing processes. Emission after transformation of their precursors; is referred to as indirect emission (Buck *et al.*, 2011). The PFAS source into a water environment can also be classified as either point or nonpoint (diffuse) sources (Ahrens & Bundschuh, 2014). Major point sources include wastewater treatment plants (WWTPs) (Ahrens *et al.*, 2009), manufacturing plants (Boiteux *et al.*, 2017), landfills (Hamid *et al.*, 2018) and airfields. Nonpoint sources include; dry or wet atmospheric deposition (Taniyasu *et al.*, 2013) and surface runoff from contaminated streets and fields (Zhao *et al.*, 2013).

2.5 Water treatment techniques

Many studies have proved the presence of PFASs in tap water (e.g Llorca *et al.*, 2012; Boiteux *et al.*, 2017). This is due to the inefficiency of most of these conventional drinking water treatment methods. Examples of these methods include; coagulation, physical separation, aeration, chemical separation and use of GAC (Rahman *et al.*, 2014; Boiteux *et al.*, 2017; Appleman *et al.*, 2014).

Aside from the conventional water treatment methods, several treatment methods have been developed, these include resin treatment, membrane technologies and advanced oxidation processes (Rahman *et al.*, 2014).

Membrane technologies are a highly dependable means of water treatment as they are easy to operate, effective and produce a constant water quality (Daal *et al.*, 2015). These technologies include; reverse osmosis, nanofiltration, ultrafiltration and microfiltration. They can be classified into high pressure (reverse osmosis and nanofiltration) and low pressure (ultrafiltration and microfiltration) membranes (Khan *et al.*, 2009; Singh & Hankins, 2016). High pressure membranes are often operated at 5-100 bar while the low-pressure membranes are often operated at 8 bars (Khan *et al.*, 2009). The major component of these technologies are highly semi permeable membranes that permit the infiltration of some substances and not others. The rejected substances are concentrated on the inflow side while the outgoing solvent will have low concentrations of the rejected substances (Singh & Hankins, 2016). This leads to the production of a water residue (waste), referred to as; membrane reject or brine or brine reject or hypersaline discharge or concentrate. There is a high variation in the components and composition of membrane reject water depending on the water source, pre-treatment or other substances that could have been added to clean or optimise the performance of the membranes. Due to the higher concentration of various contaminants in this water, proper disposal of this water has become has posed a major challenge to the utilisation of this method (Khan *et al.*, 2009; Appleman *et al.*, 2014).

Advanced oxidation processes (AOPs) are water treatment techniques that utilise strong oxidizing and non-selective radicals like $\bullet\text{OH}$, O_2^\bullet , $\text{SO}_4^{\bullet-}$, and $\text{CO}_3^{\bullet-}$ that destroy contaminants (Merino *et al.*, 2016). These radicals react with organic species to form a carbon centred radical that can easily be broken down through subsequent reactions. The $\bullet\text{OH}$ radical is the most common species that has been associated with the action of this method (Rahman *et al.*, 2014). AOPs have been used in the treatment of compounds like pharmaceuticals, phenols, dyes (Nidheesh *et al.*, 2018) and pesticides (Alves *et al.*, 2012). AOPs include methods like electrochemical oxidation, use of ultraviolet light, ozonation, Fenton and others (Niu *et al.*, 2016).

Electrochemical oxidation methods are AOPs that use the principle of electrolysis in water treatment. Electrolysis is a process in which electrons are transferred between conductors (electrodes). Electrodes comprise of the anode and cathode at which oxidation and reduction occur respectively (Sillanpää & Shestakova, 2017). Examples of anodes that have been used in water treatment include; Pt, PbO₂, doped SnO₂, IrO and BDD electrodes. During electrochemical oxidation, water is oxidised to produce •OH that are then used to degrade PFASs (Oturán & Aaron, 2014). Complete oxidation of water leads to the production of O₂ that in turn leads to low decomposition of PFASs. For this reason, it is advantageous to utilise electrodes with high O₂ overvoltage (Anglada *et al.*, 2009; Oturan & Aaron, 2014). Treatment of PFASs by electrochemical oxidation is influenced by the electron transfer capacity, formation of •OH, and the oxygen potential of anode materials (Carter & Farrell, 2008; Ochiai *et al.*, 2011; Zhuo *et al.*, 2012).

Electrochemical oxidation utilises direct anodic and indirect mechanisms to destroy contaminants. During direct anodic oxidation, contaminants are adsorbed to the anode and then destroyed by electron transfer reactions. On the other hand, the anode can produce oxidants that destroy contaminants in solution, referred to as an indirect mechanism (Rahman *et al.*, 2014).

In a comprehensive review by Merino *et al.* (2016), the BDD electrodes were referred to as the most promising electrochemical water treatment technique. This could be a result of advantageous characteristics over other electrode types (Anglada *et al.*, 2009). These include wide working potential, high chemical stability and longevity (Carter & Farrell, 2008; Zhuo *et al.*, 2012). It has been proved that degradation of PFASs by the BDD electrode is a decarboxylation process in which one carbon is removed at a time (Zhuo *et al.*, 2012).

The rate of reaction is often controlled by the current density (intensity per unit area of electrode) (Anglada *et al.*, 2009). Various studies to establish the effect of current density have been done with 0-50 mA cm⁻² with various PFAS types and experimental conditions. From these experiments, a positive correlation has been established between an increase in current density and PFAS degradation (Carter & Farrell, 2008; Ochiai *et al.*, 2011; Schaefer *et al.*, 2017). High current densities produce more charge that increases •OH production that degrade the PFASs (Zhuo *et al.*, 2014). Although this trend was established, an increase in current does not necessarily increase PFAS removal as other factors might limit the rate of reaction (Anglada *et al.*, 2009; Zhuo *et al.*, 2014). Extremely high current densities would lead to further oxidation of •OH to oxygen (O₂), decomposition with H₂O₂ and competitive production with other radicals like ozone (Hamza *et al.*, 2009).

A few studies have been done to establish the effect of temperature on removal efficiency. It has been demonstrated that PFOS and PFOA removal between 17-47°C increased with increasing temperature (Carter & Farrell, 2008; Urriaga *et al.*, 2015).

The electrolytes improve the conductivity of electricity, reducing voltage drop and resistance of the reactor (Anglada *et al.*, 2009; Zhuo *et al.*, 2012). However, there are ongoing debates on the effect of the nature and concentration of the electrolyte. For example, in an experiment using NaClO₄ (1.4 and 8.4 g L⁻¹) and Na₂SO₄ (5 g L⁻¹), Urriaga *et al.* (2015), demonstrated that the nature of electrolyte did not influence PFOA removal. On the other hand, Zhuo *et al.* (2014) demonstrated that the removal of 6:2 FTSA declined in the order of NaClO₄>NaCl>Na₂SO₄ when using Ti/SnO₂-Sb₂O₅-Bi₂O₃ as the electrode. Both chloride (Cl⁻) and sulfate (SO₄²⁻) are adsorbed to the anode reducing the generation of •OH. However, Cl⁻ can be oxidised into active forms like Cl₂, HClO and ClO⁻ which can lead to increased removal of 6:2 FTSA. The use of ClO⁻ should be avoided as it is also a contaminant leading to toxic products (Urriaga *et al.*, 2015).

pH indirectly affects the removal of PFASs on the electrode by influencing •OH generation concentrations, oxygen overpotential as well as anodes' lifespan (Zhuo *et al.*, 2012). Studies with PFOA while using electrodes made from different materials, demonstrated that degradation increased with the reduction of pH (Lin *et al.*, 2012a; Zhuo *et al.*, 2012). Low pH suppressed oxygen evolution while high pH inhibited PFOA decarboxylation. However, extremely low pH has been noted to suppress PFAS degradation as well (Zhuo *et al.*, 2012).

In a comprehensive literature review by Niu *et al.* (2016), plate distance, type of reactor and initial PFAS concentration were described to influence PFAS removal. Increased plate distance reduced removal efficiency of PFASs. However, Lin (*et al.*, 2012) discovered an increase in PFOA removal with increasing plate distance.

3 Materials and Methods

All experiments were done on a laboratory scale. They were performed at the Department of Aquatic Sciences and Assessment at the Swedish University of Agricultural Science (SLU), Uppsala, Sweden.

3.1 Materials

3.1.1 PFAS target compounds

In total, 16 target PFASs were analysed in this study including 6:2 FTSA, 8:2 FTSA, FOSA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA, PFTeDA, PFHxDA, PFBS, PFHxS and PFOS. Spiking was done with a mix of 14 PFASs that were categorised into 3 groups; precursors, PFSAs and PFCAs. Precursors included; FOSA, 6:2 FTSA and 8:2 FTSA. PFSAs included: PFBS, PFHxS and PFOS. PFCAs included: PFBA, PFHxA, PFOA, PFDA, PFDoDA, PFTeDA, PFHxDA and PFOcDA. However, PFBA and PFOcDA were not studied in this thesis due to difficulties in their quantification. A detailed list of these compounds with their respective manufacturer and purity is presented in Table A1. The internal standards (IS) used for internal calibration is comprised of 10 mass labelled internal PFASs (> 98% purity, Wellington laboratories, Canada) shown in Table A2.

3.1.2 Chemicals

Methanol (99.9% hyper grade for LC-MS, LiChrosolv[®], Merck, Germany) was used for cleaning and sample preparation for ultrahigh performance liquid chromatography tandem mass spectrometry (UHPLC-MS/MS) analysis. Experiments were done using Millipore (Millipak[®] Express 20, 0.22µm filter, Merck Millipore), DOC, tap or Nano filter reject (membrane reject) water. Anhydrous sodium sulphate

(99.9%, WR International, Belgium) was used as the electrolyte for the DOC and Millipore water experiments. Methylene blue (Certistain®, Merk KGaA, Darmstadt, Germany) was used in the pre-tests that aimed to monitor the efficiency of the BDD electrode. Experiments that were aimed at evaluating the effect of pH were done using hydrochloric acid (30%, Suprapure®, Merk KGaA, Darmstadt, Germany) and ammonium hydroxide (30% NH₃ basis, ACS reagent Sigma-Aldrich, St Louis, USA).

3.1.3 Equipment

The setup was comprised of the electrochemical cell (Nova diamont BDD electrode), a power supply (EA -PS 2084-10B, EA-PSI 5200 – 02A and Manson switching power supply HCS 3604), pump (MASTERFLEX® L/S®), magnetic stirrer, pH meter and conductometer as shown in Figure A3.

Variety of other equipments were used and are shown in Table A3.

3.2 Electrolysis system

All experiments were performed in batch mode as shown in Figure 1. Batch mode means that water from a single feed tank was circulated through a closed system. The electrochemical cell was comprised of 6 electrodes, each with an effective area of 70 cm². They were made of boron-doped diamond coating 0.1mm thick Niobium sheets. The electrode plates were 3.3 mm apart separated by nylon spacers and a treaded pin. These electrodes are connected in series and were made from the same material making them bipolar i.e each of them could act as the anode as well as the cathode. The electrodes were enclosed in a frame made by polyvinyl chloride (PVC) material.

The experiments carried out can be categorised into experimental preparations, the intended tests (the study) and quality assurance. For all sets of tests, the set up involving the electrochemical cell consisted of a power supply, the electrochemical cell, the feed beaker and a cooling bath. The cooling bath was used for experiments performed at 11.9 mA cm⁻² as these had high temperatures. The feed beaker was a 1L glass beaker containing either the test solution or a cleaning solvent. The feed beaker stood on a magnetic stirrer to ensure uniformity in the mixture. These components were organised to form a system shown in Figure 1.

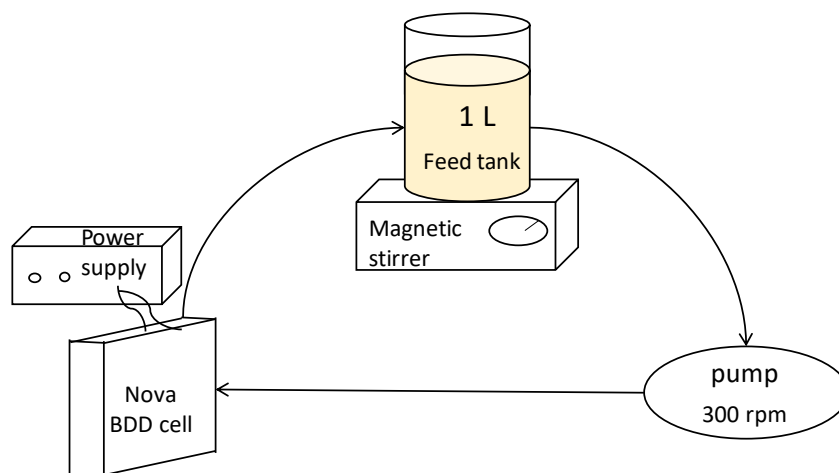


Figure 1. Illustration of a general experimental set up that used.

3.3 Experimental preparations

Prior commencing the study, several tests were done to monitor the performance of the electrochemical cell (section 3.6.1), determine the concentration of electrolyte to use, prepare the DOC water and determine the volume of acid and base used to achieve predetermined pH values for a quality control test (section 3.6.3).

3.3.1 Electrolyte tests

Anhydrous sodium sulphate (Na_2SO_4) was selected as the electrolyte for the experiments to avoid production of Cl_2 if NaCl were to be used. However, there was a need to determine the appropriate amount of this salt that could be used to apply the highest current possible. For this purpose, a sample of 1.42 g and 4 samples of 0.71 g were measured. A cleaned system, like the one described in section 3.2. was set up in a hood. The feed beaker was then set to contain 1L of Millipore water. The pump was adjusted to 300 rpm. Current was then applied, and the 1.42 g sample of the salt added first to the feed tank. The power supply was adjusted to obtain the highest possible current. Both the voltage and current obtained were recorded. The remaining 4 samples were added, one at a time and former steps repeated after each addition. The total mass of electrolyte of 2.84 g (20 mM), at which addition of more electrolyte did not lead to a change in current, was obtained.

3.3.2 Preparation of DOC water

DOC water was prepared by mixing 150 mL of Millipore water for every 1.33 g dry weight of organic soil. This organic soil was obtained from a remote site in Risberget, Sweden and sieved through a 2mm mesh. The mixture was shaken for 48 hours and then centrifuged at ≥ 3000 rpm for ≥ 30 minutes. The supernatant was then filtered through a $0.45 \mu\text{m}$ filter paper to obtain the DOC water.

A sample was obtained from the batch and sent to the chemical analysis laboratory at SLU to determine the DOC concentration of the water. The samples were analysed using an accredited method described at <https://www.slu.se/globalassets/ew/org/inst/vom/laboratorier/ackrediterade-vattenanalyismetoder.pdf>. The water was reported to have 28.8 mg L^{-1} DOC. A dilution factor of approximately 3 was used to obtain the final batch of DOC water that was used throughout the experiment. A sample was extracted from this batch, analysed and reported to have 10.8 mg L^{-1} DOC concentration which is a typical DOC concentration found in membrane reject water and other surface waters.

3.4 The study

A set up similar to that described in section 3.2 was set in a cleaned fume hood together with a pH meter and a conductivity meter.

Preparation of an experiment included; ensuring the system was properly cleaned and empty of any solvents. 1 litre of the test solution was then set. Three water types were used as test solution; DOC (10.8 mg L^{-1}), Millipore and membrane reject water. Both the Millipore and DOC water (each 1 L) were spiked with $872 \mu\text{L}$ of a mix of 14 selected PFASs ($10,000 \text{ ng L}^{-1}$ for each PFAS) resulting in a theoretical initial concentration of 1400 ng L^{-1} in the test solution. The mix was intended to contain only compounds with an even carbon number. This was done to easily monitor if the compounds with the odd carbon number i.e. PFPeA, PFHpA, PFNA and PFUnDA had been created. 20 mM of the electrolyte (Na_2SO_4) was added to both DOC and Millipore experiments. On the other hand, the membrane reject water was not spiked with PFASs and no electrolyte was added to it. This is because this water was already proved in earlier studies to be contaminated with PFAS. *Table 2* shows a summary of all the trials that were performed with their variables and aim.

Table 2. Summary of all trials performed

Sample ID	Water type		Membrane Reject water	Current Density (mAcm ⁻²)	Spiked	Aim
	Milli-pore	DOC				
Negative blanks						
B	Yes	–	–	–	No	Account for contaminants
pH test						
A	Yes	–	–	–	Yes	Account for variation in pH
Degradation trials						
M1	Yes	–	–	0.95	Yes	
M2	Yes	–	–	4.8	Yes	Evaluate the effect of current
M3	Yes	–	–	11.9	Yes	
M5	Yes	–	–	16.7	Yes	
D3	–	Yes	–	0.95	Yes	Evaluate effect of DOC
D1	–	Yes	–	4.8	Yes	
D2	–	Yes	–	11.9	Yes	
R	–	–	Yes	0.95	No	Treatment of reject water

After an experimental set up was ready, the test solution was then circulated through the system by turning on the pump. Two samples were picked: at least 10 minutes and 1 hour from the time the pump had been turned on. The experiment was then left to stand overnight to ensure the mix reached equilibrium. The following day, two samples were collected within at least 30 minutes time difference to prove that there was an equilibrium in the system. The power supply was then set to an intended current. On the application of current, samples were extracted in duplicates at time points: 0, 5, 10, 15, 30, 60, 90 and 120 minutes. For the trial done with reject water, two more samples were collected 150 and 180 minutes. 5 mL samples were collected into 10 mL vials. The samples were collected using 6 mL samples plastic syringes and syringe filters rinsed with methanol. An extra cleaning step of the syringes was done with Millipore water during the DOC and reject water trials. This

cleaning step was done to reduce methanol contamination of these test solutions since they would later be analysed for DOC. At each sampling occasion, the pH, conductivity, temperature, current and voltage were recorded. An IS mixture (0.05 ng mL⁻¹) of 20 µl was added to each sample at the time of sampling. During the experiment, the polarity was switched every after 30 minutes as a way of cleaning the electrodes. The studied current densities were varied from 0.95-16.67 mA cm⁻². The aim had been to test up to 50 mA cm⁻² but all trials set up to use current densities > 16 mA cm⁻² were unsuccessful due to unidentified technical issues. For the DOC and membrane reject water trials, water samples were collected at the end of each trial and handed over to the chemical analysis laboratory lab to measure the remaining DOC in the water. The method used by the laboratory is mentioned in section 3.3.2.

After each experiment, the system was rinsed twice with Millipore water and twice with methanol. The vials and stirring bars were each time sonicated twice in methanol for 15 minutes.

Two concepts are used to describe the changes in the concentration of the PFAS: % residual and % removal concentration calculated using the equations below.

$$\% \text{ residual} = \left(\frac{C}{C_0} \right) \times 100 \quad (1)$$

$$\% \text{ removal} = \left(1 - \frac{C}{C_0} \right) \times 100 \quad (2)$$

Where C is the concentration at a given time and C₀ is the initial concentration.

To determine the energy of the study, the energy consumption (W, kWhm⁻²) Eq 3 below was used.

$$W = \frac{AVt}{v} \quad (3)$$

Where A is the current (A), t is the time (h), v is the volume of the feed beaker (L), and V the cell Voltage (V).

3.5 Analytical method

All samples collected during the experiment and pre-tests were analysed using the online solid phase extraction (SPE) and ultra-high-performance liquid chromatography tandem spectrometry (UHPLC-MS/MS). Analysis was carried out using TSQ Quantiva (Thermo Scientific, Waltham, MA, USA).

All samples extracted during the experiment were analysed via ultra-performance liquid chromatography-tandem mass spectrometry with negative electron spray ionization (UPLC-(-ESI)-MS/MS; TSQ Quantiva, San Jose, CA, USA, ThermoScientific). An Acquity UPLC BEH-C18 column (Waters, 100 mm \times 2.1 i.d., 1.7 μ m particle size from Waters Corporation, Manchester, UK) was used as the analytical column. A Hypersil GOLD aQ column (20 mm \times 2.1 mm i.d, 12 μ m particles, from Thermo Fisher Scientific, San Jose, CA, USA) was used as an extraction column for on-line solid phase extraction. Injection volumes were 1.0 mL for all samples. The mobile phase solutions consisted of 5 mM ammonium acetate that was gradually changed to 100% acetonitrile during the run. A triple-stage quadrupole MS/MS TSQ Quantiva (Thermo Fisher Scientific) was used for the detection of compounds. Data were evaluated using TraceFinder™ 3.3 software (Thermo Fisher).

The limit of quantification (LOQ) for simultaneous analysis was determined by measuring aqueous standard solution at concentrations ranging from 0.1 ng L⁻¹ to 1000 ng/L, as the lowest calibration point in the linear range (relative standard deviation average response factor < 30%) if the S/N ratio was higher than 10. In case compounds were detected in blank samples, the average of the blank samples + 8* standard deviation was taken as LOQ for the respective compound. Internal quantification was used.

3.6 Quality control and assurance

3.6.1 Methylene blue experiments

To monitor the performance of the electrochemical cell, two tests were done: one at the beginning of the study and another during the study. In these tests, the degradation efficiency of methylene blue by the electrochemical cell was determined and

compared between the tests. A system like that described in section 3.2 was used, however, a photo spectrometer was included in the set up measure the wavelength.

Millipore water was used to clean the system and the flow rate was set to 190 mL min⁻¹ at 150 rpm. All the water was removed, and procedures aimed at preparing the photo spectrometer for the analysis were done. A feed beaker containing a methylene blue solution was then set for analysis to commence. The solution was made of 9.5 mg of methylene blue and 500 g of tap water. The methylene blue solution was then run through the system, giving the system time to equilibrate. After > 10 minutes, a current density of 0.95 mA cm⁻² was applied to the electrochemical cell. The applied voltage and current were recorded every 10 minutes. The voltage was often adjusted to maintain a constant current. The tests were run for at least 30 minutes following the application of current. Absorbance measures were made in real time within an integral range of 600-700 nM. The data, in form of time series, was exported to an excel sheet for further analysis.

Prior the experiments and in between replicates, the system was flushed twice with tap water, polarity switched and then flushed twice with Millipore water.

3.6.2 Negative blanks

Negative blanks on Millipore water were conducted with procedures like the actual trial. However, they were not spiked with PFASs and no current was applied.

3.6.3 pH tests

To determine whether pH change influenced the results obtained, a trial was carried out with procedures like those used for the negative blanks. However, in this trial, pH was adjusted from 9 to 1 and Millipore water had been spiked. pH adjustments were made by addition of either hydrochloric acid or ammonium hydroxide. A sample was collected 20 minutes after attaining pH 7, 9, 5, 3 and 1. This pH range was selected as it was typical pH ranged observed during the trials. The 20 minutes were given to allow time for the system to equilibrate.

4 Quality assurance

4.1.1 Methylene blue experiments

Trials aimed at monitoring the degradation efficiency of the electrode by using the electrode treat methylene blue proved that the method was equally efficient throughout the experiment as shown in *Figure 2*.

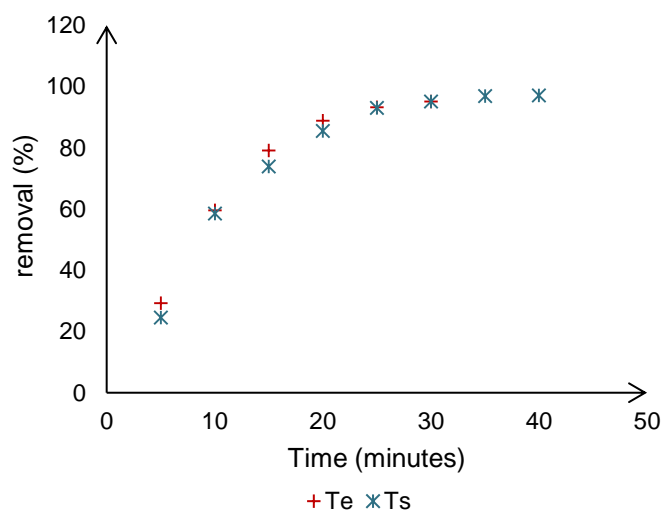


Figure 2. Degradation of methylene blue with time when treated with BDD electrode at the start (Ts) and end (Te) of the study.

4.1.2 Negative blanks

Negative blanks showed no contamination with PFASs (all peaks were below the concentration of the lowest calibration curve point). The only exception was 6:2 FTSA that was found to a concentration of $<5 \text{ ng L}^{-1}$ in three of the blank vials.

4.1.3 Limit of quantification

The limits of quantification for the different compound can be seen in the Table A4. Please note, that most compounds were not detected in the blanks and therefore the lowest calibration point was taken for which the signal to noise ratio was larger than 10. Please note, that in case the lowest quantifiable calibration point was different for different batches, the highest value was taken for all samples in this study.

4.1.4 pH experiments

The trial A1 was used to further observe the effect of pH on the removal of individual PFASs by applying no current for the BDD cells.

The residual concentration of PFASs due to pH change is shown in *Figure 3*. The detected concentration of PFASs was pH dependent except for PFHxS and PFPeA. PFDoDA, PFOS and FOSA whose detected concentration decreased at $\text{pH} < 7$. PFDA concentration increased at $\text{pH} < 5$. While PFOA and 8:2 FTSA concentration increased at $\text{pH} < 3$. On the other hand, PFBS and 6:2 FTSA concentration reduced $\text{pH} < 7$. PFASs are weak acids that form uncharged species when the pH is below their pKa. PFCAs with $\leq 11\text{Cs}$ have < 3.5 pKa while PFSA with the same carbon chain length have much lower pKa values (Higgins & Luthy, 2006). Therefore, lower pH ranges lead to the dominance of uncharged PFAS species. These species have a greater tendency to adsorb to surfaces. Thus, the increase in removals with decreasing pH. This may also imply that low pH facilitates PFAS removal when using the BDD (Zhuo *et al.*, 2012).

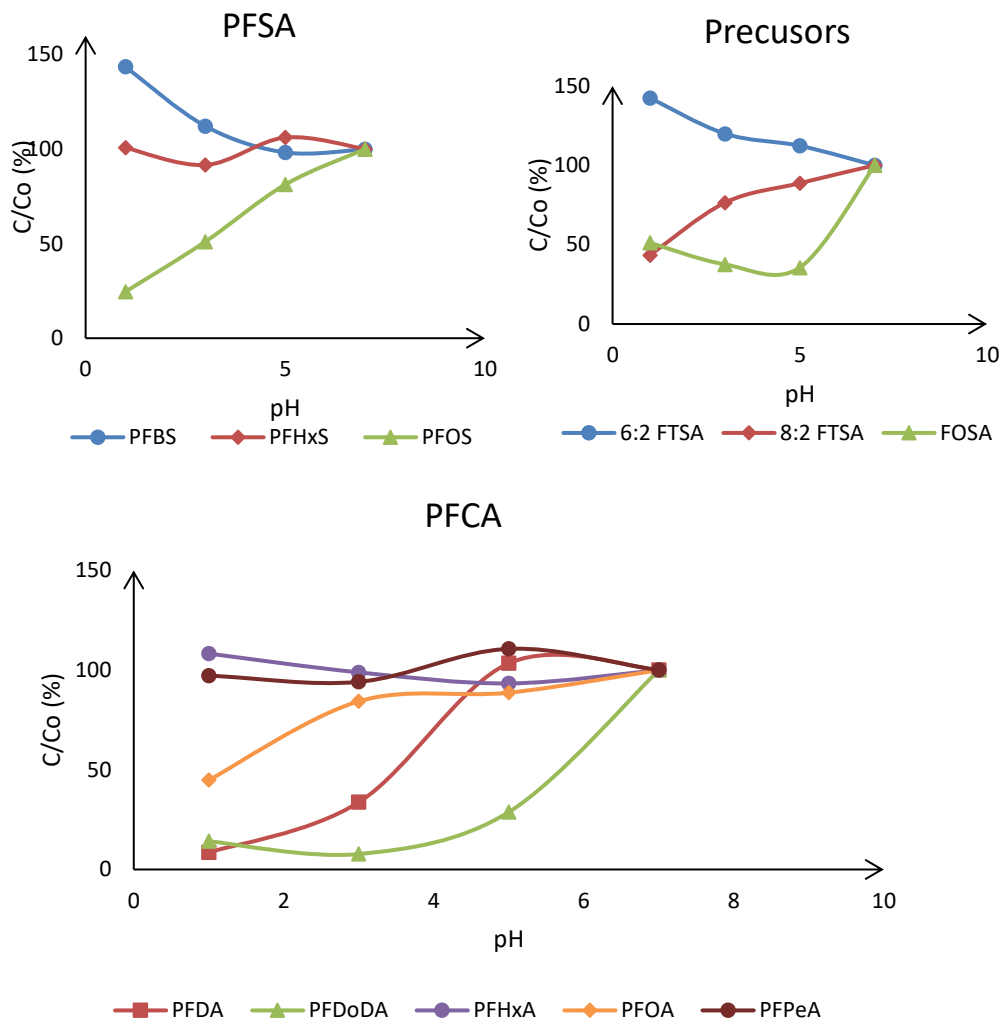


Figure 3. Effect of pH on the removal of different PFASs on spiked Millipore water but no applied current

5 Results and Discussion

5.1 Effect of current

To study the effect of current density on the removal efficiency of the 12 studied PFASs, the current density was varied while using Millipore as the test solution as shown in *Table 2*. The current densities of 0.95 (M1), 4.8 (M2) and 11.9 (M3) were tried.

Physical parameters: temperature, conductivity and pH varied throughout the experiment as shown in *Table 3*.

Table 3. Voltages used to attain the different current densities and their respective temperature, conductivity and pH ranges in trials done with Millipore water. pH reduces while conductivity and temperature increases.

Water type	Current density (mA cm ⁻²)	Voltage (V)	Temperature (°C)	Conductivity (mS)	pH
Millipore	0.95 (M1)	21.8±0.6	23-26	3.9-4	3.5-7
	4.8 (M2)	33±0.8	24-46	1.9-3	2.8-9.4
	11.9 (M3)	43±2.78	25-69	4.9-9.2	2.7-7.4

On the application of current, the temperature increased in all trials. High current densities corresponded to high temperatures. The highest temperature recorded was 68.8°C at 11.9 mA cm². This could be due to increased resistive heating (Schaefer et al., 2017). There was a direct correlation between temperature and conductivity

as shown in *Figure 4* and therefore, a similar trend to that of temperature was observed for the conductivity.

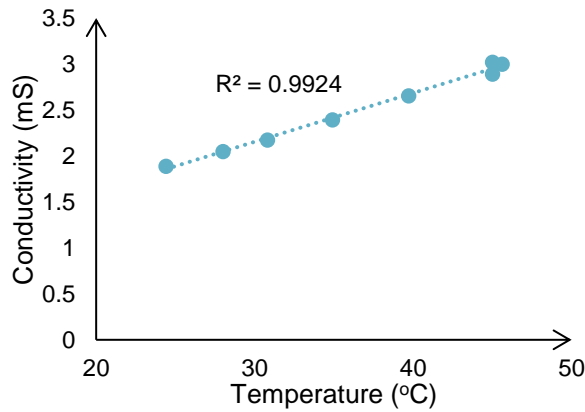


Figure 4. Relationship between conductivity and temperature when using a trial with Millipore water treated with 4.8 mA cm^{-2} as an example.

On the application of current, pH rapidly declined in all trials as shown in *Figure 5*. High current densities corresponded to a high magnitude in pH change. The reduction in pH while using this treatment can be associated with the production protons at the electrodes during the formation of $\bullet\text{OH}$ that are later used for PFAS degradation (Luong *et al.*, 2009). Also, the product of complete PFAS degradation is CO_2 . The faster rate of CO_2 formation could imply a faster rate of degradation of PFASs and thereby higher efficiency. The formed CO_2 may be hydrolysed to form carbonic acid that leads to reduced pH (Liao & Farrell, 2009). As a result, the higher the current density used, the lower the pH obtained.

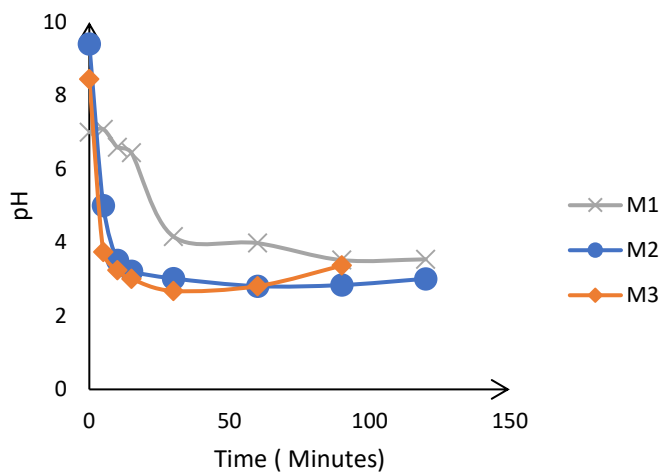


Figure 5. Change in the pH of Millipore water with time at the different current densities (0.95 , 4.8 and 11.9 mA cm^{-2}).

As noted in section 4.1.4, reduction pH affects the detected PFAS concentration, therefore reported results should be interpreted with caution.

Figure 6 shows the % residual concentration of the different PFASs when treated with three current densities: M1, M2 and M3. PFXX_br refers to the branched isomer while PFXX refers to the linear isomer. Shorter chained PFASs had lower removals compared to longer chained PFASs. M3, which was also the highest applied current density recorded the highest removals. While M1 had the least removals of the different PFASs. Therefore, increase in current density led to increased removal of PFASs. PFAS treatment involves the action of $\bullet\text{OH}$ (Lin *et al.*, 2012b; Zhuo *et al.*, 2012). The higher the current density the more $\bullet\text{OH}$ that are produced which in turn leads to increased PFAS removals (Zhuo *et al.*, 2012). Similar results were obtained by Carter & Farrell (2008) and Schaefer *et al.* (2017). It could also be noted from the results that linear PFASs had higher removals in comparison to their branched isomers.

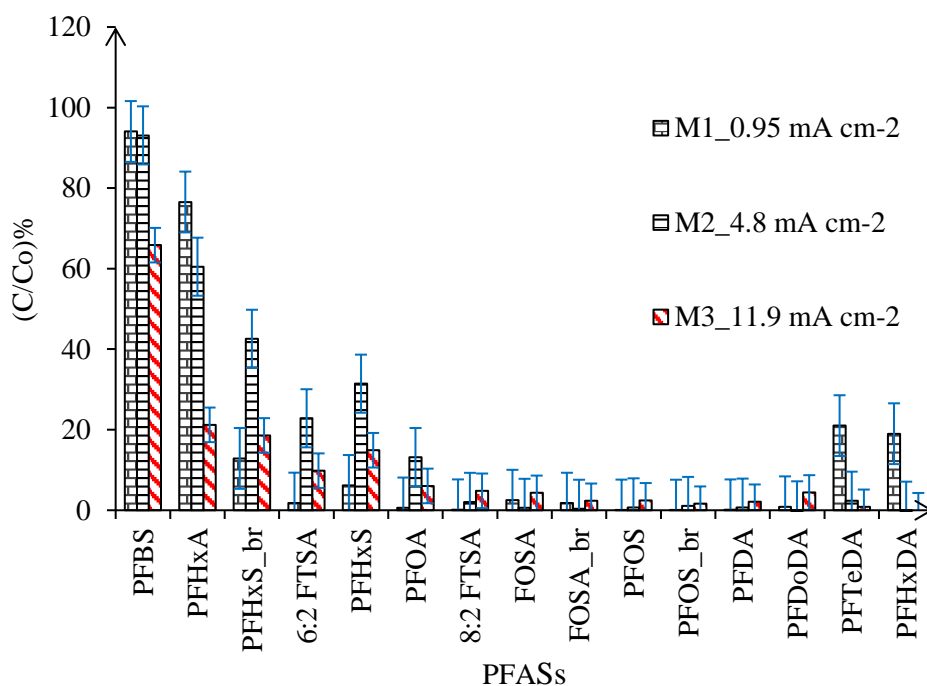


Figure 6. Percentage remaining concentration for each compound after 2 hours for both Millipore water at (0.95-11.9) mA cm⁻².

Interestingly, in all trials carried out with ≥ 4.8 mA cm⁻², including the trial done with 16.7 mA cm⁻² current density, there was a 10-fold increase in the molar concentration of PFPeA to approximately 3.04 E⁻⁷ mM. It is important to note that PFPeA was not spiked in this study although there were traces of this compound in the spiking mix (98% purity) due to contamination.

Table 4 shows the statistical significance of using the three current densities on the concentration of the PFASs and their removals after two hours. It could be observed that there was no statistical significant difference between the initial and residual concentrations for compounds (PFBS and PFDoDA) at 0.95 mA cm⁻² (M1) while rest of the compounds recorded significant removals. At 4.8 mA cm⁻² (M2), PFBS, PFHxA, PFHxS, 6:2 FTSA, PFDoDA were not significantly removed. At 11.9 mA cm⁻² (M3), PFBS, PFDoDA, PFTeDA and PFHxDA were not significantly removed while other compounds were significantly removed. Although PFDoDA in M1 and M2 as well as PFDoDA, PFTeDA, PFHxDA in M3 display no statistically

significant change in between their initial and residual concentrations according to the t-test performed, they recorded high removals (> 95%). This controversy could be due to a high variance in the data of these compounds.

PFPeA in M3 appears to be lower after 2 hours compared M1 and M2, however, PFPeA concentration was noted to have increased within one hour and then started to decline as shown in *Figure 7*.

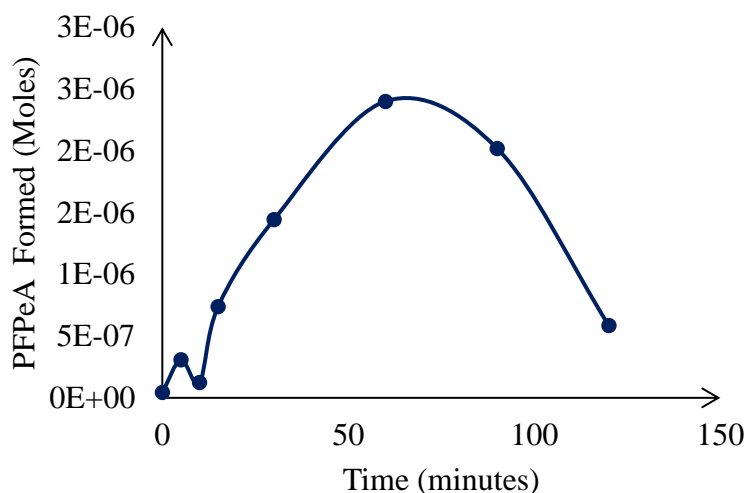


Figure 7. Changes in the concentration of PFPeA with time at 11.9 mA cm⁻² on Millipore water.

In M1 the change in PFPeA concentration was relatively lower than the rest of the experiments. However, it was noted that this trial had lower PFHxA removals. This could imply that PFPeA was being formed during the experiments and that the higher the current density the more PFPeA that is formed. The increment and then decline in PFPeA formation in M3 could imply that PFPeA was formed and then degraded. It could be noted that trials with higher PFPeA formation had lower PFHxA % removals. However, M3 had higher removals of both compounds compared to M1 and M2. Using this line of thought, M3 had a higher removal efficiency. PFAS removal using this treatment is a step by step decarboxylation process that may lead to formation of shorter chained PFASs (Lin *et al.*, 2012a; Zhuo *et al.*, 2012). Therefore, a current density with which high or complete removals of both long chained and short chained PFASs especially PFCAs are attained could have higher overall removal efficiency of PFASs. A detailed discussion of this can be found in section 5.4. It was also noted that at both M2 and M3 attained $\geq 98\%$

removal of PFTeDA and PFHxDA but M1 had lower removal efficiencies of both compounds after two hours.

Table 4. Results of a two-sample t-test (95% confidence interval, one sided) and % removals ($1-(C/C_0)$) for all quantifiable PFASs during treatment of spiked Millipore water with BDD electrode. * symbolises significant difference $p < 0.05\%$, ** at $p < 0.01\%$ and x symbolises no significant difference between initial and residual concentrations of each of the PFASs. PFXX_br refers to the branched isomer while PFXX refers to the linear isomer.

Compound	Millipore_0.95 mA cm ⁻²		Millipore_4.8 mA cm ⁻²		Millipore_11.9 mA cm ⁻²	
	effect	% removal	effect	% removal	effect	% removal
PFBS	x	6	X	7	x	34
PFPeA	x	-70	*	-2704	x	-55
PFHxA	*	23	X	40	*	79
PFHxS_br	*	87	X	57	*	81
PFHxS	*	94	X	69	*	85
6:2 FTSA	*	98	X	77	*	90
PFOA	*	99	*	87	**	94
FOSA	*	98	*	99	*	96
FOSA_br	*	98	*	100	*	98
PFOS	*	100	*	99	*	98
PFOS_br	*	100	*	99	*	98
8:2 FTSA	*	100	*	98	*	95
PFDA	*	100	*	99	*	98
PFDoDA	x	99	X	100	x	96
PFTeDA	*	79	*	98	x	99
PFHxDA	**	81	*	100	x	100

The effect of current density on the removal of different PFASs greatly varied as illustrated in *Figure 8*. For example, PFBS, PFHxA, PFTeDA and PFHxDA recorded an increase in their removal with increasing current density. PFASs like PFOS and 8:2 FTSA and PFDA recorded slight decreases in their removals. The removals of these compounds are still high i.e. > 95 . This could, therefore, be due to measurement errors and the variability in the data shown by the large error bars in *Figure 6*.

On the other hand, many trials previously done to determine the effect of current on removal efficiency were done on PFBS (Carter & Farrell, 2008; Liao & Farrell, 2009), PFHxA (Soriano et al., 2017), PFOS (Carter & Farrell, 2008; Schaefer et al., 2017) and PFOA (Urriaga et al., 2015; Schaefer et al., 2017) revealed an increase in removal efficiency with increasing current density.

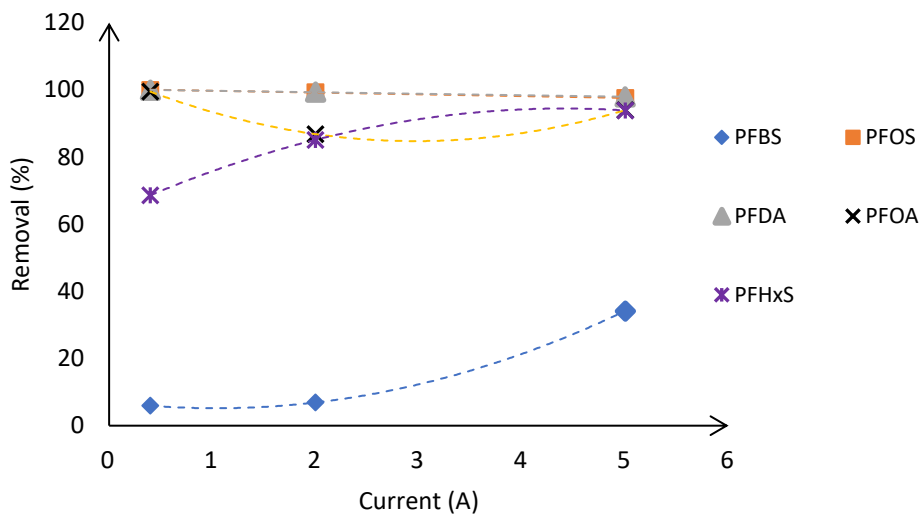


Figure 8. Illustration to show the effect of current densities on a few selected PFASs in Millipore water.

5.2 Influence of chain length

Degradation of PFASs was dependent on the perfluorinated chain length i.e. PFASs with longer chain lengths exhibited higher removal efficiencies after 2 hours than those with shorter chain lengths as shown in *Figure 9*. For trials carried out at ≥ 4.8 mA cm⁻², removal efficiency increased with an increase in the number of per fluorinated chain length. This is due to the increase in hydrophobicity of these compounds with an increase in perfluorinated chain length.(Krafft & Riess, 2015). As result, the water solubility of these compounds decreases with increasing chain length. Both of these characteristics make PFASs with longer chain length to adsorb or attach themselves to surfaces. It could, therefore, occur that longer chained PFAS were adsorbing on to the electrode faster than shorter chained PFASs leading to a faster destruction of longer chained PFASs. Similar results were obtained by (Zhuo *et al.*, 2012). Contrary to (Zhuo *et al.*, 2012) findings, PFCAs in this study exhibited lower removal efficiencies compared to FTSAAs and PFSAAs of the same carbon length. This could be due to degradation mechanisms of PFASs by the treatment that could have created shorter chained PFCAs but also the difference in the number of CF₂. This will be discussed further in section 5.4. The current density applied influenced the trend i.e. in trials M1, PFTeDA and PFHxDA had lower removal compared to those on M3 and M2. Both compounds had a lower removal efficiency after two hours.

Linear isomers generally had higher removals compared to the branched isomers.

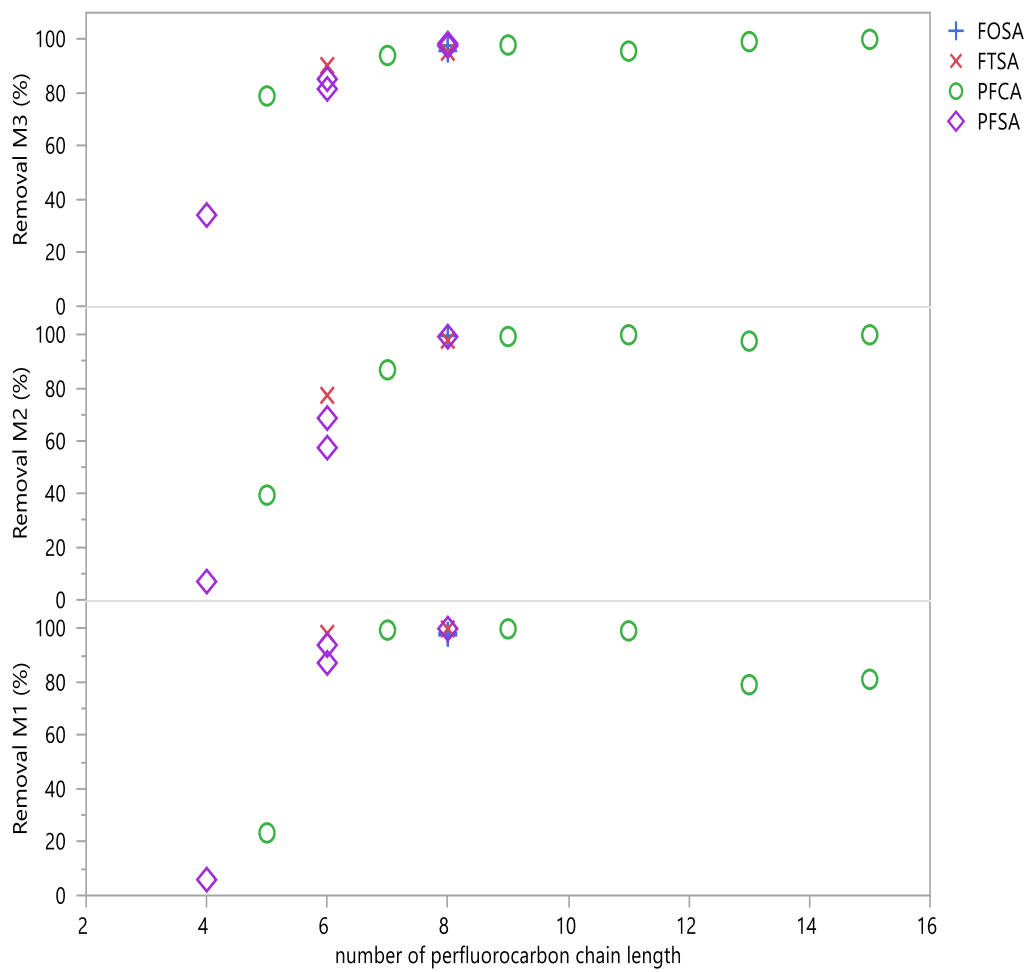


Figure 9. Effect of perfluorinated chain length on the removal efficiency of the different PFASs on M1 (0.95 mA cm⁻²), M2 (4.8 mA cm⁻²) and M3 (11.9 mA cm⁻²) after two hours.

5.2 Effect of water type

On the application of current to any of the water types, gas bubbles were continuously evolved. However, water containing DOC was noted to get frothy and the brown solution turned clear and transparent by the end of the trial as shown in Figure A4.

Similar changes in the physical parameters; temperature, pH, conductivity described in section 5.1 were noted in trials with DOC water as shown in *Table 5*. Where in, increase in current density used, led to increasing temperature, conductivity and voltage used as well as a reduction in pH.

R obtained the least changes in pH and conductivity. This could be due to the presence of a wide variety of material in the water, for example, organic matter and ions that contribute to the high buffer capacity of the water.

The voltage used for both the DOC and reject water trials was higher than that used trials done with Millipore water.

Table 5. Voltages used to attain the different current densities and their respective temperature, conductivity and pH ranges in all trials.

Water type	Current density (mA cm ⁻²)	Voltage (V)	Temperature (°C)	Conductivity (mS)	pH
Millipore	0.95 (M1)	21.8±0.6	23-26	3.9-4	3.5-7
	4.8 (M2)	33±0.8	24-46	1.9-3	2.8-9.4
	11.9 (M3)	43±2.78	25-69	4.9-9.2	2.7-7.4
DOC	0.95 (D3)	—	—	—	—
	4.8 (D1)	33.5±1.3	23-43	4.2-6.1	1.7-6.9
	11.9 (D2)	45.5±4.3	24-68	4.1-8.7	1.5-7.2
Reject	0.95 (R)	32±0.6	23-28	1.1-1.2	7.6-8.6

Table 6 shows the effect of variation of current density on DOC water and % removal attained after 2 hours. The table also shows the removal of the different PFASs in the membrane reject water after 3 hours. It could be observed that there was no statistical significant difference between the initial and residual concentrations for compounds (PFBS, PFH_xA, PFH_xS, PFH_xS br, PFOA and PFH_xDA) at 0.95 mA cm⁻² (D3) while rest of the compounds recorded significant differences in

their concentrations. At 4.8 mA cm⁻² (D1), PFBS, PFPeA, PFDoDA and PFTeDA did not record statistically significant changes in concentration. At 11.9 mA cm⁻² (D2), PFBS, PFPeA, PFDoDA, PFTeDA and PFHxDA did not record significant changes in concentration. In trial R, PFBS, PFPeA, PFDoDA and PFTeDA displayed no significant changes in their concentrations according to t-test. Although PFDoDA and PFTeDA in R recorded no statically significant change in their concentrations, they recorded high removals (> 84%). This controversy could be due to the a variation in the data used for these compounds.

Table 6. Results of a two-sample t-test (95% confidence interval, one sided) and % removals (1-(C/C₀)) for all quantifiable PFASs during treatment of membrane reject water and spiked Millipore and DOC water with the BDD electrode. * symbolises significant difference p < 0.05%, ** at p < 0.01% and x symbolises no significant difference between initial and residual concentrations of each of the PFASs.

Compound	R_0.95		DOC_0.95		DOC_4.8		DOC_11.9	
	effect	removal (%)	effect	removal (%)	effect	removal (%)	effect	Re- moval (%)
PFBS	x	22	x	9	x	20	x	37
PFPeA	x	44	x	-13	x	-934	x	-1215
PFHxA	*	-1	x	10	*	38	*	58
PFHxS_br	*	58	x	8	*	39	*	58
PFHxS	*	76	x	14	*	37	x	66
6:2 FTSA	*	100	*	26	*	73	*	83
PFOA	*	92	x	24	**	85	*	79
FOSA	*	100	*	97	*	97	*	93
FOSA_br	*	100	*	98	*	97	*	96
PFOS	*	99	*	88	**	95	**	97
PFOS_br	*	100	*	82	**	95	*	96
8:2 FTSA	*	99	*	92	*	91	*	91
PFDA	*	99	*	94	*	97	*	98
PFDoDA	x	95	*	94	*	100	*	99
PFTeDA	x	85	*	78	**	100	*	100
PFHxDA	*	87	x	76	*	100	*	99

Figure 10 demonstrates the effect of DOC on the removal efficiency of the applied PFASs after 2 hours. A 1:1-line was added to the reveal if there was a difference in the removal efficiency after 2 hours between DOC and Millipore water for the different PFASs i.e points lying on the 1:1 line will have the same removal both in Millipore and DOC water.

In the figures, the points are clumped towards the end of the line which may imply a positive correlation. It could also be noticed that the points lie close but below the line. This may imply that although removals in Millipore water were higher than those of DOC water, the presence of DOC did not cause a large effect the removal. However, a statistical test would be required to confirm this.

For long chained PFASs in all experiments, the presence of DOC had no major effect on their removal compared to shorter chained PFASs. However, in all trials, PFHxS (both linear and branched) removal appeared to have been reduced due to the presence of DOC. Longer chained PFASs have been proved to be adsorbed to organic matter more than shorter chained PFASs (Ahrens et al., 2010). Therefore, PFASs could have adsorbed to the organic matter leading both PFASs and organic matter being degraded at the same rate. Sorption of PFASs on to organic matter could lead to increased movement of PFASs to the electrode surface and hence higher removal of longer chained PFASs compared to shorter ones.

The effect of DOC on the individual PFASs can further be studied. At current density, 11.9 mA cm^{-2} , M3 had higher removals than D2 except for compounds PFBS, PFDoDA and PFTeDA. Although, the rest of PFASs had lower removals in DOC water compared to Millipore water at this current, PFHxA and PFHxS had much lower removals.

At 4.8 mA cm^{-2} , all PFASs in M2 had higher removals compared to D1 except for PFBS and PFTeDA. PFHxS (both branched and linear) was the most affected by the presence of DOC.

At 0.95 mA cm^{-2} , all PFASs had higher removals in M1 compared to D3. Although, the rest of PFASs had lower removals in DOC water compared to Millipore water at this current density, shorter PFASs had much lower removals in DOC water. Low removal efficiencies of M1 compared to D3 could be due to less production of charge that is insufficient for both DOC break down and PFAS removal.

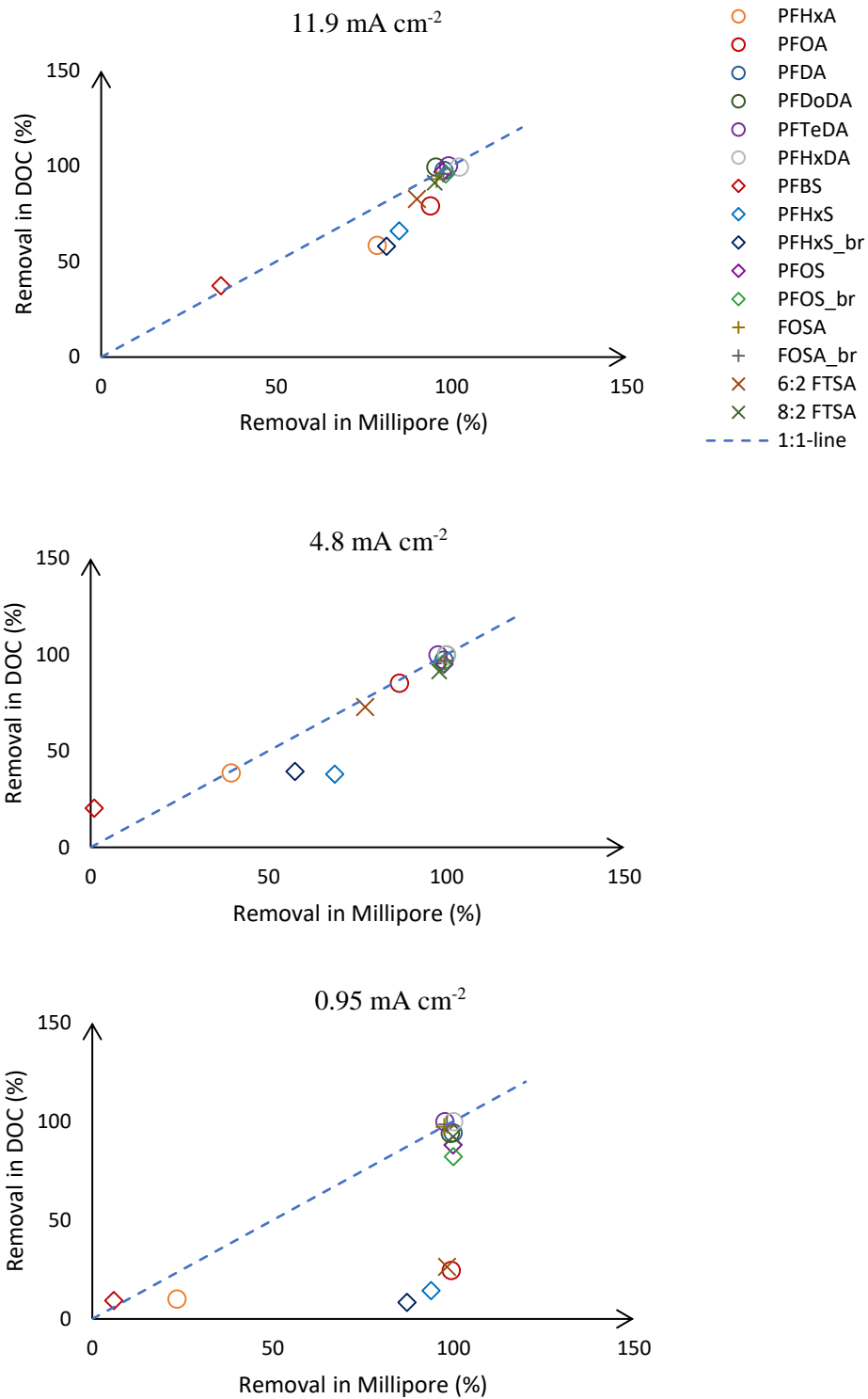


Figure 10. Effect of DOC on the removal efficiency of the Electrochemical cell after 2 hours for the different current densities 12 mA cm⁻², 4.8 mA cm⁻² and 0.95 mA cm⁻².

A comparison of the removals of three water types with the same current density was done. Reject water had the highest removals for PFBS, 8:2 FTSA, FOSA, PFTeDA and PFHxDA as compared to all water types. On the other hand, Reject water had the least removal for PFHxA. For the rest of the compounds Reject water obtained higher removals compared to DOC water. These differences are visualised in *Figure 11*. The higher removals of PFASs in reject water compared to Millipore water may be due to the high variation in chemical composition (like ions and DOC content) that could increase removal. PFAS removal in the membrane reject water could also be better than that in DOC and Millipore water trials because there is a negligible influence of pH. The pH in all trials except that of reject water greatly reduced but as demonstrated in *Figure 3*, low pH increased PFAS adsorption to surfaces. If the PFASs increasingly adsorbed on to the electrode plates, then it would be advantageous. However, if they adsorbed on to other surfaces then they would not be degraded. The observed PFAS removal in the reject water could solely be due to PFAS degradation.

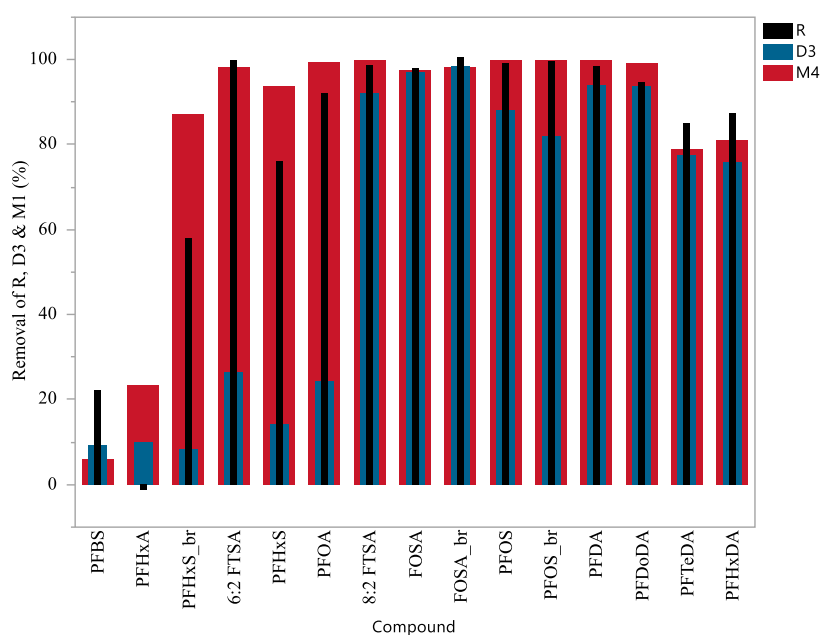


Figure 11. Comparison of % removals for 15 PFAS in 3 water types: Millipore, DOC and reject water using 0.95 mA cm^{-2} current density after 2 hours.

In comparison with Millipore water, DOC did not affect the trends explaining the relationship between perfluorinated carbon chain length and removal of the different PFASs as illustrated in both *Figure 9* and *Figure 12*.

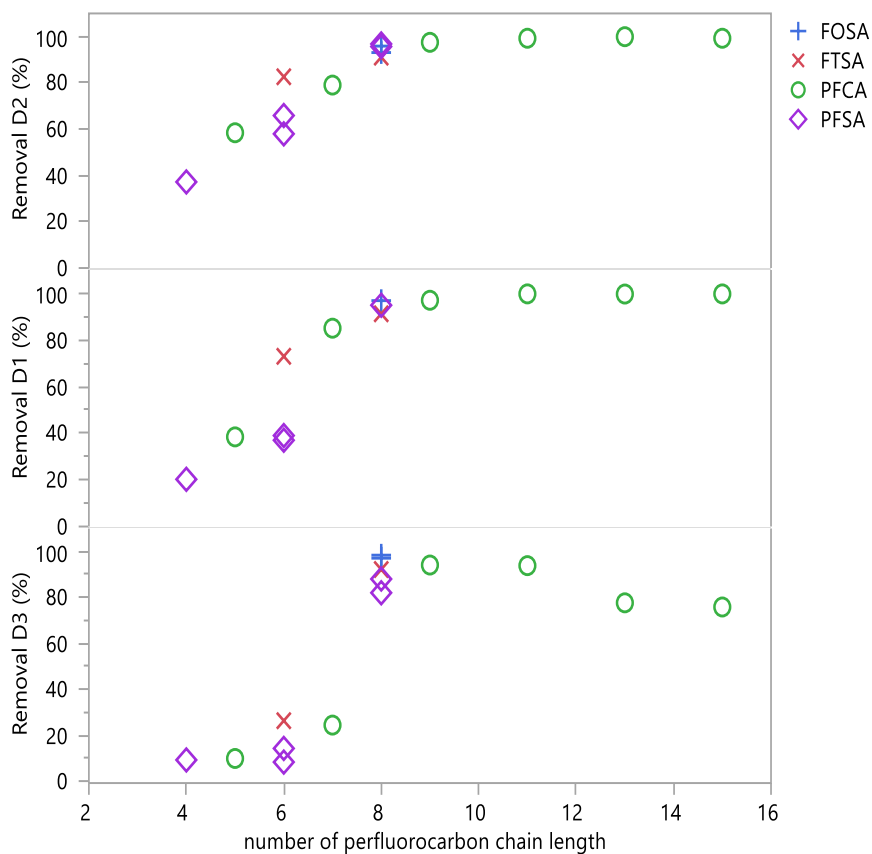


Figure 12. Effect of perfluorinated chain length on the removal efficiency of the different PFASs on D2 (0.95 mA cm^{-2}), D1 (4.8 mA cm^{-2}) and D3 (11.9 mA cm^{-2}) after 2 hours.

5.3 Energy consumption

One of the aims of the study was to determine how much energy was utilised during the trials as well as compare the energy efficiency between trials. The energy utilised within 2 hours for each experiment was considered. Although the possible drawback to this approach could be that at high current density, energy applied was being wasted as PFAS degradation had could have already been completed. However,

there were still some PFASs present after 2 hours especially the shorter chained PFASs.

The energy required to degrade 1ng of PFASs after 2 hours increased with an increase in current density used with exception of the reject water as shown in *Table 7*. This decline in energy efficiency with increasing current density used could be due to an increase in oxygen production (Hamza *et al.*, 2009). This reduces PFAS removal efficiency. Similar results were obtained by Schaefer *et al.* (2017). It had been hypothesised that PFAS removal would decrease in the presence of DOC, surprisingly, DOC water recorded higher energy use efficiency as compared to Millipore water. Urtiaga *et al.* (2015) demonstrated a similarity in the removal efficiency of PFOA with TOC removal. Presence of organic matter could have provided an increased surface area for adsorption on PFASs. As organic matter is transported to the anodes for degradation, more PFASs are degraded in turn.

It can be noted that the reject water consumed more energy per ng of PFASs removed compared to the energy utilised in both Millipore and DOC water treated with the same current density and duration. This could have been due to the high variation in the constituents of reject water such as salts and varying types of organic matter. In all experiments performed with DOC, it was visually confirmed that DOC was degraded by the end of the experiment due change in colour as can be seen in figure A4. 4.17 kWhm⁻³ was consumed per mg of DOC removed. However, this did not completely remove all the DOC at the end of the 3-hour experiment as only 40% DOC removal was attained. This low DOC removal can be associated with the use of low current density. However, several studies have confirmed that DOC could be efficiently degraded by the BDD electrode (Carter & Farrell, 2008; Liao & Farrell, 2009; Urtiaga *et al.*, 2015; Soriano *et al.*, 2017).

Table 7. Summary of the different water types, current densities used and their respective energy utilisation efficiencies.

Water type	Current density [mAcm ⁻²]	Sum PFAS removed [ng]	Sum DOC removed [ng]	Sum consumed energy after 2h [kWhm ⁻³]	Energy consumed per ng PFAS removed [kWh/ng _{removed}]	Energy consumed per mg DOC removed [kW/mg _{removed}]
MQ	0.95	4.17 E4		1.7 E1	4.0 E-4	
	4.8	4.67 E4		1.3 E2	2.8 E-3	
	12	3.75 E4		4.3 E2	1.2 E-2	
DOC	0.95	8.52 E4	–	1.8 E1	2.0 E-4	–
	4.8	6.54 E4	–	1.3 E2	2.0 E-3	–

	12	1.44 E5	–	4.6 E2	3.1 E-3	–
Reject water	0.95	1.89 E3	9.2	2.6 E1	1.4 E-2	4.17

5.4 Influence of time

Figure 13 shows the behaviour of PFCAs in M2 (Millipore water, 4.8 mA cm^{-2}) trial as an example to illustrate the changes observed with time for the different compounds. Generally, there was an increased removal with time for most PFAS. All PFASs with $>10\text{Cs}$ obtained $>90\%$ removal after 30 minutes of current application in all trials except reject water. Degradation of PFASs appeared to occur in the order of $>10\text{Cs}$, 10Cs , 8Cs , 6Cs and 4Cs . However, there was a steady in PFPeA concentration with time which indicates faster degradation of longer chained PFASs while forming shorter ones. This trend was common in all the trials despite the difference in water type or current density used. It is, however, important to note that the amount of PFPeA formed in trial M2 steadily increased during the trial while that in M3 increased and then decreased (Figure 7).

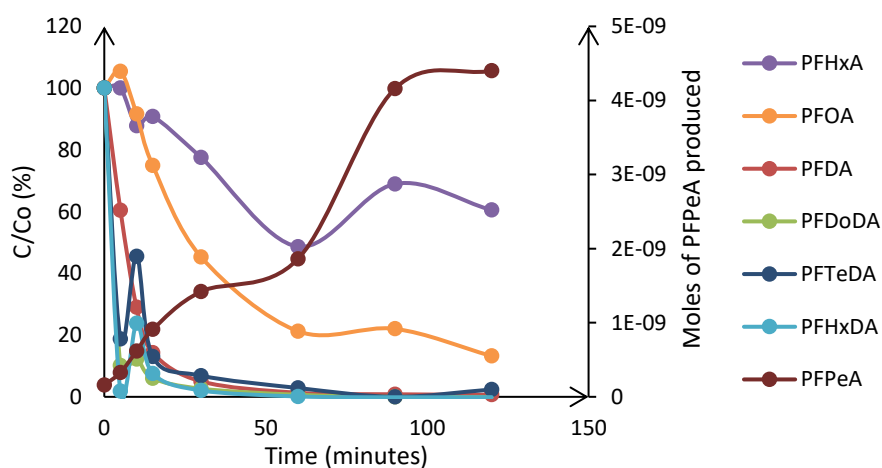


Figure 13. Illustration of PFAS removal with time using PFCA removal from Millipore water at 4.8 mA cm^{-2} current density as an example.

Figure 14 below shows the effect of time on the removal efficiency of the different investigated PFASs while using the M2 (Millipore water and 4.8 mA cm^{-2}) trial as an example. Long chained PFASs except PFOA obtained $> 80\%$ removal within the first 30 minutes of this trial. For the rest of the PFASs, removal increased with increase in time. PFHxA was noted to have a lower removal efficiency after two hours (40%) than after 1 hour (51%). While PFBS, had the least removal after two hours compared to after 0.5 and 1 hour. The reduction of PFBS removal with time may be the result of reduction pH with time since PFBS removals notably affected by reductions in pH as illustrated in Figure 3. Similar trends were observed in all trials.

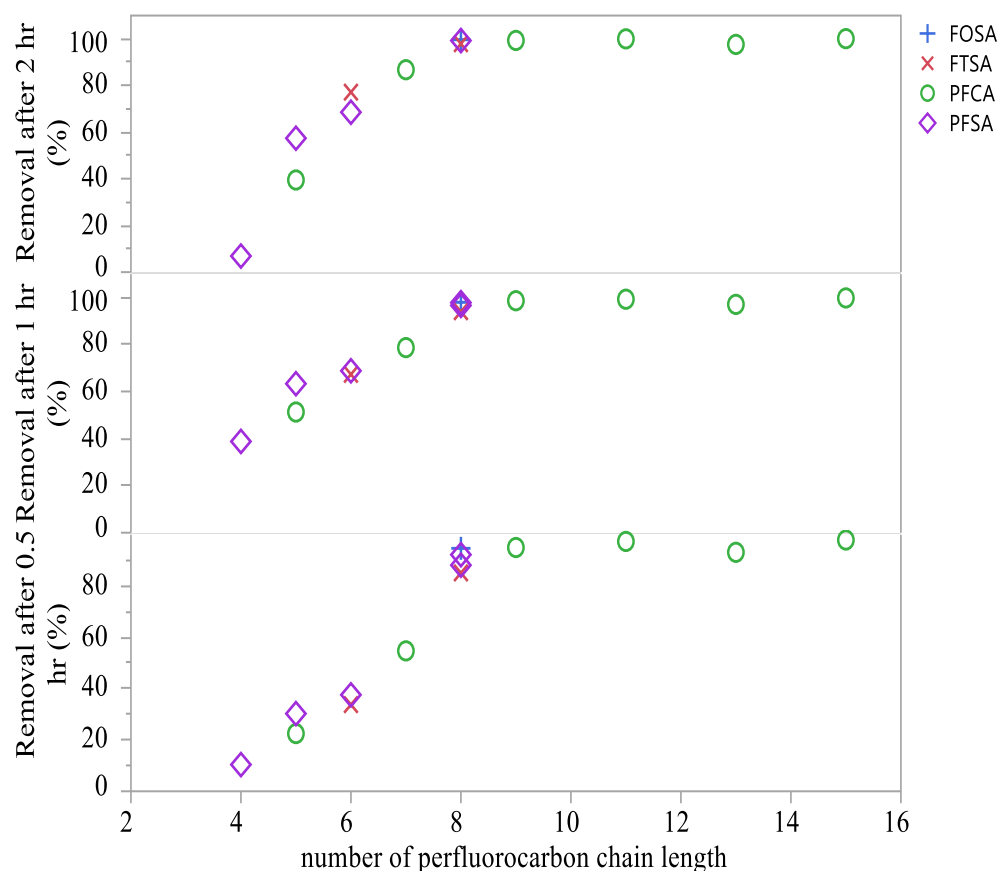
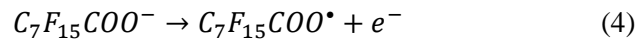


Figure 14. Variations of % removal (1-C/C₀) with fluorinated chain length at different durations of the experiment demonstrated using a Millipore trial at 4.8 mA cm^{-2} .

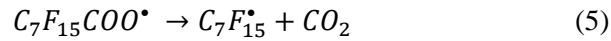
These findings imply longer chained PFASs could have been degraded early in the experiment forming shorter chained PFCAs. This is due to the mechanisms that degrade PFASs in the cell (Zhuo *et al.* 2012).

An accumulation of shorter chained PFCAs indicates that they were being formed during the experiment because of the treatment pathway that occurs for PFASs. The mechanism is a step by step decarboxylation process i.e. one CF₂ is lost at a time. The described pathway below is the most commonly proposed pathway used to best describe PFAS degradation that is characterised by the formation of shorter chained PFASs (Niu *et al.*, 2016).

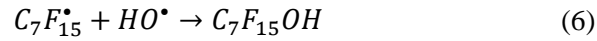
Degradation of PFOA has been used as an example of to demonstrate the mechanism. The process starts with the loss of an electron to the anode from the functional group to form a PFAS radical (Eq 4).



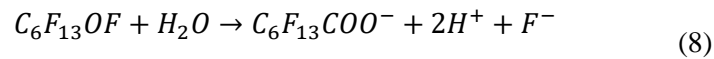
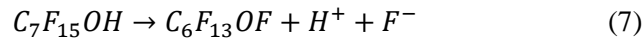
The PFAS radical would then undergo decarboxylation or desulfonation to form perfluoroalkyl radicals (Eq 5).



These then react with OH to form alcohols (Eq 6).



The alcohols react to form perfluoro carbonyl fluoride which is hydrolysed to a shorter chained PFCAs and HF (Eq 7 & 8).



This process can be repeated until the PFASs are completely degraded (Lin *et al.*, 2012; Zhuo *et al.*, 2012). As shown in this pathway accumulation of PFASs cannot

occur. The generally low removals of PFASs at the different time could have been due to the length of their chain as well their functional group.

All in all these observed trends could imply that although there may be a preferential removal of long chained PFASs because of their physiochemical characteristics, it is also important to consider that shorter chained PFASs were being formed during the treatment.

6 Conclusions

Findings from this study demonstrate the treatment of 12 selected PFASs using a BDD electrode in spiked Millipore and DOC water as well as membrane reject water. Few studies have investigated the removal of multiple PFAS types using this treatment as well as the effect water type on the treatment which is the aim of this master thesis.

It can be concluded that the current density of 11.9 mA cm^{-2} has overall high removal efficiencies of all tested PFASs. At all current densities, traces of PFPeA were formed, strongly suggesting that PFAS degradation and underlining the proposed step-wise degradation mechanisms of PFASs. A strong indicator for this was also the fact that, at high current densities, the formed PFPeA was degraded after it had been formed. The removal of different PFASs was affected differently by the current density used. The magnitude of changes in pH, temperature and conductivity increased with time.

Although PFAS removal was influenced by perfluorinated chain length, the PFAS degradation mechanism may explain the lower removals of short chained PFASs. Overall, PFASs were better removed compared to PFCAs over a given time of 2 hours.

The effect of DOC on removal varied with PFAS type and current density used. At 11.9 mA cm^{-2} , removal of long chained PFAS was influenced by the presence of DOC. On the other hand, the presence of DOC had a greater effect on PFAS removal at different current densities especially the short chained PFASs. Interestingly in all trials, the presence of DOC increased PFBS removal and yet PFHxS removal was greatly reduced. The treatment efficiently removed all PFASs in reject water compared to DOC water. Reject water recorded the least removals of PFHxA.

Energy efficiency after 2 hours decreased with increase current density used. Reject water had the least energy efficiency.

This study can be considered an essential pilot study to take this promising treatment method from the laboratory to application scale. More studies can be carried out with wider ranges of DOC concentrations to conclusively establish the effect of this parameter on the treatment.

Further studies can also;

- measure fluoride and evolved CO₂ concentrations to make a mass balance of the possible reactions.
- Measure other organic pollutants in reject water at the same time to draw conclusions on the treatment efficiency for problematic reject water in general.
- Perform toxicological studies to ensure that no toxic by-products are formed in case this treatment will be made ready for drinking water applications.
- Test other water types like landfill leachate to determine the efficiency of the treatment in different field applications.

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Appendix

Table A1. *Details on the analytical standards used*

Compound	Abbreviation	Manufacturer	Purity (%)
Perfluorobutyric acid	PFBA*	Sigma-Aldrich Sweden AB	98
Perfluorohexanoic acid	PFHxA	Sigma-Aldrich Sweden AB	97
Perfluorooctanoic acid	PFOA	Sigma-Aldrich Sweden AB	96
perfluorodecanoic acid	PFDA	Sigma-Aldrich Sweden AB	98
Perfluorododecanoic acid	PFDODA	Sigma-Aldrich Sweden AB	95
Perfluorotetradecanoic acid	PFTeDA	Sigma-Aldrich Sweden AB	97
Perfluorohexadecanoic acid	PFHxDA	Alfa Aesar GmbH & Co.KG	95
Perfluorooctadecanoic acid	PFOcDA*	Alfa Aesar GmbH & Co.KG	97
Potassium nonafluoro-1-butanesulfonate	PFBS-K	Sigma-Aldrich Sweden AB	98
Potassium tridecafluorohexane-1-sulphonate	PFHxS-K	Sigma-Aldrich Sweden AB	98
Potassium heptadecafluorooctanesulphonate	PFOS-K	Sigma-Aldrich Sweden AB	98
1H,1H,2H,2H-Tridecafluorooctane-1-sulfonic acid	6:2 FTSA	Apollo Scientific Ltd	98
1H,1H,2H,2H-Perfluorodecanesulfonic acid	8:2 FTSA	Apollo Scientific Ltd	100
Perfluorooctanesulfonamide	FOSA	Sigma-Aldrich Sweden AB	100

*compound spiked but was not considered for in the study due problems with quantification.

Table A2. IS composition and their corresponding PFASs they were used for.

<u>Internal standard</u>	<u>Calibrated PFASs</u>
¹³ C ₄ -PFBA	PFBA
¹³ C ₂ -PFH _x A	PFBS, PFPeA, PFH _x A
¹³ C ₄ -PFOA	PFHpA, PFOA
¹³ C ₅ -PFNA	PFNA
¹³ C ₂ -PFDA	PFDA
¹³ C ₂ -PFUnDA	PFUnDA
¹³ C ₂ -PFDoDA	PFDoDA, PFTeDA, PFH _x DA, PFOcDA
¹⁸ O ₂ -PFH _x S	PFH _{xs} , 6:2 FTSA
¹³ C ₄ -PFOS	PFOS, 8:2 FTSA
¹³ C ₈ -FOSA	FOSA

Table A3. *Equipment used*

Equipment used	Company
electrochemical cell	Nova diamant AB, Uppsala Sweden
power supply	EA-PS 2084-10B
power supply	EA-PSI 5200-02A
power supply	Manson switching power supply. HCS 3604
pump	MASTERFLEX® L/S®
Magnetic stirrer	Heidolph, REAX 2000
Filter paper	Munktell Ahlstrom, quantitative filterpaper, Grade 00H
Syringe filters	VWR International, VWR®syringe filters, 0.45µm pore size, Nylon membrane, USA
Syringe	HENKE SASS WOLF, 10mL HSW NORM-JECT®
Online SPE vials	Thermo scientific, Autoselect™ Polyvial™, 10 mL, Polystyrene
500 mL volumetric flask	Lenz
Glass coated Magnetic stirrer	Cowie®, Stirring magnet, length: 19 mm, diameter: 6mm
pH- meter	VWR International, pHenomenal®1000H, Germany
Conductometer	VWR International, EC 300
Precision balance	Mettler Toledo, Switzerland
Vortexer	Heidolph, REAX 2000
Vials	SULPECO
Vial-caps	SULPECO
pipettes	VWR International
Ultra-sonic bath	Branson
Centrifuge	Eppendorf, Centrifuge 5810



Figure A1. Set up used for the methylene blue experiments.

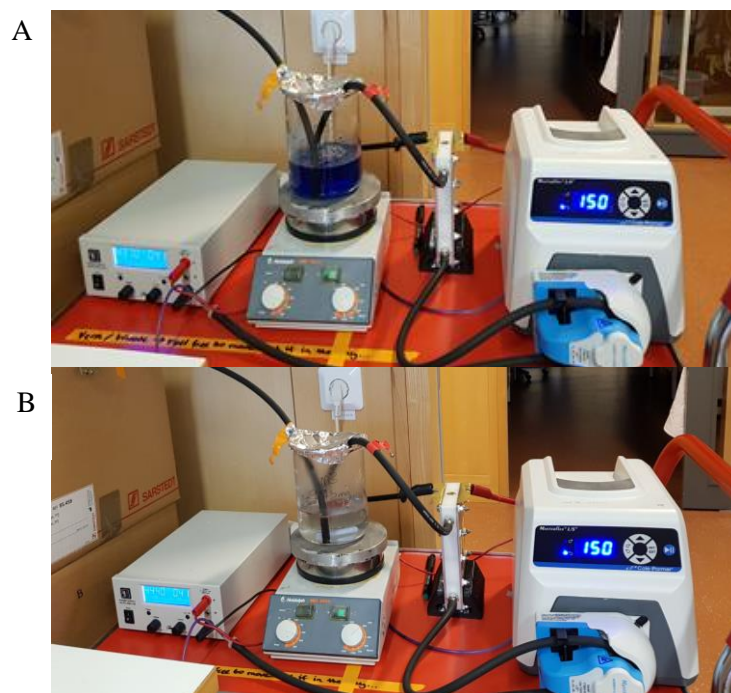


Figure A2. Illustration of the methylene blue solution before (A) and after (B) treatment with the BDD electrode.



Figure A3. Shows the set up used in to treat PFASs in Millipore, DOC and Membrane reject water.

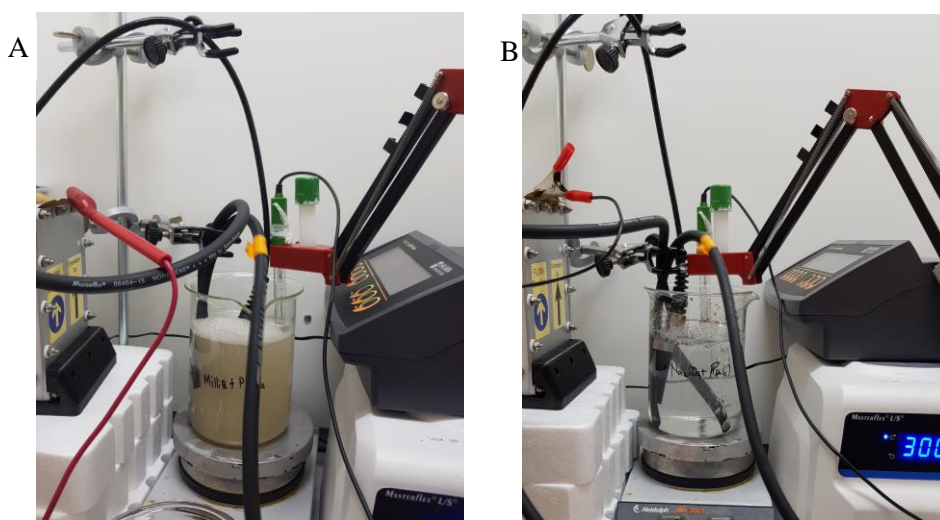


Figure A4. Illustration of DOC water during (A) and at the end (B) of the treatment with BDD electrode when using 12 mA cm^{-2} .

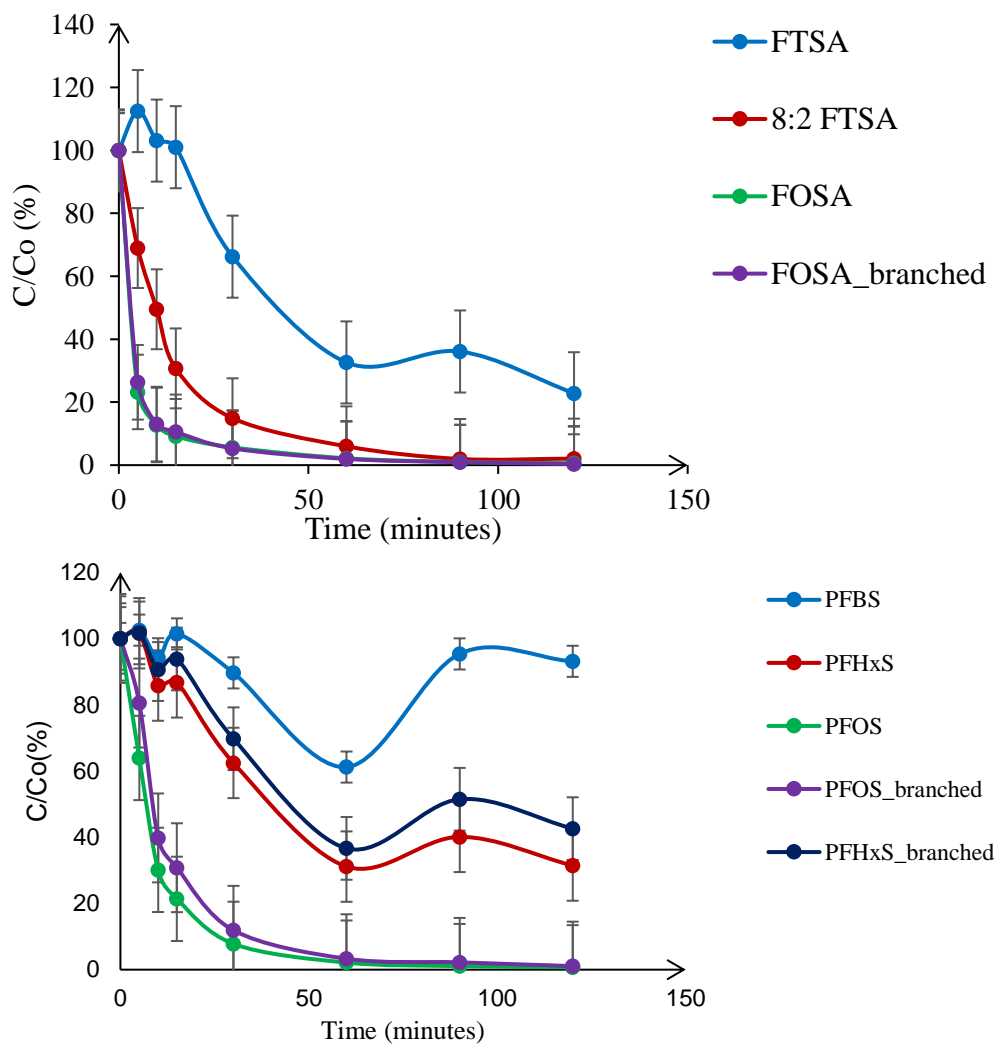
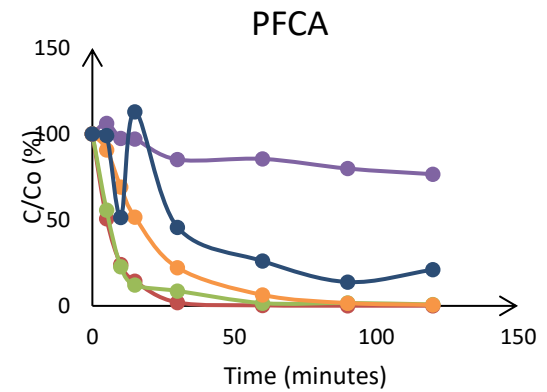
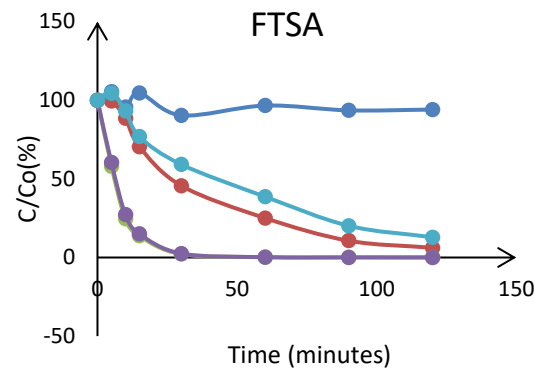
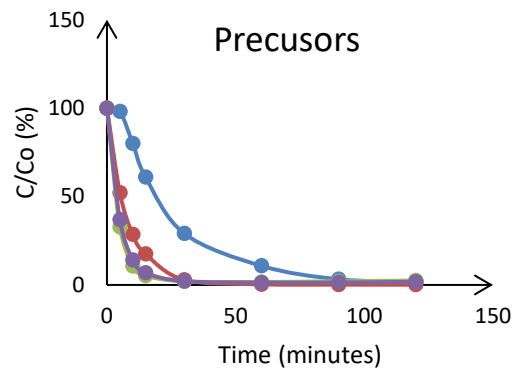
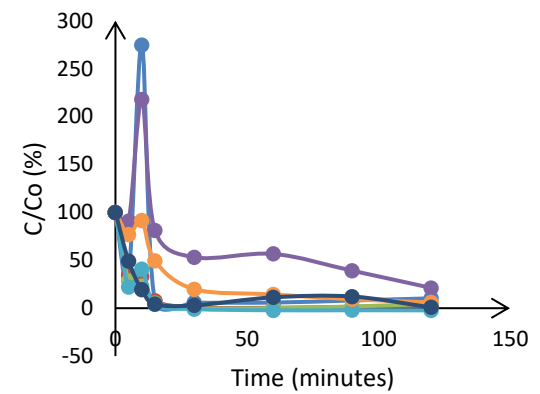
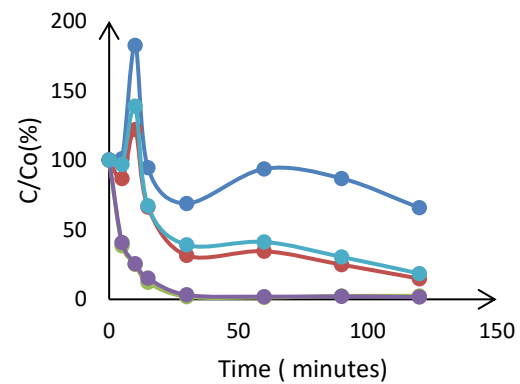
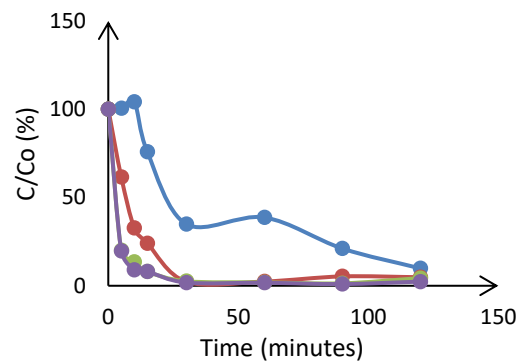


Figure A5. Illustration of PFAS removal with time from Millipore water at 4.8 mA cm⁻² current density as an example.

Millipore water_0.95 mA cm⁻²



Millipore water_11.9 mA cm⁻²

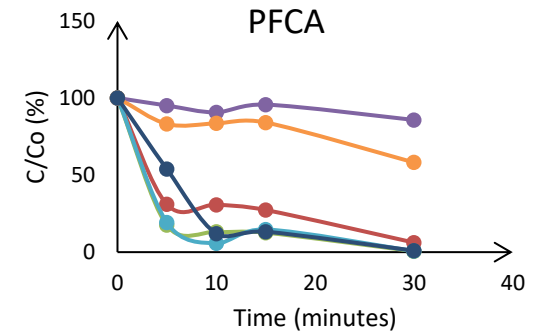
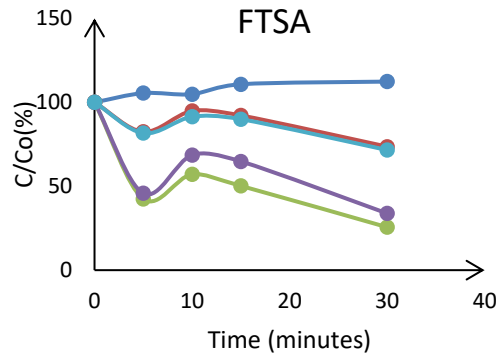
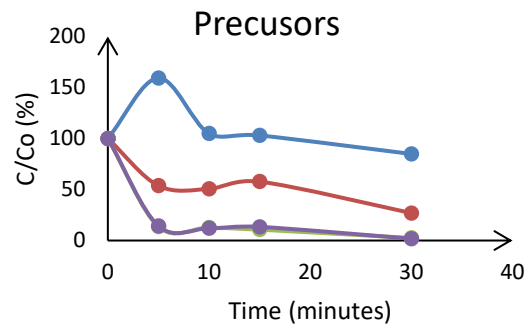


● FTSA ● 8:2 FTSA
● ● FOSA_branched

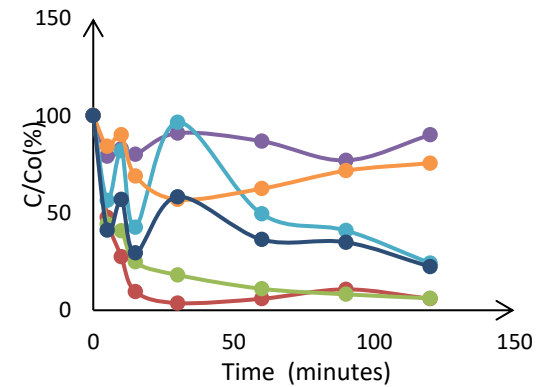
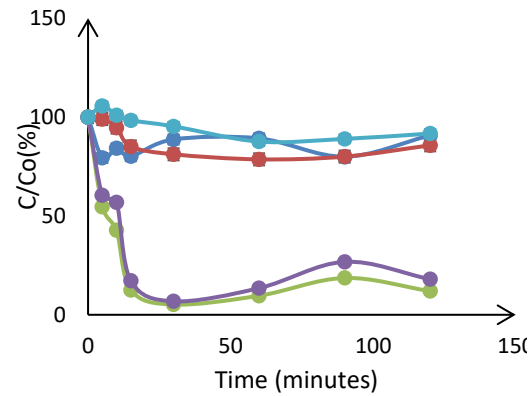
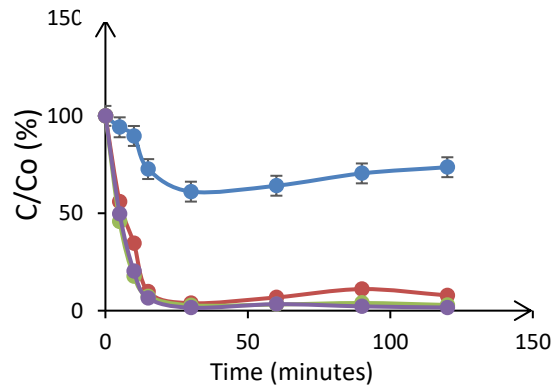
● PFBS ● PFHxS
● PFOS ● PFOS_branched

● PFBA ● PFDA ● PFDODA
● PFHxA ● PFHxDA ● PFOA

Millipore water_16.7 mA cm⁻²



DOC water_0.95 mA cm⁻²

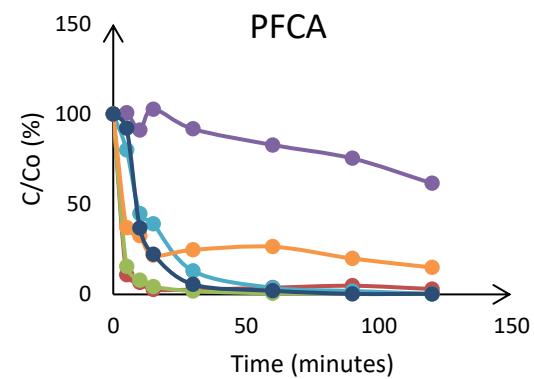
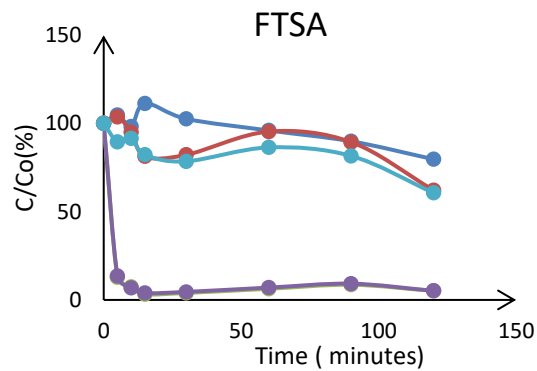
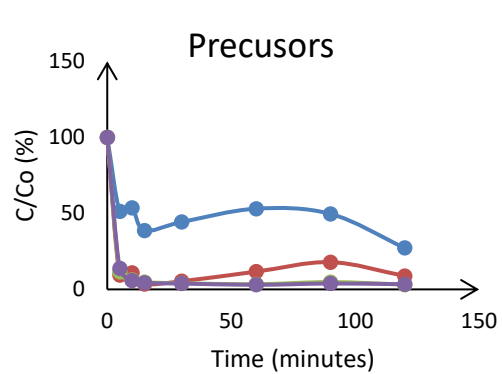


● FTSA ● 8:2 FTSA
● FOSA ● FOSA_branched

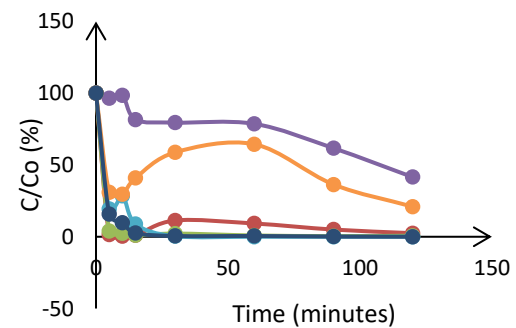
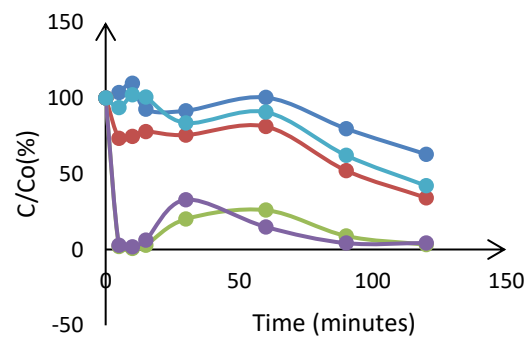
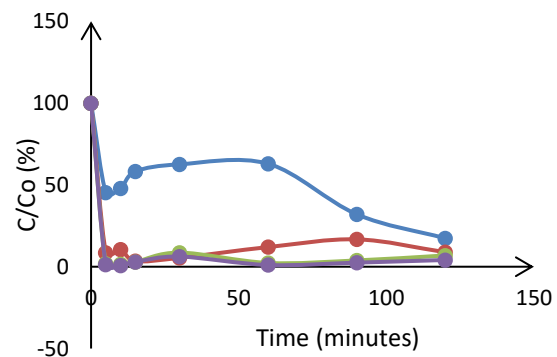
● PFBS ● PFHxS
● PFOS ● PFOS_branched

● PFDA ● PFDoDA ● PFHxA
● PFHxDA ● PFOA ● PFTeDA

DOC water_4.8 mA cm⁻²



DOC water_11.9 mA cm⁻²



● FTSA ● 8:2 FTSA
● FOSA ● FOSA_branched

● PFBS ● PFHxS
● PFOS ● PFOS_branched
● PFHxS_branched

● PFDA ● PFDoDA ● PFHxA
● PFHxDA ● PFOA ● PFTeDA

Membrane reject water_ 0.95 mA cm⁻²

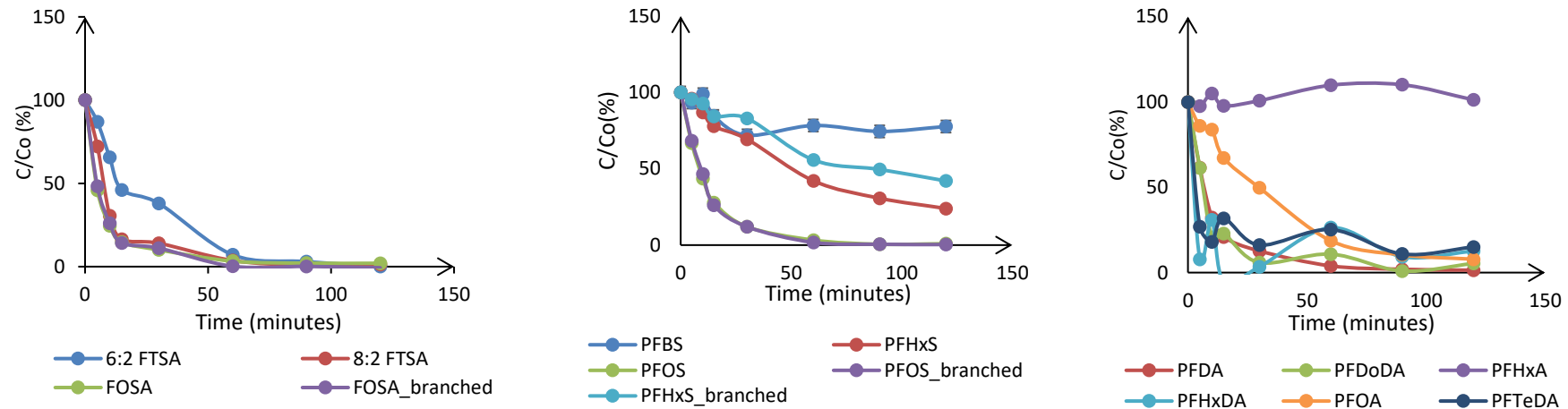


Figure A6. Residual PFAS concentration with time in the different water types at different densities.

Table A4. LOQs for the different analysed PFASs.

Abbreviation	LOQ [ng/L]
PFBA	N/A could not be quantified
PFPeA	5
PFHxA	1
PFHpA	1
PFOA	0.5
PFNA	0.5
PFDA	0.5
PFUnDA	1
PFDoDA	1
	5
PFTeDA	
	5
PFHxDA	
PFOcDA	N/A could not be quantified
	1
PFBS	
	1
PFHxS	
	1
PFOS	
	1
6:2 FTSA	
	5
8:2 FTSA	
	1
FOSA	
	1
Et-FOSA	

Table A5. Recoveries (%) of analysed PFASs during treatment the Acid test to correct the IS.

names	IS_FOSA	IS_PFDA	IS_PFDODA	IS_PFHxA	IS_PFHxS	IS_PFNA	IS_PFOA	IS_PFOS	IS_PFUnDA
A1 7	27	13	85	208	72	28	46	15	21
A1 6	27	34	37	249	109	86	69	39	26
A1 5	43	28	76	258	88	73	63	33	48
A1 4	109	46	108	256	80	91	58	46	81
A1 3	71	41	76	257	100	97	63	44	54
A1 2	33	27	37	243	86	73	57	29	31
A1 1	32	26	42	202	69	76	53	33	32
std_batch	31	11	28	24	14	22	7	10	21

Table A6. Recoveries (%) of analysed PFASs during treatment of Millipore water to correct the IS at 12 mA cm⁻².

names	IS_FO SA	IS_PF DA	IS_PFD _o DA	IS_PFH xA	IS_PF HxS	IS_PF NA	IS_PF OA	IS_PF OS	IS_PFU _n DA
M3 13A	63	117	265	345	132	110	117	96	205
M3 13B	38	82	223	220	105	68	88	74	140
M3 12A	47	68	111	212	100	80	82	65	84
M3 12B	30	57	52	224	95	73	83	57	50
M3 11A	44	53	71	205	92	75	80	53	51
M3 11B	44	49	70	218	99	68	79	50	54
M3 10A	197	190	321	937	409	273	324	202	207
M3 10B	46	43	86	226	101	61	75	45	44
M3 9A	53	59	91	312	131	98	94	60	63

M3 9B	63	65	113	254	94	86	72	63	81
M3 8A	35	39	80	167	69	56	48	40	58
M3 8B	15	11	11	334	156	113	93	45	4
M3 7A	62	54	136	237	94	97	64	65	82
M3 7B	46	47	87	225	78	74	63	50	50
M3 6A	52	32	58	207	72	61	46	30	51
M3 6B	77	33	93	188	69	64	51	34	64
M3 4	84	38	84	229	81	70	52	37	60
M3 3	71	45	95	216	79	78	53	39	64
M3 2	62	45	138	225	84	91	55	43	90
M3 1	49	35	84	217	78	74	52	31	60
Average batch	59	58	113	270	111	89	84	59	78
std_batch	36	38	75	163	74	46	60	37	51

Table A7. Recoveries (%) of analysed PFASs during treatment of Millipore water and reject water to correct the IS at various current densities.

Com- pound	IS_FOSA	IS_PFDA	IS_PFD _o DA	IS_PFH _x A	IS_PFH _x S	IS_PFNA	IS_PFOA	IS_PFOS	IS_PFUnDA
M2_12A	27	26	31	180	91	43	61	36	20
M2_12B	31	23	51	221	103	44	67	32	24
M2_11A	21	18	31	192	97	42	60	26	17
M2_11B	25	23	35	186	89	50	60	29	20
M2_10A	32	53	56	316	173	115	117	68	45
M2_10B	35	60	60	294	148	111	95	68	38
M2_09A	25	29	39	236	105	59	68	36	18
M2_09B	29	30	37	189	79	58	58	36	24
M2_08A	23	24	35	188	77	46	50	27	18
M2_08B	16	26	30	183	74	61	50	27	14
M2_07A	31	31	64	196	80	64	44	41	31
M2_07B	26	26	33	186	80	63	51	31	25
M2_06A	20	23	42	175	74	55	43	28	23
M2_06B	20	18	38	161	66	49	43	25	21
M2_05A	53	23	44	178	74	58	46	29	27
M2_05B	31	23	28	198	85	60	57	24	19
M2_04	30	19	22	184	79	52	48	20	21
M2_03	112	41	73	270	110	100	64	53	60
M2_02	47	27	50	196	67	61	44	26	45

M2_01	2	3	1	18	6	6	3	2	0
M3 13A	63	117	265	345	132	110	117	96	205
M3 13B	38	82	223	220	105	68	88	74	140
M3 12A	47	68	111	212	100	80	82	65	84
M3 12B	30	57	52	224	95	73	83	57	50
M3 11A	44	53	71	205	92	75	80	53	51
M3 11B	44	49	70	218	99	68	79	50	54
M3 10A	197	190	321	937	409	273	324	202	207
M3 10B	46	43	86	226	101	61	75	45	44
M3 9A	53	59	91	312	131	98	94	60	63
M3 9B	63	65	113	254	94	86	72	63	81
M3 8A	35	39	80	167	69	56	48	40	58
M3 8B	15	11	11	334	156	113	93	45	4
M3 7A	62	54	136	237	94	97	64	65	82
M3 7B	46	47	87	225	78	74	63	50	50
M3 6A	52	32	58	207	72	61	46	30	51
M3 6B	77	33	93	188	69	64	51	34	64
M3 4	84	38	84	229	81	70	52	37	60
M3 3	71	45	95	216	79	78	53	39	64
M3 2	62	45	138	225	84	91	55	43	90
M3 1	49	35	84	217	78	74	52	31	60
M1 12A	49	56	76	171	120	69	97	51	61
M1 12B	40	42	59	166	112	58	94	48	45

M1 11A	41	52	81	175	100	57	82	49	56
M1 11B	45	48	74	160	106	57	80	50	59
M1 10A	42	53	74	160	92	54	76	52	62
M1 10B	33	49	69	163	87	62	77	50	48
M1 9A	36	48	50	170	83	55	58	48	49
M1 9B	28	35	51	174	72	50	58	37	39
M1 8B	32	36	75	139	67	51	45	46	64
M1 7A	29	25	50	135	51	40	34	30	37
M1 7B	37	32	52	192	75	58	51	36	36
M1 6A	40	30	73	175	63	53	46	31	53
M1 6B	30	21	41	139	57	36	34	22	32
M1 5A	40	27	80	170	67	53	43	31	53
M1 5B	44	31	77	175	73	60	53	32	56
M1 4	39	20	57	144	55	46	30	24	42
M1 3	53	35	91	189	73	60	48	38	73
M1 2	35	24	55	203	75	61	45	25	38
M1 1	45	26	47	204	74	56	49	29	49
M5 9A	21	21	37	177	66	40	43	22	20
M5 9B	20	28	37	175	73	63	51	34	26
M5 8A	17	37	23	171	69	74	47	36	28
M5 8B	11	15	18	187	70	50	47	18	9
M5 7A	22	21	28	184	62	49	46	21	21
M5 7B	22	28	42	189	72	68	48	27	32

M5 6A	33	34	53	208	89	98	52	47	46
M5 6B	20	23	26	174	70	56	48	26	20
M5 5A	38	36	53	175	64	75	44	36	39
M5 5B	63	26	36	196	67	76	45	34	42
M5 4	56	32	51	197	80	73	50	36	40
M5 3	2	51	53	224	94	102	54	52	66
M5 2	101	45	42	203	79	92	53	47	47
M5 1	60	28	63	198	74	69	49	32	49
average	42	39	67	208	89	68	63	42	48

Table A8. Recoveries (%) of analysed PFASs during treatment of reject water to correct the IS at 0.95 mA cm⁻².

names	IS_FOSA	IS_PFDA	Is_PFD _o DA	IS_PFH _x A	IS_PFH _x S	IS_PFNA	IS_PFOA	IS_PFOS	IS_PFU _n DA
R 14A	129	106	182	523	198	111	145	99	156
R 14B	144	134	265	506	184	119	135	109	194
R 13A	141	121	212	487	213	121	156	100	160
R 13B	142	103	197	543	199	99	140	97	151
R 12A	147	113	158	439	186	94	128	99	149
R 12B	107	76	120	419	184	76	117	70	105
R 11A	109	76	119	461	189	87	129	77	103
R 11B	96	67	93	436	191	80	125	69	70
R 10A	105	85	136	398	182	95	127	85	119
R 10B	100	57	79	468	199	79	127	57	58
R 9A	14	65	126	421	164	78	118	71	87
R 9B	17	85	93	399	187	111	133	95	74
R 8A	105	69	118	326	188	84	117	79	79
R 8B	114	66	96	297	182	73	99	80	93
R 7A	101	51	62	260	154	56	89	53	50
R 7B	117	58	107	256	159	63	86	67	92
R 6A	131	45	56	218	153	57	90	59	44
R 6B	132	47	84	233	148	54	77	65	86
R 5A	111	28	39	169	123	1	60	39	31
R 5B	111	29	64	194	129	38	60	40	47
R 4	105	27	33	197	143	0	72	38	37
R 3	109	24	44	213	150	41	75	36	36

R 2	107	31	44	198	125	39	66	38	32
R 1	126	33	56	228	143	50	82	45	43

Table A9. Recoveries (%) of analysed PFASs during treatment of DOC water to correct the IS for various current densities.

Compound	IS_ FOSA	IS_ PFDA	IS_ PFDODA	IS_ PFHxA	IS_ PFHxS	IS_ PFNA	IS_ PFOA	IS_ PFOS	IS_ PFUnDA
D1 12A	39	40	64	135	65	44	46	38	49
D1 12B	32	30	46	119	62	38	44	29	33
D1 11A	36	31	50	128	57	40	46	32	39
D1 11B	36	40	78	107	55	48	49	40	45
D1 10A	31	30	46	103	53	35	43	31	35
D1 10B	48	41	95	124	56	51	45	45	44
D1 9A	34	37	66	106	62	49	47	45	45
D1 9B	33	29	46	110	65	42	46	29	29
D1 8A	17	36	33	104	62	51	52	37	25
D1 8B	21	23	42	99	61	37	45	29	28
D1 7A	20	33	51	142	62	56	44	47	29
D1 7B	27	41	52	103	57	62	48	51	34
D1 6A	20	22	31	113	53	36	42	22	0
D1 6B	20	24	35	114	65	42	44	27	24
D1 5A	25	19	37	98	55	46	31	22	24
D1 5B	30	29	42	123	58	63	36	30	37
D1 4	32	26	33	110	62	63	31	27	35
D1 3	36	38	46	108	61	62	33	37	42
D1 2	28	23	41	136	65	61	41	27	29
D1 1	19	31	32	92	55	57	29	31	26
D2 12A	55	34	57	160	76	44	50	36	36
D2 12B	60	35	69	169	78	58	53	35	56
D2 11A	18	13	23	130	53	31	34	16	12

D2 11B	24	23	50	108	58	32	33	25	30
D2 10A	11	11	17	140	60	26	32	12	9
D2 10B	9	13	15	94	44	29	28	15	9
D2 9A	9	11	14	130	61	36	32	16	10
D2 9B	7	14	11	114	57	33	33	16	8
D2 8A	7	16	8	126	60	39	43	18	9
D2 8B	7	12	11	121	53	33	34	18	8
D2 7A	7	21	11	116	68	46	48	28	9
D2 7B	3	9	6	99	52	25	38	12	5
D2 6A	10	19	20	109	58	39	41	29	13
D2 6B	11	50	35	107	61	71	49	50	28
D2 5A	13	16	21	100	46	43	25	18	12
D2 5B	17	24	18	93	58	56	30	31	0
D2 4	12	19	6	112	74	60	38	23	13
D2 3	15	32	13	128	61	70	37	32	26
D2 2	9	22	9	145	77	60	35	25	14
D2 1	11	25	18	126	58	55	33	30	22
D3 12A	34	54	53	260	107	85	60	58	52
D3 12B	17	51	28	261	108	89	71	52	32
D3 11A	12	39	26	235	104	76	62	43	28
D3 11B	11	34	22	259	104	77	60	39	27
D3 10A	9	53	20	225	111	91	69	58	25
D3 10B	12	42	18	208	103	78	63	48	22
D3 9A	7	35	6	202	92	77	61	33	14
D3 9B	34	49	49	240	106	78	66	56	42
D3 8A	36	47	41	223	106	93	65	60	38
D3 8B	15	42	23	258	101	85	64	47	22
D3 7A	18	43	13	211	98	80	59	51	23

D3 7B	21	50	26	262	96	86	55	50	28
D3 6A	33	42	38	270	99	88	64	52	34
D3 6B	23	52	24	260	96	97	64	55	30
D3 5A	33	37	19	226	106	105	60	52	30
D3 5B	17	50	21	243	105	96	59	53	31
D3 4	16	45	13	273	113	94	63	51	28
D3 3	22	45	9	232	101	92	66	45	27
D3 2	11	44	12	229	110	99	57	53	27
D3 1	21	43	15	278	108	105	68	54	29
average	22	32	31	159	75	61	47	36	26

Table A10. Detected concentrations at different pH (9-1) during the pH test-trial.

Compound		–	–	9	7	5	3	1
	corr_factor	1.07	0.97	0.99	0.99	0.98	0.99	0.99
6:2 FTSA	cal_amt	3299.29	2591.02	3107.22	2569.77	2921.80	3095.07	3645.41
	corr_amt	3514.00	2510.70	3085.47	2544.12	2857.17	3051.12	3625.72
8:2 FTSA	cal_amt	1778.46	1130.27	2202.53	1475.03	1325.83	1132.90	636.05
	corr_amt	1894.19	1095.23	2187.11	1460.31	1296.50	1116.81	632.62
FOSA	cal_amt	2570.68	1491.81	1725.90	1160.21	418.08	437.56	591.27
	corr_amt	2737.97	1445.56	1713.81	1148.63	408.83	431.34	588.08
FOSA_br	cal_amt	339.96	228.96	226.96	204.84	63.97	78.25	84.62
	corr_amt	362.08	221.87	225.37	202.80	62.55	77.14	84.16
PFPeA	cal_amt	141.67	55.75	25.54	18.36	27.98	23.80	24.59
	corr_amt	136.85	55.64	25.29	18.80	27.96	26.25	23.73
PFHxA	cal_amt	4681.77	3818.39	3936.30	3868.23	3718.71	3907.82	4242.51
	corr_amt	4986.45	3700.02	3897.02	3841.16	3636.45	3852.33	4219.60
PFOA	cal_amt	8271.73	7432.30	7441.76	7818.73	6679.89	6303.55	3317.16
	corr_amt	8810.02	7201.89	7367.49	7764.00	6532.13	6214.04	3299.24
PFDA	cal_amt	3571.79	2676.96	3249.16	3308.17	3402.19	1099.67	276.58
	corr_amt	3804.23	2593.97	3216.73	3285.02	3326.93	1084.06	275.09
PFDoDA	cal_amt	504.27	303.40	297.45	398.90	86.72	23.15	41.88
	corr_amt	537.08	293.99	294.48	396.11	84.80	22.82	41.65
PFTeDA	cal_amt	433.90	195.31	43.21	18.38	16.69	19.29	132.21
	corr_amt	462.14	189.25	42.78	18.25	16.32	19.02	131.50
PFHxDA	cal_amt	7948.93	5073.41	1958.69	328.13	480.49	266.53	764.16
	corr_amt	8466.21	4916.13	1939.14	325.83	469.86	262.74	760.03
PFBS	cal_amt	8258.98	7137.32	6896.65	6454.74	6859.87	7766.66	9856.49
	corr_amt	8796.44	6916.07	6827.82	6409.56	6708.13	7656.37	9803.26
PFHxS	cal_amt	6269.67	4847.54	4199.36	5393.35	4513.18	3863.31	4212.20
	corr_amt	6677.68	4697.26	4157.45	5355.60	4413.35	3808.45	4189.45
PFHxS_br	cal_amt	1474.80	1186.55	1028.92	1186.48	1127.04	905.40	1117.00
	corr_amt	1570.77	1149.77	1018.65	1178.17	1102.11	892.54	1110.97
PFOS	cal_amt	4594.58	3904.73	4140.42	3769.70	3407.05	2124.27	1014.89
	corr_amt	4893.58	3783.69	4099.09	3743.32	3331.68	2094.10	1009.41
PFOS_br	cal_amt	5545.79	4842.87	4615.62	4422.73	3942.86	3136.37	1538.03
	corr_amt	5906.69	4692.74	4569.55	4391.77	3855.64	3091.84	1529.72

Table A11. Concentrations (ng L⁻¹) of the studied PFASs detected at different durations during the treatment in the Millipore water at 0.95 mA cm⁻²-trial.

Time_ minutes	6:2 FTSA			8:2 FTSA		FOSA		FOSA_br	
	corr_factor	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
-12h	0.9835	2682.13	2637.87	1371.99	1349.35	2898.94	2851.10	339.37	333.77
-12h	1.0345	2792.72	2889.10	1468.69	1519.37	2791.03	2887.35	330.66	342.07
-3h	1.0002	3164.01	3164.51	1982.64	1982.96	1597.38	1597.64	265.26	265.30
-3:30h	1.0161	4137.99	4204.68	2545.41	2586.43	2087.27	2120.90	313.09	318.13
0	0.9609	3459.83	3324.40	2053.71	1973.31	1559.42	1498.37	249.59	239.82
0	1.0563	3141.79	3318.67	1947.68	2057.33	1424.79	1505.00	213.84	225.88
5	1.0011	3233.84	3237.40	1200.71	1202.03	462.02	462.52	78.84	78.93
5	1.0615	3424.41	3634.95	981.55	1041.90	602.53	639.58	114.65	121.70
10	1.0067	3355.99	3378.35	794.10	799.39	250.28	251.94	47.74	48.06
10	0.9949	2244.72	2233.33	430.75	428.56	106.15	105.61	26.29	26.16
15									
15	0.9514	2243.92	2134.87	396.23	376.98	91.64	87.18	17.86	16.99
30	0.9923	994.53	986.87	58.84	58.39	34.46	34.19	4.66	4.63
30	1.0170	1035.24	1052.84	64.19	65.28	33.46	34.02	6.43	6.54
60	0.9658	379.18	366.23	8.59	8.30	27.65	26.70	3.43	3.31
60	1.0008	388.16	388.48	6.52	6.53	29.25	29.28	3.56	3.56
90	1.0128	118.39	119.91	3.69	3.74	35.39	35.85	3.62	3.66
90	0.9694	108.76	105.43	3.09	2.99	34.68	33.62	3.66	3.55
120	1.0005	72.59	72.63	1.93	1.93	37.70	37.72	4.33	4.33
120	0.9478	55.59	52.69	3.00	2.84	48.68	46.14	4.95	4.69

Corr_factor (Correction factor): value for correcting for vial weight. Cal_amt (Calculated amount): Calculated concentration obtained from Quantiva. Corr_amt (corrected amount): calculated amount corrected for vial weight.

PFHxA		PFOA		PFDA		PFDODA		PFTeDA		PFHxDA	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
4155.25	4086.68	7594.60	7469.26	2915.78	2867.66	388.22	381.81	26.68	26.24	1001.73	985.20
4236.33	4382.53	8561.76	8857.24	3610.22	3734.82	465.97	482.05	176.99	183.09	6768.95	7002.56
4681.32	4682.07	8338.67	8340.00	3644.70	3645.28	305.05	305.09	10.71	10.71	550.59	550.68
6177.12	6276.67	12925.37	13133.67	5985.81	6082.27	488.33	496.20	17.79	18.08	665.22	675.94
5058.33	4860.32	9334.71	8969.30	4307.20	4138.59	113.61	109.16	2.31	2.22	308.06	296.00
5102.95	5390.25	7637.53	8067.53	3813.13	4027.81	330.44	349.04	22.14	23.38	709.72	749.68
4772.52	4777.78	7338.02	7346.10	2053.24	2055.50	137.65	137.80	16.52	16.54	935.00	936.03
j6110.92	6486.62	9547.60	10134.59	2336.03	2479.65	200.38	212.70	9.79	10.39	2094.25	2223.01
6044.28	6084.56	7809.92	7861.97	1344.73	1353.69	125.34	126.17	9.12	9.18	1483.56	1493.45
4270.53	4248.86	5466.57	5438.83	805.57	801.48	17.14	17.05	4.81	4.79	658.33	654.99
-	-	-	-	-	-	-	-	-	-	-	-
5404.35	5141.71	5220.00	4966.32	676.45	643.57	40.24	38.29	16.12	15.34	837.24	796.55
4493.24	4458.64	2203.28	2186.31	89.52	88.83	29.49	29.27	8.18	8.12	918.27	911.20
4487.14	4563.44	2053.82	2088.74	87.10	88.58	25.08	25.50	4.25	4.32	1126.00	1145.15
4662.25	4503.03	631.20	609.64	15.58	15.04	6.86	6.62	2.24	2.16	539.74	521.30
4556.86	4560.60	611.94	612.45	11.58	11.59	3.63	3.64	4.92	4.92	524.50	524.93
4100.26	4152.92	158.41	160.44	1.70	1.72	4.52	4.58	2.27	2.30	244.23	247.37
4449.69	4313.39	162.50	157.53	7.97	7.73	6.21	6.02	1.52	1.47	214.03	207.48
4056.90	4058.93	55.43	55.46	N/F	#VALUE!	4.54	4.54	2.50	2.50	166.15	166.23
4282.44	4058.95	58.54	55.49	5.14	4.87	0.94	0.89	3.39	3.21	49.81	47.21

PFBS		PFHxS		PFHxS_br		PFOS		PFOS_br	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
7344.68	7223.47	5116.56	5032.12	1266.37	1245.47	4612.91	4536.78	5240.54	5154.06
6854.70	7091.27	5158.51	5336.54	1264.79	1308.44	5107.18	5283.44	6014.90	6222.48
7844.65	7845.91	5456.50	5457.37	1293.24	1293.44	4359.57	4360.27	4969.83	4970.62
10707.82	10880.38	6964.18	7076.41	1763.07	1791.48	6601.13	6707.51	7020.92	7134.07
9051.29	8696.98	5680.19	5457.84	1419.02	1363.47	4498.41	4322.32	5358.08	5148.33
8806.49	9302.30	5337.39	5637.89	1270.04	1341.55	4633.42	4894.29	5260.31	5556.46
8714.64	8724.24	5559.07	5565.19	1432.97	1434.55	2719.99	2722.98	2997.52	3000.82
10913.90	11584.90	5829.69	6188.11	1494.65	1586.54	2979.55	3162.73	3658.13	3883.04
10708.68	10780.05	6093.28	6133.89	1586.32	1596.89	1484.75	1494.65	1681.55	1692.76
7671.90	7632.97	4345.57	4323.52	1107.79	1102.17	995.01	989.97	1425.38	1418.15
10582.20	10067.93	4376.77	4164.07	1169.65	1112.81	735.58	699.83	902.68	858.82
8852.65	8784.48	2584.73	2564.82	804.04	797.85	106.52	105.70	141.00	139.92
8477.37	8621.52	2779.15	2826.41	899.62	914.92	106.15	107.95	143.74	146.18
9497.07	9172.72	1472.74	1422.44	564.71	545.42	10.42	10.06	17.11	16.52
9419.94	9427.67	1539.17	1540.43	574.40	574.87	10.72	10.73	5.97	5.97
8786.26	8899.10	649.47	657.81	300.31	304.16	4.54	4.59	2.50	2.53
9404.95	9116.86	619.99	601.00	288.29	279.46	7.66	7.42	2.56	2.48
9472.73	9477.47	355.00	355.18	180.95	181.04	3.51	3.51	2.20	2.21
9108.14	8632.82	393.43	372.90	202.12	191.57	3.43	3.25	2.13	2.02

Table A12. Concentration (ng L⁻¹) of studied PFASs at different durations during the treatment in Millipore water at 4.8 mA cm⁻²-trial.

Time_ minutes	corr_factor	6:2 FTSA		8:2 FTSA		FOSA		FOSA_br	
		cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
-12h	0.9660	42162.78	40729.04	15432.51	14907.73	29964.96	28946.00	4667.14	4508.44
-12h	0.9981	3536.34	3529.49	1427.56	1424.79	1608.92	1605.81	235.58	235.13
-3h	0.9904	2482.47	2458.70	1019.27	1009.51	1363.28	1350.23	215.06	213.00
-3:30h	1.0239	3549.03	3633.95	959.25	982.20	2107.10	2157.52	338.88	346.99
0	0.9990	3840.26	3836.46	1354.18	1352.84	2059.07	2057.03	321.45	321.13
0	1.1027	3322.08	3663.41	1015.94	1120.32	1676.91	1849.21	270.83	298.66
5	0.9652	3915.36	3779.21	844.18	814.82	519.23	501.18	103.55	99.95
5	0.9252	4178.60	3866.00	836.60	774.01	474.23	438.76	75.34	69.70
10	0.8615	4059.64	3497.32	744.53	641.40	324.71	279.74	51.16	44.07
10	0.9836	3568.82	3510.30	507.75	499.42	240.52	236.58	40.66	40.00
15	0.9556	3516.16	3359.97	324.21	309.81	184.92	176.71	33.54	32.05
15	0.9686	3618.82	3505.10	411.26	398.33	200.83	194.52	37.24	36.07
30	0.9864	2039.19	2011.53	121.63	119.98	103.62	102.22	15.64	15.43
30	0.9121	2729.84	2489.95	244.61	223.11	137.55	125.46	20.68	18.86
60	0.9693	1046.96	1014.79	55.65	53.94	39.73	38.51	6.04	5.85
60	0.9629	1249.85	1203.42	87.05	83.81	51.24	49.33	7.14	6.87
90	0.9372	1247.06	1168.68	19.99	18.73	22.51	21.09	2.04	1.91
90	0.9403	1367.15	1285.52	28.28	26.59	20.82	19.58	4.45	4.19
120	1.0292	895.96	922.09	32.27	33.21	12.80	13.18	1.27	1.30

120	0.9698	650.02	630.39	15.18	14.72	11.53	11.18	1.09	1.05
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Corr_factor (Correction factor): value for correcting for vial weight. Cal_amt (Calculated amount) in ng L⁻¹: Calculated concentration obtained from Quantiva. Corr_amt (corrected amount):
calculated amount corrected for vial weight.

PFHxA		PFOA		PFDA		PFDODA		PFTeDA		PFHxDA	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
42356.05	40915.73	131252.17	#####	20464.71	19768.81	6430.23	6211.57	8474.38	8186.21	191393.94	184885.60
4042.47	4034.64	8599.34	8582.69	3053.85	3047.94	550.55	549.49	434.71	433.87	8237.26	8221.31
2885.71	2858.07	6252.65	6192.77	2519.18	2495.05	280.73	278.05	55.80	55.26	4349.14	4307.49
4231.31	4332.57	8192.60	8388.64	3607.66	3693.99	731.51	749.01	241.04	246.80	19822.26	20296.59
4462.44	4458.02	8756.06	8747.38	4175.05	4170.92	456.65	456.19	102.04	101.94	8964.67	8955.78
3856.71	4252.98	6720.96	7411.52	2844.65	3136.92	225.90	249.11	135.08	148.96	12099.56	13342.75
4430.73	4276.65	8798.15	8492.21	2279.35	2200.09	37.54	36.24	8.60	8.30	539.40	520.64
4777.33	4419.94	8334.38	7710.89	2414.59	2233.95	67.34	62.30	47.17	43.64	-25.54	-23.63
4078.25	3513.36	8656.09	7457.10	1288.85	1110.33	54.52	46.97	59.81	51.52	2412.20	2078.08
4186.41	4117.76	6732.30	6621.90	1035.83	1018.84	72.31	71.12	75.38	74.14	4347.15	4275.86
4073.92	3892.95	5887.05	5625.54	547.87	523.53	30.55	29.19	19.60	18.73	2192.99	2095.58
4128.74	3998.99	6089.47	5898.10	544.67	527.55	30.22	29.27	17.86	17.30	-37.09	-35.92
3167.68	3124.71	3315.99	3271.01	157.77	155.63	6.16	6.07	5.11	5.04	624.29	615.82
3962.98	3614.73	4043.69	3688.35	231.27	210.95	21.26	19.39	15.27	13.93	-37.04	-33.79

2084.52	2020.47	1488.89	1443.14	44.62	43.25	2.37	2.30	5.06	4.90	-28.88	-28.00
2295.58	2210.31	1895.21	1824.80	55.10	53.06	4.30	4.14	3.12	3.01	65.41	62.98
3118.07	2922.11	1790.65	1678.11	35.54	33.31	N/F	#VALUE!	0.02	0.02	-25.43	-23.83
3269.08	3073.88	1815.59	1707.18	29.14	27.40	-0.33	-0.31	N/F	N/F	-16.35	-15.37
2897.99	2982.54	1149.97	1183.52	28.29	29.11	-0.10	-0.10	N/F	N/F	2.46	2.53
2347.61	2276.71	873.17	846.79	19.42	18.84	-0.15	-0.15	3.38	3.28	-33.06	-32.06

PFBS		PFHxS		PFHxS_br		PFOS		PFOS_br	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
86037.11	83111.42	72679.79	70208.32	16362.94	15806.52	47115.43	45513.27	60540.24	58481.57
8491.53	8475.09	6232.25	6220.19	1457.93	1455.11	4455.17	4446.54	5343.08	5332.73
5969.35	5912.18	3851.77	3814.88	854.81	846.62	2638.41	2613.14	3421.62	3388.85
9033.79	9249.96	5400.75	5529.99	1225.75	1255.08	4114.10	4212.55	5006.42	5126.22
9293.83	9284.62	5877.67	5871.85	1345.07	1343.74	4298.06	4293.80	5310.75	5305.48
8251.43	9099.25	4898.40	5401.70	1138.14	1255.08	3286.38	3624.05	4212.37	4645.18
9724.07	9385.94	5716.95	5518.15	1331.35	1285.05	2893.86	2793.23	4308.18	4158.37
10267.21	9499.13	6333.21	5859.43	1434.58	1327.26	2567.51	2375.44	3538.62	3273.89
9327.00	8035.08	5463.48	4706.71	1280.41	1103.06	1482.85	1277.45	2183.33	1880.91
9474.99	9319.61	4984.08	4902.34	1245.36	1224.94	1177.87	1158.56	1821.73	1791.85
9635.65	9207.62	4984.85	4763.42	1243.25	1188.02	833.78	796.75	1368.96	1308.15
9774.74	9467.56	5113.92	4953.20	1261.71	1222.06	962.26	932.02	1583.74	1533.97
7759.52	7654.27	3141.07	3098.47	814.15	803.11	272.25	268.55	504.63	497.79
9706.23	8853.28	4268.81	3893.69	1083.67	988.44	396.31	361.48	656.77	599.06
5748.64	5572.00	1673.03	1621.63	460.76	446.60	84.94	82.33	153.68	148.96
5917.07	5697.27	1936.23	1864.31	513.27	494.21	93.73	90.25	162.07	156.05
9122.26	8548.95	2262.43	2120.24	673.16	630.86	46.53	43.61	101.74	95.35
9585.47	9013.11	2521.37	2370.81	734.79	690.91	46.83	44.03	114.88	108.02
9380.77	9654.45	1956.57	2013.65	598.17	615.62	39.99	41.16	61.79	63.59
7728.94	7495.50	1554.64	1507.68	493.33	478.43	17.47	16.95	36.45	35.35

Table A13. Concentrations (ng L⁻¹) of the studied PFASs detected at different durations during the treatment in the Millipore pore water at 11.9 mA cm⁻²-trial.

Time_ minutes	6:2 FTSA			8:2 FTSA		FOSA		FOSA_br	
	corr_factor	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
-12h	0.9418	2941.85	2770.72	1424.16	1341.31	2163.72	2037.85	257.35	242.38
-12h	1.0274	2755.07	2830.62	1692.93	1739.35	1240.63	1274.65	176.54	181.38
-3h	0.9895	2888.71	2858.48	1581.04	1564.50	772.31	764.23	135.39	133.97
-3:30h	1.0334	2809.89	2903.72	1380.02	1426.09	839.06	867.07	123.78	127.91
0	0.9809	3429.54	3364.09	1916.97	1880.38	988.04	969.18	139.79	137.12
0	0.9900	3311.86	3278.82	1507.41	1492.37	1027.28	1017.03	147.14	145.67
5	1.0103	3221.04	3254.07	766.75	774.61	149.91	151.45	19.45	19.65
5	0.9978	2995.82	2989.15	1185.43	1182.79	210.51	210.04	34.24	34.16
10	—	—	—	—	—	—	—	—	—
10	1.5247	2118.92	3230.65	341.69	520.97	80.11	122.14	16.05	24.47
15	1.3939	2382.73	3321.17	445.41	620.83	77.48	108.00	10.87	15.15
15	0.9434	1470.47	1387.22	154.25	145.52	39.53	37.29	7.00	6.60
30	1.1870	1527.03	1812.59	49.20	58.40	31.77	37.71	3.29	3.90
30	1.0364	340.86	353.26	13.03	13.50	8.26	8.56	0.97	1.00
60	0.9960	1148.71	1144.10	33.69	33.55	15.64	15.58	2.09	2.08
60	0.9807	1280.78	1256.00	43.43	42.59	19.85	19.46	2.54	2.49
90	0.9900	630.90	624.61	77.25	76.48	11.48	11.36	1.80	1.79
90	1.0193	671.04	683.98	89.93	91.67	13.40	13.66	0.81	0.82
120	0.9945	334.95	333.12	81.88	81.43	48.01	47.75	3.92	3.90
120	0.9820	281.82	276.73	73.52	72.20	30.91	30.36	2.52	2.48

PFHxA		PFOA		PFDA		PFDODA		PFTeDA		PFHxDA	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
3645.32	3433.27	8593.88	8093.96	2417.37	2276.74	271.40	255.61	105.94	99.77	2545.57	2397.49
3466.05	3561.10	8066.74	8287.96	2638.03	2710.37	339.04	348.33	57.61	59.19	2355.04	2419.63
3831.10	3791.01	8199.13	8113.32	2131.58	2109.27	99.62	98.58	10.91	10.79	851.92	843.00
3426.00	3540.40	8181.01	8454.18	2122.23	2193.10	120.75	124.78	5.24	5.41	448.30	463.27
4148.84	4069.66	8546.44	8383.34	2855.10	2800.61	233.13	228.68	30.83	30.24	2715.12	2663.30
3734.69	3697.44	8936.88	8847.75	2513.30	2488.24	228.29	226.02	38.41	38.03	2838.49	2810.18
3448.47	3483.83	6222.40	6286.22	655.90	662.63	21.79	22.01	9.79	9.89	279.01	281.87
3381.12	3373.59	6724.71	6709.73	1030.62	1028.33	74.54	74.37	10.85	10.83	464.09	463.06
-	-	-	-	-	-	-	-	-	-	-	-
5393.69	8223.59	5079.94	7745.23	521.57	795.22	25.65	39.11	2.68	4.08	691.73	1054.66
2834.85	3951.37	4138.73	5768.78	197.26	274.95	11.00	15.33	0.87	1.21	59.57	83.03
2307.91	2177.25	2712.25	2558.70	100.23	94.55	2.76	2.60	0.65	0.61	77.13	72.76
2850.19	3383.20	2364.16	2806.27	31.94	37.91	1.31	1.55	1.03	1.22	-0.39	-0.46
605.46	627.50	521.24	540.22	6.05	6.27	-0.73	-0.75	0.00	0.00	-30.21	-31.31
2121.79	2113.26	1221.66	1216.74	10.47	10.43	0.52	0.52	1.29	1.28	-34.94	-34.80
2206.14	2163.47	1225.20	1201.50	11.67	11.45	-0.49	-0.48	3.57	3.50	-38.41	-37.67
1407.96	1393.93	717.71	710.56	27.73	27.45	2.92	2.89	3.44	3.41	-29.04	-28.75
1530.03	1559.54	846.10	862.42	42.25	43.06	3.34	3.41	1.70	1.74	-43.36	-44.20
966.59	961.30	579.38	576.21	64.27	63.92	9.42	9.37	0.13	0.13	-37.05	-36.84
651.51	639.75	452.90	444.73	38.24	37.55	5.71	5.61	0.24	0.23	-38.99	-38.29

PFBS		PFHxS		PFHxS_br		PFOS		PFOS_br	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
7843.54	7387.27	5539.47	5217.24	1402.51	1320.93	4894.09	4609.39	5695.38	5364.08
7364.44	7566.40	5067.46	5206.43	1196.31	1229.12	4612.37	4738.86	5318.87	5464.73
7950.11	7866.91	5413.09	5356.44	1221.89	1209.10	3853.23	3812.91	4672.96	4624.06
7650.18	7905.63	5137.84	5309.40	1180.67	1220.10	3420.65	3534.87	3983.86	4116.88
9312.97	9135.24	6249.14	6129.87	1348.81	1323.07	4321.64	4239.16	4993.28	4897.99
7838.99	7760.81	5773.70	5716.11	1272.47	1259.78	4202.54	4160.63	4813.93	4765.92
8396.33	8482.44	5227.02	5280.63	1343.50	1357.28	1285.97	1299.16	1729.84	1747.58
8055.33	8037.39	4502.83	4492.81	1071.88	1069.49	1731.89	1728.03	2006.81	2002.34
-	-	-	-	-	-	-	-	-	-
9776.65	14906.15	4502.33	6864.56	1139.94	1738.03	651.01	992.57	775.22	1181.95
7241.25	10093.24	3681.69	5131.74	804.61	1121.51	517.64	721.52	724.63	1010.02
5662.51	5341.93	2467.01	2327.34	594.65	560.98	254.34	239.94	410.39	387.16
7896.08	9372.69	2484.89	2949.58	685.54	813.74	108.39	128.66	204.77	243.06
1813.93	1879.94	580.71	601.85	160.93	166.79	23.74	24.61	49.81	51.63
7605.86	7575.29	1854.36	1846.91	502.61	500.59	54.07	53.86	83.79	83.45
7891.74	7739.08	2086.49	2046.12	543.39	532.88	55.24	54.17	96.61	94.74
6820.37	6752.42	1338.72	1325.38	363.62	359.99	85.80	84.94	87.70	86.83
7293.93	7434.62	1450.06	1478.03	395.69	403.32	103.82	105.82	106.91	108.97
6433.71	6398.53	947.12	941.94	252.14	250.76	117.29	116.65	90.51	90.02
4434.33	4354.31	748.94	735.43	218.81	214.86	79.12	77.69	60.61	59.52

Table A14. Concentration (ng L⁻¹) of studied PFASs at different durations during the treatment in Millipore water at 16.7 mA cm⁻²-trial.

Time_ minutes	6:2 FTSA			8:2 FTSA		FOSA		FOSA_br	
	corr_factor	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
-12h	1.0377	3170.93	3290.58	2135.40	2215.97	4535.63	4706.77	4667.14	579.00
-12h	1.0181	3667.59	3733.90	3104.68	3160.82	1890.47	1924.65	235.58	220.89
-3h	1.1132	2943.39	3276.48	2902.50	3230.96	6571.24	7314.86	215.06	2657.33
-3:30h	1.0309	3428.65	3534.62	2486.09	2562.92	5217.25	5378.49	338.88	682.24
0	0.9340	5341.41	4988.99	4118.55	3846.81	5744.31	5365.30	321.45	797.21
0	0.9941	4181.34	4156.81	2773.73	2757.46	4600.15	4573.17	270.83	548.17
5	0.9654	9838.91	9498.30	2188.21	2112.46	643.92	621.63	103.55	75.81
5	0.9801	4042.47	3962.20	1243.45	1218.75	779.63	764.15	75.34	117.95
10	0.9395	4811.67	4520.46	1636.34	1537.31	612.39	575.32	51.16	78.82
10	0.9938	4361.59	4334.37	1605.53	1595.51	717.74	713.26	40.66	83.34
15	1.0304	4479.85	4616.12	2461.79	2536.68	563.17	580.30	33.54	107.43
15	1.0057	4069.45	4092.61	1037.30	1043.20	507.28	510.16	37.24	73.79
30	1.0076	3383.61	3409.31	750.78	756.48	135.14	136.17	15.64	14.25
30	1.1563	3254.00	3762.46	787.21	910.22	102.21	118.18	20.68	9.90

Corr_factor (Correction factor): value for correcting for vial weight. Cal_amt (Calculated amount) in ng L-1: Calculated concentration obtained from Quantiva. Corr_amt (corrected amount): calculated amount corrected for vial weight.

PFHxA		PFOA		PFDA		PFDODA		PFTeDA		PFHxDA	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
5008.83	5197.82	8550.96	8873.61	3778.18	3920.73	1060.68	1100.71	825.86	857.02	11289.24	11715.20
4930.05	5019.19	8761.89	8920.32	5719.75	5823.17	2021.36	2057.90	3820.74	3889.82	43434.37	44219.71
4360.42	4853.86	8823.58	9822.10	5054.61	5626.61	1095.84	1219.85	661.94	736.85	17846.92	19866.56
5294.76	5458.40	8964.70	9241.77	5676.96	5852.42	1381.41	1424.11	702.03	723.73	19988.64	20606.42
5996.43	5600.79	11025.23	10297.80	7070.22	6603.73	1270.15	1186.35	446.00	416.57	14722.32	13750.95
5198.58	5168.09	9945.51	9887.17	6486.41	6448.37	1302.10	1294.46	633.15	629.44	24473.55	24330.01
4898.81	4729.22	8459.36	8166.51	1643.49	1586.59	235.16	227.02	553.96	534.78	3641.38	3515.32
5669.63	5557.04	8312.09	8147.03	2367.94	2320.92	232.03	227.42	102.23	100.20	3883.63	3806.51
5102.01	4793.23	8528.65	8012.48	2053.86	1929.55	194.23	182.47	11.62	10.92	311.03	292.20
5042.69	5011.21	8417.24	8364.71	1955.32	1943.12	159.94	158.95	131.74	130.92	1928.12	1916.09
5361.57	5524.66	8188.24	8437.31	1672.35	1723.21	163.68	168.66	38.16	39.32	1151.60	1186.62
4799.93	4827.25	8012.08	8057.69	1711.57	1721.31	158.87	159.77	116.42	117.08	4613.90	4640.16
4178.19	4209.93	5664.03	5707.06	357.89	360.61	8.98	9.05	7.21	7.27	117.31	118.20
4380.31	5064.76	4933.39	5704.26	365.12	422.17	5.70	6.59	3.67	4.25	140.34	162.27

PFBS		PFHxS		PFHxS_br		PFOS		PFOS_br	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
8332.35	8646.74	5586.64	5797.43	1434.01	1488.11	5184.10	5379.71	6024.08	6251.38
8065.38	8211.21	5662.35	5764.73	1497.34	1524.41	5890.56	5997.07	6611.93	6731.48
7474.65	8320.51	4685.37	5215.59	1162.62	1294.18	5362.59	5969.44	5273.99	5870.82
8816.44	9088.93	5511.21	5681.54	1414.39	1458.10	5812.59	5992.23	6508.29	6709.43
10039.96	9377.53	7115.19	6645.73	1853.23	1730.96	7936.57	7412.92	8371.99	7819.61
8796.71	8745.12	6553.83	6515.39	1642.83	1633.19	6284.19	6247.33	7190.29	7148.12
8991.75	8680.47	4966.76	4794.82	1231.02	1188.40	2555.77	2467.30	2537.47	2449.62
10669.47	10457.60	5681.07	5568.26	1466.02	1436.91	3161.31	3098.53	4253.58	4169.11
10047.72	9439.62	6346.82	5962.70	1625.72	1527.33	3955.75	3716.35	5228.73	4912.28
9642.57	9582.39	5993.04	5955.64	1420.65	1411.78	3788.52	3764.88	5031.72	5000.31
10192.13	10502.16	5663.56	5835.83	1438.32	1482.07	3193.24	3290.37	4286.23	4416.61
9542.82	9597.14	5713.10	5745.62	1402.46	1410.45	3271.97	3290.59	4924.20	4952.23
9281.90	9352.42	4385.14	4418.45	1132.61	1141.21	1640.11	1652.57	2422.32	2440.72
9540.53	11031.29	4175.25	4827.65	1003.54	1160.35	1470.84	1700.67	2115.92	2446.54

Table A15. Concentration (ng L⁻¹) of studied PFASs at different durations during treatment in the DOC water at 0.95 mA am⁻²- trial.

Time_ minutes	corr_factor	6:2 FTSA		8:2 FTSA		FOSA		FOSA_br	
		cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
-12h	0.97	3832.00	3701.69	2391.33	2310.01	3136.75	3030.08	4667.14	342.39
-12h	1.00	3802.76	3795.40	2658.40	2653.25	2477.07	2472.27	235.58	384.65
-3h	0.99	4254.28	4213.53	2719.71	2693.66	1637.07	1621.39	215.06	295.02
-3:30h	1.02	3744.19	3833.79	2228.89	2282.23	1356.36	1388.81	338.88	250.48
0	1.00	3912.54	3908.67	2228.88	2226.67	1375.07	1373.71	321.45	181.20
0	1.10	4105.26	4527.06	2509.08	2766.88	1411.74	1556.79	270.83	261.33
5	0.97	4073.90	3932.24	1309.62	1264.08	700.15	675.80	103.55	117.26
5	0.93	4135.04	3825.70	1562.88	1445.96	692.54	640.73	75.34	112.51
10	0.86	3604.06	3104.85	491.28	423.23	254.05	218.86	51.16	38.95
10	0.98	4357.45	4285.99	1273.81	1252.92	293.93	289.11	40.66	54.46
15	0.96	2932.57	2802.30	270.21	258.20	117.84	112.61	33.54	16.44
15	0.97	3291.35	3187.92	224.92	217.85	102.63	99.41	37.24	13.28
30	0.99	2819.27	2781.03	31.49	31.06	35.75	35.27	15.64	0.76
30	0.91	2471.25	2254.09	169.90	154.97	48.04	43.82	20.68	6.18
60	0.97	2559.68	2481.03	134.70	130.57	26.86	26.04	6.04	2.17
60	0.96	2912.41	2804.22	206.94	199.25	66.90	64.41	7.14	13.13
90	0.94	3140.32	2942.96	280.99	263.33	68.73	64.41	2.04	7.50
90	0.94	3046.20	2864.31	290.60	273.25	51.58	48.50	4.45	2.64
120	1.03	3029.50	3117.89	190.26	195.81	54.83	56.43	1.27	5.51
120	0.97	3042.83	2950.93	190.50	184.74	28.68	27.82	1.09	1.94

Corr_factor (Correction factor): value for correcting for vail weight. Cal_amt (Calculated amount) in ng L-1: Calculated concentration obtained from Quantiva. Corr_amt (corrected amount): calculated amount corrected for vail weight.

PFHxA		PFOA		PFDA		PFDODA		PFTeDA		PFHxDA	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
3003.48	2901.35	5869.67	5670.07	3985.91	3850.37	1973.02	1905.92	3466.96	3349.07	124800.55	120556.72
3741.78	3734.53	7279.57	7265.48	4038.88	4031.06	1618.97	1615.84	2869.45	2863.89	148054.83	147768.16
3667.00	3631.88	6028.87	5971.13	3948.17	3910.35	1623.98	1608.43	1593.69	1578.42	167412.43	165809.06
3344.01	3424.03	5981.36	6124.49	3773.49	3863.78	1051.83	1077.00	1540.52	1577.39	107796.75	110376.24
4084.33	4080.28	6668.26	6661.66	4677.21	4672.57	1317.03	1315.73	1027.01	1025.99	77863.01	77785.85
3863.01	4259.93	6489.80	7156.61	3801.91	4192.54	912.69	1006.47	685.05	755.44	60584.72	66809.64
3303.15	3188.29	5838.90	5635.87	2302.83	2222.75	427.47	412.61	434.05	418.96	34033.59	32850.13
3259.95	3016.08	5710.47	5283.28	1978.23	1830.24	637.41	589.72	645.41	597.13	61748.28	57128.94
3692.40	3180.96	5535.67	4768.91	713.19	614.40	631.61	544.13	1104.43	951.45	96822.77	83411.53
3370.42	3315.15	7027.49	6912.25	1744.42	1715.81	385.94	379.61	461.20	453.64	42509.12	41812.03
3492.79	3337.64	4549.89	4347.78	471.31	450.38	296.35	283.18	281.30	268.81	22628.48	21623.30
3044.01	2948.34	4733.62	4584.86	375.93	364.12	287.61	278.57	472.15	457.31	49692.66	48131.00
4107.79	4052.07	3977.17	3923.23	38.41	37.89	279.24	275.45	1287.02	1269.56	147957.86	145951.03
3380.74	3083.65	3779.97	3447.81	302.81	276.20	148.65	135.59	185.43	169.14	16197.59	14774.21
3327.59	3225.35	3898.07	3778.30	179.50	173.99	97.43	94.43	427.45	414.32	41797.29	40513.03
3723.54	3585.22	4481.07	4314.62	339.70	327.08	161.55	155.55	500.40	481.82	42296.23	40725.06
3384.09	3171.41	4993.13	4679.32	500.90	469.42	90.96	85.24	460.25	431.33	30951.70	29006.46
3046.85	2864.91	4901.92	4609.22	470.76	442.65	106.49	100.13	360.60	—	38668.78	36359.79
3665.74	3772.69	5134.26	5284.05	259.54	267.11	84.63	87.10	189.54	—	13271.22	13658.40
3393.70	3291.19	4644.79	4504.50	241.16	233.88	54.24	52.60	284.37	275.78	27796.23	26956.69

PFBS		PFHxS		PFHxS_br		PFOS		PFOS_br	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
6857.13	6623.96	4586.58	4430.61	1034.11	998.94	3376.73	3261.91	3103.82	2998.27
9697.94	9679.17	4585.57	4576.69	1060.39	1058.34	3679.99	3672.87	3246.61	3240.32
8191.29	8112.84	4950.54	4903.13	1129.07	1118.25	3951.15	3913.31	3705.44	3669.96
7999.30	8190.72	4389.67	4494.71	1019.07	1043.46	3558.54	3643.69	3375.19	3455.95
9313.42	9304.19	4442.19	4437.79	1062.14	1061.09	3459.41	3455.98	3351.06	3347.74
9067.86	9999.56	4644.94	5122.19	1055.92	1164.41	3680.73	4058.92	3382.06	3729.56
7629.41	7364.11	4825.15	4657.36	1185.27	1144.05	2368.24	2285.89	2388.19	2305.14
7760.01	7179.49	4989.47	4616.22	1250.06	1156.54	1982.83	1834.49	2147.14	1986.52
9294.85	8007.39	4573.76	3940.23	1152.35	992.73	822.07	708.20	1038.01	894.23
7546.23	7422.48	5012.23	4930.03	1227.25	1207.12	2554.53	2512.64	3195.19	3142.80
8179.44	7816.10	3936.41	3761.55	1046.39	999.91	549.84	525.42	705.99	674.63
7111.27	6887.79	4350.89	4214.16	1180.95	1143.84	437.84	424.08	566.55	548.74
9579.24	9449.31	4266.83	4208.95	1105.31	1090.32	80.64	79.55	160.58	158.40
7464.24	6808.32	3721.97	3394.89	1081.80	986.74	341.15	311.17	356.92	325.55
8089.48	7840.92	3639.77	3527.93	973.97	944.04	288.58	279.71	398.04	385.81
8840.83	8512.42	3984.98	3836.95	1001.93	964.71	463.00	445.80	592.64	570.62
8334.83	7811.01	4097.72	3840.19	1052.40	986.26	800.44	750.13	1047.03	981.22
7280.12	6845.41	3886.95	3654.85	1012.78	952.31	694.18	652.73	980.09	921.57
8664.35	8917.14	4068.03	4186.71	992.48	1021.44	463.81	477.34	621.35	639.48
7950.62	7710.49	3962.84	3843.15	1006.08	975.69	438.77	425.51	657.03	637.19

Table A16. Concentration (ng L⁻¹) of studied PFASs at different durations during the treatment in DOC water at 4.8 mA cm⁻²-trial.

Time_ minutes	corr_fac- tor	6:2 FTSA		8:2 FTSA		FOSA		FOSA_br	
		cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
-12h	1.0360	5067.13	5249.72	3114.29	3226.51	3739.58	3874.33	397.65	411.98
-12h	1.1190	4151.05	4644.90	1936.25	2166.61	1986.43	2222.75	237.66	265.93
-3h	1.0151	4774.48	4846.40	3442.83	3494.69	1366.99	1387.58	179.05	181.74
-3:30h	1.0195	4624.61	4714.66	2504.65	2553.42	1224.88	1248.73	188.14	191.81
0	1.0193	4871.27	4965.32	2320.84	2365.64	1244.90	1268.93	188.94	192.58
0	1.0335	4826.27	4987.88	2608.13	2695.46	1105.63	1142.65	156.20	161.43
5	1.0025	2664.15	2670.72	176.81	177.25	54.92	55.06	9.36	9.38
5	1.0829	2153.64	2332.09	316.63	342.87	216.02	233.92	37.87	41.01
10	1.0059	2758.82	2775.03	380.40	382.63	104.65	105.26	13.53	13.61
10	1.0144	2426.06	2460.96	214.93	218.02	50.00	50.72	7.23	7.33
15	0.9944	1814.53	1804.43	49.67	49.39	30.40	30.23	3.96	3.94
15	1.0267	1926.17	1977.51	144.89	148.75	86.67	88.98	11.31	11.61
30	1.0036	2758.83	2768.69	224.91	225.71	64.90	65.13	9.39	9.42
30	1.0031	1545.36	1550.16	72.09	72.31	36.25	36.37	4.65	4.66
60	1.0037	2236.12	2244.42	206.41	207.18	33.00	33.12	4.40	4.42
60	1.0169	2886.09	2934.74	432.89	440.18	51.50	52.37	6.42	6.53
90	1.0395	1966.91	2044.65	337.75	351.10	56.45	58.68	7.12	7.40
90	1.0182	2752.35	2802.40	632.88	644.39	61.66	62.78	6.52	6.64
120	0.9450	1456.21	1376.10	315.45	298.09	41.58	39.29	6.38	6.03
120	1.0149	1264.96	1283.76	191.08	193.92	39.55	40.14	6.25	6.34

PFHxA		PFOA		PFDA		PFDoDA		PFTeDA		PFHxDA	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
5249.02	5438.16	9725.98	10076.44	4519.29	4682.13	3016.21	3124.90	3599.57	3729.27	43164.44	44719.79
3539.60	3960.70	6764.21	7568.94	4123.22	4613.75	1959.45	2192.57	2033.49	2275.42	29868.79	33422.25
4414.89	4481.39	8608.28	8737.95	4146.08	4208.53	2034.49	2065.13	1017.50	1032.83	24583.52	24953.83
4218.63	4300.78	9283.30	9464.06	4493.91	4581.41	1415.91	1443.48	828.01	844.13	29486.96	30061.12
4905.25	4999.94	8964.08	9137.13	5062.52	5160.25	1377.45	1404.04	953.25	971.65	26134.98	26639.53
3893.81	4024.20	7718.07	7976.51	4161.07	4300.40	1516.89	1567.69	806.13	833.12	22862.38	23627.93
4422.96	4433.86	3200.02	3207.91	276.50	277.18	156.39	156.78	893.06	895.26	21805.93	21859.71
4171.61	4517.27	3077.82	3332.85	665.62	720.77	321.49	348.13	740.56	801.93	20292.22	21973.64
3380.96	3400.82	3470.24	3490.63	387.79	390.06	130.86	131.63	381.27	383.51	11891.49	11961.35
4645.88	4712.71	2220.99	2252.93	204.52	207.46	119.65	121.37	288.69	292.84	11662.36	11830.11
4537.12	4511.85	1623.60	1614.56	32.12	31.94	49.77	49.49	191.22	190.16	11315.13	11252.11
4501.60	4621.57	2157.40	2214.89	212.35	218.01	89.12	91.50	213.61	219.30	9255.82	9502.50
4052.51	4066.99	2794.97	2804.96	156.59	157.15	28.84	28.94	44.56	44.72	3101.30	3112.38
4083.27	4095.97	1547.31	1552.12	82.26	82.51	30.92	31.02	57.23	57.41	3758.56	3770.24
3934.46	3949.08	1837.41	1844.24	115.08	115.51	9.45	9.49	24.09	24.18	1200.35	1204.81
3365.65	3422.39	2774.03	2820.80	219.73	223.44	10.04	10.20	12.69	12.90	733.68	746.04
3036.10	3156.09	1525.24	1585.52	162.50	168.93	9.98	10.37	2.62	2.73	564.75	587.07
3489.21	3552.66	1891.37	1925.77	263.46	268.25	7.99	8.13	2.92	2.97	443.35	451.42
2738.95	2588.26	1455.53	1375.45	153.28	144.85	2.97	2.80	1.75	1.65	66.30	62.65
2850.10	2892.44	1246.40	1264.92	125.95	127.83	4.93	5.01	4.20	4.26	74.27	75.37

PFBS		PFHxS		PFHxS_br		PFOS		PFOS_br	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
11823.70	12249.75	5752.14	5959.41	1630.35	1689.09	6665.31	6905.48	7125.80	7382.57
8279.80	9264.84	4849.88	5426.87	1389.57	1554.89	5513.33	6169.25	6423.83	7188.07
10582.55	10741.96	4909.25	4983.20	1418.48	1439.85	5506.45	5589.39	6229.03	6322.86
9893.11	10085.75	4788.98	4882.23	1314.98	1340.59	5192.30	5293.40	6484.91	6611.18
11298.65	11516.78	5395.75	5499.92	1483.45	1512.08	5902.28	6016.23	6809.62	6941.09
9049.66	9352.69	2.00	2.07	1361.51	1407.10	4996.73	5164.05	5880.65	6077.56
10662.52	10688.81	4311.02	4321.65	1391.71	1395.14	443.21	444.30	597.72	599.19
10322.03	11177.32	3365.66	3644.54	1069.92	1158.58	899.37	973.90	1071.33	1160.10
8499.77	8549.70	3730.50	3752.41	1246.95	1254.27	490.26	493.14	562.32	565.63
11787.09	11956.63	3502.86	3553.25	1335.34	1354.54	308.46	312.89	322.28	326.92
11256.79	11194.10	3202.06	3184.23	1204.94	1198.23	75.32	74.90	128.64	127.92
11711.94	12024.08	2986.02	3065.60	1115.85	1145.59	272.51	279.77	367.49	377.28
10799.89	10838.47	3615.05	3627.97	1171.15	1175.34	296.00	297.06	420.68	422.19
10530.90	10563.65	2681.20	2689.54	1060.40	1063.70	140.54	140.97	165.76	166.28
10740.59	10780.47	3404.68	3417.32	1179.71	1184.09	223.71	224.54	318.27	319.45
9090.34	9243.60	3850.52	3915.43	1258.11	1279.32	464.03	471.86	575.33	585.03
8480.92	8816.11	3066.94	3188.16	1040.20	1081.31	302.42	314.37	421.91	438.59
9752.73	9930.08	3619.11	3684.92	1222.00	1244.22	622.31	633.63	741.28	754.76
7968.39	7530.00	2512.68	2374.44	903.38	853.68	351.79	332.44	407.83	385.39
8964.98	9098.18	2365.37	2400.51	862.28	875.09	227.65	231.04	281.06	285.24

Table A17. Concentration (ng L⁻¹) of studied PFASs at different durations during the treatment in the DOC water at 11.9 mA cm⁻²-trial.

Time_ minutes	corr_factor	6:2 FTSA		8:2 FTSA		FOSA		FOSA_br	
		cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
-12h	1.0118	4841.26	4898.27	3114.29	3150.97	3854.71	3900.11	509.04	515.04
-12h	1.2419	3636.23	4515.94	1936.25	2404.68	2025.55	2515.59	293.79	364.87
-3h	1.0959	4958.22	5433.54	3442.83	3772.88	1434.93	1572.49	262.20	287.34
-3:30h	1.1143	4013.29	4472.13	2504.65	2791.01	1421.17	1583.65	228.87	255.04
0	0.9981	6649.69	6636.95	2320.84	2316.39	2185.97	2181.78	354.46	353.78
0	1.0153	5420.71	5503.71	2699.53	2740.86	1997.43	2028.02	336.98	342.14
5	1.0279	2432.95	2500.77	176.81	181.74	40.36	41.49	3.69	3.79
5	0.9972	2514.64	2507.67	316.63	315.76	26.54	26.46	4.17	4.16
10	1.0221	2244.90	2294.61	380.40	388.82	31.12	31.80	3.82	3.90
10	1.0313	2890.40	2980.96	214.93	221.66	25.29	26.08	1.25	1.29
15	1.0134	2877.36	2915.91	49.67	50.33	59.22	60.02	10.11	10.24
15	1.0335	3385.97	3499.42	144.89	149.74	43.05	44.49	7.70	7.96
30	1.0835	3045.07	3299.32	224.91	243.69	135.57	146.89	15.37	16.65
30	0.9927	3624.11	3597.70	72.09	71.56	171.97	170.71	21.81	21.65
60	1.2856	2442.38	3139.86	206.41	265.36	28.65	36.83	3.73	4.79
60	0.9978	3803.38	3794.88	432.89	431.92	48.58	48.47	1.69	1.69
90	1.0086	1797.06	1812.43	337.75	340.64	83.06	83.77	10.11	10.19
90	0.9967	1721.80	1716.11	632.88	630.78	58.02	57.83	5.29	5.27
120	1.0193	951.07	969.39	315.45	321.52	116.75	119.00	11.72	11.94
120	1.0193	926.68	944.53	191.08	194.76	132.55	135.10	13.27	13.53

Corr_factor (Correction factor): value for correcting for vail weight. Cal_amt (Calculated amount) in ng L-1: Calculated concentration obtained from Quantiva. Corr_amt (corrected amount): calculated amount corrected for vail weight.

PFHxA		PFOA		PFDA		PFDODA		PFTeDA		PFHxDA	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
3501.54	3542.78	9334.13	9444.06	4154.67	4203.60	1649.48	1668.90	3402.85	3442.92	59431.91	60131.85
3018.97	3749.34	8306.52	10316.09	3557.89	4418.65	1486.06	1845.58	5982.87	7430.28	127728.85	158629.97
3440.72	3770.57	8665.47	9496.19	3686.31	4039.71	1161.59	1272.95	2004.85	2197.05	72633.47	79596.57
3863.32	4305.01	8221.16	9161.09	4568.05	5090.32	2243.70	2500.22	4820.33	5371.44	156459.19	174347.22
4292.35	4284.13	12574.93	12550.83	5641.24	5630.42	1189.34	1187.06	1734.60	1731.28	46071.46	45983.17
4517.57	4586.73	10391.84	10550.95	5159.30	5238.30	1518.17	1541.41	2016.50	2047.37	53392.38	54209.86
4060.27	4173.45	3310.32	3402.59	55.96	57.52	70.50	72.46	545.88	561.10	21838.26	22447.02
4024.37	4013.21	3051.39	3042.93	93.15	92.89	54.32	54.17	336.33	335.40	13453.80	13416.51
3833.40	3918.27	2775.94	2837.39	26.22	26.80	36.69	37.50	149.70	153.02	18043.26	18442.73
4304.26	4439.12	3252.70	3354.61	17.39	17.93	38.46	39.66	383.43	395.45	34152.57	35222.64
3230.55	3273.83	3751.52	3801.78	66.87	67.76	12.91	13.08	76.15	77.17	8433.40	8546.39
3524.35	3642.44	4597.01	4751.04	31.35	32.40	20.62	21.31	66.02	68.23	7753.80	8013.60
2965.36	3212.95	5651.26	6123.11	567.80	615.21	42.09	45.60	12.25	13.27	318.17	344.74
3552.09	3526.20	6207.40	6162.17	523.40	519.58	26.65	26.46	16.43	16.31	329.17	326.77
2352.35	3024.13	5211.41	6699.68	360.76	463.78	11.52	14.81	12.83	16.49	-12.54	-16.13
3651.51	3643.35	6777.06	6761.91	460.14	459.11	14.60	14.56	12.74	12.71	18.31	18.27
2414.89	2435.54	3648.28	3679.48	281.21	283.61	7.85	7.92	4.96	5.01	-3.64	-3.67
2801.35	2792.08	3932.93	3919.91	216.37	215.65	7.63	7.60	2.87	2.86	-31.38	-31.27
1781.96	1816.29	2174.51	2216.40	114.79	117.00	12.45	12.69	2.11	2.15	-21.94	-22.36
1672.45	1704.67	2116.20	2156.96	127.98	130.44	10.50	10.71	0.32	0.32	-22.75	-23.19

PFBS		PFHxS		PFHxS_br		PFOS		PFOS_br	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
9642.02	9755.58	5838.37	5907.13	1469.83	1487.14	6612.83	6690.71	10172.82	10292.62
8208.84	10194.79	4339.74	5389.64	1113.83	1383.29	6144.98	7631.62	2265.60	2813.71
9465.63	10373.06	5373.18	5888.29	1342.35	1471.04	5868.01	6430.56	7724.27	8464.77
10646.56	11863.79	4437.46	4944.79	1215.39	1354.34	6581.25	7333.69	7418.29	8266.43
12224.19	12200.77	7141.71	7128.03	1794.23	1790.79	8303.56	8287.65	7981.46	7966.17
13306.82	13510.56	5663.78	5750.50	1416.00	1437.68	6193.49	6288.31	7186.88	7296.92
12118.39	12456.20	4350.61	4471.88	1460.68	1501.40	96.76	99.45	203.33	208.99
12389.66	12355.31	4251.75	4239.96	1362.53	1358.75	177.22	176.73	238.03	237.37
11689.94	11948.75	3710.88	3793.03	1234.15	1261.47	53.48	54.66	132.82	135.76
13884.74	14319.78	4918.49	5072.59	1796.57	1852.86	55.29	57.02	140.50	144.90
10630.95	10773.37	4136.01	4191.42	1354.15	1372.29	255.37	258.79	607.76	615.90
11037.88	11407.72	4892.95	5056.90	1641.34	1696.34	148.94	153.93	366.59	378.87
9771.31	10587.16	3927.24	4255.14	1129.91	1224.25	1238.06	1341.43	1978.93	2144.16
11424.44	11341.19	4745.05	4710.48	1334.57	1324.84	1508.44	1497.45	3129.20	3106.40
8692.75	11175.21	3530.28	4538.45	1011.74	1300.66	1343.97	1727.78	1035.33	1331.00
12885.80	12857.00	5104.75	5093.34	1470.63	1467.35	1955.48	1951.11	1050.20	1047.85
8773.25	8848.28	3162.58	3189.63	965.02	973.28	632.71	638.12	295.96	298.49
10299.18	10265.10	3008.02	2998.06	927.81	924.74	632.13	630.03	381.78	380.51
7505.39	7649.98	1988.76	2027.07	647.75	660.23	188.94	192.58	295.96	301.66
7266.79	7406.78	1987.27	2025.55	612.17	623.96	252.60	257.47	381.78	389.13

Table A18. Concentration (ng L⁻²) of studied PFASs at different durations the treatment in reject water at 0.5 mA am⁻².

Time_ minutes	corr_fac- tor	6:2 FTSA		8:2 FTSA		FOSA		FOSA_br	
		cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
-12h	0.9844	13.43	13.22	20.35	20.03	52.12	51.31	2.28	2.24
-12h	1.0216	16.21	16.56	24.10	24.62	133.43	136.31	7.17	7.33
-3h	1.0854	18.38	19.95	34.94	37.92	484.47	525.84	36.87	40.01
-3:30h	1.0546	20.49	21.61	51.85	54.68	575.13	606.52	45.64	48.13
0	0.9551	25.71	24.55	60.33	57.62	706.59	674.88	59.80	57.12
0	1.0117	24.77	25.06	55.19	55.83	646.76	654.35	53.07	53.69
5	1.0221	19.25	19.68	30.68	31.36	276.73	282.84	23.72	24.25
5	0.9994	19.97	19.96	43.07	43.05	282.14	281.97	23.78	23.76
10	0.9996	15.38	15.38	18.19	18.18	188.70	188.62	16.98	16.98
10	1.0126	14.39	14.57	13.13	13.29	112.48	113.90	8.81	8.92
15	1.0246	9.98	10.23	5.98	6.13	82.86	84.90	6.72	6.89
15	1.0520	10.25	10.78	10.24	10.77	91.09	95.83	6.93	7.29
30	1.0343	7.28	7.52	6.76	6.99	62.56	64.70	5.14	5.32
30	0.9967	9.83	9.80	7.51	7.48	59.33	59.14	5.76	5.75
60	0.9976	2.02	2.01	2.14	2.14	24.12	24.06	0.27	0.26
60	1.0582	1.16	1.23	1.55	1.64	15.26	16.15	-0.08	-0.08
90	0.9910	0.79	0.78	0.69	0.68	14.78	14.65	0.21	0.21
90	1.0092	0.58	0.59	0.14	0.14	10.96	11.06	-0.09	-0.09
120	0.9861	0.01	0.01	0.97	0.95	10.98	10.83	-0.40	-0.40
120	1.0406	0.00	0.00	0.29	0.30	13.70	14.25	-0.25	-0.25
150	0.9683	-0.11	-0.11	0.24	0.23	10.69	10.35	-0.63	-0.61
150	1.0165	0.03	0.03	0.20	0.20	9.69	9.85	-0.33	-0.33
180	1.0924	-0.28	-0.30	0.04	0.04	11.92	13.02	-0.04	-0.04
180	0.9730	-0.17	-0.17	0.02	0.02	12.41	12.07	-0.16	-0.16

PFHxA		PFOA		PFDA		PFDODA		PFTeDA		PFHxDA	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
50.18	49.40	47.17	46.44	59.81	58.88	10.27	10.11	1.35	1.33	15.25	15.01
64.00	65.38	73.29	74.88	86.76	88.64	9.17	9.37	4.10	4.18	11.42	11.66
50.71	55.04	101.23	109.88	171.57	186.22	14.91	16.19	9.85	10.69	18.71	20.31
60.78	64.10	114.02	120.25	180.65	190.51	31.56	33.28	23.94	25.25	20.33	21.44
67.19	64.18	150.79	144.02	199.78	190.81	12.70	12.13	7.46	7.12	27.57	26.33
60.44	61.14	139.51	141.15	202.69	205.07	20.41	20.65	2.31	2.34	9.77	9.88
51.11	52.24	101.20	103.43	103.30	105.58	14.73	15.06	4.74	4.84	2.95	3.01
71.01	70.96	118.31	118.23	131.81	131.73	10.15	10.14	1.27	1.27	0.04	0.04
65.08	65.05	109.06	109.01	72.93	72.89	7.02	7.01	3.24	3.24	7.70	7.70
66.66	67.50	105.66	106.99	51.11	51.76	1.49	1.51	0.83	0.84	4.29	4.34
63.67	65.23	80.12	82.09	32.51	33.30	4.14	4.24	2.16	2.21	-1.18	-1.21
55.41	58.29	86.67	91.18	45.14	47.48	4.94	5.20	4.75	5.00	-0.92	-0.96
58.59	60.60	60.15	62.21	22.84	23.62	1.42	1.47	2.71	2.81	2.77	2.87
66.86	66.64	66.10	65.89	25.42	25.33	0.95	0.94	0.86	0.85	-1.56	-1.55
73.05	72.88	25.39	25.33	8.60	8.58	1.01	1.01	1.60	1.59	0.69	0.69
62.16	65.78	21.49	22.74	6.19	6.55	3.25	3.44	3.90	4.13	9.04	9.57
68.35	67.73	13.67	13.55	3.90	3.87	0.05	0.05	0.79	0.78	-1.16	-1.15
70.64	71.28	13.04	13.16	3.56	3.59	0.32	0.33	1.68	1.69	4.73	4.78
62.50	61.63	10.40	10.26	2.55	2.51	1.26	1.24	1.26	1.25	-0.49	-0.48
63.59	66.17	9.55	9.94	2.78	2.90	0.93	0.97	2.08	2.16	5.19	5.40

65.23	63.16	7.34	7.11	2.49	2.41	0.38	0.36	0.48	0.46	1.65	1.60
52.34	53.20	5.77	5.86	1.74	1.76	0.79	0.81	1.60	1.62	2.04	2.07
56.74	61.98	6.53	7.13	2.68	2.93	0.47	0.52	0.96	1.05	2.17	2.37
63.59	61.87	7.24	7.05	2.40	2.34	0.25	0.24	N/F	N/F	-1.05	-1.02

PFBS		PFHxS		PFHxS_br		PFOS		PFOS_br	
cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt	cal_amt	corr_amt
72.90	71.76	326.37	321.29	86.79	85.44	4515.59	4445.36	152.97	150.59
83.55	85.35	383.48	391.76	80.97	82.72	149.09	152.31	189.54	193.64
113.07	122.72	302.16	327.96	67.21	72.95	160.78	174.50	175.85	190.87
122.62	129.31	333.47	351.67	79.01	83.32	164.14	173.10	202.44	213.49
158.62	151.50	399.07	381.17	87.92	83.98	224.17	214.11	249.71	238.50
154.63	156.44	364.23	368.50	81.87	82.83	203.94	206.33	230.51	233.22
134.76	137.74	336.56	343.99	78.14	79.86	126.86	129.66	159.78	163.31
123.77	123.69	342.01	341.80	74.51	74.46	126.90	126.82	136.22	136.14
127.21	127.16	318.39	318.25	72.88	72.85	95.92	95.88	122.72	122.67
147.78	149.64	299.13	302.91	76.01	76.97	70.88	71.78	80.45	81.47
106.04	108.65	269.82	276.46	60.93	62.43	48.63	49.82	54.59	55.94
121.85	128.18	265.88	279.69	70.03	73.67	54.40	57.23	55.38	58.26
100.38	103.82	248.94	257.47	63.53	65.70	18.95	19.60	22.50	23.27
97.81	97.49	239.00	238.22	68.67	68.44	26.65	26.56	29.25	29.16
115.65	115.38	158.02	157.64	47.82	47.71	7.03	7.02	5.67	5.66
98.25	103.97	135.41	143.29	40.07	42.40	5.26	5.56	1.84	1.95
97.66	96.79	111.52	110.52	40.67	40.30	1.29	1.27	1.27	1.25
110.67	111.69	107.90	108.89	39.39	39.75	0.82	0.82	1.00	1.01
103.00	101.57	86.14	84.94	34.28	33.81	1.75	1.73	0.34	0.33
111.35	115.86	82.89	86.25	32.72	34.05	1.70	1.77	1.13	1.18

107.39	103.99	60.33	58.41	25.86	25.04	0.90	0.87	0.22	0.22
88.62	90.09	60.52	61.52	28.60	29.07	1.71	1.74	0.20	0.21
90.39	98.74	48.52	53.01	25.22	27.55	1.61	1.75	1.59	1.73
103.85	101.04	56.36	54.84	30.99	30.16	1.47	1.43	1.04	1.01

Corr_factor (Correction factor): value for correcting for vial weight. Cal_amt (Calculated amount) in ng L-1: Calculated concentration obtained from Quantiva. Corr_amt (corrected amount): calculated amount corrected for vial weight.

Table A19. Concentrations (ng L⁻¹) of PFPeA analysed throughout the experiments done with Millipore water.

Time_ minutes	Millipore_0.9 mA cm ⁻²		Millipore_4.8 mA cm ⁻²		Millipore_11.9 mA cm ⁻²		Millipore_16.7 mA cm ⁻²	
	cal_amt	cal_amt	cal_amt	cal_amt	cal_amt	cal_amt	cal_amt	cal_amt
-12h	19.59	19.27	418.01	403.80	10.28	9.68	20.84	21.63
-12h	22.47	23.25	35.79	35.72	14.08	14.47	31.22	31.78
-3h	43.46	43.47	21.71	21.50	2.23	2.21	27.33	30.42
-3:30h	51.14	51.96	43.79	44.83	10.92	11.29	28.11	28.98
0	53.70	51.59	51.41	51.36	25.53	25.05	46.17	43.12
0	31.00	32.74	43.62	48.11	7.41	7.33	39.04	38.81
5	55.25	55.31	87.12	84.09	80.71	81.53	119.26	115.13
5	71.66	76.06	96.98	89.72	81.19	81.01	147.03	144.11
10	72.36	72.84	178.09	153.42	135.88	–	271.01	254.61
10	39.92	39.72	174.89	172.02	43.12	65.74	231.70	230.26
15	–	–	268.65	256.71	170.20	237.23	289.31	298.11
15	86.21	82.02	230.38	223.14	162.26	153.07	339.43	341.36
30	198.69	197.16	379.65	374.50	555.92	659.88	520.59	524.55
30	77.74	79.06	412.28	376.05	98.28	101.86	538.77	622.95
60	89.78	86.71	509.00	493.36	648.37	645.76		
60	102.39	102.47	508.81	489.91	634.26	621.99		
90	145.52	147.38	1138.22	1066.68	512.23	507.13		
90	108.64	105.31	1201.12	1129.40	548.64	559.22		
120	136.90	136.97	1263.25	1300.11	159.09	158.22		
120	214.65	203.45	1056.22	1024.32	154.38	151.59		

Cal_amt (Calculated amount) in ng L⁻¹: Calculated concentration obtained from Quantiva. Corr_amt (corrected amount): calculated amount corrected for vial weight.

Table A20. Concentrations (ng L⁻¹) of PFPeA analysed throughout the experiments done with DOC water and R.

Time_ minutes	DOC_0.95 mA cm ⁻²		DOC_4.8 mA cm ⁻²		DOC_11.9 mA cm ⁻²		R_0.95 mA cm ⁻²	
	cal_amt	cal_amt	cal_amt	cal_amt	cal_amt	cal_amt	cal_amt	cal_amt
-12h	42.14	40.71	139.71	144.75	139.71	141.36	85.036	83.71
-12h	110.64	110.42	75.72	84.72	75.72	94.04	37.720	38.53
-3h	112.06	110.99	186.37	189.17	186.37	204.23	19.400	21.06
-3:30h	78.09	79.96	136.20	138.85	136.20	151.77	25.126	26.50
0	105.84	105.74	73.53	74.95	73.53	73.39	48.540	46.36
0	8.05	8.88	55.30	57.15	55.30	56.15	38.984	39.44
5	37.87	36.55	212.98	213.51	212.98	218.92	30.835	31.52
5	31.50	29.14	229.46	248.47	229.46	228.82	17.403	17.39
10	136.97	118.00	243.27	244.70	243.27	248.66	9.190	9.19
10	98.38	96.77	315.78	320.33	315.78	325.68	32.387	32.80
15	105.91	101.21	438.39	435.95	438.39	444.26	17.294	17.72
15	14.12	13.68	343.20	352.35	343.20	354.70	37.869	39.84
30	28.37	27.99	664.55	666.92	664.55	720.03	45.734	47.30
30	87.43	79.75	540.35	542.03	540.35	536.41	28.374	28.28
60	58.44	56.64	965.10	968.69	965.10	1240.71	28.640	28.57
60	127.58	122.84	819.10	832.91	819.10	817.27	24.699	26.14
90	167.71	157.17	1022.50	1062.91	1022.50	1031.24	21.017	20.83
90	57.40	53.98	1175.20	1196.57	1175.20	1171.31	15.809	15.95
120	95.30	98.08	1075.13	1015.98	1075.13	1095.84	14.653	14.45
120	78.27	75.90	1343.49	1363.45	1343.49	1369.37	21.797	22.68

150		34.103	33.02
150		13.684	13.91
180		19.823	21.66
180		13.628	13.26

Cal_amt (Calculated amount) in ng L-1: Calculated concentration obtained from Quantiva. Corr_amt (corrected amount): calculated amount corrected for vial weight.

