Ministry of Environment
of Denmark
Environmental
Protection Agency

Derivation of cut-off values for PFAS in sewage sludge

Environmental Project
no. 2232
February 2023

Publisher: The Danish Environmental Protection Agency

Editor:
John Jensen,
Patrik Fauser,
Hans Sanderson,
Katrin Vorkamp,
Rikke Andersen,
Dorte Rasmussen

ISBN: 978-87-7038-488-9

Contents

Foreword **5**

Short summary **6**

Resumé **8**

Glossary **11**

1.	**Introduction**	**13**
1.1	Scope	13
1.2	Definition of relevant exposure scenarios	13
1.3	PFAS – Characteristics as a chemical group	14
1.4	Sources and environmental fate	15
1.5	International and national regulation of PFAS	16
1.6	Sludge in Denmark	17
1.7	Risk assessment frameworks	18
2.	**Chemical-physical properties of PFAS**	**20**
2.1	Sorption of PFAS	20
2.2	K_{oc} values	23
2.2.1	Input K_{oc} for calculations and modelling	24
3.	**Fate: Degradation, ageing, bioavailability, extractability and leaching of PFAS**	**26**
3.1	Degradation of PFAS in soil (DT_{50})	26
3.2	Fate of PFAS in soils over time as influenced by ageing	26
3.3	Non-Extractable Residues (NER)	27
3.3.1	Model validation of NER for PFAS.	28
3.4	Leaching studies with PFAS	29
3.5	PFAS in groundwater	31
3.6	Conclusions on the Fate of PFAS	33
4.	**Calculation methods and equations**	**35**
4.1	Introduction to REACH methodologies and basic assumptions	35
4.2	Concentration in soil after sludge application	35
4.3	Realistic sludge application rates	36
4.4	Long-term accumulation in sludge amended soils	37
4.5	PFAS partitioning between soil and pore water	38
5.	**Exposure of soil ecosystems**	**40**
5.1	Environmental Threshold Concentration for soil dwelling organisms (ETC_{soil})	40
5.2	Prediction of sludge threshold concentration	40
6.	**Exposure of groundwater**	**43**
6.1	Environmental Threshold Concentration for groundwater (ETC_{gw})	43

6.2	Screening assessment for threshold concentration in sludge protecting groundwater	43
6.3	Elaborated assessment of threshold concentrations in sludge protecting groundwater	46
6.4	Groundwater model descriptions	46
6.5	Model outputs	46
6.6	Alternative modelling of leaching	49
6.6.1	Box Model description	49
6.6.2	Results from Box Model	50
6.6.3	PFAS composition in sludge and leaching potential	51
6.6.4	Modelled groundwater concentrations	52
6.6.5	Incorporation of NER in the Box Model	53
6.7	Conclusions on groundwater scenario	57
7.	**Exposure of freshwater recipients**	**59**
7.1	Environmental Threshold Concentration for freshwater ecosystems (ETC_{fw})	59
7.2	Screening assessment for threshold concentration in sludge protecting freshwater	59
7.3	More realistic assessment of sludge load and background concentrations of PFOS in freshwater recipients	61
7.3.1	Application rate of sludge	61
7.3.2	Background concentration of PFOS in Danish freshwater recipients	62
7.3.3	Assessment of the current level of PFOS in Danish sludge	62
7.4	Alternative assessment of threshold concentration of PFOS in sludge protecting freshwater ecosystems	64
7.4.1	Point Source calculations	64
7.4.2	Calculation for a reference area	64
7.5	Conclusions on freshwater recipients	66
8.	**Human exposure**	**68**
8.1	Calculating maximum concentration in sewage sludge protecting humans	70
8.2	Conclusion on human exposure	71
9.	**Summary, conclusions and recommendations**	**73**
9.1	Conclusions	77
9.2	Recommendations	78
10.	**References**	**80**

Appendix A: Chemical-Physical properties of PFAS
Appendix B: Terrestrial Ecotoxicity data
Appendix C: PFAS concentrations in Danish Sludge

Foreword

The Danish Environmental Protection Agency has commissioned this report as part of the work on establishing a scientifically justified and risk-based limit value for PFAS in sewage sludge for agricultural purposes. In October 2021, the Danish Environmental Protection Agency published indicative cut off values for PFAS in sewage sludge for agricultural purposes.

The indicative limit values were based on a literature study carried out by the Danish Environmental Protection Agency. It was decided to set the indicative limit values at the level of the soil quality criterion for $PFAS_4$ and $PFAS_{22}$. This was due to the presumption that the soil quality criterion was sufficiently low to protect, in the short term, soil, surface water, groundwater and crops when using sewage sludge for agricultural purposes.

This report constitutes the scientific contribution to the work on determining a cut off value that can be implemented in the statutory order on waste to agricultural purposes.

The Environmental Protection Agency, Ministry of Environment,
Copenhagen, February 2023

This work is the result of several months of literature research and calculation procedures. With more than 25 years of experience in ecotoxicology and risk assessment covering heavy metals and multiple groups of organic pollutants, the assessment of PFAS as a group has undoubtedly come up on top with regard to their complexity, limitation in information and their global omnipresence. The work is aiming at increasing the knowledge and elucidating the environmental impact and fate processes important for deriving safe and protective cut-off values for PFAS in Danish sewage sludge.

John Jensen, Aarhus University
Aarhus, February 2023

Short summary

By the use of calculations and modelsimulation, this report aims to derive approximations for cut-off values for per- and polyfluoroalkyl substances (PFAS) in sewage sludge that protect a predefined set of targets via four specified exposure routes. The main conclusion is that such approximations are associated with a number of uncertainties hampering a solid determination of a safe absolute upper limit for PFAS in sludge. Instead, it is concluded that a sludge concentration of 15µg $PHAS_4$/kg is very likely to be in full compliance with current environmental thresholds in soil, freshwater and groundwater.

The major targets of protection have been biota in soil and adjacent freshwater systems as well as humans exposed via food and drinking water. Where possible, environmental threshold concentrations (ETC) have been used as limits for exposure. These may be existing national or international Environmental Quality Standards (EQS) or new calculated estimations for safe no-effect concentrations. The following exposure scenarios are considered in this report:

Sludge → soil → soil dwelling microorganisms, invertebrates and plant species
Sludge → soil → soil pore water → freshwater (streams) → aquatic organisms
Sludge → soil → soil pore water → groundwater → drinking water → humans
Sludge → soil → crops for animal feed → livestock →food (meat and dairy products) → humans

The methodology used in this report is based upon acknowledged risk assessment procedures and models from European authorities like ECHA, EFSA and EMA, but whereas these typically base their assessments on predicted no effect concentrations and exposure routes from source to recipient, the calculations in this report are based upon established (national) environmental threshold concentrations in fresh water and ground water and reversed exposure linkages starting in the recipient and ending in the source, i.e. sewage sludge.

Essential parameters in the calculations and modelling are the fate and removal processes of PFAS in soil. PFAS are a large group of substances deviating widely in the environmental fate and behavior. The report mainly focuses on four PFAS, i.e. PFOS, PFOA, PFNA and PFHxS, as these make up the ground water quality criteria. The adsorption-desorption distribution coefficient (K_d) is an important parameter for understanding the mobility of a compound in the environment and its distribution between water, sludge, soil compartments. K_d is often normalized to the organic content of the matrix in order to obtain the organic carbon-water partition coefficient (K_{oc}). In most of the scenarios, a median K_{oc} is used. Very few studies have determined the degradation half-life of PFAS. For precautionary reasons, the DT_{50} is, hence, set at 100 years in the majority of the calculations. Besides removal from the soil by leaching and degradation, the report incorporates removal of PFAS to the pool characterized as Non-Extractable Residues (NER), as this fraction has been shown to be largely immobile and not easily available for leaching in long-term semi-field studies.

Using realistic sludge application rates and median K_{oc} and k_{NER} values, calculations predict maximum concentrations of PFAS in sludge that ensure compliance with existing ETC for ground water as 5.1, 44.9, 9.4 and 5.2 µg/kg for PFOA, PFOS, PFNA and PFHxS, respectively. Model predictions showed that sludge concentrations corresponding to approximately the 90th percentile found in Danish sludge would not result in ground water concentrations exceeding the ETC_{gw} of 2 ng/L even in a long term perspective.

For the protection of freshwater recipients, calculations predicted maximum PFOS concentrations in sludge significantly higher than what is typically found in Danish sludge, i.e. 175 µg/kg. For protection of terrestrial ecosystems, draft ETC_{soil} are derived and presented for PFOA and PFOS. Calculations predicted safe maximum PFOS concentrations in sludge significantly higher than what is typically found in Danish sludge, i.e. 134 and 110 µg/kg for PFOA and PFOS, respectively.

It was concluded infeasible to calculate maximum sludge concentrations protecting humans from the food web scenario outlined above due to the complexity in the numerous transfer functions and the general lack of data needed in these calculations steps. However, it was shown that the predicted long-term soil concentrations of $PFAS_4$ at a steady state situation would be markedly below the existing human toxicologically-based soil quality criteria.

It has only been possible to find a single study that has quantified first order removal rates to NER in a long-term (semi) field study. To use results from a single lysimeter study alone to estimate leaching for the entire country of Denmark imposes a notable degree of uncertainty to the objective of calculating a specific upper concentration of PFAS is sludge being in compliance with the existing environmental threshold concentrations in Denmark. In that respect, it is as an alternative approach suggested that a $PFAS_4$ concentration of 15 µg/kg could form the basis for setting a regulatory cut-off value for PFAS in sludge, as it, under the assumption of normal sludge application rates and median K_{oc} and K_{NER}, is observed that:

- 15 µg $PFAS_4$/kg minimum is a factor of 10 below the predicted maximum concentration in sludge that protects soil dwelling species, soil processes and the terrestrial ecosystem.
- 15 µg $PFAS_4$/kg is markedly below the predicted maximum concentration in sludge protecting groundwater by being in compliance with the ETC_{gw} of 2 ng/L.
- 15 µg $PFAS_4$/kg will as input in the FOCUS model PELMO result in predicted groundwater concentrations several orders of magnitude below the ETC_{gw} of 2 ng/L.
- 15 µg $PFAS_4$/kg is minimum a factor of 10 below the maximum concentration of PFOS in sludge predicted to protect freshwater recipients by being in compliance with the ETC_{fw} of 0.00065 µg/L.
- 15 µg $PFAS_4$/kg in sludge is predicted to result in long-term concentrations in soil pore water below the existing ETC_{fw} of 0.00065 µg/L.
- 15 µg $PFAS_4$/kg in sewage sludge will result in long-term soil concentrations at the steady state situation being at least a factor of 10 below the existing soil quality criteria for $PFAS_4$ of 0.01 mg/kg.

Based upon the presented calculations and model prediction, it is likely that a maximum concentration of $PFAS_4$ in sludge could be higher than 15 µg/kg. However, due to the relatively large uncertainty associated with the determination of K_{oc} and k_{NER}, for precautionary reasons it is recommended to use the indicative maximum concentration of 15 µg/kg presented in this report as a basis for deriving a regulatory cut-off value for $PFAS_4$.

Resumé

Indeværende rapport fremstiller beregningsmetoder og modelberegninger med henblik på at fremsætte forslag til afskæringsværdier for PFAS i spildevandsslam, som beskytter miljø og mennesker. Hovedkonklusionen er, at der er knyttet en række usikkerheder til disse beregninger, hvorfor det er vurderet uhensigtsmæssigt at forsøge at fastsætte sikre og absolutte maksimumkoncentrationer af PFAS i slam. I stedet estimeres det, at slamkoncentrationer på 15 µg $PFAS_4$/kg med stor sandsynlighed ikke i sig selv vil føre til overskridelse af gældende miljøkvalitetskrav.

PFAS anvendes bredt i samfundet og kan derfor havne i affaldsstrømmen, hvor en andel derved ankommer med spildevand til de kommunale og private rensningsanlæg. Her vil en fraktion binde sig til den organiske fraktion og på den vis kunne måles i spildevandsslammet. I Danmark anvendes næsten 2/3 af al slam som organisk gødning på landbrugsjorder, hvorfra det teoretisk kan sprede sig til recipienter, grundvand, den agrobiologiske fødekæde og, i sidste indstans, til mennesker.

I denne rapport er det kvantitativt tilstræbt at regne baglæns fra allerede eksisterende grænseværdier i miljøet til sikre afskæringsværdier i spildevandsslam. Hertil er brugt det gældende vandkvalitetskrav for PFOS på 0,65 ng/L, de gældende grænseværdier i grund- og drikkevand på 2 ng/L for $PFAS_4$ og 100 ng/L for $PFAS_{22}$. Desuden er gældende jordkvalitetskriterier for beskyttelse af mennesker på 0,1 ($PFAS_4$) og 0,4 mg/kg ($PFAS_{22}$) indraget. Endelig er der i rapporten beregnet nye forslag til økotoksikologiske jordkvalitetskriterier for PFOS og PFOA med henblik på beskyttelse af jordbundsorganismer.

Beregningsmetoderne bygger på metoder allerede benyttet i EU til risikovurdering af industrikemikalier, pesticider og lægemidler. Forskelen er, at de bliver brugt bagvendt til at beregne slamkoncentrationer, som ikke forventes at udgøre en risiko for de nævnte mål. Vigtige parametre i beregningerne og modellerne er adsorptionskoefficienten i jord, K_d, og denne normaliseret til jordens organiske indhold, K_{oc}. Derudover er der indarbejdet aspekter af ældning, da det er dokumenteret at være et vigtigt element for biotilgængelig, bioakkumulering og mobilitet af PFAS under langvarige bindingsforhold i jord. Den rate, hvorved PFAS bliver immobil eller ikke-estraherbar, kaldet NER[1], indrages derfor på linje med nedbrydningsraten og udvaskningsraten i en samlet tabsrate for PFAS i jordmaricen. Foruden de nævnte beregningsmetoder er der anvendt flere eksponeringsmodeller udviklet i EU regi, dvs. FOCUS modellerne PELMO og MACRO, samt en mere forsimplet nybeskrevet såkaldt box model. Modellerne kan ikke køres bagvendt, hvorfor de er anvendt med et arealbaseret input af PFAS, som svarer til de teoretiske værste scenarier, der dog i praksis fomodentlig aldrig vil forekomme for PFAS forbundet til spildevandsslam.

Resultaterne viser, at PFAS i spildevandsslam ikke, selv på langt sigt, forventes at udgøre et problem for jordlevende organismer. For grundvand viser beregningerne, at man ved en realistisk slamudbringning og en realistisk antagelse om tabsrater til den ikke-mobile fraktion (NER)[1] kan beregne teoretiske afskæringsværdier på 5,01, 44,9, 9,4 og 5,2 µg/kg for henholdsvis PFOA, PFOS, PFNA og PFHxS. Det anerkendes dog samtidigt, at der foreligger en betragtelig usikkerhed i disse beregninger. Derfor er udvaskningen testet i andre modeller med et meget højt input af PFAS, som svarer til en slamudbringning, der er cirka 7 gange højere

[1] Non-Extractable Fraction (NER) – Læs Kapitel 3.

end gennemsnittet og PFAS koncentrationer, som ligger i den allerhøjeste ende af målte værdier (cirka 90% fraktilen). Efter den maksimale simuleringstid på 20 års slamudbringning forudser PELMO modellen under de nævnte forudsætninger grundvandskoncentrationer, som ligger minimum en faktor 1000 under grundvandskriteriet på 2 ng/L. Den simple box model kan simulere i flere århundrede og har desuden en række meget konservative forudsætninger indbygget. Her forudser modellen, når der indarbejdes fjernelse via NER, fremtidige grundvandskoncentrationer, som mindst ligger en faktor 50-100 under grundvandskriteriet på 2 ng/L. Ved en realistisk og gennemsnitlig slamudbring forudses grundvandskoncentrationer, der er syv gange lavere.

Med henblik på beskyttelse af vandkvalitetskriteriet for PFOS er der beregnet afskæringsværdier i spildevandsslam, der varierer markant, alt efter hvilke forudsætninger og input data man bruger. Ved en medianværdi for K_{oc} og NER-dannelse samt en realistisk årlig arealtilførsel af spildevandsslam er det vurderet, at en eventuelt afskæringsværdi kan ligge på 175 µg PFOS/kg, hvilket er langt over, hvad man finder i dansk spildevandsslam i dag. Det forudsætter en fortynding af porevandet med en faktor tre i vandløbet. Med andre ord forudsættes det, at der i et opland til en ferkvandsrecipient maksimalt anvendes spildevandsslam på 1/3 af det samlet oplandsareal (ikke kun landbrug). Udelades fortyndingsaspektet, er afskæringsværdien i slam tilsvarende lavere, dvs. omtrent 58 µg PFOS/kg.

Med hensyn til at beskytte mennesker fra eksponering til PFAS gennem optag i foderafgrøder og siden produktionsdyr og kød og mælk har det ikke været muligt at lave troværdige ekstrapoleringer, idet der mangler central viden inden for mange af optagelsesprocesserne gennem fødekæden fra slamgødet jord til mennekser. En simpel sammenligning af de beregnede ligevægtskoncentrationer af PFAS i jord efter årtier eller århundredes slamudbringning viser, at disse er væsentligt under de humantoksikologiske jordkvalitetskriterier, der er fastsat til at beskytte mennesker mod PFAS indtag, herunder jordspisende børn.

Grundet den relativt store usikkerhed, der er forbundet med mange af de centrale parametre, som indgår i beregningerne, f.eks. K_{oc} og K_{NER}, er det ikke anbefalet at anvende de beregnede maksimumkoncentrationer af PFAS direkte som afskæringsværdier i spildevandsslam uden nærmere evaluering og overvejelser. Det kan dog entydigt konkluderes, at $PFAS_4$ koncentrationer i den øvre ende af, hvad der findes i dansk spildevandsslam, ikke forventes at udgøre et problem i forhold til de miljøkvalitetskrav, der findes for grundvand og overfladevand. Det er således ved den såkaldte ligevægtssituation, hvor den årlige til- og fraførsel af PFAS er ens (ofte mange årtier eller århundrede ude i fremtiden), beregnet, at en maksimumkoncentration på 15 µg $PFAS_4$/kg i slam med stor sandsynlighed vil være tilstrækkeligt beskyttende i forhold til at overskride gældende kvalitetskrav i jord, ferskvand og grundvand, idet at:

- 15 µg $PFAS_4$/kg er minimum en faktor 10 under den beregnet grænseværdi for PFOA og PFOS i slam, der beskytter den generelle jordkvalitet samt jordlevende planter og dyr.
- 15 µg $PFAS_4$/kg er markant under de koncentrationer af $PFAS_4$, som efter realistisk slamudbringning forventes at kunne overskride de gældende grænseværdier i grundvand på 2 ng $PFAS_4$/L.
- 15 µg $PFAS_4$/kg vil som input i FOCUS modelberegninger resultere i grundvandskoncentrationer, som ligger minimum 1000 gange under grænseværdien på 2 ng $PFAS_4$/L efter en 20 årig simuleringsperiode.
- 15 µg $PFAS_4$/kg er minimum en faktor 10 under den slamkoncentration, der ved realistisk slamudbringning er beregnet for PFOS til at beskytte overfladevand ift gældende vandkvalitetskrav.
- 15 µg $PFAS_4$/kg er beregnet til at resultere i porevandskoncentrationer, som ligger under det gældende vandkvalitetskrav for PFOS på 0,00065 µg/L.
- 15 µg $PFAS_4$/kg er beregnet til ved normal slamudbringning, at resultere i fremtidige jordkoncentrationer, der ligger minimum en faktor 10 under det gældende humantoksikologiske jordkvalitetskriterium for $PFAS_4$ på 0,01 mg/kg.

Det er som nævnt overvejende sandsynligt, at en grænseværdi for $PFAS_4$ i spildevandsslam ifølge beregninger og modelkørsler teoretisk kan være højere end 15 µg $PFAS_4$/kg uden negative konsekvenser for overfladevand og grundvand, men af forsigtighedsgrunde knyttet op til persistensen af PFAS i miljøet og en usikkerhed i fastsættelsen af K_{oc} og k_{NER} anbefales det, at bruge den indikative maximumkoncentration på 15 µg $PFAS_4$/kg som udgangspunkt for en endelig fastsættelse af en myndighedsbaseret afskæringsværdi for $PFAS_4$ i spildevandsslam.

Det har ikke været muligt at finde data og lave beregninger for alle de restrende PFAS i gruppen af $PFAS_{22}$, men et ikke fuldt videnskabelig funderet overslag vil være, at en grænseværdi for $PFAS_{22}$ i spildevandsslam med en stor sikkerhedmargin kunne fastsættes på mellem 50 og 100 µg $PFAS_{22}$/kg ud fra kendskab til eksisterende slamkoncentrationer, mobilitet og giftighed for mennesker i forhold til $PFAS_4$.

Glossary

6.2 FTS	n:2 fluorotelomer sulfonic acid [C= 8]
AFFF	Aqueous Film-Forming Foam
AMAP	Arctic Monitoring and Assessment Programme
BfR	The German Federal Institute for Risk Assessment
CFX	CF = Carbon-Fluoride bond; X = the carbon chain length (using the same naming conventions as hydrocarbons based on the number of carbons
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ECHA	European Chemical Agency
EFSA	European Food Safety Authority
EMA	European Medicinal Agency
ETC	Environmental Threshold Concentration(s)
FDA	U.S. Food and Drug Administration
FOCUS	FOrum for Co-ordination of pesticide fate models and their USe
FTOH	Fluorotelomers alcohols
ITRC	Interstate Technology and Regulatory Council
LOD	Limit of Detection
LOQ	Limit of Quantification
MACRO	A physically based one-dimensional numerical model of water flow and reactive solute transport in field soils
NER	Non-Extractable Residues
NOVANA	The National Monitoring Program for Water and Nature in Denmark
PCB	Polychlorinated biphenyls
PEC	Predicted Environmental Concentration
PELMO	A one-dimensional simulation model simulating the vertical movement of pesticides in soil by chromatographic leaching
PFAS	Per- and polyfluoroalkyl substances
$PFAS_{22}$	Sum of PFBS, PFPeS, PFHxS, PFHpS, PFOS, PFNS, PFDS, PFUnS, PFDoS, PFTrS, PFOSA, 6:2 FTS, PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA and PFTrDA
$PFAS_4$	Sum of PFOS, PFOA, PFNA and PFHxS
PFBA	Perfluorobutanoate / Perfluorobutanoic acid [C= 4]
PFBS	Perfluorobutane sulfonate / Perfluorobutane sulfonic acid [C= 4]
PFCA	Perfluorinated carboxylic acids
PFDA	Perfluorodecanoate / Perfluorodecanoic acid [C= 10]
PFDo(D)A	Perfluorododecanoate / Perfluorododecanoic acid [C= 12]
PFDo(D)S	Perfluorododecane sulfonate / Perfluorododecane sulfonic acid [C=12]
PFDS	Perfluorodecane sulfonate / Perfluorodecane sulfonic acid [C= 10]
PFHpA	Perfluoroheptanoate / Perfluoroheptanoic acid [C= 7]

PFHpS	Perfluoroheptane sulfonate / Perfluoroheptane sulfonic acid [C= 7]
PFHxA	Perfluorohexanoate / Perfluorohexanoic acid [C= 6]
PFHxS	Perfluorohexane sulfonate / Perfluorohexane sulfonic acid [C= 6]
PFNA	Perfluorononanoate / Perfluorononanoic acid [C= 9]
PFNS	Perfluorononane sulfonate / Perfluorononane sulfonic acid [C= 9]
PFOA	Perfluorooctanoate / Perfluorooctanoic acid [C= 8]
PFOS	Perfluorooctane sulfonate / Perfluorooctane sulfonic acid [C= 8]
(P)FOSA	Perfluorooctane sulphonamide [C= 8]
PFP(e)A	Perfluoropentanoate / Perfluoropentanoic acid [C= 5]
PFSA	Perfluorinated sulfonic acids
PFTr(D)A	Perfluorotridecanoate / Perfluorotridecanoic acid [C= 13]
PFTr(D)S	Perfluorotridecane sulfonate / Perfluorotridecane sulfonic acid [C= 13]
PFUn(D)A	Perfluoroundecanoate / Perfluoroundecanoic acid [C= 11]
PFUn(D)S	Perfluoroundecane sulfonate / Perfluoroundecane sulfonic acid [C= 11]
PNEC	Predicted No Effect Concentration
REACH	The registration, evaluation, authorisation and restriction of chemicals within EU
SVHC	Substances of Very High Concern
STP	Sewage Treatment Plant
UNEP	United Nations Environmental Programme
WWTP	Waste Water Treatment Plant

1. Introduction

1.1 Scope

This report aims to derive approximations for cut-off values for per- and polyfluoroalkyl substances (PFAS) in sewage sludge that protect a predefined set of targets via pre-defined exposure routes. The major targets of protection have been biota in soil and adjacent freshwater systems as well as humans exposed via food and drinking water. Where possible, environmental threshold concentrations (ETC) have been used as limits for exposure. These may be existing national or international Environmental Quality Standards or new calculated estimations for safe no-effect concentrations.

1.2 Definition of relevant exposure scenarios

To safeguard the use of sewage sludge, the potential for adverse effects on terrestrial and aquatic organisms as well as humans must be evaluated. In this context, it is necessary to describe the exposure pathways of PFAS compounds from sludge to uptake/intake scenarios for terrestrial and aquatic species as well as humans. Hence, the following exposure scenarios are considered in this report:

Sludge → soil → soil dwelling microorganisms, invertebrates and plant species
Sludge → soil → soil pore water → groundwater → drinking water → humans
Sludge → soil → soil pore water → freshwater (streams) → aquatic organisms
Sludge → soil → crops for animal feed → livestock →food (meat and dairy products) → humans

Due to the legislation and current practice for sewage sludge application to land in Denmark, it is not considered relevant to evaluate the direct exposure scenario of human intake via vegetables or fruit grown in sludge-amended soils, since sewage sludge is not used directly on fields used for production of food for human consumption. Direct uptake by grazing animals is also omitted, as sewage sludge application on grassland is not relevant in a Danish legal context. Human intake of fish or shellfish is not considered specifically, as it is believed to be included in the aquatic ETC_{fw} used to protect the freshwater environment by secondary poisoning scenarios.

Simple conservative (worst-case) distribution, adsorption and partitioning relationships that are described in the Exposure Guidance Documents published by the European Chemical Agency (ECHA, 2016[2]), The European Food Safety Authority (EFSA, 2019) and the European Medicinal Agency (EMA, 2007) are used. In ECHA R.16[2] (ECHA, 2016), guidelines for calculating Predicted Environmental Concentrations (PECs) for soil, groundwater and surface water are given and can be calculated generically at local scale.

The concentration in groundwater is calculated below an agricultural area subject to sludge amendment and is used directly as proxy for exposure of humans through drinking water. In the initial screening, the concentration in pore water of agricultural soil is used as an indication for potential groundwater levels. It should be noted that this may be a worst-case assumption, neglecting transformation and possible dilution in deeper soil layers or from leached water from adjacent fields and from the groundwater reservoir to the drinking water tap.

[2] Guidance on information requirements and Chemical Safety Assessment, Chapter R.16: Environmental exposure assessment

Exposure assessment in risk assessment frameworks like the ones described in this report can be an iterative process (ECHA, 2016). If risk is identified in the initial phase, the exposure assessment may need to be refined. This refinement is possible at every step in the workflow, including compartment specific properties such as leaching rate, soil density, soil porosity, organic fraction in soil, degradation half-life of PFAS and sorption coefficients. For refinement of leaching to freshwater and groundwater, alternative models to the simple partitioning equations found in R.16 are presented in the respective chapters.

1.3 PFAS – Characteristics as a chemical group

The group of per- and polyfluoroalkyl substances (PFAS) has become a major environmental and health concern. PFAS molecules consist of an alkane chain that is either fully ("per") or partly ("poly") fluorinated, and a functional group, such as -OOH or $–SO^{-3}$. Figure 1.1 shows the chemical structures of perfluorooctane sulfonate (PFOS), perfluorooctanoic acid (PFOA), perfluorohexane sulfonate (PFHxS) and perfluorononanoic acid (PFNA), the four individual PFAS compounds mainly addressed in current EU legislation.

Some characteristics of PFAS distinguish them from other, better-studied organic contaminants, such as polyaromatic hydrocarbons (PAH) and polychlorinated biphenyls (PCBs):

- The carbon-fluorine bond in PFAS molecules is the strongest in organic chemistry, resulting in half-lives of years. Environmental half-lives for PFOS were summarized by UNEP (2006), for example including a half-life of 41 years in water.
- The long alkane chain (Figure 1.1) makes this part of the molecule hydrophobic, while an acid group or other polar functional groups add a hydrophilic part to the molecule. This combination of hydrophobic and hydrophilic properties affects the fate of PFAS in the environment, disenabling analogies to PCBs or other highly persistent compounds. Furthermore, the parameters typically used for describing chemical properties and predicting its environmental behaviour, e.g. especially octanol-water-partition coefficients (K_{ow}) and, to some extent, also K_{oc}, are not applicable to PFAS.
- PFAS may exist in both a neutral and a charged form, and results have shown that the sorption affinity of cationic and zwitterionic PFAS to sediment/soil is much stronger than that of anionic PFAS (Lyu et al. 2022).
- PFAS are an extremely large compound group of over 4,700 individual substances (Glüge et al., 2020). For comparison, 209 PCB congeners are possible. The initial work on PFOS and PFOA has constantly been extended to now also involving multi-analyte or screening methods (Figure 1.2).

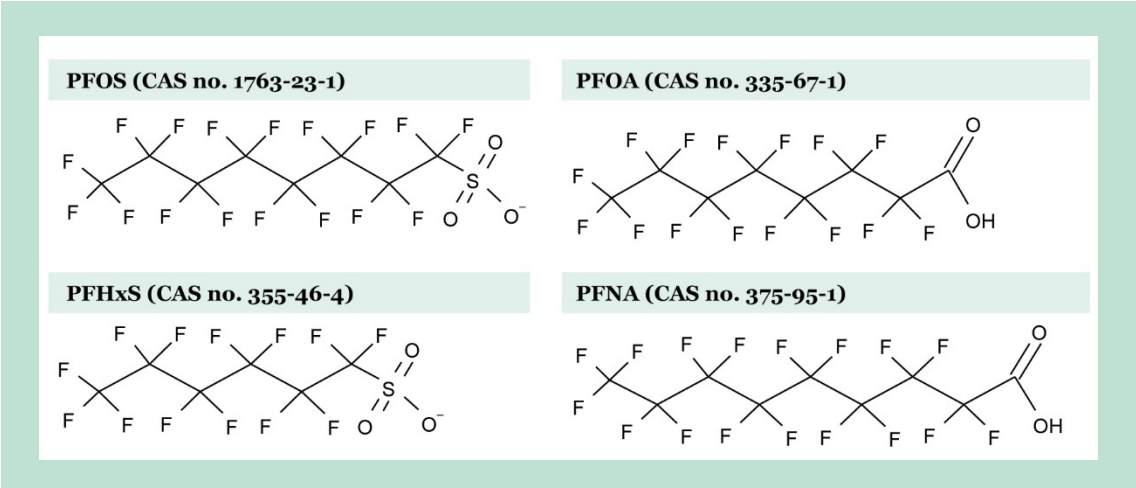

FIGURE 1.1. Chemical structures for perfluorooctane sulfonate (PFOS), perfluorooctanoic acid (PFOA), perfluorohexane sulfonate (PFHxS) and perfluorononanoic acid (PFNA).

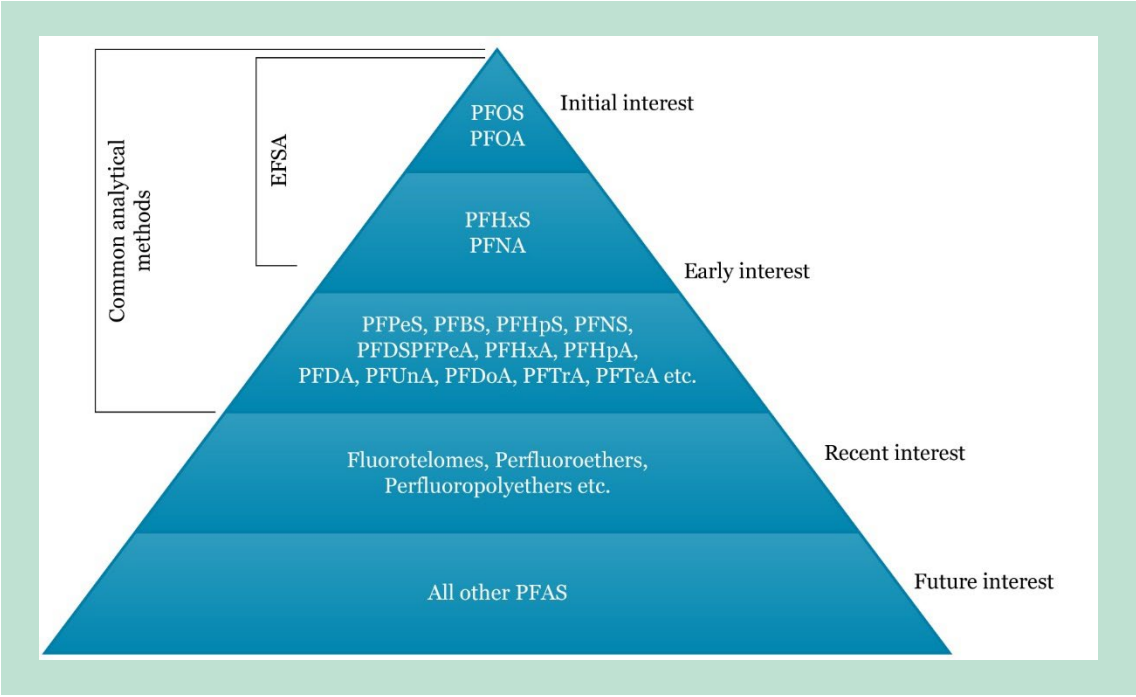

FIGURE 1.2. Schematic overview of the PFAS universe. See text for more details. Modified after ITRC (2020).

The unique PFAS characteristics, including their stability at elevated temperatures and UV light, have led to a wide application of PFAS in a number of industrial branches and consumer products. Glüge et al. (2020) described more than 200 applications for approximately 1400 PFAS chemicals. For the Nordic countries, they listed the plastic and rubber industry, the electronic industry and the building and construction sectors as the main PFAS users among the industrial PFAS uses, also including fluorine-containing polymers. For consumer products, the main categories were coating and paints as well as lubricants and greases. This information was taken from the SPIN database[3]. PFAS are widely used as stain repellents, in functional outdoor clothing, non-sticking cookware and other applications where their water- and oil repellent characteristics are useful (Glüge et al., 2020). PFOS was the main PFAS component in firefighting foams and replaced by fluorotelomer alcohols in the early 2000s (ITRC, 2020).

1.4 Sources and environmental fate

The extensive use of PFAS has led to their widespread occurrence in the environment, favoured by their environmental persistence. Besides direct emissions of perfluorosulfonic acids (PFSAs) and perfluorocarboxylic acids (PFCAs), they can be formed in the environment and in organisms from precursors, such as fluorotelomers alcohols (FTOHs) that can be oxidised to PFCAs (Ellis et al., 2004; Butt et al., 2014). The use of PFOS in firefighting foams has led to a number of contaminated hotspots in many countries, including Denmark (Banzhaf et al., 2017). Levels of selected PFAS compounds in the Danish environment are monitored in the NOVANA programme, including fish and water samples (Miljøstyrelsen, 2017).

PFAS can be transported over long distances and reach remote areas such as the Arctic and Antarctic (Casal et al., 2017; Muir et al., 2019, Boisvert et al. 2019). PFSAs and PFCAs can be transported in their ionic forms with ocean currents, while volatile neutral precursors, such as FTOHs, can be transported with the atmosphere and oxidise to PFCAs during the process or

[3] Substances in Preparations in Nordic Countries, (SPIN). http://spin2000.net/

after uptake in organisms (Ellis et al., 2004; Butt et al., 2014). Measurements within the Danish-Greenland contaminant monitoring programme (AMAP Core Programme) have documented the presence of FTOHs in Arctic air and the accumulation of PFSAs and PFCAs in Arctic animals, with recent decreases of PFOS and PFOA (Rigét et al., 2013; Bossi et al., 2016). Bioaccumulation of PFAS is different from that of e.g. PCBs, as PFAS molecules bind to proteins, while PCBs partition to lipid phases (De Silva et al., 2021).

1.5 International and national regulation of PFAS

The Stockholm Convention on Persistent Organic Pollutants included PFOS and PFOA in 2009 and 2019, respectively, aiming at global restrictions (PFOS) and elimination (PFOA) based on persistence, bioaccumulation, adverse effects and long-range transport. Recently, PFHxS has been reviewed and recommended to the Conference of the Parties for addition to the Stockholm Convention (UNEP, 2019). Long-chain PFCAs have now been nominated by Canada for review under the Stockholm Convention.

EU legislation has restricted the use of long-chain PFCAs with nine to 14 carbon atoms under REACH. In addition, PFBS, PFHxS and hexafluoropropylene oxide-dimer acid (HFPO-DA; GenX), a replacement for PFOA, are included in the list of Substances of Very High Concern. The European Food Safety Agency (EFSA) re-assessed exposure to PFAS from food in 2020 and lowered the tolerable weekly intake (TWI) for humans to 4.4 ng/kg body weight for the sum of PFOS, PFOA, PFHxS and PFNA (EFSA, 2020). The EU Drinking Water Directive sets a limit of 0.1 µg/L for the sum of 20 individual PFAS compounds (PFCAs and PFSAs with four to 13 carbon) and 0.5 µg/L for "total PFAS", which still needs to be defined (EU, 2020a). PFOS and PFOA are priority substances of the Water Framework Directive, to which the Danish environmental monitoring programme NOVANA is linked.

Denmark, Sweden, Norway, Germany and the Netherlands have announced to issue a proposal to the European Chemicals Agency (ECHA) on a restriction of all PFAS[4] based on the reasoning that a chemical-by-chemical assessment will not be sufficiently protective against PFAS exposure given the high number of individual compounds. The European Chemicals Strategy for Sustainability also includes plans of banning all PFAS in firefighting foams and other uses, provided the uses are not essential for society, and addressing PFAS with a group approach (EU, 2020b).

In 2021, the Danish Environmental Protection Agency established new legal quality standards for PFAS in drinking water, groundwater and soil. The soil QS was targeted towards protecting humans from exposure at hot-spots, e.g. contaminated sites or old dump sites. These new QS were based on updated information and recommendations from the European Food safety Authority (EFSA), leading to a revised Tolerable Weekly Intake (TWI). Experts considered the decreased response of the immune system to vaccination of toddlers and children to be the most critical human health effect when determining the TWI. This differs from EFSA's previous opinion on PFAS from 2018, which used increased cholesterol levels as the main critical effect. More information about the toxicity of PFAS can be found in Chapter 8.

In October 2021, the Danish Environmental Protection Agency (EPA, Miljøstyrelsen) launched a set of (temporary) cut-off criteria for PFAS in sewage sludge used for agricultural purposes. These cut-off criteria were on dry-weight basis and equal to the EQS established for contaminated soils (see Text Box 1.1).

It is common practice in Denmark to incorporate sewage sludge in soil. However, the new sludge criteria did not consider any dilution resulting from soil incorporation or the fact that the

[4] https://echa.europa.eu/da/registry-of-restriction-intentions/-/dislist/details/0b0236e18663449b

EQS_{soil} typically are based on a scenario of protecting children from direct soil ingestion, which is an unlikely scenario for arable land. The Danish EPA therefore initiated the present study with the aim to recommend new risk-based cut-off values for PFAS in sewage sludge, aiming to protect the following four protection goals: Drinking- and groundwater; Ecosystems in freshwater recipients; Soil ecosystems; Humans exposed via food uptake.

Text Box 1.1. Environmental Threshold Concentrations (ETC) or Quality Standards of PFAS in Denmark.

Sewage sludge: 0.4 mg/kg (dw) as sum of PFBS, PFPeS, PFHxS, PFHpS, PFOS, PFNS, PFDS, PFUnS, PFDoS, PFTrS, PFOSA, 6:2 FTS, PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA and PFTrDA (in this report named $PFAS_{22}$).

Sewage sludge: 0.01 mg/kg (dw) as sum of PFOA, PFOS, PFNA and PFHxS (in this report named $PFAS_4$).

Soil: 0.4 mg/kg (dw) as $PFAS_{22}$

Soil: 0.01 mg/kg (dw) as $PFAS_4$

Groundwater: 0.1 µg/L as $PFAS_{22}$

Groundwater: 0.002 µg/L as $PFAS_4$

Drinking Water: 0.1 µg/L as $PFAS_{22}$

Drinking Water: 0.002 µg/L as $PFAS_4$

Freshwaters (Annual Average): 6.5×10^{-4} µg PFOS/L

Freshwaters (Maximum): 36 µg PFOS/L

Marine waters (Annual Average): 1.3 x 10-4 µg PFOS/L

Marine waters (Maximum): 7.2 µg PFOS/L

Biota: 9.1 µg PFOS/kg (ww)

1.6 Sludge in Denmark

Sewage sludge has been used as organic fertilizer on arable land since the initiation of wastewater treatment. It has many beneficial effects on soil fertility due to its content of minerals, organic carbon, nitrogen and phosphorous, which are all essential for intensive crop production. At the same time, it was recognized early on that these beneficial sludge effects may appear along elevated concentrations of heavy metal in potential toxic concentrations.

Furthermore, sewage sludge often reflects human activities, which is why numerous organic manmade chemicals can be found in sewage sludge. The quality of Danish sludge has steadily improved since the middle of the 1980s, when the first set of quality criteria for heavy metals was introduced. In 1997, cut-off criteria for the organic pollutants LAS, DEHP, nonylphenol and PAHs were introduced (Jensen and Jepsen, 2005). In 2010, new cut-off criteria for PCB were introduced due to an on-going debate about the general safety of using sludge on arable land. In combination with the need of municipalities to secure long-term agreements with farmers or other users, the increased quality demand has in time led to a reduction in the use of sewage sludge as organic fertilizer. Today, more than 60% of the produced Danish sludge is used directly as fertilizer on arable land, whereas the remainder is used for other recycling purposes or incinerated (10%) (Miljøstyrelsen 2022).

1.7 Risk assessment frameworks

The European Chemicals Agency (ECHA) manages the technical and administrative aspects of the implementation of the European Union regulation called “Registration, Evaluation, Authorisation and Restriction of Chemicals” (REACH) and has developed numerous technical guidance documents, of which R.16 – Environmental Exposure Assessment (ECHA, 2016) is most relevant for this report. With regard to derivation of environmental threshold concentrations, EU has published a technical guidance document supporting the derivation of Environmental Quality Standards in support of the common Implementation Strategy for the Water Framework Directive (2000/60/EC)[5].

The European Food Safety Authority (EFSA) manages food safety aspects for example associated to the use of plant protection products and feed additives, of which the latter is most relevant in the context of this report, as feed additives end up in manure entering soil in a manner familiar to sewage sludge. EFSA has published a guidance document used in the risk assessment of feed additives (EFSA, 2019).

The European Medicinal Agency (EMA) fosters scientific excellence in the evaluation and supervision of veterinary and human medicines in the European Union (EU). Medicines can potentially end up in sewage sludge (humans and pets) or manure (husbandry) via disposal or excretion. EMA has therefore developed technical guidance documents for risk assessment of human (EMA 2006) and veterinary (EMA 2007) medicinal products.

Typically, the risk assessment approach mentioned above operates by comparing a calculated or modelled prediction of an environmental exposure to a predicted “environmentally safe” level of a chemical, typically denoted Predicted No Effect Concentration (PNEC). PNEC values used in regulative aspects, for example to indicate good environmental standards or determine emissions ceilings, are often named Environmental Quality Standards (EQS). EQS can, for example, be drinking water standards or freshwater quality standards.

If the predicted environmental concentration (PEC) is higher than the predicted no-effect concentration, a potential risk is present, i.e. if PEC>PNEC or PEC/EQS>1. The PEC/PNEC ratio is typically denoted risk quotient (RQ) or risk characterization ratio (RCR). This report applies the same principle, but in a different and reverse procedure. The starting point is the EQS or PNEC, as it is used as a threshold environmental (exposure) concentration. Based upon this, a set of calculations and equations are used to calculate backwards towards a safe concentration in soil and, ultimately, in sewage sludge.

[5] Guidance Document No. 27; Technical Guidance For Deriving Environmental Quality Standards. Technical Report - 2011 – 055. DOI : 10.2779/43816

To the extent possible, this report uses the same equations, terms, abbreviations, denotations, etc. as used in the risk assessment frameworks described above. Calculated environmental concentrations are, however, often abbreviated as “C” and not “PEC”. Furthermore, the term PNEC is replaced by the term Environmental Threshold Concentration (ETC). The same goes for the term EQS, unless these are derived and published in the context of national or international regulatory frameworks, such as the Water Frame Directive.

2. Chemical-physical properties of PFAS

Appendix A summarizes a review of relevant chemical-physical properties of PFAS. Since adsorption to soil is of principal influence, the data govern the adsorption, i.e. predominantly adsorption to organic carbon (K_{oc}) is discussed in more details below

2.1 Sorption of PFAS

The sorption kinetics of PFAS in sludge and soils are very important parameters when aiming to predict the transport from soil to freshwater recipients and groundwater.

The fate of PFASs entering the soil environment from e.g. sludge application depends on the sorption behavior of a given chemical to a specific soil under given environmental conditions, such as pH and temperature. The soil sorption coefficient, or K_d value, is a widely used equilibrium partitioning coefficient of chemicals used to predict their mobility from the soil to groundwater or adjacent freshwater systems.

The distribution coefficient (K_d), which is the ratio of the concentration in the solid phase (soil) to the liquid phase (pore water) once an equilibrium is reached, is defined in Eq. 2.1.as:

$$K_d = \frac{Concentration\ in\ solid\ phase\ (\frac{mg}{kg}\ dw)}{Concentration\ in\ liquid\ phase\ (\frac{mg}{l})} \qquad \text{Eq.2.1}$$

If K_d is high, it means a larger portion of the substance is adsorbed to soil particles and, hence, the substance is less mobile, while a lower value means that the contaminant is more prone to leaching. In reality, the K_d value varies with the physiochemical properties of the contaminant and the soil properties. The mobility may also vary over time with biological and chemical degradation and evaporation. Organic substances generally have a high affinity for organic carbon. Therefore, the K_d can be calculated with the formula in Eq. 2.2.

$$Kd = Koc \times foc \qquad \text{Eq.2.2}$$

Where K_{oc} (L/kg) is the distribution coefficient between organic carbon and water, i.e. C_{oc}/C_w, and f_{oc} is the fraction of organic carbon in soil (0-1).

K_{oc} are typically estimated from so-called sorption batch studies, for example the OECD 106 Guideline. Known volumes of solutions of the test substance, non-labelled or preferably radiolabelled, are added to soil samples of known dry weight. The mixture is agitated for an appropriate time. The soil suspensions are then separated by centrifugation and filtration, and the aqueous phase is analysed. The amount adsorbed may be determined indirectly by calculating the difference between the amount of test substance initially present in solution and the amount remaining at the end of the experiment, or it may be determined directly quantifying the test substance adsorbed by analysis of soil. The latter makes the analytical procedure more troublesome and time consuming and involves stepwise soil extraction with appropriate solvent(s).

K_{oc} and, hence, K_d values can vary substantially, depending on soil type, soil pH, the acid-base properties of the PFAS and the type of organic matter in the soil. For some substances, the relationship between K_d and K_{oc} are strong, whereas for others there is less correlation.

For instance, in a collation of numerous published sorption data for a range of PFAS and various soil and sediment properties, Li et al. (2018) found generally weak relationships between K_d values and organic carbon. Simple regression relationships between literature K_d values for numerous PFASs and soil properties are given in Table 2.1 (Li et al. 2018). Significant ($P < 0.05$) relationships for chemicals with more than 10 data points were found for PFOS (n =178), PFOA (n =147), PFNA (n= 87), PFDA (n = 57), PFHpA (n = 54), PFHxA (n = 50) and FOSA (n=26). However, for all these relationships the R^2 values were ≤0.35, except for (P)FOSA, where R^2= 0.70.

TABLE 2.1. Relationship between K_d values and content of organic carbon. Table redrafted from Li et al. (2018, supplementary information) for a number of PFAS and organic carbon content (% OC). Significant level is indicated as: *P<0.05; **P<0.01; ***P<0.001

PFAS	#Carbon	R^2	P level
PFBA	3	0.04	0.181
PFBS	4	0.01	0.527
PFPeA	4	0.08	0.124
PFHxA	6	0.10	0.029 *
PFHxS	6	0.05	0.321
PFHpA	6	0.22	0.0003 ***
PFOA	7	0.07	0.002 **
PFOS	8	0.05	0.003 **
(P)FOSA	8	0.70	1.1E-07 ***
EtFOSAA	8	0.87	0.02 *
MeFOSAA	8	0.98	0.004 **
PFNA	8	0.34	2.4E-09 ***
PFDA	9	0.35	1.4E-06 ***
PFDS	10	0.38	0.140
PFUnDA	10	0.13	0.253
PFUdA	10	0.80	0.003 **

Li et al. (2019) found solid and statistical significant correlations between K_d and total organic carbon (TOC) for PFOA and PFOS with R^2 of 0.6972 and 0.9180 and p values of 0.0386 and 0.0026, respectively. However, there were no significant correlations ($p > 0.05$) between the contents of TOC and the K_d of PFPeA, PFDA, and PFBS, indicating that TOC was not a dominant soil parameter affecting the adsorption of these compounds onto soils.

Miao et al. (2017) calculated the K_{oc} of PFOA from the slope of the K_d vs. F_{oc} relationship obtained for ten Chinese soils, as there was a strong correlation between the K_d values and the soil organic carbon (R^2 =0.977), which showed a log K_{oc} of 5.615 L/kg.

Other parameters than organic carbon have been shown to alter sorption of PFAS to soil and sediments, e.g. Li et al. (2018) suggested that the contribution of multiple soil properties must be considered. For example, changes in solution pH or exchangeable cations could affect the partitioning of PFAS.

Campos Pereira et al. (2018) investigated the effect of solution pH and calculated soil organic matter (SOM) net charge on the sorption of 14 PFAS onto an organic soil as a function of pH and added concentrations of Al^{3+}, Ca^{2+} and Na^{+}. The K_{oc} showed a negative relationship to both pH and the SOM bulk net negative charge. The effects of cation treatment and SOM bulk

net charge were evident for many PFASs with low to moderate sorption (C5-C8). However, for most long-chained PFASs (>C9), smaller effects of cations were seen, and instead sorption was more strongly related to the pH value. This suggests that the most long-chained PFAS, similarly to other hydrophobic organic compounds, are preferentially adsorbed to the highly condensed domains of the humic fraction, while shorter-chained PFASs to a larger extent are bound to humic and fulvic acid, where cation effects are significant. Generally, shorter-chain PFAS bind less strongly to soil than longer-chain PFAS.

In a batch experiment, Li et al. (2019) also found that the fraction that partitioned to solid soil surfaces increased with chain length of the substance for PFDA, PFOS, PFOA, PFBS and PEPeA. PFBS and PEPeA have the same number of carbon atoms (four), however, PFBS has a sulfonic functional group, which gives the molecule a higher sorption capacity. Within a relatively high organic (3.28% OC) soil type, equilibrium was reached within less than 48 hours. The fraction remaining in the aqueous phase at equilibrium differed from almost 75% for the 4-carbon-PFAS (PFPeA) to 25% for the 9-carbon-PFAS (PFDA). They concluded that the content of protein, rather than TOC, affects the adsorption of PFAs onto soils. In addition, anion exchange capacity and iron oxides were dominant soil properties affecting the adsorption.

Higgens and Luthy (2006) investigated the sorption of a number of PFAS on five different field collected sediments. Organic carbon, rather than sediment iron oxide content, was the dominant sediment-parameter affecting sorption, indicating the importance of hydrophobic interactions. However, sorption also increased with increasing solution [Ca^{2+}] and decreasing pH, suggesting that electrostatic interactions play a role. Perfluorocarbon chain length was the dominant structural feature influencing sorption, with each CF2 moiety contributing 0.50-0.60 log units to the measured distribution coefficients. The sulfonate moiety contributed an additional 0.23 log units to the measured distribution coefficient, when compared to carboxylate analogs.

Pettersson et al. (2015) investigated 19 PFAS with the aim of setting guideline values for K_{oc}. They ended up only suggesting a preliminary guideline K_{oc} value for PFOS, as they concluded that the scientific knowledge was insufficient to determine K_{oc} for all other PFAS.

The calculated or measured fraction in pore water in laboratory batch studies may change in the field over a very long perspective due to ageing processes (See also Chapter 3). In the field, higher K_{oc} coefficients have therefore typically been measured compared to laboratory derived K_{oc} coefficients. Zareitalabad et al. (2013) found log K_{oc} to be approximately 2.8 for PFOA and 3.0 for PFOS in laboratory experiments. In field collected sediments and sludge, the median log K_{oc} was calculated as 3.7 for PFOA and 4.2 for PFOS. The deviation is most likely due to varying and/or smaller concentrations in the field, ageing processes in the field (the contact time in laboratory is short relative to the contact time in the field) and sorption hysteresis that may increase the binding in field samples (Zareitalabad et al., 2013; Li et al., 2019). Applying laboratory derived distribution coefficients in risk assessment can therefore cause overestimation of PFAS concentrations in pore water and, consequently, also underestimate the residence time of the contaminants in soil (Zareitalabad et al., 2013).

McLachlan et al. (2019) studied the fate of C4-C14 perfluorinated carboxylic acids (PFCA) and two perfluorinated sulfonic acids (PFSA) in a field lysimeter experiment using an agricultural soil spiked with PFAS at four different levels (0.1 mg/kg, 1 mg/kg, 5 mg/kg, and 10 mg/kg of each PFAS). The lysimeters were planted with crops. Concentrations in soil were measured at the beginning and end of the growing season, and Lysimeter drainage water was collected and analysed. Under these (semi) field conditions, K_d values were measured. There was a strong positive correlation between K_d and nFC. A linear regression of log K_d for the PFCAs against nFC gave correlation coefficients of 0.97 and 0.96 for the upper and lower layer soils, respectively.

Enevoldsen and Juhler (2010), concluded that adsorption for six PFAS compounds in two Danish agricultural top soils (Jyndevad, a sandy soil, and Sjællands Odde, a clay soil) was characterised by linear Freundlich isotherms. Variability in sorption characteristics for soil types as well as compound properties were found, and correlation between the organic carbon normalised sorption coefficient (K_{oc}) and PFAS molecular weight was demonstrated. The K_d values were in the range 0.1 to 33 (l/kg) and 0.3 to 65 (l/kg) for sorption and desorption, respectively. The corresponding K_d values for adsorption are listed in Table 2.2. The soil types Jyndevad (OC of 1%, and pH of 6.1) and Sjællands Odde (OC of 0.42% and pH of 7.6) are two soil types relatively similar to the Karup and Langvad soil types used in the FOCUS models (Chapter 6).

TABLE 2.2. K_d values determined in two Danish agricultural soils Enevoldsen and Juhler (2010).

PFAS (soil:water ratio)	K_d – Sand Jyndevad	K_d - Clay Sj.Odde
PFHpA (12:25)	0.63	0.63
PFOA (12:25)	1.1	1.5
PFOA (3:14)	1.5	1.8
PFNA (12:25)	4.2	n.a.
PFNA (3:14)	5.2	7.7
PFDA (3:14)	30	33
PFBS (12:25)	0.41	0.07
PFOS (3:14)	15	17

2.2 K_{oc} values

Despite the challenges and limitations presented above, this project must derive useful K_{oc} or K_d values, as these are mandatory and essential for the calculations presented with regard to leaching of PFAS from soil into pore water and, subsequently, into freshwater or groundwater. It is often recommended to use median values of log K_{oc} values if data from more than five soils are available, which is the case for all of the $PFAS_{22}$ where data could be identified (Table 2.4).

Commonly, the K_{ow} describing the partition of a substance in between octanol and water (reflecting the hydrophobic versus lipophobic properties of a substance) has been used to calculate the K_{oc} values for organic substances by using experimentally established relationships. QSAR models are often used in that context, e.g. Sabljić et al. (1995) established simple relationships between K_{ow} and K_{oc} for a wide number of groups of organic substances.

PFAS are surfactants by nature, with both hydrophobic and lipophobic properties that prevent them from fully dissolving into either of the two liquids. They therefore tend to concentrate at interfaces, including solid-water interfaces, air-water interfaces or interfaces between organic liquids and water (Le et al., 2021). Consequently, K_{ow} values for PFAS are not a meaningful tool for estimating environmental fate and transport studies of PFAS. Instead, only measured K_{oc} values, preferably established on the basis of measured K_d values, are used.

Sewage sludge is normally used only for arable land in Denmark. These are (often by liming) pH-optimised for crop growth, resulting in pH typically in the range of 6.5 and 7.5, and rarely outside a pH range of 6-8. Nevertheless, it has been decided to include all available and valid K_{oc} values, even if studies were performed at lower pH, as the persistent nature of PFAS enables them to persist in soils for decades or even centuries, in which land use changes may occur. For example, change of land use from arable land to forest may over time reduce soil pH

to 3-4. In the case of PFOS and PFOA, reduced pH had influence – although not dramatically - on the log K_{oc} values as indicated in Table 2.3, where data from batch studies covering pH from 2.8 to 8.3 are included. However, it is noted that ionclusion of low pH data will increase the K_{oc} and hence reduce the predicted mobility of PFAS (see for example Table 7.1).

TABLE 2.3. The PFOS and PFOA log K_{oc} values for subsets of data as split up in all data (pH >2.8) versus only data from studies performed at pH > 6.0 (see Appendix A).

PFAS	pH (N)	10th percentile	50th percentile	90th percentile
PFOS	> 2.8 (N=83)	2.84	3.60	4.80
PFOS	≥ 6.0 (N=30)	2.80	2.98	3.66
PFOA	> 2.8 (N=74)	1.77	2.30	3.00
PFOA	≥ 6.0 (N=22)	1.75	2.24	2.99

2.2.1 Input K_{oc} for calculations and modelling

Two key batch studies form the basis of the input of K_{oc} for the modelling presented in this report, i.e. Campos Periera et al. (2018) and Nguyen et al. (2020). Both are batch studies, which is why K_{oc} values are estimated based upon adsorption to soil (K_d values) and not extrapolated from K_{ow} values. In Campos Periera et al. (2018), the sorbed amount of PFAS was determined indirectly by calculating aqueous loss. Furthermore, all PFAS sorption was attributed to the organic carbon content of the organic rich soil (f_{oc} = 0.45), and sorption to mineral phases was thus assumed to be negligible. Nguyen et al. (2020) determined K_d value (C_s/C_w) directly by measured concentration of PFAS measured in the soil phase (C_s) and the concentration of the PFAS measured in the aqueous phase (C_w). Based upon knowledge about the OC content in each soil, the K_d values were converted to K_{oc} values. All K_d and K_{oc} values can be found in Appendix A, and Table 2.4 below contains a summary of the data. The median K_{oc} is used as input data to the leaching calculations and modelling.

TABLE 2.4. The log K_{oc} value used in the leaching calculations and models and the data foundation behind those. For comparison with K_{oc} determined in batch studies in references A-D, K_{oc} values estimated on the basis of K_d values measured in semi-field condition (Lysimeter study) from McLaclan et al. (2019) are included. The K_{oc} in McLaclan et al. (2019) is the average of two values determined in the upper and the lower soil layer of the Lysimeter. The presented log K_{oc} are all median data from the data set, except for PFOS, where the 10th percentile of log K_{oc} is presented as well. All K_{oc} values can be found in Appendix A. $PFAS_4$ are highlighted in bold.

PFAS	# Data (N)	log K_{oc}	References^	McLaclan et al. (2019)
PFBS	58	1.80	A, B	1.89
PFPS	40	1.85	A	*
PFHxS	71	2.31	A, B	2.24
PFHpS	40	2.76	A	*
PFOS [Median]	86	3.60	A, B, C, D	3.35
PFOS [10th percentile]	86	2.84	A, B, C, D	3.35
PFNS	40	3.76	A	*
PFDS	40	4.23	A	*
PFUnS	0	*	*	*
PFDoS	0	*	*	*
PFTrS	0	*	*	*
(P)FOSA	71	4.36	A, B	*
6.2 FTS	40	2.28	A	*
PFBA	40	1.90	A	1.28
PFPeA	55	1.38	A, B	1.56
PFHxA	71	1.50	A, B	1.73
PFHpA	73	1.91	A, B, C	2.04
PFOA	77	2.30	A, B, C	2.37
PFNA	74	2.90	A, B, C	2.98
PFDA	73	4.00	A, B, C	3.68
PFUn(D)A	70	4.30	A, B	4.20
PFDo(D)A	69	4.77	A, B	4.65
PFTr(D)A	0	*	*	5.02

*No data

^ References: A= Nguyen et al. 2020; B= Campos Periera et al. 2018; C= Enevoldsen and Juhler 2010, D= Pettersson et al. 2015.

3. Fate: Degradation, ageing, bioavailability, extractability and leaching of PFAS

3.1 Degradation of PFAS in soil (DT_{50})

The REACH Annex XV restriction dossier (ECHA, 2014) and REACH proposal for identification of PFOA as an SVHC (ECHA 2013) state that PFOA is not biodegradable and that, based on high persistence, it is not possible to calculate half-lives in soil or sediment. Moreover, there are many precursors that degrade in soil forming PFOS and PFOA.

Zhang et al. (2022) reviewed degradation studies with PFAS and concluded that recent research outcomes have shown that an increasing number of PFAS species in fact are biodegradable to some extent. Both mixed culture and pure microbial species show potential in degrading certain PFAS species, though they typically cannot be degraded completely through a single biodegradation pathway. The absence or very limited biotic degradation is associated with the recent anthropogenic origin of PFAS and high toxicity of fluoride. Evolution and gene spread is driven by natural selection, and metabolism of polyfluorinated compounds may often lack selective benefit (Wackett 2021). Without rapid export of the fluoride product, the metabolism will be counter-selected against and not be retained in populations. Thus, metabolism has not evolved over years as it may have for other organic pollutants. Since microbes have not been long-exposed to highly-fluorinated natural products, they require newly evolved metabolism.

Due to the lack of reliable DT_{50} values and the proven high resistance to biodegradation, the DT_{50} for all PFAS was set at 100 years (36,500 days) as a conservative estimate.

3.2 Fate of PFAS in soils over time as influenced by ageing

It has been observed that as soil-pollutant contact time increases, the pollutant vmobility, bioavailability and extractability decreases. This phenomenon has been termed 'ageing'. Decreased chemical extractability with increased soil-chemical contact time is evident and a result of an ongoing sorption process and sequestration. Major processes involved in ageing are diffusion into nano-pores and sorption (adsorption and absorption) to soil organic matter. Strong sorption and slow release processes are responsible for the process called sequestration of hydrophobic pollutants.

Processes and mechanisms involved in the sequestration process are mainly:

1. Adsorption onto mineral surfaces.
2. Absorption into flexible/soft natural organic matter.
3. Adsorption on condensed/hard natural organic matter.
4. Diffusion in micro-porous media.
5. Encapsulation.

The first two mechanisms are usually fast and reversible, whereas the latter three mechanisms exhibit a slow desorption rate, pronounced sorption-desorption hysteresis, and largely irreversible retention of contaminants. Moreover, normal solvent extractability is reduced significantly for the last three mechanisms. Therefore, extraction procedures using varying extraction

conditions (e.g. changing temperature, pressure or solvent type), such as sequential supercritical fluid extraction, may reveal information about the prevailing retention mechanisms (Ortega-Calvo et al. 2015). The non-extractable part is the part that causes the most challenges in risk assessment, as it can be discussed whether the remaining fractions must be considered in the risk evaluation, since they may or may not become more or less available for uptake over time. To sufficiently establish the non-extractable part, often named bound residues or non-extractable residues (NER), it will be necessary to use radio-labelled ^{14}C, as the NER by definition cannot be extracted even after the most aggressive solvent extractions have been performed. NERs remaining in soils may belong to two fractions, i.e. the intact chemical associated with mineral and/or organic matter fractions and/or the transformation products of the ^{14}C-labelled chemical incorporated within microbial biomass (biochemical components), or even ^{14}C-carbonates. These assimilated residues (known as biogenic NERs) are of no ecotoxicological or toxicological concern.

3.3 Non-Extractable Residues (NER)

Non-Extractable Residues, is a term introduced by - among others - regulatory agencies in risk assessment frameworks in order to adjust the risk assessment of persistent substances with regards to persistent, bioaccumulation and toxicity (PBT) properties. NER vary according to the chemical physical properties of the matrix and the contaminant as well as it changes over time. As a result, low ecotoxicity, reduced plant uptake or reduced leaching has been observed in the field at historically contaminated sites where laboratory studies with freshly spiked substances have indicated a significantly higher ecotoxicity or uptake rate.

The amount and characteristics of NER may have a significant impact on the derivation of degradation half-lives and, hence, on the regulatory conclusions with respect to the PBT (Persistent, Bioaccumulation and Toxicity) and vPvB (very persistent and very bioaccumulative) assessments of chemicals within REACH, for example.

Concepts and interpretations regarding NERs may be implemented in differently under various regulatory frameworks. NER can, under certain criteria, be assumed to be degraded residues of no environmental concern, or NER can be regarded as potentially bioavailable and as non-degraded. In other words, NER can be considered either a `safe sink´ or a hidden potential future hazard from a re-mobilisable repository, depending on which regulatory context it applies.

The quantification and identification of extractable residues (parent substances and transformation products) of the tested substance is a core part of performing a standard simulation test (OECD TG 307, 308 and 309) and is always needed. By default, the residues remaining in the matrix after these extractions (total NER) should be regarded as non-degraded substances. The fraction of NER must therefore be minimized by using extraction methods that on the one hand are so harsh that they extract as much as possible, but on the other hand do not modify the physicochemical nature of the extracted compounds. The extraction method therefore must be tailored to the substance tested and its degradation products, so that modification of parent substances and degradation products is avoided (ECHA 2019, ECETOC 2013). These methods may include harsh extraction methods such as Soxhlet (reflux), microwave assisted extraction (MAE), ultra-sonication and Accelerated Solvent Extraction (ASE) - also called Pressurised Liquid Extraction (PLE).

Schäffer et al. (2018), proposed an approach to experimentally discriminate three separate types of NER in environmental matrices. The approach operates with NER type I and II as well as biogenic NER (bioNER - NER Type III), as outlined below (ECHA 2019).

NER Type I: Are adsorbed or physically entrapped into the matrix, contain the parent substance, transformation products or both. NER Type I have the potential to be remobilized and therefore should be regarded as non-degraded substances when calculating the half-life. If

chemical analyses are conducted, it may be possible to distinguish whether NER Type I consist of unmodified parent substance or of transformation products.

NER Type II: Residues that are strongly bound to the matrix in surface water, soils or sediments and that are considered to have low remobilization rates. Unless there are indications from the available literature or monitoring data regarding their potential remobilization, strongly bound residues may be regarded as irreversibly bound.

NER Type III: NER Type III are incorporated into biomass and result from the anabolic formation of biomolecules (amino acids, phospholipids, and other biomass compounds) from the degradation products of the parent substance. Dead biomass, and therefore biogenic NER, are eventually fixed in organic matter derived from decaying microbial biomass. NER Type III are considered to be of no concern.

The information on the quantity of NER types (I, II, III) can be used for refining the half-life (DT_{50}). The half-life may be calculated using the sum of the concentrations of the parent substance, transformation products and NER Type I. Biogenic NER (Type III) and strongly bound NER (Type II) can be regarded as inert and removed for assessment as if they were degraded. DT_{50} should hence be regarded as a half-life for dissipation rather than for degradation. The environmental effects are, however, considered comparable.

Zhu et al. (2021) investigated the NER development during a 240-day incubation of PFOS (1.95 µg/kg) and its alternative 6:2 chlorinated polyfluorinated ether sulfonate (F-53B) (2.33 µg/kg) in a silty clay topsoil. The results confirmed the formation of NER, but whereas NER-PFOS was formed predominantly by covalent binding (via head group) and strong adsorption (via tail group), the formation of NER-F-53B was mainly driven by physical entrapment. Both compounds showed a three-stage (initial stage, (re)incorporating stage and a remobilizing stage) pattern with regards to NER formation. The remobilization of NER-PFAS was mainly attributed to the decomposition of soil organic matter by microbial activities.

Zhang et al. (2021) investigated plant uptake of five selected ether-PFAS in order to understand distribution of ether-PFAS in plant-soil systems. They found the non-extractable fractions to range from 22.8 to more than 80% after 80 days of soil-PFAS contact.

3.3.1 Model validation of NER for PFAS.

Gassmann et al. (2021) tested the ability of the FOCUS model MACRO (See Chapter 6) to simulate the leaching and plant uptake of PFOA and PFOS. The model results were compared with data from a field lysimeter using two concepts of adsorption: a kinetic two-side sorption concept usually applied for pesticide leaching (scenario I) and an alternative approach including the formation of NER (scenario II). The validation data for the model originates from a long-term lysimeter study regarding PFOA and PFOS leaching (Stahl et al. 2013) updated with sampling data from 2011-2015. These data were used to calibrate the leaching model MACRO 5.2 for both PFOA and PFOS. The breakthrough of substances could only be simulated adequately by including aspects of NER formation (scenario II), as scenario I noticeably overestimated the leaching behavior of both PFAS.

The kinetic rate of NER formation could not be taken from the literature, but was initially estimated between 0.001 and 0.014 d^{-1}. After calibration with lysimeter data, posterior parameter statistics showed that the kinetic rate of NER formation was higher for PFOA (range 0.0030-0.0066; median of 0.0047 d^{-1}) than for PFOS (range 0.0011-00.0016; median 0.0013 d-1). However, since more than 90% of both substances is in the NER pool at the end of the simulation period, there is no apparent difference in absolute NER formation of both substances. Even though PFOA has a faster NER formation, the availability of the substance for NER formation in the soil is much lower compared with PFOS, due to its lower affinity and adsorption

to e.g. organic carbon (K_{oc}), since the calculation concept of NER formation outlines that only adsorbed material can be rendered NER (Gassmann et al. 2021).

Both sampling data and model calculations showed that the breakthrough of PFOA had ended after 8 years, while the breakthrough of PFOS was still ongoing and stable at a plateau, with 2.4–8.4% of PFOS still in the mobile adsorption pool and, thus, potentially leaking out in the following years (Table 3.1).

TABLE 3.1. Simulated and sampled substance balance of PFOA and PFOS from 2007 to 2015. Table re-printed from Gassmann et al. (2021).

	Mass (g/m2)		% of applied
	PFOA	PFOS	PFOA
Leaching mass simulated	4.9–25.5	1.2–3.5	1.4–7.1
Leaching mass sampled	13.9	2.7	3.9
Plant uptake simulated	0.002–0.005	0.016–0.026	0.0006–0.0013
Plant uptake sampled	0.005	0.020	0.0013
Left in Soil (simulated)	334.5–355.1	363.9–366.2	92.9–98.6
NER pool	341.8–351.3	335.5–355.3	95.0–97.6
Reversible sorption pool	0.0–3.8	8.7–30.7	0.0–1.1

The width of the concentration uncertainty bounds of both substances was largest in the model simulations during years without lysimeter outflow.

The model results by Gassmann et al. (2021) suggest that more than 90% of PFOA and PFOS were expected to be found in the pool of NER after 8 years (Table 3.1). With a median K_{fOC} of 72 ml/g and 510 ml/g for PFOA and PFOS, respectively, the pool of PFOS for NER formation is about 7.1 times higher, but the rate is 3.6 times slower when compared with PFOA. Also, in a lysimeter study McLachlan et al. (2019) found faster NER formation for PFOA than for PFOS in soils under near-natural conditions. They also found that for the C11-C14 PFAS, most of the decrease in soil concentration was attributed to the formation of non-extractable residues, whereas for the remaining PFAS leaching was the dominant removal process. McLachlan et al. (2019) concluded that model simulations with PELMO based on measured K_d values under-predicted removal by leaching. This was attributed to mixture effects that reduced sorption to soil. Finally, McLachlan et al. (2019) noted that it may have been possible to extract more of these chemicals from the soil using a more aggressive extraction and that quantification of non-extractable-residues is relative to the extraction method employed.

The NER formation in Gassmann et al. (2021) is somehow higher than the ones reported in McLachlan et al. (2019), who found a loss of PFOA (45%) and PFOS (20%) to NER. The time-scale of the experiment of McLachlan et al. (2019) was, however, much shorter (120 days) than the 8 years of Gassmann et al. (2021). Considering that NER formation is an ongoing kinetic process, the much higher NER fraction found by Gassmann et al. (2021) may be reasonable.

3.4 Leaching studies with PFAS

A wide number of studies elucidating the potential leaching from PFAS contaminated soils have been published. It is beyond the scope of this report to review all of them. Many of these are associated with the evaluation of various physical materials used at field scale for in-situ

stabilization. Common for many of these studies is that they are very site specific and often conducted at sites historically impacted with aqueous film forming foam (AFFF), leaving very high soil concentrations as a result. These sites and PFAS concentrations are by no means comparable to the situation in arable land fertilized with sewage sludge.

Furthermore, it is evident that evaluations of the fate and leaching of historically contaminated soils are hampered by the fact that leaching is influenced both by the presence of non-transformable and transformable (precursors) PFAS (Weidemann et al. 2022). The results of contaminated field soil experiments have shown that it is a challenge to estimate PFAS leaching without knowing all occurring precursors and complex transformation dynamics. Below, a few studies are summarized that elucidate whether NER is a relevant parameter for PFAS in sludge amended soils.

Høisæter and Breedveld (2022) reported the leaching of PFAS from historically AFFF contaminated field soil under saturated conditions using up-flow columns for four soil samples with varying PFAS concentrations to quantify the long-term release potential of the source zone. PFOS was the most abundant PFAS present in the soils, varying from 358 to 1097 µg/kg, and the total organic carbon (TOC) content varied from 0.73 to 2.0%. The experiment was run with approximately 100 years of natural water infiltration. The results indicated that at the end of the experiment, between 0 and 50% of the PFOS was still left in soils, with the highest amount remaining found in the sandy low OC soil. The relative leaching potential was, however, not directly correlated to the TOC content of the soils. The removal of the other PFAS after 100 years of simulated rainfall was in the four soil types lowest for e.g. PFBS (4-18% removal) and PFBA (11-37% removal) and highest for e.g. PFOA (56-100% removal) and PFNA (39-100% removal).

Rayner et al. (2022) assess PFAS leaching for 37 aged field soils from five sites historically contaminated with PFAS over decades. Leaching from intact soil cores was taken to reflect field conditions. These were compared to two new laboratory batch tests and two standard approaches. The PFAS mass leached as a fraction of the total was 27% from the soil cores and between 30 and 90% in the four laboratory batch studies. The leaching potential (% of total) for shorter chain PFAS was higher in all tests. For the intact core experiment, near-water saturated conditions were adopted with a likely overestimation of mass release compared to unsaturated flow conditions in the field. In 25 cores, leaching of PFAS (sum of 15 PFAS) ranged between 7.3 and 67.8 %, with a mean of 27.3 % of the total concentrations found in the soil.

Kabiri et al. (2022) evaluated the leaching and desorption of a wide range of PFASs from twelve contaminated soils with three different leaching tests, including a column leaching experiment performed for 21 days, equivalent to 68 pore volumes (one pore volume is the volume of water that a saturated soil holds in its pores). All tests showed similar PFAS leaching behavior, with short-chain ($CF_2 \leq 6$) PFAS more easily desorbed and leached and long-chain PFASs more difficult to desorb. Leaching of long-chain PFAS was pH-dependent, where leaching increased at high pH, while leaching of short-chain PFASs was less sensitive to pH. The total concentration of PFAS (sum of all detected PFASs out of in total 28) in the soils ranged from 17.7 to 8.3E+05 µg/kg, with PFOS being the by far dominating PFAS in all soils. The percentage leached differed among PFAS, contamination level and among soil types, but ranged from almost nothing to 100%. PFDS and PFOS were typically lost by leaching within a range of 25-50%, whereas PFPeS and PFHxS for example, leached more than 75% and often 100%. Schaefer et al. (2022) used field-deployed lysimeters to measure the concentrations of PFAS in soil pore water at a site historically impacted with aqueous film forming foam (AFFF). The absolute measured concentration in pore water depended naturally on the concentrations found in the soil, but they found a relatively higher leaching potential of PFAS like PFBS, PFHxS, PFPeA and PFHxA than for example PFOS and PFBA.

Sepulvado et al. (2011) investigated the occurrence and fate of PFAS from land-applied sludge by evaluating the levels, mass balance, desorption and transport of PFAS in soils receiving application of sludge at various loading rates. These data suggest leaching of PFAS from the application zone to a depth, in some cases, of 120 cm. However, as expected, the longer chain-length PFAS appear to be much less mobile than the shorter chain-length.
In a mass balance evaluation of a two-year soil column study in two different field soils, which were already contaminated with a mixture of PFAS, Weidemann et al. (2022) found that 100% of the initial applied mass of PFBA, PFPeA, PFHxA, PFHpA, PFBS and PFHxS could be recovered, all of it in the percolates, whereas for PFOA only approximately 80% could be recovered – again all in the percolate. Finally, for PFAS, like PFOS, PFDA and PFNA, only between 20 and 60% could be recovered, mainly in the soil phase. Mass balances showed a significant correlation between the number of CFX groups and recovery rates. The reduced recovery could be a result of covalent binding (NER type II) and/or bioNER formation (NER type III), just as losses due to adsorption on vessel walls cannot be ruled out.

Stahl et al. (2013) studied the behavior of PFOA and PFOS in soil and the carry-over from soil to plants. A concentration of 25 mg/kg soil was applied to 1.5 m^3 monolithic soil columns of a lysimeter. Growth samples and percolated water were analyzed throughout a period of five years, where only natural rainfall and no artificial irrigation was applied. Besides PFOA and PFOS, results were are also presented regarding short chained PFAS, such as PFBA, PFBS, PFPeA, PFHxA, PFHxS and PFHpA, which were present (3.5% in total) in the technical mixtures of PFOA and PFOS. The concentration of PFOA in lysimeter leachate increased linearly (r^2 = 0.913) the first six months and then remained at a high level the next three years. The concentration of PFOS remained almost constant the first six months and then rose in a nearly linear manner (r^2 = 0.955) to a value of 622 µg/L leachate three years later. The concentration of PFOA was approximately 450 times higher than PFOS in the beginning and 60 times at the end of the study. During the study, it was estimated that in total 11,235 mg PFOA and 47.3 mg PFOS were removed by leaching. This can be compared to 360 g PFOA and 367.5 g PFOS per (1500 kg of soil) lysimeter, i.e. 3.1 and 0.01% of the applied were leached for PFOA and PFOS, respectively. After five years, 96.88% of the PFOA and 99.98% of the PFOS originally applied to the soil were still in the lysimeter. These values were obtained by subtracting the rounded off amounts lost to plant uptake (PFOA, 0.001%; PFOS, 0.004%) and to leachate (PFOA, 3.12%; PFOS, 0.013%) from the total. These results indicate that PFOA is transported rapidly by water passing through the soil, whereas PFOS travels much more slowly and was found in increasing amounts throughout the 42 months of the study. PFHxA, PFHxS and PFHpA could only be detected in lysimeter leachate the first six month, whereas PFBS could be detected in leachate the entire period. It should be noted that the used soil concentrations are at least three orders of magnitude higher than what is predicted in Danish sludge amended soils.

The overall conclusion in the above studies is that the PFAS chemical structure appeared to have a greater effect on leaching from soil than soil physicochemical properties.

3.5 PFAS in groundwater

In Denmark, monitoring of PFAS in groundwater samples revealed that findings of PFAS in more than 1000 samples varied for individual substances, ranging from 0% for PFAS like PFDS, PFOSA, PFDA and PFHpS, to approximately 15% for PFOA and 10% for PFHxS and PFOS (GEUS 2023). In total, 20-25% of all groundwater samples had detectable levels of PFAS, although only 6% were above the threshold for $PFAS_4$ of 2 ng/L.

Several monitoring studies have demonstrated findings of PFAS in groundwater (Xu et al. 2021, Liu et al. 2022). Xu et al. (2021) concluded in their review that PFOA, PFBA, PFOS and PFBS were present at high concentrations up to 21,200 ng/L, while their substitutes GenX and

F-53B were found up to 30,000 ng/L and 0.18–0.59 ng/L, respectively. At four different aqueous film-forming foam (AFFF)-impacted Canadian airports, Liu et al. (2022) found that horizontal transfer of PFASs in surface soils was limited, but vertical migration down the soil column occurred even in locations of low permeability. However, three of the sites displayed median ∑PFAS levels in the range of 1,340-2,670 µg/kg dw, which was magnitude higher than that of the 4th, i.e. 53 µg/kg dw. Such concentrations are markedly above what is likely to be found in agricultural soils receiving sewage sludge for decades (Table 8.2).

Data has shown that PFOS continues to leach in small quantities even years after the pollution with e.g. firefighting aqueous film-forming foams (AFFF) has potentially stopped. The source concentration may, however, be orders of magnitude higher at contaminated sites compared to normal sludge amended arable soils. Direct comparison between contaminated hot spots and soils fertilized with biosolids should therefore only be made with caution.

Johnson (2022) reported data for PFAS in soil and groundwater following historical land application of biosolids. In this study, the impact of land applying biosolids on the occurrence, concentration and distribution of PFAS in soils, the vadose zone, and the immediately underlying groundwater at an agricultural station with a long history of applying biosolids plus irrigation using treated wastewater effluent for planted feedstock crops was investigated. The land application of dewatered biosolids from multiple publicly owned treatment works began at the station in the mid-1990s and has continued till today. Surface soil samples were collected along a nearly 4,600 m transect of an agricultural station, with characterization of the soil concentrations and vertical distribution of twelve PFAS homologues. Furthermore, soil boring samples (n = 50) were collected through the vadose zone down to approximately 18 m during well installation at the site. Groundwater samples (n = 2) were collected from the perched aquifer located at approximately 17 m depth. All twelve targeted PFAS, homologues were detected at quantifiable concentrations in all soil samples collected near the surface (n = 34), with total PFAS (Σ 12PFAS) concentrations ranging from 73 to 196 µg/kg, which is approximately one order of magnitude higher than in a similar Danish study (Draborg and Tsitonaki 2023, see below). The soil concentration rank was PFOS>PFDA>PFOA at all sampling locations regardless of the varying annual average loading rates. The surface-soil concentrations of PFOS ranged from 36 to 100 µg/kg. With regard to transport, the results showed leaching of short-chain PFAS compounds through the soil profile. PFOA were detected above LoQ down to approximately 9 meters, whereas PFOS could only be quantified down to 3 m. However, both PFOA and PFOS were detected below LoQ down to 18 m below surface. The migration of PFAS through the soil profile is possibly related to a measured increase in soil pH through that profile, as sorption of PFAS compounds has been shown to decrease with increasing pH. Measured concentrations of PFOA and PFOS in groundwater located approximately 17 m below surface were reported as ≤ 0.029 µg/L and ≤ 0.002 µg/L, respectively. With measured groundwater concentrations 1 to 2 orders of magnitude less than soil concentrations, the significant role of retention processes in soil systems contributing to the overall transport, fate and leaching behavior of PFAS is evident.

A recent Danish study (Draborg and Tsitonaki 2023) investigated the transport and fate of PFAS in field soils amended with large quantities of sewage sludge for numerous years, i.e. since 2003, at the CRUCIAL[6] experimental site[7]. In highly sludge loaded plots, the load corresponds to 75 years of a typical Danish sludge load, while in accelerated plots the total sludge load corresponds to more than 200 years of typical sludge loads in Denmark. The trend of PFAS concentrations measured in the sewage sludge used for fertilizing the plots is depicted in Figure 3.1. The concentration has markedly decreased in the period 2003 to 2022.

[6] Closing the Rural-Urban nutrient Cycle—Investigations through Agronomic Long-term experiments

[7] https://plen.ku.dk/english/research/plant_soil/sf/crucial/

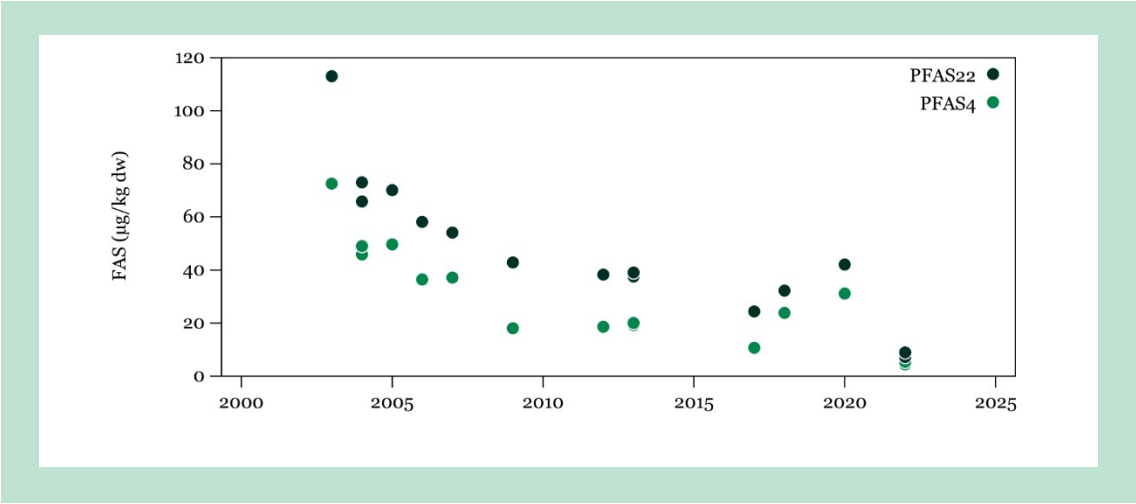

FIGURE 3.1. Measured PFAS (µg/kg dw) in sludge samples covering the period 2003-2022 from Avedøre WWTP used for soil amendment of long-term CRUCIAL research plots (See text). Solid circles are $PFAS_{22}$ and open circles are $PFAS_4$. Reprinted from Draborg and Tsitonaki (2023).

In total, 10 boreholes were made at four different mark plots covering two plots with high sludge application rate (6 drillings), one plot with accelerated (very high) sludge load (2 drillings) and one control plot (2 drillings) with no use of organic fertilizer. Soil samples were taken down to 18 meters below surface, and water samples were collected by filters located from 4.5 meters down to 18 meters. LOD for soil samples were 0.5 µg/kg for the sum of $PFAS_{22}$ and the LOD for water samples for $PFAS_{22}$ was 0.3 ng/L. No or very low levels of PFAS were detected in the control soil. Higher soil concentrations were identified in the sludge accelerated plot, and generally the highest soil concentrations were found in the top soil (30 cm), i.e. 7.2-11 µg/kg in the top soil of the accelerated plot versus <LOD-5.5 µg/kg in the top soil of the normal plots. In the accelerated plots, the soil concentrations decreased as follows at 0.3, 0.5 and 1.0 meter: 8.6/11.0 (two replicates), 1.1 and 0.28 µg/kg. In the normal plots, the soil concentrations decreased as follows at 0.3, 0.5 and 1.0 meter (two replicates): 4.7/5.5, 0.74/0.41, 0.06/0.08 µg/kg.

Generally, PFAS was not found or found at very low levels in the groundwater samples from the site. PFAS was detected in three drillings of the 10, all in plots amended with normal sludge application. Two of the filters were located in plots located next to an accelerated plot. In one of the filters, located at 4.5-5.5 meters below surface, up to 4.93 ng/L were detected for the sum of $PFAS_{22}$ and 2.69 ng/L for the sum of $PFAS_4$. In the two others plots, all detections were below 1.0 ng/L for the sum of $PFAS_{22}$. PFOA and PFOS were by far the most common of the $PFAS_{22}$, and in two of the three filters, PFOS was the only PFAS identified in water samples.

3.6 Conclusions on the Fate of PFAS

PFAS are very persistent and biological degradation is very limited over time. However, other dissipation processes may occur in the soil environment, including plant uptake, leaching and encapsulation.

On the one hand, several lysimeter-like studies have shown that the availability of (especially long chained) PFAS for leaching and plant uptake are markedly reduced, and only a minor fraction of the total concentration is leached within a time frame of 5-10 years. On the other hand, monitoring studies across the globe have been able to detect PFAS in groundwater, indicating that these substances, to some extent, are capable of leaching to groundwater.

Gassmann et al. (2021) found via model calculations and measurement from long-term Lysimeter studies that after 8 years, more than 90% of PFOA and PFOS could be considered as non-extractable residues with restricted availability and, hence, reduced potential for leaching. In a 5-year lysimeter study, Stahl et al. (2013) still found 96.88% of the PFOA and 99.98% of the PFOS originally applied to the soil. Loss to leachate was estimated to 3.12% for PFOA and 0.013% for PFOS. Shorter studies have found lower levels of NER formation, but as the predictions presented in this report all are based on very long-term accumulation of PFAS in soils to steady state situations occurring after decades or even centuries, short term studies are less relevant in this context.

A number of unknown factors for NER for PFAS are, however, still present, as this group of substances does not behave in a manner fully comparable to other very persistent organic pollutant or heavy metals.

4. Calculation methods and equations

4.1 Introduction to REACH methodologies and basic assumptions

In line with the guidance outlined in ECHA R.16, the sludge application is treated as a single event once a year. In ECHA R.16, for sludge application to agricultural soil an application rate ($APPL_{sludge}$) of 5.000 kg/ha/y dry weight is assumed, while for grassland a rate of 1.000 kg/ha/y should be used. In this report, the grassland scenario is omitted. However, as the maximum permitted load on arable land in Denmark theoretically is 7,000 kg/ha/y, this sludge load is used throughout this report, acknowledging that this is an absolute worst-case situation, which very rarely or almost never in practice will be used for sludge on arable soils in Denmark. More realistic annual application rates of sludge would be 1-2 tons dry matter per hectare, due to the legal restriction in phosphor application of a maximum annual application of 30 kg P/ha as averaged over a three-year period.

The sludge and the PFAS are assumed equally distributed on the field and subsequently incorporated (ploughed) into the soil, resulting in a homogenously mixed soil top layer theoretically 20 cm thick. The topsoil layer is assumed to have a dry bulk density of 1.7 kg/dm^3 or 1700 kg/m^3. No macro pore flow (preferential flow) is assumed in the topsoil layer. For screening purposes, it is expected that all applied PFAS will be available for uptake (bioavailable) in soil organisms and plants, which is a conservative approach, especially in cases where long-term accumulation over time is considered, as data generally shows a reduced bioavailability of persistent substances over time (see Chapter 3). In R.16, in the terrestrial ecosystem the concentration in agricultural soil is averaged over 30 days, and for human indirect exposure (exposure of humans via the environment), the concentration is averaged over 180 days. In this report, no averaging is made. Rather, the initial concentration, and not the time weighted average, in the year of steady state (the year where input of PFAS equals output) is used as a conservative estimate of soil exposure.

In the Sections below, the relevant ECHA R.16 calculations used across the various exposure scenarios are presented. The main principle is that these equations normally are used to calculate the concentration in the recipients (freshwater and groundwater) after a predefined sludge load and sludge concentration. In this report, these equations are reversed in order to calculate the maximum concentration in sludge being in compliance with the relevant environmental threshold or target concentrations, e.g. EQS for freshwater. In other words, where R.16 starts with a sludge concentration and ends with a predicted concentration in the recipients, these reversed calculations start with a threshold concentration in the recipients and end with a predicted sludge concentration.

4.2 Concentration in soil after sludge application

The estimation of the concentration in soil after sludge amendment follows the recommendation in the exposure guideline for ECHA R.16 (2016) unless otherwise stated. These recommendations are also reflected in EFSA (2019) and EMA (2007).

The top layer of the soil compartment is described as one compartment, with an average influx through aerial deposition and sludge application, and removal processes from the soil by degradation, volatilization and leaching. The time dependent concentration in the topsoil layer can be described with a simple differential equation as:

$$\frac{dCsoil}{dt} = -k\ x\ Csoil + Dair$$ Eq. 4.1

where

C_{soil}	Concentration in soil	mg/kg
D_{air}	Aerial deposition flux per kg of soil	mg/kg/d
t	Time	days
k	First order rate constant for removal from topsoil	d^{-1}

The aerial deposition of PFAS (D_{air}) is in this report considered very limited and, hence, neglected.

The removal rate constant (k) is in R.16 a summary of the first order removal rate constants for volatilization, leaching and biodegradation. Due to the intrinsic properties of PFAS, the removal by volatilization is typically negligible and, hence, neglected in this report. Therefore, k = k(leaching) + k(biodegradation). As studies have shown the importance of the formation of non-extractable residues in predicting leaching of PFAS from soils (see Chapter 3), this report also operates with a removal of PFAS from the bioavailable and mobile fraction in soil caused by NER formation, which is why k_{NER} is added to the equation as:

$k = k_{leaching} + k_{biodegradation} + k_{NER}$

The initial concentration, $C_{soil(0)}$, is governed by the input of the substance through sludge application. The concentration just after one sludge application (t=0) can be calculated as:

$$Csoil(0) = \frac{Csludge\ x\ APPLsludge}{DEPTHsoil\ x\ RHOsoil(dw)}$$ Eq. 4.2

where

$C_{sludge(0)}$	Concentration in sludge at time zero^		mg/kg
$APPL_{sludge*}$	Application rate of sludge (dw)	0.7	$kg/m^2/y$
$DEPTH_{soil}$	Mixing depth of soil	0.2	m
$RHO_{soil(dw)}$	Bulk density of dry soil	1700	kg/m^3

* The recommended default value for sludge application to agricultural soil in REACH R.16 is 0.5 $kg/m^2/y$, however, as the maximum theoretically permitted load in Denmark is 0.7 $kg/m^2/y$, this is used throughout this report unless otherwise stated. ^Concentration in soil at time zero is the concentration immediately after sludge amendment the first year.

4.3 Realistic sludge application rates

Sewage sludge in Denmark is regulated based on the "Waste-to-Soil Act" (Bek. nr. 1001 af 27/06/2018), where §25 states that no more than 7 tons of dry matter may be applied annually per hectare as calculated as an average over a ten-year period. However, application of biowaste is also regulated according to the "Fertiliser Act" (Bek. Nr. 1142 af 10/07/2022), where a maximum soil application of 30 kg P/ha (calculated as an average over three years) is stated. The actual sludge application hence in practise depends on the P content of the sludge in question. In Miljøstyrelsen (2009, 2022), the average P content of Danish sludge is reported as approximately 29 kg/t dw. This corresponds very well with the average P content of 28.85 kg/t reported in Miljøstyrelsen (2013). With an average annual ceiling of 30 kg P/ha and a median P content of 29 kg/t, this results in a median sludge application rate of 1.03 t/ha/y. The 10^{th} and 90^{th} percentile of P content in Danish sludge was in 2005 reported as 15 and 39 kg/t, respectively, resulting in an annual sludge load of 2 and 0.77 t/ha/y at the lowest and highest percentile of P, respectively.

4.4 Long-term accumulation in sludge amended soils

Due to the strong adsorption and limited degradation, many PFAS have the potential to accumulate in soils over time. Therefore, the long-term steady-state soil concentration ($C_{soil\text{-}ss}$) can be considered as a worst-case situation. Such steady state plateau concentrations in sludge-amended soils occurs when the annual input of PFAS equals the annual removal. A key parameter to determine the long-term accumulation is the degradation, or rather the dissipation rate, typically described by the DT_{50} value. Very limited information is available for PFAS with regard to DT_{50}. For precautionary reasons, the biodegradation half-life is set to a default at 100 years (see Chapter 3.1 for discussion).

According to the details described in ECHA R.16, the soil concentration at the steady state situation ($C_{soil\text{-}ss}$) is calculated as:

$$Csoil - ss = Csoil(0)\ x\ \frac{1}{1-Facc} \qquad \text{Eq. 4.3a}$$

The concentration in soil after a fixed sludge application period (*n* years) can also be calculated by equations found in ECHA R.16 [Eq.16.52], where the initial soil concentration in year *n* $C_{soil(yn)}$ is calculated as:

$$Csoil(yn) = Csoil(0)\ x\ [1 + \sum_1^n Facc^n] \qquad \text{Eq.4.3b}$$

where

$C_{soil\text{-}ss}$	Initial soil concentration in a steady-state situation	mg/kg
$C_{soil(0)}$	Concentration in soil after the first sludge amendment in year 1, t=0	mg/kg
$C_{soil(yn)}$	Concentration in soil after the first *n* sludge amendments, i.e. soil concentration in year *n*	mg/kg
F_{acc}	Fraction of PFAS accumulation in one year	

where

$$Facc = e^{-365\ x\ k} \qquad \text{Eq. 4.4}$$

In Eq. 4.4, the overall first order removal rate *k* is defined as the combined removal by leaching, biodegradation and formation of immobile and non-extractable residues (NER), as removal by volatilization (k_{volat}) is omitted in the case of PFAS, i.e.:

$$k = k_{removal} = k_{leaching} + k_{biodegradation} + k_{NER} \qquad \text{Eq. 4.5a}$$

$$k\text{leaching} = \frac{Finf\ x\ RAINrate}{Ksoil\text{-}water\ x\ DEPTHsoil} \qquad \text{Eq. 4.5b}$$

$$k\text{biodegradation} = \frac{ln2}{DT50} \qquad \text{Eq. 4.5c}$$

and k_{NER} is the removal rate by NER formation (see Chapter 3). Studies have unequivocally shown that for PFAS, as for PFOA and PFOS, a significant fraction of the total concentration of PFAS is to be considered as non-extractable residue irreversibly incorporated in the soil matrix and, hence, immobile.

F_{inf}	Fraction of rainwater that infiltrates into soil	0.25	
$RAIN_{rate}$	Rate of wet precipitation	1.92E-03	m/day
DT_{50}	half-life for biodegradation in bulk soil	36500	days
$K_{soil\text{-}water}$	Soil-water partitioning coefficient	Eq.4.6	m3/m3
$DEPTH_{soil}$	Mixing depth of soil	0.2	m

and

$$Ksoil\text{-}water = (Fair\text{-}soil \cdot Kair\text{-}water) + Fwater\text{-}soil + (Fsolid\text{-}soil \cdot \frac{KPsoil}{1000} \cdot RHOsolid) \quad \text{Eq. 4.6}$$

where

$F_{air\text{-}soil}$	Fraction air in fresh field soil	0.2	m^3/m^3
$F_{water\text{-}soil}$	Fraction water in fresh field soil	0.2	m^3/m^3
$F_{solid\text{-}soil}$	Fraction solid in fresh field soil	0.6	m^3/m^3
RHO_{solid}	Bulk density of soil solids	2500	kg/m^3
$K_{air\text{-}water}$	Partition coefficient air and water in soil	Eq. 4.7	m^3/m^3
Kp_{soil}	Partition coefficient solids and water in soil (v/w)	Eq. 4.8	L/kg

and

$$Kair - water = \frac{VP \cdot MOLW}{SOL \cdot R \cdot TEMP} \quad \text{Eq. 4.7}$$

and

$$Kp\ soil = Foc \cdot Koc \quad \text{Eq. 4.8.}$$

where (see Appendix A for data and discussion)

VP	Vapor pressure	0.01*	Pa
MOLW	Molar mass	Appendix A	g/mol
SOL	Water solubility	Appendix A	mg/L
TEMP	Temperature at air-water interface	285	K
R	Gas constant	8314	Pa m^3/mol/K
F_{oc}	Fraction of organic carbon in soil (dw)	0.02	kg/kg
K_{oc}	Organic carbon partition coefficient	Appendix A, Table 2.4	L/kg

* As a conservative approach, a low vapor pressure of 0.01 Pa for all PFAS is chosen as a worst-case consideration, which as a conservative approach basically neglect evaporation as a dissipation process (Appendix A).

From the above, many of the needed parameters can be found from default values in e.g. R.16, whereas DT_{50}, K_{NER} and $K_{soil\text{-}water}$ are substances dependent. Substance-dependent values can be found for the individual PFAS in Appendix A. A summary and discussion regarding adsorption, K_d and K_{oc} values can be found in Chapter 2.

4.5 PFAS partitioning between soil and pore water

When PFAS enters the soil via sludge, it will exchange between the various phases found in the soil matrix, i.e. adsorbed to the mineral or organic part of the soil, solved in the soil pore water and vaporised in the soil air.

The partitioning to air is - by using a default vapour pressure for all PFAS of 0.01 Pa – considered of limited importance in this study. This may be a conservative and overestimating approach with regard to leaching, as Schaefer et al. (2022) found that inclusion of air-water interfacial sorption resulted in a 58% reduction in the predicted PFOS pore water concentration. Only by including the air-water interfacial sorption, they found PFOS pore water concentrations that were identical (within the 95% confidence interval) to the measured PFOS pore water concentration in a lysimeter study. Brusseau and Guo (2022) also found that both measured and simulated data indicated an importance of air-water interfacial adsorption for the distribution of longer-chain PFAS within soil samples. The soil concentrations in both studies were, however, markedly higher when compared to typically Danish sludge amended soils, as these originated from an aqueous film forming foam (AFFF) contaminated area.

Based upon R.16 [Eq.16-55], the soil pore water concentration is calculated as:

$$Cpw = \frac{Csoil-ss\ x\ RHOsoil\ (dw)}{Ksoil-water\ x\ 1000} \qquad \text{Eq. 4.9}$$

where

$C_{soil-ss}$	Soil concentration when steady state concentration is reached after numerous sludge applications	Eq. 4.3	mg/kg
$RHO_{soil(dw)}$	Bulk density of dry soil	1700	kg/m^3
$K_{soil-water}$	Partition coefficient solids and water in soil (w/w)	Eq. 4.6	m^3/m^3
1000	Conversion factor		L/m^3

By rearranging Eq. 4.9, the soil concentration at steady state can be estimated as:

$$Csoil\text{-}ss = \frac{Cpw \cdot Ksoil-water \cdot 1000}{RHOsoil(dw)} \qquad \text{Eq. 4.10}$$

5. Exposure of soil ecosystems

The first and primary environmental entrance of substances found in sewage sludge is agricultural soils fertilized with this organic waste.

No national or EU derived environmental thresholds for soil ecosystems are available. National soil quality standards for $PFAS_4$ and $PFAS_{22}$ do exist (Text Box 1.1). However, these are established for contaminated sites and focus on protecting humans from direct and indirect exposure, primarily soil ingesting children. In other words, it has not being investigated to which extent such soil concentrations are protective to soil ecosystems.

In order to derive sewage sludge concentrations protecting the group of soil dwelling organisms, it has therefore been necessary to compile relevant data (See Appendix B) and derive a soil related environmental threshold concentration (ETC). Since it is not a core activity in this project, the ETC derivation can only be seen as a first screening of data, and the associated ETC is not to be used directly as a proxy for a formal EQS for soil.

5.1 Environmental Threshold Concentration for soil dwelling organisms (ETC_{soil})

As reviewed in Ankley et al. (2021), PFAS have been shown to affect the antioxidant defense systems of aquatic and terrestrial invertebrates and cause signs of oxidative stress. Sub-lethal effects, e.g. changes in lipid peroxidation (LPO), increase in reactive oxygen species (ROS), and changes in antioxidant enzyme activities and expression have been observed. Exposure to PFAS has also been associated with genotoxic effects, including DNA strand breaks and fragmentation, chromosomal breaks and apoptosis in several invertebrate species. Furthermore, behavioral abnormalities related to, for example, feeding and filtration rates, swimming, valve closure, burrowing and locomotor endpoints, such as number and direction of movements, have been observed in invertebrate species exposed to PFAS.

In contrast to the aquatic environment, no ecotoxicological based soil quality standards exist for PFAS in Denmark. Furthermore, although some countries may have soil quality standards for PFAS, these are typically, including the Danish soil quality standards, based upon protection of humans with soil ingesting children as the most sensitive exposure pathway. A safe concentration for soil dwelling organisms used in this report is therefore based on a non-comprehensive screening of relevant literature. A relative wide-ranging dataset can only be found for PFOS and PFOA. Appendix B contains a brief review of the available data. Relevant long-term exposure data has been identified for the three trophic levels: microorganisms, plants and soil invertebrates.

In summary, based upon the data presented in Appendix B, indicative ETC_{soil} of 16 µg/kg for PFOS and 2.0 µg/kg for PFOA are chosen as estimates of soil threshold concentrations.

5.2 Prediction of sludge threshold concentration

The ETC_{soil} presented in Section 5.1 is the long-term threshold for PFAS in soil. ETC_{soil} is therefore set at the level of the steady state soil concentration in the reverse calculations (Eq. 4.3). Based upon Eq.4.3 and a long-term target soil concentration corresponding to the ETC_{soil}, the threshold concentration in soil after a single sludge application ($C_{soil(0)}$) can be calculated as:

$$Csoil(0) = Csoil(ss)\ x\ (1 - Facc) \quad \text{Eq. 5.1}$$

where $C_{soil(ss)}$ equals the derived ETC_{soil} for PFOS and PFOA, respectively. The fraction accumulating in one year (F_{acc}) depends on the biodegradation and the leaching potential and can be calculated on the basis of Eq. 4.4. As limited information is available on biological uptake and bioavailability of non-extractable residues of PFAS in soil dwelling organisms, NER is as a conservative approach neglected in the assessment for soil dwelling species.

Knowing the threshold soil concentration after a single sludge application ($C_{soil(0)}$), the corresponding threshold concentrations in sludge (C_{sludge}) can be calculated as

$$Csludge = \frac{Csoil(0)\ x\ DEPTHsoil\ x\ RHOsoil(dw)}{APPLsludge} \quad \text{Eq. 5.2}$$

The input data, the transitional outcome and the resulting sludge concentration are presented in Table 5.1.

In conclusion, it has only been possible to establish interim environmental threshold concentrations for PFOA and PFAS due to the lack of ecotoxicological data for other PFAS. Based on these targets, it is estimated that a sludge concentrations below 134 µg PFOA/kg dw and 110 µg PFOS/kg dw will not lead to unacceptable effects on soil ecosystems.

TABLE 5.1. Input data, transitional calculation results and subsequent sludge concentration for PFOA and PFOS protecting soil dwelling organisms. See also Appendix A for details regarding chemical-physical parameters and Appendix B for derivation of ETCsoil. Note that the worst case solubility with regard to soil accumulation is chosen (see Appendix A). Default values according to REACH R.16 are marked by an asterisk (*).

	PFOA	PFOS
ETC_{soil} [µg/kg]	2.0	16.0
Log K_{oc} [Table 2.4]	2.3	3.6
MOLW [g/mol]	414.1	500.1
SOL [mg/L]	64	7.7
TEMP [K]*	285	285
R [Pa m^3/mol/K]*	8314	8314
$K_{air\text{-}water}$ [d^{-1}] (Eq. 4.7)	2.7E-08	2.7E-07
$F_{air\text{-}soil}$ [m^3/m^3]*	0.2	0.2
$F_{water\text{-}soil}$ [m^3/m^3]*	0.2	0.2
$F_{solid\text{-}soil}$ [m^3/m^3]*	0.6	0.6
RHO_{solid} [kg/m^3]*	2500	2500
Kp_{soil} (Eq. 4.8)	4.0	79.6
$RAIN_{rate}$ [m/d]*	1.92E-03	1.92E-03
$K_{soil\text{-}water}$ [m^3/m^3] (Eq. 4.6)	6.19	119.6
DT_{50} [days]	36500	36500
RHO_{soil} [kg/m^3]*	1700	1700
$DEPTH_{soil}$ [m]*	0.2	0.2
$K_{leaching}$ [d^{-1}]	3.88E-04	2.0E-05
$K_{biodegradation}$ [d^{-1}]	1.90E-05	1.90E-05
K_{NER} [d^{-1}]	0	0
$k_{removal}$ [d^{-1}] (Eq.4.5)	4.07E-04	3.9E-05
F_{acc} [Eq.4.4]	0.86	0.99
$C_{soil\text{-}ss}$ = ETC_{soil} [mg/kg] (Eq. 4.3)	2.0E-03	1.60E-02
$_{Csoil(0)}$ [mg/kg] (Eq. 5.1)	2.76E-04	2.26E-04
$APPL_{sludge}$ [$kg/m^2/y$]	0.7	0.7
C_{sludge} [mg/kg] (Eq. 5.2)	1.34E-01	1.10E-01
C_{sludge} [µg/kg] (Eq. 5.2)	**134**	**110**

6. Exposure of groundwater

PFAS entering agricultural soils have the potential to leach to the groundwater with simple matrix water flow. It is, however, well established that transport of water and solutes via macropore-dominated pathways of soils, typically called preferential flow, may also occur in soils. Preferential flow is defined as water and its constituents moving by preferred pathways through a porous medium. Such preferential water flow is typically some orders of magnitude faster than flow through the remainder of the porous medium. Preferential flow can, thus, result in water and matter fluxes bypassing large parts of the vadose zone. Consequently, it influences the water cycle and can impact the quantity and quality of water leaving the vadose zone. In this report, it has not been possible to include preferential flow in the calculations.

The task of identifying threshold concentrations in sludge has been constructed in two steps, i.e. first an initial screening using simple REACH related equations and assumptions and secondly a more advanced modelling predicting leaching of PFAS from soil to groundwater used by e.g. EFSA for their risk assessment of plant protection products.

6.1 Environmental Threshold Concentration for groundwater (ETC_{gw})

In Denmark, almost all drinking water originates from groundwater. The Danish authorities have from 2022 introduced two new sets of threshold concentrations in drinking water and groundwater (TC_{gw}), i.e. 0.002 µg/L of the four PFAS: PFOA, PFOS, PFNA and PFHxS, and 0.1 µg/L as sum of PFBS, PFPeS, PFHxS, PFHpS, PFOS, PFNS, PFDS, PFUnS, PFDoS, PFTrS, PFOSA, 6:2 FTS, PFBA, PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnDA, PFDoDA and PFTrDA.

It is anticipated that groundwater must be of a quality where it can be used directly as drinking water without any further dilution or cleaning. There is no indication in the TC_{gw} with regard to the differences in toxicity or hazard of the four PFAS, e.g. toxicity equivalents, which is why they are considered equally important. In the initial screening, simple toxicity additivity (Cedergreen et al. 2014) is assumed, i.e. either 1/4 or 1/22 of the respective EQS are allocated to each of the PFAS.

6.2 Screening assessment for threshold concentration in sludge protecting groundwater

The exposure pathway for drinking water and groundwater presented by ECHA in R.16 follows an approach of setting the concentration in groundwater (C_{gw}) directly at the predicted concentration in pore water (C_{pw}) of agricultural soils, i.e. $C_{gw} = C_{pw}$. This is a very conservative approach based upon considerations that some countries have shallow groundwater reservoirs. In Denmark, large parts of the drinking water originate from deeper groundwater reservoirs.

Based upon an identified threshold concentration in pore water (C_{pw}) that correspond to the TC_{gw}/QS_{gw}, a corresponding threshold concentration in soil resulting in C_{pw} after long-term accumulation can be estimated for the steqady state situation ($C_{soil\text{-}ss}$) from Eq. 4.10. Knowing the $C_{soil\text{-}ss}$, the threshold concentration in soil after a single sludge application the first year ($C_{soil(0)}$) can be calculated from equation 5.1 using the first order removal rate (Eq.4.5-4.8) and the fraction accumulating each year (F_{acc}), Eq. 4.4. Knowing the threshold concentration in soil after a single sludge application ($C_{soil(0)}$), the corresponding threshold concentrations in sludge (C_{sludge}) can be calculated from equation 5.2.

The calculations presented above are summarized in Table 6.1a for $PFAS_4$ making up the sum-criteria of 2 ng/L. The results for the $PFAS_{22}$ are not shown, as these lead to significantly higher limits in sludge.

TABLE 6.1a. Screening results for $PFAS_4$ in the sludge-soil-groundwater-drinking water system. The chemical-physical data can be found in Appendix A. Note that the worst-case solubility with regard to leaching is chosen for PFOA and PFOS (see Appendix A for discussion). For the four individual ETC_{gw}, 0.25 x QS_{gw} is used, i.e. 0.25 x 0.002 µg/L = 5.0E-04 µg/L. The first order rate constant for NER formation in soil (k_{NER}) has only been identified for PFOS and PFOA (Chapter 3). For PFNA and PFHxS, similar k_{NER} has been used as for PFOS and PFOA, respectively. Sludge application rate is 0.7 kg/m^2/y (7 t/ha/y).

	PFOA	**PFOS**	**PFNA**	**PFHxS**
ETC_{gw} [µg/L]	5.0E-04	5.0E-04	5.0E-04	5.0E-04
Log K_{oc} (Table 2.4)	2.3	3.6	2.9	2.31
MOLW [g/mol]	414.1	500.1	464,1	400.1
SOL [mg/L]	9500	370	0.0625	2.3
TEMP [K]*	285	285	285	285
R [Pa m^3/mol/K]*	8314	8314	8314	8314
$K_{air\text{-}water}$ [d^{-1}] (Eq. 4.7)	1.84E-10	5.7E-09	3.13E-05	7.34E-07
$F_{air\text{-}soil}$ [m^3/m^3]*	0.2	0.2	0.2	0.2
$F_{air\text{-}water}$ [m^3/m^3]*	0.2	0.2	0.2	0.2
$F_{solid\text{-}soil}$ [m^3/m^3]*	0.6	0.6	0.6	0.6
RHO_{solid} [kg/m^3]*	2500	2500	2500	2500
Kp_{soil} (Eq. 4.8)	3.99	79.62	15.89	4.08
$RAIN_{rate}$ [m/d]*	1.92E-03	1.92E-03	1.92E-03	1.92E-03
$K_{soil\text{-}water}$ [m^3/m^3] (Eq. 4.6)	6.19	119.6	24.03	6.33
DT_{50} [days]	36500	36500	36500	36500
RHO_{soil} [kg/m^3]*	1700	1700	1700	1700
$DEPTH_{soil}$ [m]*	0.2	0.2	0.2	0.2
$k_{leaching}$ [d^{-1}]	3.88E-04	2.01E-05	9.99E-05	3.79E-04
$k_{biodegradation}$ [d^{-1}]	1.90E-05	1.90E-05	1.90E-05	1.90E-05
k_{NER} [d^{-1}]	4.7E-03	1.3E-03	1.3E-03	4.7E-03
$k_{removal}$ [d^{-1}] (Eq.4.5)	5.10E-03	1.34E-03	1.42E-03	5.10E-03
F_{acc}	0.16	0.61	0.60	0.16
$C_{soil\text{-}ss}$ [mg/kg] (Eq. 4.10)	1.82E-06	3.52E-01	7.07E-06	1.86E-06
$C_{soil(0)}$ [mg/kg] (Eq. 5.1)	1.54E-06	1.36E-02	2.86E-06	1.57E-06
$APPL_{sludge}$ [kg/m^2/y]	0.7	0.7	0.7	0.7
C_{sludge} [mg/kg] (Eq. 5.2)	7.47E-04	6.61E-03	1.39E-03	7.63E-04
C_{sludge} [µg/kg] (Eq. 5.2)	**0.75**	**6.61**	**1.39**	**0.76**

The calculated threshold concentrations of PFAS presented in Table 6.1 must be considered as individual threshold concentrations and cannot be summed, since their individual fate properties differ. In other words, less of some PFAS may reach groundwater compared to other PFAS, if found in the same sludge concentrations, due to their higher affinity to organic carbon and/or NER formation rates in general.

The estimated threshold concentrations found in Table 6.1 are lower than the concentrations typically found in Danish sludge. However, the assessment assumes a very worst case scenario with regard to sludge application rate, i.e. 7 t dw/ha/y. Such an application rate is in reality never occurring when considering sewage sludge from municipal waste water treatment plants, due to the relative high level of phosphor found in these biosolids. A more realistic sludge application rate can be found by taking into consideration the average annual national application ceiling of 30 kg P/ha (See Section 4.4) and a median P content of 29 kg/t in Danish sludge. This results in a median sludge application rate of 1.03 t/ha/y, in which case the threshold concentration in sludge can be similarly higher when keeping the overall PFAS load per ha the same (Table 6.1.b).

TABLE 6.1b. As for Table 6.1a, but with a sludge load (APPLsludge) of 0.103 kg/m^2/y (1.03 t/ha/y).

k_{NER} = Median	PFOA	PFOS	PFNA	PFHxS
C_{sludge} [µg/kg]	**5.07**	**44.9**	**9.43**	**5.19**

The k_{NER} has a significant impact on the calculated cut-off value of sludge, as it is decisive for the accumulation and leaching rate of PFAS in soils, the calculation presented above is repeated using k_{NER} the minimum values reported in Gassmann et al. (2021) of 0.0011 d^{-1} , and rates 25 and 50% lower than the minimum range. For PFNA and PFHxS, no NER was reported, for which reason these have been duplicated from information from PFOS and PFOA. For comparison, the calculated cut-off values are aligned together with the reported 90th percentile in Danish sludge (Appendix C). Based on this, it is concluded that even when assuming a 50% lower removal rate to NER than the lowest reported rate from a long-term semi-field study, the cut-off values for $PFAS_4$ are higher than the 90th percentile of PFAS concentration found in Danish sludge (Table 6.1.c).

TABLE 6.1c. As for Table 6.1a and 6.1b, i.e. $APPL_{sludge}$ = 0.103 kg/m^2/y (1.03 t/ha/y), but with different input of k_{NER}.

Steady state situation	PFOA	PFOS	PFNA	PFHxS
k_{NER} = minimum	0.0030	0.0011	0.0011	0.0030
C_{sludge} [µg/kg]	**4.40**	**39.5**	**8.38**	**4.36**
k_{NER} = 75% of Min.	0.00225	0.000825	0.000825	0.00225
C_{sludge} [µg/kg]	**3.84**	**31.5**	**6.80**	**3.81**
k_{NER} = 50% of Min.	0.0015	0.00055	0.00055	0.0015
C_{sludge} [µg/kg]	**3.10**	**22.5**	**5.05**	**3.07**
Measured C_{sludge} [µg/kg] (90th Percentile)	2.5	15	2.5	2.5
Max. C_{sludge} if $PFAS_4$<15 µg/kg	3.4	13.0	7.3	2.5

Even when reducing the k_{NER} to half of the lowest reported NER removal rate, predicted individual threshold concentrations in sludge become higher than the reported 90th percentile of PFAS concentrations in Danish sludge. For k_{NER} reduced by 50%, predicted individual thresholds of PFOA and PFNA in sludge are lower than the maximum concentrations measured in the fraction of Danish sludge having a summed $PFAS_4$ concentration lower than 15 µg/kg.

The calculations presented above are based on an assumption of NER formation as reported in Gassmann et al. (2021). If neglecting NER as a removal process, the sludge concentrations would have to be adjusted accordingly, as shown in Table 6.1.d.

TABLE 6.1d. As for Table 6.1a and 6.1b, but with k_{NER} = 0.

Steady state situation	PFOA	PFOS	PFNA	PFHxS
		Sludge load: 7 t/ha/y		
C_{sludge} [µg/kg]	0.12	0.24	0.15	0.12
		Sludge load 1.03 t/ha/y		
C_{sludge} [µg/kg]	0.83	1.64	0.99	0.83

A refinement of the groundwater scenario is presented in Section 6.3 and onwards.

6.3 Elaborated assessment of threshold concentrations in sludge protecting groundwater

So called higher tier exposure models for groundwater are available and used in the risk assessment frameworks of for example plant production products in EFSA and veterinary medicinal products in EMA. These have in common that they calculate exposure concentrations in the recipients after a specification of the area-based load of pesticides or medicines. In contrast to the compartment transfer functions and equations found in REACH, the models cannot be reversed. The chosen groundwater exposure models used in this project, PELMO and MACRO, are both used with FOCUS[8] scenarios and both recognized and approved fate models used by European Agencies like EFSA and EMA for predicting groundwater exposure resulting from pesticide use and leaching of feed additives and veterinary medicines in manure. The main difference is that MACRO account for leaching through macro pores, which is relevant for some soil types, e.g. clay soils, but not other, e.g. sandy soils.

6.4 Groundwater model descriptions

PELMO is a one-dimensional simulation model simulating the vertical movement of pesticides in soil by chromatographic leaching. The MACRO model calculates coupled unsaturated-saturated water flow in cropped soil, including the location and extent of perched water tables, and can also deal with saturated flow to field drainage systems. The MACRO model accounts for macro-pore flow, with the soil porosity divided into two flow systems or domains (macro-pores and micro-pores), each characterized by a flow rate and solute concentration. Both models were originally developed with the aim of assessing leaching of pesticides after agricultural use. They therefore have some boundaries, which limit their use for assessing leaching of PFAS. Pesticides are generally not granted for market authorization in Europe if they are considered very persistent with very long DT_{50}. The models therefore typically produce output covering a maximum of a 20-year period. Furthermore, the MACRO model can only use DT_{50} values less than one year, which is very unrealistic for PFAS. In this context, it has been decided to run the PELMO model for a worst-case scenario in Denmark for the longest possible period, i.e. 20 years. A sandy soil in Karup has been chosen as representative for a maximum leaching profile for PFAS, since PFAS mobility in clay soil, despite the potential of macro-pore flow, is considered to be lower than in sandy soils.

6.5 Model outputs

There is a strict linear relation between input and output of the PELMO model. This enables interpolation and prediction based upon a few model runs for each PFAS. Arbitrary input of PFAS in the higher end of what is expected in Danish sludge amended soils has therefore been used. The models have not been used for $PFAS_{22}$ due to e.g. lack of suitable K_{oc} values for some PFAS and since focus has been on $PFAS_4$ summing up the groundwater criteria of 2 ng/L, i.e. PFOS, PFOA, PFNA and PFHxS, as this by all means will lead to the lowest calculated threshold concentration in sludge.

[8] FOrum for Co-ordination of pesticide fate models and their USe

A crude sensitivity evaluation of the model output to K_{oc} and DT_{50} values has been performed for PFOS as a model substance.

As input data for the models are K_d or K_{oc} values, DT_{50} values and area-based loading (kg/ha). The log K_{oc} values used are, unless otherwise noted, the median values as shown in Table 2.4. DT_{50} values of 100 years are used in the simulations, as PFAS are considered to be very persistent and no solid data for DT_{50} values can be found. The annual input of PFAS to agricultural soils is calculated as:

$$APPL_{PFAS} = C_{sludge} \times APPL_{sludge} \qquad \text{Eq. 6.1}$$

where

$APPL_{PFAS}$	Annual application (load) of PFAS to arable land	kg/ha/y
C_{sludge}	Concentration of PFAS in sludge	kg/t
$APPL_{sludge}$	Annual (worst case) application rate of sludge to arable land	t/ha/y

The units for the application rate of PFAS is kg/ha/y, as the models are developed for pesticides and the usual application rates of these are kg active ingredient (a.i.) per ha. A calculated example of the PFOS load is presented below.

C_{sludge}	C_{sludge}	C_{sludge}	$APPL_{sludge}$	$APPL_{PFAS}$
µg PFOS/kg dw	µg PFOS/t dw	kg PFOS/t dw	t/ha/y	kg PFOS/ha/y
16.0	16.0E+03	1.60E-05	7.0	1.12E-04

Based on data covering the annual area-based input, the degradation rate (DT_{50}) and adsorption properties (log K_{oc}), the PELMO calculate the predicted groundwater concentration (C_{gw}) in the following 20 years. The maximum concentrations in this period are presented in Table 6.2.

TABLE 6.2. Input parameters and maximum output results from the PELMO model. The input concentrations are compared to the median of PFAS in Danish sludge (Appendix C). Due to model restrictions, the predicted groundwater concentrations are modelled after 20 years of sludge application, which is very far from the time needed to reach steady state.

PFAS	DT_{50}	Log K_{oc}	C_{PFAS} Median*	C_{PFAS} Input PELMO	PFAS Load**	C_{gw}	C_{gw}
	Years	kg/L	µg/kg dw	µg/kg dw	kg/ha	µg/L	ng/L
				$PFAS_4$			
PFOS	100	3.6	4,5	16	1.12E-04	1.58E-18	1.58E-15
PFOA	100	2.3	0.85	1.8	1.26E-05	1.04E-06	1.04E-03
PFNA	100	2.9	0.6	0.894	6.26E-06	1.03E-11	1.03E-08
PFHxS	100	2.31	0.19	3.91	2.74E-05	2.13E-06	2.13E-03
				Selected PFAS among the remaining $PFAS_{22}$			
(P)FOSA	100	4.36	0.85	1.73	1.21E-05	<1E-24	<1E-21
6.2 FTS	100	2.28	0.24	3.08	2.16E-05	2.55E-06	2.55E-03
PFBA	100	1.9	0.19	4.65	3.26E-05	1.87E-04	1.87E-01
PFP(e)A	100	1.38	0.24	1.7	1.19E-05	9.30E-04	9.30E-01
PFBS	100	1.8	0.19	3.9	2.73E-05	3.58E-04	3.58E-01
PFDA	100	4	2.4	4.3	3.01E-05	1.25E-24	1.25E-21
PFDoDA	100	4.77	0.85	1.6	1.12E-05	<1E-24	<1E-21

* The median of PFAS concentrations found in 215 Danish sludge samples (Appendix C). ** Based on a sludge application rate of 7.0 t dw/ha/y, which is markedly higher than the average sludge application rate used in Denmark of approximately 1.03 t/ha/y (see Section 4.3).

The sensitivity of the PELMO model calculations to variation in log K_{oc} are presented for PFOS in Table 6.3. Here, it is seen that the outputs are relatively sensitive to the value of the log K_{oc}.

TABLE 6.3. Impact of K_{oc} on the output of PELMO for PFOS after 20 years of simulations. The chosen log K_{oc} represents the 10th and the median of log K^{oc} values presented in Appendix A and Table 2.4.

C_{sludge}	DT_{50}	Log K_{oc}	C_{gw}
µg/kg dw	years	L/kg	ng/L
16	100	3.6	1.58E-15
16	100	2.84	7.00E-07

Table 6.4 shows the PELMO model sensitivity to DT_{50} for selected PFAS. Here, it is seen that only limited difference (<5%) in output, i.e. groundwater concentration, is observed between chosen half-lives of 10 and 100 years, respectively. The main reason for the limited difference between DT_{50} of 10 and 100 years is the relatively short simulation period of 20 years. If the PELMO model could simulate until steady state, the results for the two DT_{50} values would be markedly apart.

TABLE 6.4. Impact of DT_{50} on the output of PELMO for PFAS after 20 years of simulations (maximum simulation period).

PFAS	log K_{oc}	Sludge Conc.	PFAS load	C_{gw}	
				DT_{50}=100 y	DT_{50}=10 y
	L/kg	µg/kg dw	kg/ha/y	ng/L	ng/L
			$PFAS_4$		
PFOS	3,6	16	1,12E-04	1,58E-15	1,51E-15
PFOS	3,6	5,48	3,84E-05	5,41E-16	5,17E-16
PFOA	2,3	1,8	1,26E-05	1,04E-03	1,02E-03
PFNA	2,9	0,894	6,26E-06	1,03E-08	1,00E-08
PFHxS	2,31	3,91	2,74E-05	2,13E-03	2,09E-03
			Selected PFAS among the remaining $PFAS_{22}$		
(P)FOSA	4,36	1,73	1,21E-05	<1E-21	<1E-21
6.2 FTS	2,28	3,08	2,16E-05	2,55E-03	2,50E-03
PFBA	1,9	4,65	3,26E-05	1,87E-01	1,86E-01
PFP(e)A	1,38	1,7	1,19E-05	9,30E-01	9,26E-01
PFBS	1,8	3,9	2,73E-05	3,58E-01	3,55E-01
PFDA	4	4,3	3,01E-05	1,25E-21	1,19E-21
PFDoDA	4,77	1,6	1,12E-05	<1E-21	<1E-21

In summary, it can be concluded that an internationally accepted model used by Competent Authorities for regulatory purposes of pesticides predicts groundwater concentrations orders of magnitude below the threshold concentrations after twenty years of application with sludge applications having PFAS concentrations similar to at least the upper quartiles in Danish sludge. However, as the PELMO model only simulates for 20 years, and as the steady state situation

for many PFAS may be significantly further out in the future, alternative modelling has been proposed and presented in Section 6.6 and onwards.

6.6 Alternative modelling of leaching

Due to the restrictions in the FOCUS models presented above, e.g. limited years of simulation and maximum DT_{50} value of one year (MACRO), a simple alternative Box Model has been applied in order to further elucidate the leaching potential of PFAS in sludge amended soils.

6.6.1 Box Model description

The soil column was divided into five boxes with the below characteristics. The characteristics are derived from Barlebo et al. (2007) and are presented in Table 6.5.

TABLE 6.5. Characteristics for the Box Model.

Soil layer	Karup	Langvad
A (0-20)	Height: 20 cm OC: 2.2% Θ_{water}: 0.34 Θ_{air}: 0.08 Θ_{soil}: 0.58	Height: 20 cm OC: 2.1% Θ_{water}: 0.43 Θ_{air}: 0.02 Θ_{soil}: 0.55
B (20-40)	Height: 20 cm OC: 1.7% Θ_{water}: 0.32 Θ_{air}: 0.08 Θ_{soil}: 0.58	Height: 20 cm OC: 1.4% Θ_{water}: 0.34 Θ_{air}: 0.02 Θ_{soil}: 0.64
B (40-70)	Height: 30 cm OC: 0.3% Θ_{water}: 0.34 Θ_{air}: 0.1 Θ_{soil}: 0.58	Height: 30 cm OC: 0.5% Θ_{water}: 0.34 Θ_{air}: 0.02 Θ_{soil}: 0.66

Where:

OC:	Content of organic carbon
Θ_{water}:	Volume fraction water in soil
Θ_{air}:	Volume fraction air in soil
Θ_{soil}:	Solids fraction in soil

A constant net-precipitation of N_{net} 325 mm/year (~0.00089 $m^3/m^2/d$) was assumed.

Sludge was assumed to be applied once a year. The calculations were carried out for a substance application of 1 kg/ha/year and then scaled to the actual substance application rate (PFAS load) (Table 6.2). This is durable, as the equations are linear with respect to application rate.

A constant total 1st order biodegradation rate corresponding to a high half-life (DT_{50}) of 100 years was assumed, i.e. there was no adaption to soil depth nor to actual temperature.
As discussed, it is assessed reasonable to include a 1st order expression for the formation of NER in the model. Gassmann al. (2021) estimated 1st order rate constants, k_{NER}, for the NER information based on data from an outdoor lysimeter study with spiked PFOS and PFOA to:

PFOA: range 0.0030-0.0066 d^{-1}; median of 0.0047 d^{-1}

PFOS: range 0.0011-0.0016 d^{-1}; median 0.0013 d^{-1}

A mass balance was formulated for each box:

$$\Delta m_i = \Delta m_{leached,i-1} - \Delta m_{leached,i} - m_i \cdot k_{deg} \cdot \Delta t - m_i \cdot k_{NER} \cdot \Delta t \quad \text{Eq. 6.2}$$

For box 1 (the upper layer) a dosage of 1 kg/ha was added to the box once a year.

where:

m_i is the mass of the substance in box I (kg)

k_{deg} is the first order biodegradation rate constant (d^{-1})

k_{NER} is the first order rate constant for the formation of NER (d^{-1})

$\Delta m_{leached,i}$ is the amount of substance leached from box I in the time step Δt (d) (kg)

$$\Delta m_{leached,i} = N_{net} \cdot C_{porewater,i} \cdot \Delta t \quad \text{Eq.6.3}$$

Within each box, the pore water concentration was calculated from:

$$C_{porewater,i}\left(\frac{kg}{m^3}\right) = \frac{m_i}{V_i \cdot (\theta_{water,i} + \theta_{soil,i} \cdot \rho_{soil,matrix} \cdot K_{d,i})} \quad \text{Eq.6.4}$$

where

V_i is the volume of the box i (m^3/m^2)

K_{di} is the soil water partition coefficient in box i calculated from the substance K_{oc} and the content of organic carbon in the soil (OC_i) ($K_{di}=K_{oc}/1000 \cdot OC_i$) ($m^3/kg$)

6.6.2 Results from Box Model

Calculations with the Box Model were performed for a predefined time period (up to >1000 years) until a steady-state concentration was derived. The time step, Δt, was set to 10 days. A check of sensitivity of the time step was investigated by calculation with a time step of 5 days. This gave only very minor differences in the calculation results.The concentration in groundwater was set equal to the percolate water concentration in box 4 at steady-state.

The results at steady state are presented in Table 6.6. Here, it can be seen that the modelled maximum concentrations are predicted to occur in the very far future, i.e. often > 1000 years from now. Therefore, the predicted groundwater concentrations are also modelled after 10, 50 and 100 years of sludge application. These results are presented for PFOS, PFHxS, PFOA and PFNA in Table 6.6. In contrast to the output from the PELMO model (Table 6.4), it can be seen that DT_{50} in the simplified Box Model has a marked influence on the groundwater concentration of PFOS due to the long simulation period.

TABLE 6.6. Calculated groundwater concentrations (ng/L) at steady state (SS) using a simplified Box Model for two Danish soils, i.e. Karup, a sandy soil, and Langvad, a clay soil. The results are presented for sludge scenarios representing realistic worst-case situations, i.e. approximately the 90th percentile sludge concentration in Denmark (Appendix C). The period until

95% of steady state ranges from approximately 200 to more than 1000 years if using a DT_{50} of 100 years. Formation of NER is not included in the calculations.

PFAS	PFAS load	$logK_{oc}$	DT_{50}	$K_{removal}$	C_{gw} (Karup)	C_{gw} (Langvad)	Time to 95% of SS
	kg/ha/y	L/kg	Years	d^{-1}	ng/L	ng/L	Years
PFOS	1.12E-04	3.6	100	1.90E-05	14,7	13,2	200-500
PFOS	1.12E-04	3.6	10	1.90E-04	0,27	0,17	70-80
PFOS	1.12E-04	2.84	100	1.90E-05	61	49,8	200-500
PFOS	3.84E-05	3.6	100	1.90E-05	4,94	4,45	200-500
PFBS	2.73E-05	1.8	100	1.90E-05	66,8	55,4	200-500
PFHxS	2.74E-05	2.31	100	1.90E-05	35,6	28,0	200-500
(P)FOSA	1.21E-05	4.36	100	1.90E-05	0,099	0,067	500-1000
6.2 FTS	2.16E-05	2.28	100	1.90E-05	29,3	23,1	200-500
PFBA	3.26E-05	1.9	100	1.90E-05	72	58,9	200-500
PFP(e)A	1.19E-05	1.38	100	1.90E-05	39,3	34,8	200-500
PFOA	1.26E-05	2.3	100	1.90E-05	16,7	13,1	200-500
PFNA	6.26E-06	2.9	100	1.90E-05	3,07	2,53	200-500
PFDA	3.01E-05	4	100	1.90E-05	1,23	1,03	200-500
PFDoDA	1.12E-05	4.77	100	1.90E-05	0,007	0,004	500-1000

Since the formation of non-extractable residues has been shown to have significant impact on the leaching potential of PFAS from soils (See Chapter 3), this has been incorporated in the calculations presented in Section 6.6.5.

6.6.3 PFAS composition in sludge and leaching potential

The calculations and extrapolations made in this report must represent as many scenarios for sludge application in Denmark as possible and not only worst-case situations like the one presented in Table 6.6. Large variation in PFAS composition exists between different WWTP and between each batch produced within a WWTP across the year. Especially for a group of substances like PFAS, where precursors may be an important parameter. Since each PFAS behaves differently after reaching the soil environment, some pragmatic approaches must be made, since the groundwater criteria is a sum of 4 and 22 PFAS, respectively.

Based on an internal database for PFAS levels in Danish sludge (see Appendix C), the concentrations can be summarized as listed in Table 6.7. Main focus in this report is on $PFAS_4$ forming the groundwater criteria of 2 ng/L, as the $PFAS_4$ concentrations in average (median) make up more than 30% of the $PFAS_{22}$ concentrations, whereas the groundwater criteria for $PFAS_4$ is 50 times lower than the criteria for $PFAS_{22}$, i.e. 2 vs 100 ng/L. Many of $PFAS_{22}$ are only found above analytical quantification limits in relatively few cases. In the 215 sludge samples available, only PFOSA, PFDA, PFUnDS and PFDoDA were, besides the $PFAS_4$, quantified in more than 50 samples. All other PFAS was quantified in less than 15% of the 215 samples (see Appendix C).

TABLE 6.7. The summarized concentration of $PFAS_4$ and $PFAS_{22}$, respectively, and the percentage of $PFAS_4$ compared to $PFAS_{22}$. There are 215 samples (See Appendix C for details). Furthermore, the percentage of each of the four PFAS are compared to the sum of 4 and 22

PFAS, respectively. Both median and the 10th and 90th percentiles are shown. The median (50th percentile) ratios (in bold) are used in Table 6.8.

	$PFAS_4$	$PFAS_{22}$	$PFAS_4$:$PFAS_{22}$	PFOS:$PFAS_4$ PFOS:$PFAS_{22}$	PFOA:$PFAS_4$ PFOA:$PFAS_{22}$	PFNA:$PFAS_4$ PFNA:$PFAS_{22}$	PFHxS:$PFAS_4$ PFHxS:$PFAS_{22}$
	µg/kg	µg/kg	%	%	%	%	%
50P	7.49	22.94	31.60	**73.53** 22.89	**12.14** 3.63	**8.42** 2.64	**3.81** 1.25
10-90P	3.40-17.83	12.48-56.35	16.53-56.63	25.00-87.63 4.55-47.47	5.02-25.00 1.47-6.08	3.37-25.00 1.18-4.55	1.11-25.00 0.61-4.15

The comparison of the leaching potential of the various PFAS is a combination of the sludge concentrations and the chemical-physical properties (log K_{oc}) of the substance. PFOS are by far found in the highest concentrations, whereas PFOA, PFHxS and PFNA each typically (>90% of samples) compose less than a quarter of $PFAS_4$ (Table 6.7). However, PFOS are also significantly less mobile than e.g. PFOA and PFHxS. As a precautionary approach, the groundwater criteria of 2ng $PFAS_4$/L can therefore be split evenly between the four PFAS, i.e. 0.5 ng/L (Scenario A, Table 6.8). If instead of an even distribution of the groundwater criteria, the criteria are distributed unevenly according to the median individual PFAS concentration in sludge, the individual threshold will differ accordingly (Scenario B, Table 6.8). These median ratios are summarized numbers from 215 sludge samples and, hence, do not sum up to 1.0. In the individual sludge samples, the sum of the four ratios will always sum up to 1. Based on these results and this approach, the individual groundwater thresholds, i.e. the allocated ratio of the groundwater criteria of 2 ng/L, can be used in the calculation of threshold concentrations in sludge presented below.

TABLE 6.8. Suggestion to threshold concentration for groundwater for the four individual PFAS making up the sum criteria for $PFAS_4$ of 2 ng/L. Two different approaches or scenarios have been shown. See text for discussion.

PFAS	Even ratio of PFAS:$PFAS_4$	Uneven ratio of PFAS:$PFAS_4$ (Table 6.7)	Scenario A: Even distribution of the groundwater criteria of 2 ng/L	Scenario B*: Uneven distribution of the groundwater criteria of 2 ng/L
PFOS	0.25	0.74	0.5	1.48
PFOA	0.25	0.12	0.5	0.24
PFNA	0.25	0.08	0.5	0.16
PFHxS	0.25	0.04	0.5	0.08

*Calculated as: PFAS:$PFAS_4$ ratio x 2 ng/L, e.g. 0.74 x 2 ng/L = 1.48 ng/L for PFOS

6.6.4 Modelled groundwater concentrations

The PFAS concentration in groundwater calculated by the simplified Box Model is shown in Table 6.9.

The predicted PFAS groundwater concentrations shown in Table 6.9 from the Box Model are multiple orders of magnitude, i.e. approx.10E+13, higher after 10 years of simulation than the output from PELMO after 20 years of simulation (Table 6.2). This demonstrates that the simplified Box Model within comparable time frames (simulation periods) is a far more conservative and overestimating tool than more advanced FOCUS models, such as PELMO used by European competent authorities like EFSA and EMA in their chemical regulation. The use of the Box Model will therefore introduce a high surplus of precautionary aspects to the predicted threshold of PFAS in sewage sludge.

6.6.5 Incorporation of NER in the Box Model

The calculations presented in Table 6.9 do not incorporate reduced leachability and mobility of the non-extractable residues (NER), as discussed in Chapter 3. The same is true for other leaching models, e.g. MACRO and PELMO. As concluded in Chapter 3, data indicates that over a ten year period a significant fraction, i.e. >90%, of PFAS such as PFOS and PFOA, are likely to be bound to the soil matrix as NER. This is also supported by relevant field studies monitoring leaching of PFAS in Denmark and other countries, as shown in Chapter 3.

Gassmann et al. (2021) compared the measured leaching of spiked PFOS and PFOA from a long time running outdoor lysimeter study with the outcome of the focus model MACRO and concluded that the observed leaching was significantly lower than the model predictions. Only by incorporating the formation of NER in the MACRO model could they obtain alignment between model results and observed measured leaching. The kinetic rate of NER formation could not be taken from the literature, but was initially estimated between 0.001 and 0.014 1/d. After calibration with lysimeter data, posterior parameter statistics showed that the kinetic rate of NER formation was higher for PFOA (range 0.0030-0.0066; median of 0.0047 d^{-1}) than for PFOS (range 0.0011-00.0016; median 0.0013 d^{-1}). These median rates for NER formation of 0.0047 d^{-1} and 0.0013 d^{-1} are used in the Box Model. As no data could be found with regard to the NER formation rate for PFNA and PFHxS, the NER formation rate published by Gassmann et al. (2021) for PFOA and PFOS are adopted to include the two other PFAS substances of the $PFAS_4$ according to their similarity in log K_{oc} (Table 2.4), i.e. median NER for PFOS=PFNA=0.0013 and PFOA=PFHxS=0.0047.

The following observations and conclusions can be made from the data in Table 6.9 and 6.10, i.e. with or without the formation of NER.

- The inclusion of NER has a large effect on the predicted C_{gw}, with C_{gw} of PFOS being one order magnitude lower after 10 years of simulation and more than four orders of magnitude lower at steady state.
- If including NER, steady state is predicted to occur after maximum 20 years as compared to more than 500 years without the incorporation of NER.
- The reported variation in k_{NER} has an influence of the C_{gw} of up to an order of magnitude between the lowest and the highest estimate of k_{NER}.

The individual PFAS concentrations used to calculate predictions of groundwater concentrations for $PFAS_4$ shown above do not enable a prediction for the sum of all four, as each sludge sample is unique in its relative distribution between the four PFAS (See Appendix C). The comparison with arbitrary individual threshold (Table 6.8) shows that, if omitting NER in the calculations, the predicted groundwater concentrations may be one order of magnitude (Table 6.11) above the individual thresholds. If including NER in the calculations, the predicted C_{gw} are between one and three orders of magnitude below the individual thresholds (Table 6.11). In the calculations presented in Table 6.9-6.11, a sludge application of 7 t/ha/y is used. In practice, this will normally be significantly lower, i.e. an average 1.03 t/ha/y (Section 4.3), for which reason the predicted groundwater concentrations will be similarly reduced in Table 6.9, 6.10 and 6.11.

TABLE 6.9. The calculated groundwater concentrations (ng/L) of selected PFAS using a simplified Box Model, a DT_{50} of 100 years and worst case individual PFAS loads (approximating the 90th percentile of PFAS in Danish sludge and an annual worst case sludge application rate of 7t/ha/y) shown in Table 6.4. The predicted groundwater concentrations are shown after 10, 50 and 100 years of sludge application and at the year of steady state, which is predicted 200-500 years ahead for most PFAS and 500-1000 years for (P)FOSA and PFDoDA. Karup is a Danish sandy soil, and Langvad a Danish clay soil. NER is not incorporated in the calculations.

PFAS:		**PFOS**	**PFOS**	**PFOA**	**PFNA**	**PFHxS**	**(P)FOSA**	**6.2 FTS**	**PFBA**	**PFP(e)A**	**PFBS**	**PFDA**	**PFDoDA**
Log K_{oc}:		**3,6**	**3,6**	**2,3**	**2,9**	**2,31**	**4,36**	**2,28**	**1,9**	**1,38**	**1,8**	**4**	**4,77**
Sludge Conc. (µg/kg dw):		**5,48**	**16**	**1.8**	**0.894**	**3.91**	**1.73**	**3.08**	**4.65**	**1.7**	**3.9**	**4.3**	**1.6**
Karup	10 years	4,55E-03	1,32E-02	2,59E+00	1,19E-01	5,47E+00	1,88E-06	4,50E+00	1,09E+01	5,36E+00	9,77E+00	1,15E-04	4,05E-08
Karup	50 years	5,82E-01	1,70E+00	6,47E+00	1,38E+00	1,39E+01	6,26E-04	1,13E+01	2,62E+01	1,38E+01	2,40E+01	2,89E-02	1,60E-05
Karup	100 years	2,14E+00	6,25E+00	9,59E+00	1,94E+00	2,05E+01	5,61E-03	1,68E+01	4,02E+01	2,16E+01	3,71E+01	1,91E-01	1,70E-04
Karup	Steady State	4,94E+00	1,47E+01	1,67E+01	3,07E+00	3,56E+01	9,89E-02	2,93E+01	7,20E+01	3,93E+01	6,68E+01	1,23E+00	6,74E-03
Langvad	10 years	2,02E-03	5,85E-03	2,42E+00	7,61E-02	5,09E+00	7,43E-07	4,22E+00	1,04E+01	5,07E+00	9,29E+00	4,69E-05	1,58E-08
Langvad	50 years	3,63E-01	1,06E+00	5,61E+00	1,31E+00	1,20E+01	2,70E-04	9,80E+00	2,26E+01	1,25E+01	2,08E+01	1,41E-02	6,47E-06
Langvad	100 years	1,68E+00	4,90E+00	7,90E+00	1,76E+00	1,69E+01	2,65E-03	1,39E+01	3,37E+01	1,93E+01	3,14E+01	1,10E-01	7,16E-05
Langvad	Steady State	4,45E+00	1,32E+01	1,31E+01	2,53E+00	2,80E+01	6,71E-02	2,31E+01	5,89E+01	3,48E+01	5,54E+01	1,03E+00	3,51E-03

TABLE 6.10. The calculated groundwater concentrations (ng/L) of selected PFAS using a simplified Box Model, a DT_{50} of 100 years and worst-case individual PFAS loads (approximating the 90th percentile of PFAS in Danish sludge) shown in Table 6.4. Otherwise, same input as in Table 6.9, except for the inclusion of NER formation. The data shows the influence k_{NER} covering the span of removal rates by NER (k_{NER}) reported in Gassmann et al. (2021) (See Chapter 3). The first order rate constant for NER formation in soil (k_{NER}) has only been identified for PFOS and PFOA (Chapter 3). For PFNA and PFHxS, a similar k_{NER} has been used as for PFOS and PFOA, respectively.

PFAS:		**PFOS**			**PFNA**			**PFOA**			**PFHxS**		
k_{NER} (d^{-1})		**0.0011**	**0.0013**	**0.0016**	**0.0011**	**0.0013**	**0.0016**	**0.0030**	**0.0047**	**0.0066**	**0.0030**	**0.0047**	**0.0066**
Karup	10 years	7,03E-04	4,42E-04	7,94E-05	7,97E-03	5,29E-03	3,01E-03	3,69E-02	1,06E-02	3,67E-03	7,62E-02	2,17E-02	7,51E-03
Karup	50 years	1,02E-03	5,57E-04	8,85E-05	9,32E-03	5,80E-03	3,13E-03	3,70E-02	1,06E-02	3,67E-03	7,62E-02	2,17E-02	7,51E-03
Karup	Steady	<20	<20	<20	<20	<20	<20	<10	<10	<10	<10	<10	<10
Langvad	10 years	3,05E-04	1,91E-04	3,40E-05	4,68E-03	3,05E-03	1,68E-03	2,56E-02	6,76E-03	2,24E-03	5,26E-02	1,38E-02	4,55E-03
Langvad	50 years	4,60E-04	2,46E-04	3,84E-05	5,74E-03	3,45E-03	1,78E-03	2,56E-02	6,76E-03	2,24E-03	5,26E-02	1,38E-02	4,55E-03
Langvad	Steady	<20	<20	<20	<20	<20	<20	<10	<10	<10	<10	<10	<10

TABLE 6.11. The calculated groundwater concentrations (C_{gw}) (ng/L) of selected PFAS using a simplified Box Model, a DT_{50} of 100 years and worst-case individual PFAS loads (approximating the 90th percentile of PFAS in Danish sludge and a sludge application rate of 7t/ha/y) shown in Table 6.4. Otherwise, same input as in Table 6.9 and 6.10. The calculated individual C_{gw} is compared with the individual groundwater threshold concentrations (TC_{gw}) (ng/L) for the two scenarios A and B presented in Table 6.8. Ratios (C_{gw}:TC_{gw}) above one are in bold and indicate that the used worst case exposure scenario potentially can lead to an exceedance of the groundwater threshold. Data in italics indicate scenarios with ratios above one, even if using a normal realistic sludge application rate of 1 t/ha/y. A time span of 50 years representa the steady state situation.

		C_{gw}	C_{gw}:TC_{gw}	C_{gw}:TC_{gw}	C_{gw}	C_{gw}:TC_{gw}	C_{gw}:TC_{gw}	C_{gw}	C_{gw}:TC_{gw}	C_{gw}:TC_{gw}	C_{gw}	C_{gw}:TC_{gw}	C_{gw}:TC_{gw}
		PFOS			PFOA			PFNA			PFHxS		
Scenario (Table 6.8):			**A**	**B**		**A**	**B**		**A**	**B**		**A**	**B**
GwTC:			0,5	1,48		0,5	0,24		0,5	0,16		0,5	0,08
						No NER							
Karup	10 years	1,32E-02	2,64E-02	8,92E-03	2,59E+00	**5,18E+00**	***1,08E+01***	1,19E-01	2,38E-01	7,44E-01	5,47E+00	***1,09E+01***	***6,84E+01***
Karup	50 years	1,70E+00	**3,40E+00**	1,15E+00	6,47E+00	**1,29E+01**	***2,70E+01***	1,38E+00	**2,76E+00**	***8,63E+00***	1,39E+01	***2,78E+01***	***1,74E+02***
Langvad	10 years	5,85E-03	1,17E-02	3,95E-03	2,42E+00	**4,84E+00**	***1,01E+01***	7,61E-02	1,52E-01	4,76E-01	5,09E+00	***1,02E+01***	***6,36E+01***
Langvad	50 years	1,06E+00	**2,12E+00**	7,16E-01	5,61E+00	**1,12E+01**	***2,34E+01***	1,31E+00	**2,62E+00**	***8,19E+00***	1,20E+01	***2,40E+01***	***1,50E+02***
						With median NER							
Karup	10 years	4,42E-04	8,84E-04	2,99E-04	5,29E-03	1,06E-02	2,20E-02	1,06E-02	2,12E-02	6,63E-02	2,17E-02	4,34E-02	2,71E-01
Karup	50 years	5,57E-04	1,11E-03	3,76E-04	5,80E-03	1,16E-02	2,42E-02	1,06E-02	2,12E-02	6,63E-02	2,17E-02	4,34E-02	2,71E-01
Langvad	10 years	1,91E-04	3,82E-04	1,29E-04	3,05E-03	6,10E-03	1,27E-02	6,76E-03	1,35E-02	4,23E-02	1,38E-02	2,76E-02	1,73E-01
Langvad	50 years	2,46E-04	4,92E-04	1,66E-04	3,45E-03	6,90E-03	1,44E-02	6,76E-03	1,35E-02	4,23E-02	1,38E-02	2,76E-02	1,73E-01

6.7 Conclusions on groundwater scenario

Various approaches and models have been used to predict safe concentration in sewage sludge protecting groundwater from PFAS leached from sludge amended soils. Due to the very high persistence and the long time for reaching a steady state, the potential maximum leaching is predicted to occur several centuries in the future.

Calculations using sludge concentration from the higher end of the measured concentrations in Danish sludge generally predict groundwater concentrations below the threshold concentrations. This is, for example, demonstrated in a 20-year simulation with the advances PELMO model, which predicted groundwater concentrations multiple orders of magnitude below the threshold concentrations. Different simplified calculations and models shows that due to the very high persistence, elevated groundwater concentrations can be predicted at steady state, typically occurring several centuries ahead if neglecting the removal of PFAS from the mobile pool by the formation of non-extractable residues.

Several field and semi-field studies have, however, shown leaching of PFAS that is lower than anticipated based solely on their normal adsorption kinetics. It is therefore concluded that PFAS may form non-extractable residues (NER) that are removed from the mobile pool of soil-associated PFAS (Gassmann et al., 2021, Stahl et al., 2013). The fraction of NER will be dependent on contact time, soil properties and PFAS characteristics, which adds to the complexity. The occurrence and magnitude of this is not well studied for most PFAS, but studies with PFOA and PFOS suggest it can exceed 90% after years of ageing.

So, on the one hand scientific data clearly demonstrate that NER should be taken into account when assessing leaching on a long perspective. On the other hand, it has only been possible to find one study presenting first order removal rates to NER (Gassmann et al. 2021). To use results from a single lysimeter study alone to estimate leaching for the entire country of Denmark imposes a large degree of uncertainty. Consequently, it is concluded to be unachievable to estimate fixed numerical, solid and science-based upper concentration or cut-off values for PFAS in Danish sludge protecting groundwater. Instead, based on a qualitative weight of evidence approach, it is concluded that the current 90% percentile of $PFAS_4$ in Danish sludge (Appendix C, Table 6.12) could be used as an indicative threshold concentration, i.e. 17.8 µg/kg, as data from a wide set of different calculations and models shows that these concentrations are very unlikely to result in situations with an exceedance of the groundwater concentrations above the threshold in a long-term perspective. In a short and medium time frame, e.g. 20-50 or even 100 years, the margin of protection is significantly higher in such predictions, taking into consideration that steady state will occur several centuries in the future.

For the sake of simplicity and for adding an extra margin of precaution, it could be suggested to have a threshold of in total 15 µg/kg for $PFAS_4$. In the data presented for Danish sludge in Appendix C, this threshold is exceeded in 30 of 215 samples, i.e. 14%. Using the same approach for $PFAS_{22}$ would call for a threshold in the range of 50-100 µg/kg. Since there are examples of relatively high $PFAS_4$ concentrations in the fraction of sludge samples having a total $PFAS_{22}$ concentration below e.g. 50 µg/kg (Appendix C), it may be recommended to have both sludge thresholds in operation, as this also reflects the thresholds for as well $PFAS_4$ as $PFAS_{22}$ in groundwater.

Miljøstyrelsen also published data from 384 sludge samples in Denmark (Miljøstyrelsen, 2022). Here the average and median concentrations were reported as 8.1 and 5.2 µg/kg, respectevily, for $PFAS_4$, and 12.2 and 9.4 µg/kg for $PFAS_{22}$.

TABLE 6.12. Percentiles of the individual PFAS and $PFAS_4$ as measured in 215 Danish sludge samples from 45 different wastewater treatment plants (Appendix C).

µg/kg	$PFAS_4$	PFOS	PFOA	PFNA	PFHxS
MIN	0.36	0.043	0.085	0.07	0.05
10P	3.40	2.4	0.3	0.185	0.137
50P	7.49	4.5	0.85	0.6	0.19
90P	**17.83**	**15**	**2.5**	**2.5**	**2.5**
MAX	65.15	55	19	7.4	4.3
N Total	215	215	215	215	215
N > LOQ	215	183	154	99	12
Max C_{PFAS} if $PFAS_4$<15 µg/kg (N=185)	-	13	3.4	7.3	2.5

7. Exposure of freshwater recipients

7.1 Environmental Threshold Concentration for freshwater ecosystems (ETC_{fw})

In Denmark, freshwater quality standards exist for one PFAS, i.e. PFOS. PFOS is on the EU list of priority substances, which is why the Danish water quality standards are aligned with the EU Environmental Quality Standards (EQS) associated to the Water Framework Directive (WFD). This EQS represents targets for good chemical and ecological status of freshwater ecosystems. Both an EQS for a long-term (annual average, AA) and a short-term (maximum acceptable concentration, MAC) exposure scenario is established for PFOS and its derivate at 6.5×10^{-4} and 36 µg/L for AA-EQS and MAC, respectively.

For the calculations made in this report, the EU and Danish EQS for freshwater organisms of 6.5×10^{-4} µg PFOS/L is chosen as an environmental threshold concentration for freshwater systems (ETC_{fw}).

7.2 Screening assessment for threshold concentration in sludge protecting freshwater

ECHA R.16 does not contain a relevant exposure scenario for leaching and run-off from sludge-amended soils to freshwater recipients. However, frameworks for estimating the exposure of freshwater organisms after land application of manure are established by EFSA (2019) and EMA (2007) in their assessment of feed additives and veterinary medicinal products, respectively. In EFSA (2019) and EMA (2007), the predicted environmental concentration for surface freshwater (C_{fw}) resulting from run-off or drainage is based on an assumption that one part of run-off/drainage water will be diluted by two parts receiving water, which corresponds to a dilution factor of three (Eq. 7.1a). When setting the concentration in run-off/drainage water equal to the concentration in soil pore water (C_{pw}) in the sludge amended top layer of the soil, C_{pw} can be found in Eq. 7.1b by re-arranging Eq. 7.1a:

$$Cfw = \frac{Cpw}{3} \qquad \text{Eq.7.1a}$$

$$Cpw = 3 \cdot Cfw \qquad \text{Eq. 7.1b}$$

where

$C_{fw} = ETC_{fw} = AA\text{-}EQS_{fw} = 6.5 \times 10^{-4}$ µg PFOS/L

In the calculation presented in this Section, it is assumed that the background concentration in the receiving water is zero, as PFAS from other potential sources in this generic assessment is neglected, since these will differ markedly across the country. In areas with known exposure from other sources, e.g. contaminated hot spots, the calculated threshold in sewage sludge can be adjusted according to the documented exposure from these sources, and/or the emission from these sources can be reduced by e.g. remediation activities.

Based on a threshold concentration in pore water (C_{pw}) corresponding to three times the EQS_{fw} (due to dilution factor of 3), a resultant steady state concentration of PFOS in soil after long-term accumulation ($C_{soil\text{-}ss}$) can be estimated from Eq. 4.10, taking the formation rate of non-extractable residues (NER) into account (Eq. 4.5, see Chapter 3).

Knowing the $C_{soil\text{-}ss}$, the threshold concentration in soil after a single sludge application the first year ($C_{soil(0)}$) can be calculated from equation 5.1. Knowing the threshold concentration in soil after a single sludge application ($C_{soil(0)}$), the corresponding threshold concentrations in sludge (C_{sludge}) can be calculated from equation 5.2.

Based on the data and calculations presented above, results can be found for PFOS in Table 7.1. To investigate the influence of K_{oc}, the 10th, 50th (median) and 90th percentile values of log K_{oc} from Appendix A are presented.

The 10th percentile K_{oc} value represents high freshwater exposure, meaning that PFOS has high leaching potential, which yields a minimum (worst-case) sludge concentration as cut-off value. $K_{air\text{-}water}$ is not as significant for PFOS, therefore the variability in reported vapor pressure and water solubility is not included as a variable in Table 7.1. In Table 7.2, the sensitivity of the calculation to the selected NER formation rate is presented as the range and median values found in Gassmann et al. (2021). The variation in the reported k_{NER} is relatively minor in the study by Gassmann. As no other reliable long-term k_{NER} has been identified, the impact of a using a k_{NER} being 50% lower than the median, i.e. 0.00055 d^{-1}, is tested (Table 7.2).

TABLE 7.1. Calculated threshold concentration in sludge for PFOS using percentiles of log K_{oc} data found in Appendix A and a DT_{50} of 100 years.

	Eq. / Cpt.	**Log K_{oc} = 2.84 (10th percentile) (L/kg)**	**Log K_{oc} = 3.6 (median) (L/kg)**	**Log K_{oc} = 4.68 (90th percentile) (L/kg)**
$K_{soil\text{-}water}$ [m^3/m^3]	4.6	20.95	119.6	1436.1
$k_{leaching}$ [d^{-1}]	4.5b	1.15E-04	2.00E-05	1.67E-06
$k_{biodegradation}$ [d^{-1}]	4.5c	1.90E-05	1.90E-05	1.90E-05
k_{NER} [d^{-1}]	Cpt.3	0.13E-02	0.13E-02	0.13E-02
$k_{removal}$ [d^{-1}]	4.5a	1.43E-03	1.34E-03	2.07E-05
$C_{fw} = ETC_{fw}$ [µg/L]		6.5E-04	6.5E-04	6.5E-04
$C_{pw} = 3 \times C_{fw}$ [µg/L]	7.1b	1.95E-03	1.95E-03	1.95E-03
$C_{soil\text{-}ss}$ [µg/kg]	4.10	2.40E-02	1.37E-01	1.65E00
F_{acc}	4.4	0.59	0.61	0.62
$C_{soil}(0)$ [µg/kg]	5.1	9.79E-03	5.31E-02	6.30E-01
$APPL_{sludge}$ [t/ha/y]		7.0	7.0	7.0
C_{sludge} [µg/kg]	**5.2**	**4.76**	**25.8**	**306**

TABLE 7.2. Calculated threshold concentration in sludge for PFOS using the range of NER formation rates found in Gassmann et al. (2021), as well as no NER formation and a k_{NER} 50% of the minimum reported in Gassmann et al. (2021), and a DT_{50} of 100 years.

	Eq.	k_{NER} = 0	50% k_{NER} 0.00055 d^{-1}	Min. k_{NER} 0.0011 d^{-1}	Median k_{NER} 0.0013 d^{-1}	Max. k_{NER} 0.0016 d^{-1}
Log K_{oc}		3.6	3.6	3.6	3.6	3.6
$K_{soil\text{-}water}$ [m^3/m^3]	4.6	119.6	119.6	119.6	119.6	119.6
$k_{leaching}$ [d^{-1}]	4.5b	2.00E-05	2.00E-05	2.00E-05	2.00E-05	2.00E-05
$k_{biodegradation}$ [d^{-1}]	4.5c	1.90E-05	1.90E-05	1.90E-05	1.90E-05	1.90E-05
$K_{removal}$ [d^{-1}]	4.5a	3.91E-05	5.89E-04	1.14E-03	1.33E-03	1.64E-03
$C_{fw} = ETC_{fw}$ [µg/L]		6.50E-04	6.50E-04	6.50E-04	6.50E-04	6.50E-04
$C_{pw} = 3 \times C_{fw}$ [µg/L]	7.1b	1.95E-03	1.95E-03	1.95E-03	1.95E-03	1.95E-03
$C_{soil\text{-}ss}$ [µg/kg]	4.10	1.37E-01	1.37E-01	1.37E-01	1.37E-01	1.37E-01
$C_{soil}(0)$ [µg/kg]	5.1	1.94E-03	2.65E-02	4.67E-02	5.31E-02	6.18E-02
$APPL_{sludge}$ [t/ha/y]		7.0	7.0	7.0	7.0	7.0
C_{sludge} [µg/kg]	**5.2**	**0.94**	**12.9**	**22.7**	**25.8**	**30.0**

The calculated sludge concentration presented above is under the provision that maximum a third of all water in a stream within a catchment area originates from leaching from soils amended with sludge, i.e. one unit of soil pore water from these soils is diluted by two units of pore water arriving from other agricultural soils or non-agricultural soils. In reality, it will most likely be rare that one third of all soils, not only agricultural soils, in a catchment are amended with sewage sludge annually for a period of decades or even centuries. A dilution factor of three is therefore considered relatively conservative in the context of normal land use and normal agricultural practice in most catchments.

A further elucidation of the freshwater scenario is conducted in the following sections.

7.3 More realistic assessment of sludge load and background concentrations of PFOS in freshwater recipients

The assessments presented above is, on the one hand, based upon a very conservative worst-case approach with regard to using a sludge load of 7 t/ha/y (see Section 4.3) and, on the other hand, based upon a premise of sewage sludge being the only source of PFOS in freshwater recipients, i.e. the background concentration of PFOS is zero. These two aspects are elucidated further below.

7.3.1 Application rate of sludge

With an average annual ceiling of 30 kg P/ha and a median P content of 29 kg/t, this results in a median sludge application rate of 1.03 t/ha/y (see Section 4.3). If using this sludge application rate in the calculation presented in section 7.2, threshold concentrations in sludge can be calculated as shown in Table 7.3.

TABLE 7.3. Calculated threshold concentration in sludge for PFOS using a range of P content found in Danish sludge (see text for discussion) and a log K_{oc} of 3.6 and a DT_{50} of 100 years.

	Eq. / Cpt.	10th percentile 15 kg P/t d.w.	50th percentile 29 kg P/t d.w.	90th percentile 39 kg P/t d.w.
$K_{soil\text{-}water}$ [m^3/m^3]	4.6	119.6	119.6	119.6
$k_{leaching}$ [d^{-1}]	4.5b	2.00E-05	2.00E-05	2.00E-05
$k_{biodegradation}$ [d^{-1}]	4.5c	1.90E-05	1.90E-05	1.90E-05
k_{NER} [d^{-1}]	Cpt.3	0.13E-02	0.13E-02	0.13E-02
$k_{removal}$ [d^{-1}]	4.5a	1.33E-03	1.33E-03	1.33E-03
$C_{fw} = ETC_{fw}$ [µg/L]		6.5E-04	6.5E-04	6.5E-04
$C_{pw} = 3 \times C_{fw}$ [µg/L]	7.1b	1.95E-03	1.95E-03	1.95E-03
$C_{soil\text{-}ss}$ [µg/kg]	4.10	1.37E-01	1.37E-01	1.37E-01
$C_{soil}(0)$ [µg/kg]	5.1	5.31E-02	5.31E-02	5.31E-02
$APPL_{sludge}$ [t/ha/y]	4.2	2.0	1.03	0.77
C_{sludge} [µg/kg]	**5.2**	**90.2**	**175**	**234**

If neglecting NER formation, the calculated sludge concentration in the three scenarios presented above in Table 7.3 would be 3.3, 6.41 and 8.58 µg/kg.

If aiming at having the pore water in compliance with the ETC_{fw} directly, i.e. omitting dilution, the threshold for sludge concentrations in Table 7.3 is three times lower, i.e. approximately 30, 58 and 78 µg PFOS/kg.

7.3.2 Background concentration of PFOS in Danish freshwater recipients

In the calculations presented above, it is anticipated that PFOS from sludge will leach into recipient waters having no previous contamination from other sources, e.g. contaminated hot spots or atmospheric deposition. This may not always be the case. In Boutrup et al. (2021), the latest monitoring data from the national programme NOVANA was reported for a wide set of hazardous substances in the aquatic environment, including PFOS. In streams, PFOS has been monitored since 2008. The median concentrations in 140 samples from 12 monitoring stations were in the first monitoring period (2008-2013) below the detection limit, whereas the average concentration was reported as 0.0034 µg/L and the 90th percentile as 0.0042 µg/L. In the latest monitoring period (2014-2019), the average, the median and the 90th percentile of the measured PFOS concentration were reported as 0.0027, 0.0012 and 0.0076 µg/L in 324 samples from 28 monitoring stations, keeping in mind the ETC_{fw}/EQS_{fw} of 0.00065 µg/L. It is, however, not possible directly to compare concentrations in individual samples with the EQS, which is defined as the annual average of a set of monthly samples, i.e. 12 samples per year. Furthermore, it is not clear to what extend the chosen monitoring stations represent background concentrations typically found in arable land, or if they are selected on the basis of the occurrence of hot-spots, e.g. local waste water treatment plants or contaminated hot-spots. Data does, however, clearly indicate that multiple sources to PFOS in freshwater streams may be found and that more information with regard to background concentrations in receiving waters would be beneficial for the final evaluation of the concentration in sludge protecting freshwater recipients.

7.3.3 Assessment of the current level of PFOS in Danish sludge

As discussed in Chapter 6 for groundwater, scientific data clearly demonstrate that NER should be taken into account when assessing leaching on a long perspective. On the other hand, it has only been possible to find one study presenting first order removal rates to NER

(Gassmann et al. 2021). To use results from a single lysimeter study alone to estimate leaching for the entire country of Denmark imposes a large degree of uncertainty. Consequently, it may be concluded that it is unachievable to estimate a fixed numerical, solid and science-based upper threshold concentration or cut-off values for PFAS in Danish sludge protecting groundwater and freshwater. Instead, the indicative threshold of 15 µg $PFAS_4$/kg outlined for the groundwater scenario in Chapter 6 can be tested in the calculation method and principles presented in Chapter 4. As a conservative approach for such calculations, the entire concentration of 15 µg/kg is thought to be allocated to PFOS as a worst case scenario. In practise, this is never 100% and in average only approximately 73.5% (Table 6.7). The predicted freshwater concentration resulting from a long-term sludge application with PFOS reaching a steady state in soils is presented in Table 7.4 with and without inclusion of NER formation.

Data in Table 7.4 shows that if NER is incorporated in the calculations, the predicted freshwater concentration will - not even in a long perspective - be in conflict with the ETC_{fw} for PFOS, except in receiving waters with background concentrations above approximately 6.0E-04 µg/L. If neglecting NER in the calculations, the predicted freshwater concentration exceeds the ETC_{fw} in a long perspective. In perspective, calculations (Eq. 4.3b) show that in scenarios neglecting NER, the accumulated soil concentrations after 25, 50 and 100 years of sludge application, $C_{soil(25y)}$, $C_{soil(50y)}$ and $C_{soil(100y)}$ are estimated to be 9.6E-05, 1.64E-05 and 2.4E-04 µg/kg, which, when using the methods described above and in Chapter 4, leads to predicted freshwater concentrations of 4.6E-07, 7.8E-07 and 1.2E-06 µg/L, respectively. These calculations clearly indicate that any potential conflict with the ETC_{fw} will occur in more than 100 years from now, even if assuming no NER will be formed during that period, which is very unlikely.

TABLE 7.4. Calculated freshwater concentration after sludge application until steady state including and excluding the first order removal of PFOS to NER (k_{NER}). The chosen sludge concentration is comparable to the 90th percentile of PFOS in Danish sludge (Appendix C, Table 6.12), and the sludge application rate is the average sludge application rate in Denmark- (Chapter 4.3). The maximum background concentration is the difference between the threshold concentration in freshwater and the predicted freshwater concentration coming from long-term sludge application. As $C_{fw} > ETC_{fw}$ for the no-NER scenario, maximum C_{bg} is per definition 0. Log K_{oc} is 3.6.

	No NER	NER
C_{sludge} [µg/kg]	15	15
$APPL_{sludge}$ [t/ha/y]	1.03	1.03
$K_{soil\text{-}water}$ [m^3/m^3]	119.6	119.6
$k_{leaching}$ [d^{-1}]	2.00E-05	2.00E-05
$k_{biodegradation}$ [d^{-1}]	1.90E-05	1.90E-05
k_{NER} [d^{-1}]	0	0.13E-02
$K_{removal}$ [d^{-1}]	3.90E-05	1.34E-03
$C_{soil(0)}$ [µg/kg]	4.54E-03	4.54E-03
F_{acc}	0.99	0.61
$C_{soil\text{-}ss}$ [µg/kg]	3.21E-01	1.18E-02
C_{pw} = [µg/L]	4.56E-03	1.67E-04
Dilution Factor	3	3
C_{fw} [µg/L] (C_{pw}/3)	1.52E-03	5.57E-05
ETC_{fw}	6.5E-04	6.5E-04
Maximum C_{bg} [µg/L]	0	5.94E-04

Table 7.4 shows that, if assuming a realistic sludge application rate based upon the median P content of Danish sludge, a median removal rate to NER observed in a long-term semi-field study, and the entire 15 µg/kg of the suggested $PFAS_4$ cut-off value allocated to PFOS alone, the predicted pore water in soils will, before dilution, be below the ETC_{fw} of 6.5E-04 µg/L, i.e. 1.67E-04 µg/L.

7.4 Alternative assessment of threshold concentration of PFOS in sludge protecting freshwater ecosystems

7.4.1 Point Source calculations

In this section, an alternative approach to the one used in section 7.3 is used to elucidate the use of sewage sludge and the threshold concentration of PFOS. The principle is the same, i.e. the threshold concentration in pore water is estimated, and from this the equations in ECHA R.16 (ECHA 2016) are used for reverse calculation to the threshold concentration in soil at a steady state situation. From this soil steady-state level, the soil threshold concentration after the first sludge application can be calculated. Based on this, the threshold concentration in sludge can be predicted.

In the context of calculating potential risk from contaminated hot spots to recipients, the following equation is commonly used in Denmark (Miljøstyrelsen 2016).

$$Cfw = \frac{Flux\ of\ contaminant}{Water\ flow\ in\ recipient} = \frac{A\ x\ I\ x\ Cpw}{Q} \qquad \text{Eq. 7.2}$$

7.4.2 Calculation for a reference area

In the context of contaminated hot spots, the flux of contaminants is coupled to the concentration in the contaminated plume or polluted aquifer from a site with a known specific area. In the context of leaching from soil amended with biosolids such as sewage sludge, it is anticipated that the flux of contaminants is coupled with the concentration in soil pore water, and as it is not possible upfront to find a fixed generic area of sludge amended soils within catchments across Denmark, a contaminated reference area is instead set arbitrarily at one ha, i.e. 10,000 m^2, since the sludge application rate in the Danish regulation is controlled by a hectare-based norm and dosing. The calculation for 1.0 ha can only be seen as a reference situation, since the specific are of arable land fertilized with sewage sludge within a catchment depends on the local situation and results must be scaled accordingly.

The infiltration rate of water from a non-sealed area is also defined as the net precipitation. The gross precipitation is the term for the total amount of precipitation (both rain and snow) that falls on the landmass, whereas the net precipitation is the precipitation that remains on the landmass and is available for the lakes, watercourses and groundwater. The average freshwater flow from land to sea in Denmark was in 2020 estimated to 359 mm, whereas the average over the past three decades (1990-2019) was estimated as 324 mm or 324 L/m^2 (Thodsen et al. 2020). The value of 324 L/m^2 is used in Eq. 7.3 as an estimate of the infiltration rate of the reference area.

The water flow in streams differs widely across Denmark and across the year and depends on the size of the stream, other physical conditions in the stream, the size of the catchment, extent of drainage and the rate of net precipitation within the catchment. In Miljøstyrelsen (2016), the recommended default value for Q was 130 L/s for smaller streams and 2,300 L/s for larger streams in Jutland and 10 and 200 L/s in Zealand. As a realistic, yet precautionary value, a Q_{ref} of 100 L/s is used as reference flow in this report.

Provided that leaching from a reference area of 1 ha is targeted to result in a concentration in the stream comparable to the threshold concentration, the corresponding concentration in pore water is calculated by rearranging Eq. 7.2, as:

$$Cpw = \frac{EQSfw\ x\ Q}{A\ x\ I} \qquad \text{Eq.7.3a}$$

where:

C_{fw}	Concentration in the freshwater recipient. Here set at the EQS_{fw} for PFOS	6.5 x 10^{-4}	µg/L
A	Reference area receiving PFOS via sewage sludge	10,000*	m^2
I	Infiltration rate	324	L/m^2/year
C_{pw}	Concentration in leaching water source (pore water)	Eq.6.2b	µg/L
Q_{sec}	Water flow in streams	100	L/s
Q_{year}	Water flow in streams	3.15E+09**	L/year

* The Danish sludge regulation is based upon an annual (average) input ceiling of 7 tons per hectare, i.e. per 10,000 m^2. **100 L/s = 100 x 60 s/min x 60 min/hour x 24h/day x 365 day/year = 3.15E+09 L/year.

or

$$Cpw = \frac{0.00065\ \frac{\mu g}{L}\ x\ 3.15\ E{+}09\ L/year}{10{,}000\ m2\ x\ 324\ \frac{L}{m2\ x\ year}} = 0.63\ \mu g/L \qquad \text{Eq. 7.3b}$$

In other words, leaching of pore water from 1.0 ha with a concentration of 0.63 µg/L will result in a freshwater concentration of 6.5E-04 µg/L in a stream with a flow of 100L/s.

Having established the soil pore water concentration (C_{pw}) in Eq. 7.3 for the reference area, the soil concentration at steady state leading to that pore water concentration ($C_{soil(ss)}$) is found in Eq. 4.10. Knowing the $C_{soil\text{-}ss}$, the threshold concentration in soil after a single sludge application the first year ($C_{soil(0)}$) can be calculated from equation 5.1. Knowing the threshold concentration in soil after a single sludge application ($C_{soil(0)}$), the corresponding threshold concentrations in sludge (C_{sludge}) can be calculated from equation 5.2. The outcome of these calculations is seen in Table 7.5.

TABLE 7.5. Calculation of a threshold concentration in sludge for a theoretical reference area of 1.0 ha. See text for more details.

$C_{soil\text{-}ss}$	PFOS concentration in soil at steady state	44.3	µg/kg
$C_{soil(0)}$	Concentration in soil in first year d.w.	17.1	µg/kg
k_{NER}	NER formation rate (see Chapter 3)	0.0013	d^{-1}
F_{acc}	Fraction of PFOS accumulation in one year - Eq. 4.4	0.61	-
C_{sludge}	The concentration in sewage sludge d.w.	8,360	µg/kg

In conclusion, for a reference area of 1.0 ha, any sludge concentration below 8,360 µg PFOS/kg dw will result in freshwater concentrations below the ETC_{fw} - provided it is the only source of contamination and leaching arrives to running water with no PFAS. As this is only a theoretical reference area, the threshold concentration in sludge must be scaled according to the specific area amended with sewage sludge within a specific catchment as:

$$Csludge\ \left(\frac{\mu g}{kg}\right) = \frac{Aref\ (ha)}{Asludge\ (ha)}\ x\ 8{,}360\ \frac{\mu g}{kg} \qquad \text{Eq. 7.4}$$

In Eq. 7.4, A_{ref} is 1.0 ha and A_{sludge} is the area (ha) fertilized with sewage sludge within a catchment. In other words, if, as an example, 1000 ha within a catchment are fertilised annually with the theoretical reference sludge load of 7t/ha/y, the average concentration in this sewage sludge should be below 8.36 µg/kg dw.

If knowing the average phosphor concentration in sludge used as fertiliser within the catchment area, Eq. 7.4 can be adjusted to the reference application rate of 7 t/ha/y ($APPL_{sludge\text{-}ref}$) as:

$$Csludge\ \left(\frac{\mu g}{kg}\right) = \frac{Aref\ (ha)}{Asludge\ (ha)}\ x\ \frac{APPLsludge{-}ref\ (t/ha)}{APPLsludge{-}average\ (t/ha)}\ x\ 8{,}360\frac{\mu g}{kg} \qquad \text{Eq. 7.5}$$

In Eq. 7.5, $APPL_{ref}$ is an application rate of 7t/ha/y and $APPL_{sludge\text{-}average}$ is the average sludge application rate (t/ha/y) within the catchment calculated on the basis of the actual P content in the used sludge, acknowledging an annual average maximum load of 30 kg P/ha.

If knowing the background concentration of PFOS in the stream receiving leachate from the sludge amended soils within the catchment, Eq. 7.5 can be adjusted to the background concentration of PFOS as:

$$Csludge\ \left(\frac{\mu g}{kg}\right) = \frac{Aref\ (ha)}{Asludge\ (ha)}x\ \frac{APPLsludge{-}ref\ (t/ha)}{APPLsludge{-}average\ (t/ha)}x\frac{(EQS{-}Cbg)(\frac{\mu g}{L})}{EQS\ (\frac{\mu g}{L})}x\ 8{,}360\ \frac{\mu g}{kg} \qquad \text{Eq.7.6}$$

In Eq. 7.6, C_{bg} is the (background) concentration in the stream, measured as an average of 12 yearly samples (i.e. monthly sampling), and the EQS is the environmental threshold concentration for PFOS in Denmark, i.e. 0.00065 µg/L.

As an example, included for illustration only, the maximum concentration in sludge applied at a rate of 1.0 t/ha/y (i.e. average phosphor content of 30 kg P/t) used on 5000 ha within a catchment of a stream having a background concentration of 2.0E-04 µg PFOS/L, can be calculated as:

$$Csludge\ \left(\frac{\mu g}{kg}\right) = \frac{1\ (ha)}{5000\ (ha)}\ x\ \frac{7\ (t/ha)}{1\ \ (t/ha)}\ x\ \frac{(0.00065 - 0.0002)(\frac{\mu g}{L})}{0.00065\ (\frac{\mu g}{L})}\ x\ 8{,}360\frac{\mu g}{kg} = 8.1\ \mu g/kg$$

Finally, if information is available about local infiltration rate and water flow at the catchment, Eq. 7.6 can be scaled further with the remaining variables as I_{ref}/I_{local} and/or Q_{local}/Q_{ref}, where I_{ref} and Q_{ref} are 324 L/m^2/year and 100 L/s, respectively, i.e.:

$$Csludge - max\ \left(\frac{\mu g}{kg}\right) = \frac{A(ref)}{A(sludge)}x\frac{APPLsludge(ref)}{APPLsludge}x\frac{(EQS - Cbg)}{EQS}x\frac{Q}{Qref}x\frac{Iref}{I}x\ 8{,}360\ \frac{\mu g}{kg}$$

7.5 Conclusions on freshwater recipients

Calculations predicting thresholds of PFOS in sludge protecting freshwater all conclude that such thresholds should be found in the range of approximate 20 to more than 200 µg/kg, depending on the input data and assumptions made. If omitting this removal pathway of NER formation, the predicted threshold concentration for PFOS in sludge is estimated to be below 1 µg/kg.

Calculations using median and realistic data with regard to annual sludge application rates, formation rate of non-extractable residues and K_{oc} values, show that a sludge concentration of 15 µg PFOS/kg, corresponding to the 90th percentile in Danish sludge, is likely to be protective for freshwater recipients, as the predicted concentration of PFOS in pore water before potential dilution in the stream is below the ETC_{fw}. In situations where other sources of PFOS within the catchment of a stream have enhanced the background concentration above approximately

6.0E-04 µg/L, the addition of leached PFOS from sludge amended fields may in the long-term results in exceedance of the ETC_{fw}.

8. Human exposure

Humans can be exposed to PFAS from multiple sources and via several pathways (De Silva et al., 2021), as summarized in Figure 8.1. Exposure can take place through food, from environmental accumulation of PFAS in food chains, from food processing or migration from food packaging materials. Drinking water can be a source of PFAS exposure, especially in contaminated hot spot areas. Several PFAS sources exist in the indoor environment, and uptake can occur with dust and indoor air, the latter mainly for neutral, volatile compounds, such as FTOHs. Exposure is also possible from direct contact with consumer products.

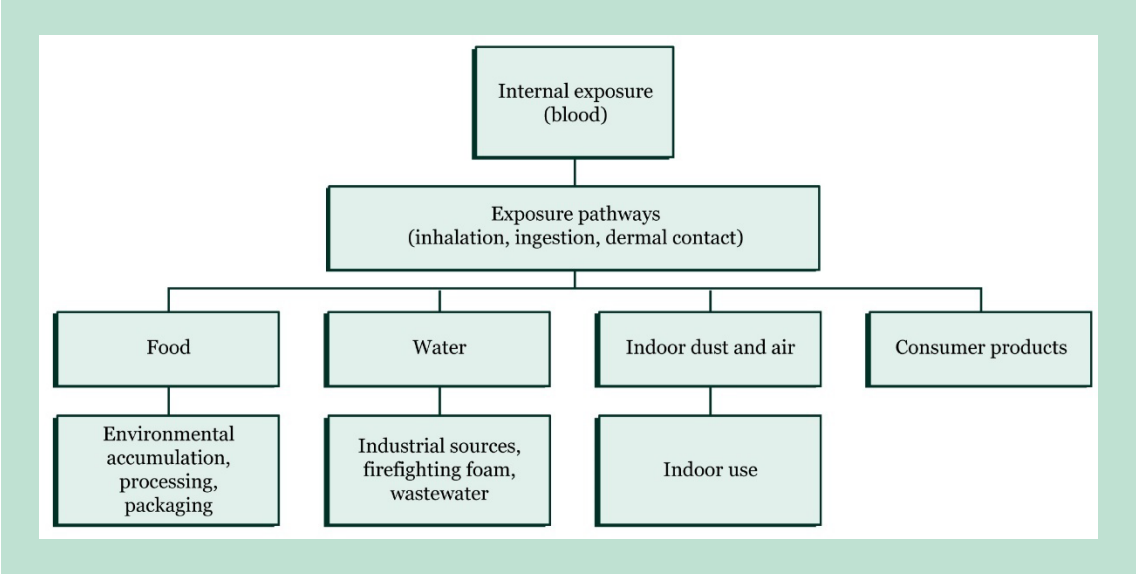

FIGURE 8.1. Potential human exposure to PFAS. Modified after De Silva et al. (2021).

As a consequence of multiple exposure sources and routes, PFAS have been widely detected in humans. They are included in human biomonitoring studies, such as the European Human Biomonitoring Initiative HBM4EU (Vorkamp et al., 2021) and the National Health and Nutrition Examination Survey (NHANES) of the USA (Kato et al., 2011). The US measurements, conducted since 1999/2000, have documented decreasing serum levels for PFAS, while long-chain PFAS, such as PFNA, have shown increasing concentrations (Kato et al., 2011). Human exposure to PFAS has been associated with altered immune and thyroid function, liver and kidney disease, lipid and insulin dysregulation, reproductive and developmental toxicity and cancer (Fenton et al., 2021). However, Fenton et al. (2021) point out that toxicity data are only available for few PFAS compounds, mainly PFOS and PFOA.

Today's scientific research has indicated that exposure to high levels of certain PFAS may lead to adverse health outcomes (Fenton et al. 2021). However, research is still ongoing to further elucidate how different levels of exposure to different PFAS may lead to a diversity of potential adverse effects on human health. Special attention is allocated to how low exposure to PFAS over long periods of time may affect especially children.

Based on human studies, EFSA (2020) concluded that effects on the immune system were critical for the risk assessment. Other endpoints, which had been assessed previously, include increased serum total and LDL cholesterol being a risk factor for cardiovascular disease, and increased alanine aminotransferase (ALT) levels, indicating effects on liver cells and liver disease.

As mentioned, effects on the immune system turned out to be the most critical, as they were observed at the lowest serum PFAS levels in both animals and humans. In contrast to previous evaluations focusing on PFOS and PFOA, EFSA combined the exposure and toxicity assessment for the sum of four PFASs (PFOS, PFOA, PFHxS, PFNA), which share toxicokinetic properties and exert similar toxicological effects when studied in animal tests. Current data do not allow the derivation of all compounds' specific potency factors, which is why equal potency for effects of all these four PFASs on immune outcomes was default assumed by EFSA (2020).

The lowest, and therefore most conservative, Bench-Mark Dose for the 10th centile ($BMDL_{10}$) was determined to be serum concentrations of 17.5 ng/mL for $PFAS_4$ in one-year-old toddlers. This was based on the inverse association between serum levels of the sum of these four PFAS and antibody titres against diphtheria found in a German study. The $BMDL_{10}$ was used to estimate the daily intake by mothers that would result in this critical serum concentration at 1 year of age in breastfed children. Using PBPK modelling, this serum level of 17.5 ng/mL in children was estimated to correspond to long-term maternal exposure of 0.63 ng/kg bw per day, i.e. an acceptable daily intake (ADI) of 0.63 ng/kg bw per day. To account for accumulation over time, a tolerable weekly intake (TWI) of 7 * 0.63 = 4.4 ng/kg bw per week was established for the sum of PFOA, PFNA, PFHxS and PFOS. This TWI is also considered protective for the other potential critical toxicological endpoints (EFSA, 2020).

Maximum acceptable levels of PFAS in meat and animal based food products are presently published by the EU[9]. According to EFSA (2020), 'Fish meat', 'Fruit and fruit products' and 'Eggs and egg products' contributed most to the human exposure for four PFAS of concern (PFOA, PFNA, PFHxS and PFOS). These four compounds represent 90.7% of plasma levels in adults and 87.1% of total PFAS measured in human serum, and they show similar accumulation and long half-lives in humans.

The US Food and Drug Administration (US FDA) has addressed the question whether the general food supply is a significant source of exposure to PFAS for U.S. consumers. Since 2019, they have sampled a broad range of products covering what the average U.S. consumer eats. However, The US FDA found that sample sizes for the specific types of foods are limited and therefore cannot be used to draw definitive conclusions. The FDA also tests foods grown or produced in areas with known PFAS contamination. Their analyses showed that environmental PFAS contamination does not necessarily mean contamination of the food itself at detectable PFAS levels. They note that this is because the amount of PFAS taken up by crops depends on many factors, including the specific type of PFAS and characteristics of the food[10].

Australian and New Zealand health authorities (Food Standard Australia and New Zealand (FSANZ[11])) have provided trigger values of concern for investigation - the lowest were determined for milk (0.4 µg/kg). Trigger points for fruit and vegetables were determined to be between 0.6 and 1.1 µg/kg, respectively. For finfish 5.2 µg/kg; for mammalian meat (3.5 µg/kg) and eggs (11 µg/kg).

Death et al. (2021) published a review of PFAS in livestock and game. They found that there have been relatively few investigations of PFAS in livestock. The tissue concentration in cattle rank decreases in the following order: liver > back fat > kidney > intraperitoneal fat > lung >

[9] https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32022R2388&qid=1671539058153&from=EN

[10] https://www.fda.gov/food/chemical-contaminants-food/testing-food-pfas-and-assessing-dietary-exposure

[11] https://www1.health.gov.au/internet/main/publishing.nsf/Content/ohp-pfas-hbgv.htm

spleen > muscle. They showed that PFOA concentrations in muscle in some studies were 1% of the liver concentration for PFOA and 10% for PFOS. Table 8.1 summarizes the maximum detected values from the literature.

TABLE 8.1. Maximum values reported (Death et al. 2021).

Tissue	PFOS µg/kg ww	PFOA µg/kg ww
Beef (liver)	4.5	Na
Pork (liver)	11.3	Na
Beef (muscle)	2.7	0.1
Pork (muscle)	0.29	10.7
Chicken (egg)	86.9	Na

Death et al. (2021) conclude that due to the low sample size and few studies there is uncertainty with respect to the tissue distribution and clearance information of PFAS in animals and livestock and it is hence difficult to assess human health risk associated exposure to humans via the consumption of meats. The transfer of PFAS in the trophic levels from soil to feed and the meat is not yet quantified or modelled. This needs to be done before responsible authorities can take appropriate risk-based measures to inform and protect consumers, and a precautionary approach is hence currently advisable.

8.1 Calculating maximum concentration in sewage sludge protecting humans

Reverse modelling of maximum sludge concentration of PFAS can theoretically be calculated using equations found in for example the EU TDG (EC, 2003, Part 1, Appendix III, page 250 onwards). However, as it includes a wide number of exposure pathways and default input parameters that are not available for the vast majority of PFAS forming the human toxicological sum-criteria ($PFAS_4$ and $PFAS_{22}$), it has not been deemed feasible or reliable to arrive at reliable cut-off values in sludge protecting humans. One of the main obstacles in the extrapolation method described in e.g. EC (2003), besides the many stages in the trophic food web ranging from soil to feed crop to meat, milk or egg consumed by humans, is the use of log K_{ow} in some of the transfer functions. It is generally accepted that, due to the chemical-physical properties of PFAS, it is not feasible to generate reliable K_{ow} values for PFAS via for example QSAR.

The German Federal Institute for Risk Assessment (BfR, 2021) estimated the maximal possible PFAS levels in feed for laying hens, dairy cows and fattening pigs, which would not lead to an exceedance of the maximum levels proposed by the EU Commission for eggs, cow's milk, pork and pork liver when feeding. For laying hens, dairy cows and fattening pigs, the maximum concentration in feed was estimated as 0.31, 0.03 and 0.04 µg/kg dw, respectively.

In summary, there are currently a very large number of uncertainties and generic assumptions in the chain of modelling steps necessary to calculate exposure of humans to PFAS originating from sludge amended soils. Together with the uncertainty of the validity of the log K_{ow} for PFOS, it makes the final prediction of a cut-off value for PFOS in sludge very uncertain. Furthermore, there is not sufficient experimental data to accurately evaluate and validate such predictions.

The German Federal Institute for Risk Assessment (BfR 2021) concluded - in line with the US FDA recommendations and the conclusions from Death et al. (2021) - that:

- *No background levels of PFAS in feedstuffs can be established on the basis of the available data from feedstuff investigation programs and the present performance of the analytical methods for PFAS in feedstuffs.*
- *The knowledge base concerning the transfer of PFAS from the feed should be expanded, so that reliable statements can also be made in the future for substances other than PFOS and PFOA.*
- *That the assessment of the maximum possible PFAS levels in feedstuffs that prevent exceedance of the proposed maximum levels in foods of animal origin shows that the current analytical detection limits in feed should be significantly improved. Hence, the BfR recommends, as a first step, the development of more sensitive PFAS analytical methods, on which basis PFAS background levels can be estimated from feed monitoring as a pre-requisite for the derivation of maximum levels.*

8.2 Conclusion on human exposure

EU thresholds for PFAS in food for human consumption have been published by EU[12], but yet knowledge and data is lacking to predict safe sewage sludge concentration based upon reverse food web calculations. Based on the great uncertainties and the recommendations from BfR, it is concluded to be out of scope in this report to derive reliable thresholds and cut-off value for PFAS in sludge that protects humans from exposure via meat, egg or milk products from husbandry being fed with fodder grown on sludge-amended soils.

From this perspective, it should be noted that this by no means leads to a conclusion on whether or not the current levels of PFAS in sludge pose a risk to humans, but rather that it has not been possible to collect enough and reliable information available to establish solid threshold concentrations of PFAS for this specific scenario. In order to be able to present such a calculation with more certainty, the following data are needed:

1. National or internationally accepted maximum concentration in plant-based feed for husbandry
2. Reliable estimates of bioaccumulation/bioconcentration factors (BAF/BCF) from soil to crops
3. The influence of NER on bioconcentration and bioaccumulation in plants.

The first set of data cannot be established within the scope of this report, whereas some information has been collected with regard to the latter two sets of data. Pot and lysimeter studies (Stahl et al. 2013, Krippner et al. 2015) have, for example, shown that plant uptake of long chained PFAS like PFOA and PFOS generally is limited, with BCF well below one, i.e. concentrations in the plants are lower than in the soil at soil concentrations relevant for most sludge amended soils. The limited uptake may be due to the formation of NER over time, as discussed in Chapter 3.

In conclusion, thresholds for sewage sludge protecting cannot be established due to lack of data and great uncertainties in a long cascade of food web transfer functions, however, it can be mentioned that the calculated steady state concentration in soil after normal sludge application with PFAS concentrations corresponding to their individual 90th percentile measured in Danish sludge is estimated to be well below the current soil quality standard of 10 µg/kg for $PFAS_4$ established to protect humans from exposure, including soil ingesting children (Table 8.2).

[12] https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32022R2388&qid=1671539058153&from=EN

If making an arbitrary and theoretical summation of the four individual calculated steady state soil concentrations, it adds up to 0.34 (no NER) and 0.02 (NER) µg/kg, respectively, i.e. approximately a factor 30 and 500 below the QS_{soil} for $PFAS_4$.

The theoretical added steady state soil concentration above was a result an summed $PFAS_4$ sludge concentration of 22.5 µg/kg (15.0+2.5+2.5+2.5 µg/kg), as compared to the 90th percentile of $PFAS_4$ measured as 17.8 mg/kg (Table 6.12). In such aspects, it is considered very unlikely that normal agricultural sludge application with a threshold of 15 µg $PFAS_4$/kg will result in soil concentrations exceeding the current QS_{soil} in Denmark of 10 µg/kg, even in a long-term perspective.

TABLE 8.2. Estimated steady state concentration of individual $PFAS_4$ in soils amended with sludge containing individual PFAS concentration corresponding to 90th percentile in Danish sludge (Table 6.12). The four individual $C_{soil\text{-}ss}$ are compared to the Danish Soil Quality Standard (QS_{soil}) for human protection of 10 µg $PFAS_4$/kg.

	PFOS		PFOA		PFNA		PFHxS	
	No NER	NER	No NER	NER	No NER	NER	No NER	NER
C_{sludge} (µg/kg)	15	15	2.5	2.5	2.5	2.5	2.5	2.5
$APPL_{sludge}$ (t/ha/y)	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03
$C_{soil\text{-}ss}$ (µg/kg)	3.2E-01	1.2E-02	5.5E-03	9.0E-04	1.8E-02	1.9E-03	7.6E-04	5.6E-03
QS_{soil} (µg $PFAS_4$/kg)	10E+00							

9. Summary, conclusions and recommendations

The main objective of this report is to derive risk-based cut-off values for per- and polyfluoroalkyl substances (PFAS) in sewage sludge. For simplicity, the project solely focuses on sewage sludge as a source of PFAS in the environment. The report therefore does not incorporate multiple sources in the calculation of cut-off values in sewage sludge. Consequently, atmospheric (wet or dry) deposition, effluent from wastewater treatment plants and leaching from hot spots, e.g. contaminated sites, are not included in the calculations. With other known sources, it could be argued that the transport from sludge to freshwater recipients and groundwater must be reduced accordingly in order to comply with environmental quality standards, or it could be argued that the input from other sources should be reduced in order to enable a safe use of sewage sludge. It is not possible to include a general scientifically based margin of safety that incorporates other sources, as these will be site specific and differ widely in time and geographic space across the country. The potential inclusion of such an additional margin of safety is therefore a task for competent authorities to implement for precautionary reasons and/or for local authorities to implement according to local information regarding point sources or elevated background concentrations.

The group of per- and polyfluoroalkyl substances (PFAS) has become a major environmental and health concern. PFAS molecules consist of an alkane chain that is either fully ("per") or partly ("poly") fluorinated, and a functional group such as -OOH or -SO3-. The carbon-fluorine bond in PFAS molecules is the strongest in organic chemistry, resulting in half-lives of years or even decades and centuries.

Four different exposure routes and protection endpoints were identified, i.e.

Sludge → soil → soil dwelling microorganisms, invertebrates and plant species
Sludge → soil → soil pore water → groundwater → drinking water → humans
Sludge → soil → soil pore water → freshwater (streams) → aquatic organisms
Sludge → soil → crops for animal feed → livestock →food (meat and dairy products) → humans

As an initial screening, methods and equations derived from guidance documents published by ECHA and EFSA are used, primarily the report from ECHA "Guidance on information requirements and Chemical Safety Assessment, Chapter R.16: Environmental exposure assessment". The methods described in R.16 are designed to calculate environmental exposure from a set of fixed scenarios, including a sewage sludge scenario. In this report, these equations are used reversely by starting with a fixed environmental threshold concentration (ETC) and calculating backwards to an associated sludge concentration complying with the ETC in question. Important chemical-physical input parameters for evaluating the leaching potential of PFAS are degradation and adsorption kinetics and distribution coefficients between soil, organic carbon, pore water and air, the most important being the DT_{50} and the K_{oc} values. As PFAS have a very long degradation time, i.e. essentially being persistent to a degree where they often are called "forever chemicals", a theoretical DT_{50} of 100 years has been chosen as default. Literature data for K_{oc} has been reviewed and compiled for evaluation.

A large data set of K_d and K_{oc} values has been compiled, and the median K_{oc} value in the data set was used as input for the leaching models. Furthermore, data from semi-field (lysimeter)

and field studies were compiled and evaluated in order to compare monitored leaching with modelled and theoretical leaching of PFAS. Data shows that PFAS over time will be incorporated in the soil matrix, e.g. in the organic matter, to a level where leaching and plant uptake are significantly lower than expected based upon modelling and simple batch studies in the laboratory. The fraction of non-extractable residues (NER) may add up to more than 90% of PFOS and PFOA after a decade. This may explain the very low levels of PFAS reported in groundwater below sludge-amended soils in the few studies available from sludge amended fields, including a recent Danish field study monitoring the leaching of PFAS to groundwater below agricultural soils receiving large quantities of sludge. As a consequence, first order rates for NER formation have been incorporated along rates for leaching and biodegradation in the estimation of the overall removal rate of PFAS in soils.

For freshwater recipients, Danish environmental quality standards (EQS) exist for PFOS (0.00065 µg/L), and for groundwater two threshold concentrations exist for the groups of $PFAS_4$ (2.0 ng/L) and $PFAS_{22}$ (100 ng/L), respectively. These have been used as ETC_{fw} and ETC_{gw}, respectively.

In the initial screening, a dilution factor of three from soil pore water to freshwater and no dilution from pore water to groundwater is assumed. The calculated sludge concentrations complying with the ETC for freshwater (ETC_{fw}) are predicted to be 25.8 µg PFOS/kg dw in a worst case sludge application scenario (7t/ha/y) and 175 µg PFOS/kg dw in a more realistic sludge application scenario (1.03 t/ha/y). In both calculation scenarios, potential background concentrations of PFOS in freshwater have been neglected. If the pore water concentration is compared directly with the ETC_{fw}, i.e. without dilution, the threshold in sludge is reduced accordingly by a factor of three, i.e. to 58.3 µg PFOS/kg in the most realistic scenario.

In the initial groundwater screening, no dilution from pore water to groundwater is assumed. Although the ETC_{gw} is presented as a sum criteria of $PFAS_4$, the sludge concentration must be calculated individually due to the difference in chemical-physical properties and, hence, leaching behavior. If assuming a typical and realistic sludge application rate of 1.03 t dw/ha/y, the maximum sludge concentration of $PFAS_4$ was estimated to be approximately: PFOS: 44.9 µg/kg; PFOA: 3.1 µg/kg; PFNA: 9.4 µg/kg; PFHxS: 3.2 µg/kg.

The FOCUS model PELMO, an international accepted model used by competent authorities for regulatory purposes of pesticides, predicted groundwater concentrations orders of magnitude below the threshold concentrations after twenty years of sludge application with PFAS concentrations similar to the upper quartiles in Danish sludge. Due to the limited simulation period and the long-term persistence of PFAS, an alternative simplified Box Model was used to calculate groundwater concentrations after long-term sludge application, i.e. several centuries.

For soil dwelling species, no national or EU based ETC exist, wherefore a draft ETC_{soil} was derived within the project. ETC_{soil} could only be derived for PFOS and PFOA due to lack of data for other PFAS. Indicative ETC_{soil} of 16 µg/kg for PFOS and 2.0 µg/kg for PFOA were chosen as estimates of soil threshold concentrations. The resulting cut-off values in sludge protecting soil dwelling organisms were estimated as 134 µg PFOA/kg dw and 110 µg PFOS/kg dw, respectively. For the protection of soil dwelling organisms, NER was not included in the calculations, as no data could be found elucidating the quantitative importance of NER for bioaccumulation.

For exposure of humans via food intake, a number of necessary transfer functions were affected by large uncertainties and lack of data. The very large number of uncertainties and generic assumptions in the chain of modelling steps necessary to calculate exposure of humans to PFAS originating from sludge amended soils together with the uncertainty of the validity of

the log K_{ow} for PFOS make the final prediction of a cut-off value for PFOS in sludge very uncertain. Furthermore, there is not sufficient experimental data to accurately evaluate and validate such predictions.

In the calculations and predictions presented in this report, a number of assumptions have been made and a number of defaults have been chosen. Some of these and their implications are discussed below. The implications of the various choices generally point both ways, but in total they most likely point towards a conservative approach potentially overestimating the leaching potential of PFAS from sludge amended soils.

Factor	Implication	Information
Predominantly using of K_{oc} from laboratory batch studies	Conservative approach leading to lower cut-off values in sludge	Applying laboratory derived distribution coefficients in risk assessment can cause overestimation of PFAS concentrations in (pore)water and, consequently, also underestimate the residence time of the contaminants in soil (Zareitalabad et al., 2013).
Choice of K_{oc}	An average approach potentially both over- and underestimating leaching	Generally, the median log K_{oc} has been chosen for the calculations. As adsorption and, hence, leaching in the models are sensitive to the choice of K_{oc}, this approach does not represent the worst case situation.
Choice of NER	Has a significant impact on the estimations and data is very limited	The inclusion of NER has a significant impact on the calculations. However, very few – if any -studies are available that elucidate the long-term formation of NER for PFAS, especially for other PFAS than PFOS and PFOA. It has been decided to include the best reported and longest running semi-field study (Gassmann et al. 2021) in order to incorporate this important aspect, which can aid to explain the relatively low leaching reported of especially long-chained PFAS in many field studies relevant for sludge scenarios. It is, however, acknowledged that the use of a specific rate for NER is associated with notably uncertainties.
Neglecting volatilization of PFAS	Conservative approach leading to an overestimation in the leaching potential	PFAS may exist as neutral PFAS with higher volatility and lower water solubility or ionic PFAS with lower volatility and higher water solubility. Since PFAS dissociation constants decrease with decreasing pH, volatilization increases with decreasing pH with maximum volatilization at pH = 1 for PFOA (Johansson et al., 2017). Therefore, under natural soil-water conditions, volatilization of PFAS is often reported as minimal or negligible.
Assuming limited impact of air-water partitioning.	Conservative approach leading to lower cut-off values in sludge, as PFAS associated to the air phase is not available for leaching	Schaefer et al. (2022) found that inclusion of air-water interfacial sorption resulted in a 58% reduction in the predicted PFOS pore water concentration. Only by including the air-water interfacial sorption did they find PFOS pore water concentrations that were identical (within the 95% confidence interval) to the measured PFOS pore water concentration in a lysimeter study.
Mixture effect on the leaching of PFAS	May potentially underestimate the leaching of especially short chain PFAS.	Mclachan et al. (2019) tested leaching of a mixture containing equal concentrations of the 13 PFAS and found measured K_d in laboratory studies overestimated the soil/water distribution measured in the lysimeters. The longer chained PFAS may have occupied sorption sites

		and, hence, reduced the sorption capacity of the soil for the shorter chained PFAS, leading to a more rapid elution from the lysimeters.
Using a default sludge load of 7 t/ha/y according to the theoretical maximum in the Danish legislation	Conservative approach leading to markedly lower cut-off values in sludge	For some of the simple equations, results have been presented for a more realistic sludge application rate in Denmark. For the model calculations, output is linear, and the results can be scaled accordingly.
PFAS being characterised as forever chemicals. Using a default DT_{50} of 100 years	Impact uncertain, as the true DT_{50} based upon degradation is unknown, although most likely lower than 100 years.	Zhang et al. (2022) reviewed degradation studies with PFAS and concluded that recent research outcomes have shown that an increasing number of PFAS species are, in fact, biodegradable to some extent. Both mixed culture and pure microbial species show potential in degrading certain PFAS species, though they typically cannot be degraded completely through a single biodegradation pathway. Consequently, dissipation time by biodegradation from soils for most PFAS is most likely lower than 100 years.
Choice of leaching model	Conservative approach leading to lower cut-off values in sludge	Data show that the used Box Model within comparable time frames (simulation period) predicts groundwater concentrations that are multiple orders of magnitude, i.e. 10E+13, higher than more advanced FOCUS models like PELMO used by the European competent authorities EFSA and EMA in their regulation of pesticides, feed additives and medicinal products.
Limited pre-set of model sites for calculations	May not represent worst case for all of Denmark	The model calculations in this report are based on a number of pre-set sites, e.g. Karup and Langvad, which represent two different soil types, but by no means represent all Danish soil types, differences in pH and potential difference in precipitation or other weather conditions important for leaching processes.
Precursors of PFAS	Neglecting presence of precursors for e.g. $PFAS_4$ may underestimate the environmental load	Many PFAS precursors (such as alcohols, amides) may in sludge or the environment be degraded to for example PFOA and PFOS. So, although the biotransformation could effectively remove PFAA precursors, it actually may cause problems by degrading these into more persistent PFAAs, such as PFOS and PFOA (Zhang et al. 2021, Glaser et al. 2021).
Simultaneous leaching of PFAS from a catchment to a stream	Will overestimate the time-dependent load to streams as distance from source to sink play a role	In the simple REACH equations and the Box Model, leaching of PFAS from sludge amended soils is assumed to occur simultaneously from the entire catchment area treated with sludge, regardless of the distance to the stream, which is unlikely and, hence, conservative.

9.1 Conclusions

The results obtained and reported in the previous chapters lead to a wide set of conclusions, including the ones listed below:

- Fate and behavior of PFAS in the environment are substance, time and soil dependent.
- Simple methods and equations used in ECHA and EFSA context generally seem to overestimate the potential for leaching of PFAS from sludge-amended soils compared to what is measured in field studies and what more advanced groundwater models, like PELMO, predict.
- Exposure of soil dwelling organisms does not seem to be the most sensitive endpoint for protection, i.e. sludge levels that protect freshwater and groundwater will most likely also protect soil ecosystems.
- It has not been possible to estimate valid thresholds in sludge for protection of humans exposed via the food web sludge-soil-crops-animal feed-husbandry-food-humans, but calculations shows that the long-term soil concentrations at the steady state situation are likely to be well below the current human toxicological soil quality standard of 10 µg/kg.
- Over time will PFAS be incorporated as non-extractable residues (NER) in the soil matrix, reducing its mobility, immediate availability for biological uptake and potential for leaching.
- Field and semi-field (lysimeter) studies as well as model simulations predict NER being as high as >90% for PFOS and PFOA after a decade, whereas other PFAS may have lower NER fractions.
- A Danish field study with high sludge loads has demonstrated low potential for vertical transport and leaching, leading to - with a few exceptions - very low or non-detectable groundwater concentrations below sludge amended field plots.
- Existing FOCUS models, like PELMO and MACRO, are not fully suited for evaluating leaching of substances with very long half-lives, as the simulation period is too short to reach steady state. Furthermore, the flexibility with regard to input of high DT_{50} values may be too narrow as the models are developed for pesticides, which no longer are approved if they have very long DT_{50}.
- The PELMO model predicted very low groundwater concentration after 20 years of simulation, i.e. multiple orders of magnitude below the $PFAS_4$ criteria of 2.0 ng/L.
- A simplified constructed Box Model was used to predict groundwater concentrations on a very long perspective (up to 1000 years).
- The Box Model can be considered a simplified leaching model compared to e.g. PELMO and delivers significantly more conservative outputs, i.e. markedly higher predicted groundwater concentrations.
- Whereas it is not possible to incorporate the formation of NER in the PELMO model, it can be done in the Box Model.
- It has only been possible to find a single study that has quantified first order removal rates to NER in a long-term (semi) field study (Gassmann et al. 2021). To use results from a single lysimeter study alone to estimate leaching for the entire country of Denmark imposes a large degree of uncertainty.
- Consequently, due to the large uncertainty it is considered unachievable to estimate fixed upper threshold concentrations for PFAS in Danish sludge protecting groundwater and freshwater systems.
- Taking all available information into account, including the consideration that all estimations are based upon steady state scenarios often reached several centuries out in the future, it is concluded that it is unlikely that normal sewage sludge application with PFAS concentrations corresponding to the higher end of what is found in Danish sludge today in itself will result in an exceedance of the groundwater and the freshwater thresholds within a relevant time span.

- Even when assuming a 50% lower removal rate to NER than the lowest reported from a long-term semi-field study, the predicted threshold concentrations of $PFAS_4$ in sludge protecting groundwater are higher than the 90th percentile of the $PFAS_4$ concentrations found in Danish sludge, i.e. a $PFAS_4$ concentration of 17.8 µg/kg.
- In light of the above, it is concluded that **an indicative threshold concentration of 15 µg/kg dw for $PFAS_4$ in sludge** is very likely to protect groundwater and freshwater with regard to being in compliance with the respective threshold concentrations, provided there are no other sources leading to highly elevated background concentrations.
- As many of the underlying calculations presented in this report are based on a sludge application rate corresponding to adding a maximum of 30 kg P per ha, an alternative or supplement to the dry weight based threshold concentration could be a phosphor-based threshold concentration **of 0.5 µg $PFAS_4$/kg P.**
- Due to the lack of reliable data for many of the $PFAS_{22}$, it is less transparent how to recommend cut-off values for the sum of these. However, there is no indication that the current concentrations of $PFAS_{22}$ in Danish sludge will be in conflict with the groundwater threshold of 100 ng/L, as the threshold for $PFAS_{22}$ is 50 times higher than for $PFAS_4$, and the 90th percentile of the summed concentrations of $PFAS_{22}$ is 3.2 times higher than $PFAS_4$ (Appendix C). A pragmatic and non-science based threshold concentration could, hence, range from 50 to 100 µg $PFAS_{22}$/kg.
- In regional catchments or groundwater reservoirs with known elevated background concentrations of PFAS, special attention may be needed with regard to a possible local regulation of sludge application.
- Monitoring data suggest that the background concentration in many freshwater samples and at some monitoring stations may exceed the EQS for PFOS. The source of PFOS monitored at these stations are not specifically reported and/or are unknown.

9.2 Recommendations

Based on the results and information collected in this report, the following recommendations are made:

- It is recommended to obtain more and better information with regard to the presence of PFAS in Danish freshwater streams in order to validate the predictions presented in this report and to gain better insight into the background concentration of PFOS across the country. This could include more frequent collection of water samples from an increased number of NOVANA monitoring stations.
- In line with the above, it is recommended to map and quantify the sources of PFAS in the catchments of freshwater recipients having exceeded background concentration of PFAS in order to identify potential risk mitigation measures and to evaluate the potential influence of sewage sludge application.
- It is recommended to consider the use of SWAT modelling to improve the predicted PFAS transport from soil to freshwater at catchment scale. The Soil & Water Assessment Tool (SWAT) is a watershed to river basin-scale model used to simulate the transport of water and solutes to surface and ground water at different land use and land management practices. SWAT can be used to predict leaching from non-point source pollution.
- It is recommended to initiate studies and/or compile future reported data with regard to the long-term removal rate by formation of NER in soils in order to gain more information for a wider range of PFAS, more diverse soil types, the temporal changes in the NER formation rate and the importance of differences in climatic weathering conditions.
- It is recommended to gain new information derived from controlled field studies monitoring leaching of PFAS in drained and non-drained soils before and after sludge application.
- It is recommended to align the sludge regulation with the food safety regulation controlling the maximum acceptable PFAS concentration in feed to husbandry.
- It is recommended to investigate to which extend the current toxicological based soil quality standards sufficiently protect humans from exposure via the food-web based scenario

outlined in this report, e.g. by compiling available and/or obtaining new knowledge with regards to plant uptake of PFAS other than PFOA and PFOS.

- Since steady state concentrations reached several centuries in the future are significantly higher than the concentrations obtained after 10-50 years, it could, as a precautionary step, be a long-term target to reduce PFAS levels in sludge below the current level and the outlined cut-off value.
- It is recommended to collect and publicly publish the PFAS concentrations in Danish sludge from a wide set of representative Danish Waste Water Treatment Plants. This would in time allow adjustment of the conclusions made in this report, since the calculations are based on extrapolations and predictions reaching decades and even centuries in the future.
- If a more solid estimation of the soil scenario is needed, it is recommended to perform a more comprehensive derivation of ETC for soil ecosystems by performing a more wide-ranging data collection of effects on soil dwelling organisms and a formal quality assessment according to accepted criteria found in e.g. the Klimisch or CRED evaluation systems (Klimisch et al. 1997, Moermond et al. 2006).

10. References

Ankley, G.T., Cureton, P., Hoke, R.A., Houde, M., Kumar, A., Kurias, J., Lanno, R., McCarthy, C., Newsted, J., Salice, C.J., Sample, B.E., Sepúlveda, M.S., Steevens, J. and Valsecchi, S. 2021. Assessing the Ecological Risks of Per- and Polyfluoroalkyl Substances: Current State-of-the Science and a Proposed Path Forward. Environ Toxicol Chem, 40: 564-605. https://doi.org/10.1002/etc.4869

Banzhaf, S.; Filipovic, M.; Lewis, J.; Sparrenbom, C.J.; Barthel, R. 2017. A review of contamination of surface-, ground-, and drinking water in Sweden by perfluoroalkyl and polyfluoroalkyl substances (PFASs). Ambio 46, 335-346.

Barlebo HC, Rosenbom AE, Kjær J. 2007. Evaluation of Pesticide Scenarios for the Registration Procedure. Environmental Project No. 1178, 2007, Miljøstyrelsen.

BfR. 2021. Bundesinstitut für Risikobewertung. PFAS in food: BfR confirms critical exposure to industrial chemicals. BfR Opinion No 020/2021 issued 28 June, 2021. Doi: 10.17590/20210914-121236

Boisvert G, Sonne C, Rigét FF, Dietz R, Letcher RJ. 2019. Bioaccumulation and biomagnification of perfluoroalkyl acids and precursors in East Greenland polar bears and their ringed seal prey. Environ Pollut. 1335-1343. doi: 10.1016/j.envpol.2019.06.035.

Boutrup S, Kjær C, Johansson LS, Larsen MM, Poulsen MB, Bossi R, Christensen MR, Frank-Gopolos T. 2021. Miljøfarlige forurenende stoffer i vandmiljøet. NOVANA. Tilstand og udvikling 2008-2019. Aarhus Universitet, DCE – Nationalt Center for Miljø og Energi, 288 s. - Videnskabelig rapport nr. 466. http://dce2.au.dk/pub/SR466

Bossi, R.; Vorkamp, K.; Skov, H. 2016. Concentrations of organochlorine pesticides, polybrominated diphenyl ethers and perfluorinated compounds in the atmosphere of North Greenland. Environ. Pollut. 217, 4-10

Brusseau ML, Guo B. 2022. PFAS concentrations in soil versus soil porewater: Mass distributions and the impact of adsorption at air-water interfaces. Chemosphere 202:134938, ISSN 0045-6535, doi: 10.1016/j.chemosphere.2022.134938.

Butt, C.M.; Muir, D.C.G.; Mabury, S.A. 2014. Biotransformation pathways of fluorotelomer-based polyfluoroalkyl substances: A review. Environ. Toxicol. Chem. 33, 243-267.

Campos Pereira H, Ullberg M, Kleja DB, Gustafsson JP, Ahrens L. 2018. Sorption of perfluoroalkyl substances (PFASs) to an organic soil horizon - Effect of cation composition and pH. Chemosphere. 207:183-191. doi: 10.1016/j.chemosphere.2018.05.012.

Casal, P.; Zhang, Y.; Martin, J.W.; Pizarro, M.; Jiménez, B.; Dachs, J. 2017. Role of snow deposition of perfluoroalkylated substances at coastal Livingston Island (Maritime Antarctica). Environ. Sci. Technol. 51, 8460-8470.

Cedergreen N. Quantifying synergy: a systematic review of mixture toxicity studies within environmental toxicology. 2014. PLoS One 9(5):e96580. doi: 10.1371/journal.pone.0096580.

Death C, Bell C, Champness D, Milne C, Reichman S, Hagen T. 2021. Per- and polyfluoroalkyl substances (PFAS) in livestock and game species: A review, Science of The Total Environment, Volume 774, 2021, doi: 10.1016/j.scitotenv.2020.144795.

De Silva A, Armitage JM, Bruton TA, Dassuncao C, Heiger-Bernays W, Hu XC, Kärrman A, Kelly B, Ng C, Robuck A, Sun M, Webster TF, Sunderland EM. 2021. PFAS exposure pathways for humans and wildlife: A synthesis of current knowledge and key gaps in understanding. Environ. Toxicol. Chem. 40, 631-657.

Draborg H, Tsitonaki K. 2023. Undersøgelser af CRUCIAL forsøget for PFAS påvirkning fra spildevandsslam. WSP: Projektnummer 22001604.

EC, 2003. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market.

ECETOC. 2013. Development of interim guidance for the inclusion of non-extractable residues (NER) in the risk assessment of chemicals. Technical Report No. 118. ISSN-2079-1526-118 (online).

ECHA. 2013. Member State Committee support document for identification of Pentadecafluorooctanoic Acid (PFOA) as a Substance of Very High Concern because of its CMR and PBT properties. Adopted on 14 June 2013. https://echa.europa.eu/documents/10162/8059e342-1092-410f-bd85-80118a5526f5.

ECHA. 2014. Annex XV Restriction Report. Proposal for a Restriction. Perfluorooctanoic acid (PFOA), PFOA salts and PFOA-related substances.

ECHA. 2016. European Chemicals Agency. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.16: Environmental exposure assessment. ECHA-16-G-03-EN. ISBN: 978-92-9247-775-2.

ECHA. 2019. Options to address non-extractable residues in regulatory persistence assessment. Background note.

EFSA. 2019. European Food Safety Authority. Guidance on the assessment of the safety of feed additives for the environment. EFSA Journal 17(4):5648. doi: 10.2903/j.efsa.2019.5648

EFSA. 2020. Scientific Opinion on the risk to human health related to the presence of perfluoroalkyl substances in food. EFSA Journal 18:6223. doi: 10.2903/j.efsa.2020.6223

Ellis DA, Martin JW, De Silva AO, Mabury SA, Hurley MD, Andersen MPS, Wallington TJ. 2004. Degradation of fluorotelomer alcohols: A likely atmospheric source of perfluorinated carboxylic acids. Environ. Sci. Technol. 38: 3316-3321.

EMA. 2006. European Medicines Agency. Guideline on the environmental risk assessment of medicinal products for human use. Doc. Ref. EMEA/CHMP/SWP/4447/00 corr 1*

EMA. 2007. European Food Safety Authority. Guidance on environmental impact assessment for veterinary medicinal products in support of the VICH guidelines GL6 and GL38. EMEA/CVMP/ERA/418282/2005-corr

Enevoldsen R, Juhler RK. 2010. Perfluorinated compounds (PFCs) in groundwater and aqueous soil extracts: using inline SPE-LC-MS/MS for screening and sorption characterisation of perfluorooctane sulphonate and related compounds. Anal Bioanal Chem 398: 1161–1172. doi: 10.1007/s00216-010-4066-0

EU. 2020a. Directive (EU) 2020/2184 of the European Parliament and of the Council of 16 December 2020 on the quality of water intended for human consumption. Official Journal of the European Union L435/1-62

EU. 2020b. Chemicals Strategy for Sustainability – Towards a Toxic-Free Environment. Communication from the Commission to the European Parliament, the Council, the European Economic and Social Committee and the Committee of the Regions. COM(2020) 667 final, Brussels, 14 October 2020.

Fenton, S.E.; Ducatman, A.; Boobis, A.; DeWitt, J.C.; Lau, C.; Ng, C.; Smith, J.S.; Roberts, S.M. 2021. Per- and polyfluoroalkyl substance toxicity and human health review: Current state of knowledge and strategies for informing future research. Environ. Toxicol. Chem. 40, 606-630.

Gassmann M, Weidemann E, Stahl T. 2021. Combined leaching and plant uptake simulations of PFOA and PFOS under field conditions. Environ Sci Pollut Res Int. 28(2):2097-2107. doi: 10.1007/s11356-020-10594-6.

GEUS 2023. De Nationale Geologiske Undersøgelser for Danmark og Grønland. Forekomst af PFAS-stoffer i de almene vandværkers boringskontrol for periode 1/1-2022 til 31/12-2022. https://www.geus.dk/Media/638089490651606185/BK%202022%20Q4%20PFAS.pdf

Glaser D., Lamoureux E, Opdyke D, LaRoe S, Reidy D, Connolly J. 2021. The impact of precursors on aquatic exposure assessment for PFAS: Insights from bioaccumulation modeling. Integrated Environmental Assessment and Management 17: 705-715. https://doi.org/10.1002/ieam.4414

Glüge, J.; Scheringer, M.; Cousins, I.T.; DeWitt, J.C.; Goldenman, G.; Herzke, D.; Lohmann, R.; Ng, C.A.; Trier, X.; Wang, Z. 2020. An overview of the uses of per- and polyfluoroalkyl substances (PFAS). Environ. Sci. Process Impacts 22, 2345-2373.

Higgins CP, Luthy RG. 2006. Sorption of perfluorinated surfactants on sediments. Environ Sci Technol. 40(23):7251-6. doi: 10.1021/es061000n.

Høisæter Å, Breedveld GD. 2022. Leaching potential of per- and polyfluoroalkyl substances from source zones with historic contamination of aqueous film forming foam - a surfactant mixture problem. Environmental Advances 8:100222.https://doi.org/10.1016/j.envadv.2022.100222.

ITRC. 2020. History and use of per- and polyfluoroalkyl substances (PFAS). Interstate Technology Regulatory Council, Washington DC, USA.

Jensen J, Jepsen SE. 2005. The production, use and quality of sewage sludge in Denmark. Waste Manag. 25:239-47. doi: 10.1016/j.wasman.2004.08.011. PMID: 15823740.

Johansson JH, Yan H, Berger U, Cousins IT. 2017. Water-to-air transfer of branched and linear PFOA: influence of pH, concentration and water type. Emerg Contamin 3: 46-53

Johnson GR. 2022. PFAS in soil and groundwater following historical land application of biosolids. Water Res. Mar 1;211:118035. doi: 10.1016/j.watres.2021.118035.

Kabiri S, Tucker W, Navarro DA, Bräunig J, Thompson K, Knight ER, Nguyen TMH, Grimison C, Barnes CM, Higgins CP, Mueller JF, Kookana RS, McLaughlin MJ. 2022. Comparing the Leaching Behavior of Per- and Polyfluoroalkyl Substances from Contaminated Soils Using Static and Column Leaching Tests. Environ Sci Technol. 56(1):368-378. doi: 10.1021/acs.est.1c06604.

Kato, K.; Wong, L.-Y.; Jia, L.T.; Kuklenyik, Z.; Calafat, A.M. 2011. Trends in exposure to polyfluoroalkyl chemicals in the U.S. population: 1999-2008. Environ. Sci. Technol. 45, 8047-8045.

Krippner J, Falk S, Brunn H, Georgii S, Schubert S, Stahl T. 2015. Accumulation potentials of perfluoroalkyl carboxylic acids (PFCAs) and perfluoroalkyl sulfonic acids (PFSAs) in maize (Zea mays). J Agric Food Chem. 63:3646-3653. doi: 10.1021/acs.jafc.5b00012.

Le, S. T., Kibbey, T. C. G., Weber, K. P. Glamore, W. C., O'Carroll, D. M. 2021. A group-contribution model for predicting the physicochemical behavior of PFAS components for understanding environmental fate. Science of The Total Environment, 764, 142882. https://doi.org/10.1016/j.scitotenv.2020.142882.

Li Y, Oliver DP, Kookana RS. 2018. A critical analysis of published data to discern the role of soil and sediment properties in determining sorption of per and polyfluoroalkyl substances (PFASs). Sci Total Environ. 628-629:110-120. doi: 10.1016/j.scitotenv.2018.01.167.

Li F, Fang X, Zhou Z, Liao X, Zou J, Yuan B, Sun W. 2019. Adsorption of perfluorinated acids onto soils: Kinetics, isotherms, and influences of soil properties. Sci Total Environ. 2019: 504-514. doi: 10.1016/j.scitotenv.2018.08.209.

Liu M, Munoz G, Duy SV, Sauvé S, Liu J. 2022. Per- and Polyfluoroalkyl Substances in Contaminated Soil and Groundwater at Airports: A Canadian Case Study. Environmental Science & Technology 2022 56 (2), 885-895. DOI: 10.1021/acs.est.1c04798.

Lyu X, Xiao F, Shen C, Chen J, Park CM, Sun Y, Flury M, Wang D. 2022. Per- and polyfluoroalkyl substances (PFAS) in subsurface environments: Occurrence, fate, transport, and research prospect. Reviews of Geophysics, 60, e2021RG000765. https://doi.org/10.1029/2021RG000765.

McLachlan MS, Felizeter S, Klein M, Kotthoff M, De Voogt P. 2019. Fate of a perfluoroalkyl acid mixture in an agricultural soil studied in lysimeters Chemosphere 223: 180-187. Doi: 10.1016/j.chemosphere.2019.02.012.

Miao Y, Guo X, Dan Peng, Fan T, Yang C. 2017. Rates and equilibria of perfluorooctanoate (PFOA) sorption on soils from different regions of China. Ecotoxicol Environ Saf. 139:102-108. doi: 10.1016/j.ecoenv.2017.01.022.

Miljøstyrelsen. 2009. Spildevandsslam fra kommunale og private renseanlæg i 2005. Orientering fra Miljøstyrelsen Nr. 3 2009.

Miljøstyrelsen. 2013. Livscyklusvurdering og samfundsøkonomisk analyse for anvendelse af spildevandsslam. Miljøprojekt nr. 1459. ISBN: 978-87-92903-81-5.

Miljøstyrelsen. 2016. Parametervurdering i forbindelse med screening af overfladevandstruende forureninger. Editors: Roost S, Nielsen SS, Nicolajsen ES. ISBN: 978-87-93435-13-1.

Miljøstyrelsen. 2017. Det nationale overvågningsprogram for vand og natur 2017-21. ISBN 978-97-7120-862-7.

Miljøstyrelsen. 2022. Gennemførelse og anvendelse af slam-direktivet. Afrapportering. Orientering fra Miljøstyrelsen nr. 57.

Muir D, Bossi R, Carlsson P, Evans M, De Silva A, Halsall C, Rauert C, Herzke D, Hung H, Letcher R, Rigét F, Roos A. 2019. Levels and trends of poly- and perfluoroalkyl substances in the Arctic environment – An update. Emerg. Contam. 5, 240-271.

Nguyen TMH, Bräunig J, Thompson K, Thompson J, Kabiri S, Navarro DA, Kookana RS, Grimison C, Barnes CM, Higgins CP, McLaughlin MJ, Mueller JF. 2020. Influences of Chemical Properties, Soil Properties, and Solution pH on Soil-Water Partitioning Coefficients of Per- and Polyfluoroalkyl Substances (PFASs). Environ Sci Technol 54(24):15883-15892. doi: 10.1021/acs.est.0c05705.

Ortega-Calvo JJ, Harmsen J, Parsons JR, Semple KT, Aitken MD, Ajao C, Eadsforth C, Galay Burgos M, Naidu R, Oliver R, Peijnenburg WJ,, Römbke J, Streck G, Versonnen B. 2015. From Bioavailability Science to Regulation of Organic Chemicals. Environmental Science & Technology 49(17):10255. DOI: 10.1021/acs.est.5b02412

Pettersson M, Ländell M, Ohlsson Y, Berggren KD, Tiberg C. 2015. Preliminära riktvärden för högfluorerade ämnen (PFAS) i mark och grundvatten. Statens geotekniska institut, SGI Publikation 21, Linköping.

Rayner J, Slee D, Falvey S, Kookana R, Bekele E, Stevenson G, Lee A, Davis G. 2021. Intercomparison of Pfas Leaching Methods for Aged Field Soils, Inclusive of Compositional Changes, the Effects of Soil:Water Ratios, Tumbling and Ph Variations. Available at SSRN: https://ssrn.com/abstract=3995255 or http://dx.doi.org/10.2139/ssrn.3995255

Rigét F, Vorkamp K, Bossi R, Sonne C, Letcher RJ, Dietz R. 2016. Twenty years of monitoring of persistent organic pollutants in Greenland biota. A review. Environ. Pollut. 217, 114-123.

Sabljić A, Güsten H, Verhaar H, Hermens J. 1995. QSAR modelling of soil sorption. Improvements and systematics of log K_{OC} vs. log K_{OW} correlations. Chemosphere 31: 4489-4514. https://doi.org/10.1016/0045-6535(95)00327-5.

Schäffer A, Kästner M, Trapp S. 2018. A unified approach for including non-extractable residues (NER) of chemicals and pesticides in the assessment of persistence. Environ Sci Eur. 30:51. doi: 10.1186/s12302-018-0181-x.

Schaefer CE, Lavorgna GM, Lippincott DR, Nguyen D, Christie E, Shea S, O'Hare S, Lemes MCS, Higgins CP, Field J. 2022. A field study to assess the role of air-water interfacial sorption on PFAS leaching in an AFFF source area. Journal of Contaminant Hydrology 248: 104001, ISSN 0169-7722, doi: 10.1016/j.jconhyd.2022.104001.

Sepulvado JG, Blaine AC, Hundal LS, Higgins CP. 2011. Occurrence and Fate of Perfluorochemicals in Soil Following the Land Application of Municipal Biosolids. Environmental Science & Technology 45 (19), 8106-8112. DOI: 10.1021/es103903d

Stahl T, Riebe RA, Falk S, Failing K, Brunn H. 2013. Long-term lysimeter experiment to investigate the leaching of perfluoroalkyl substances (PFASs) and the carry-over from soil to plants: results of a pilot study. J Agric Food Chem. 61:1784-1793. doi: 10.1021/jf305003h.

Thodsen H, Tornbjerg H, Rolighed J, Baattrup-Pedersen A, Larsen SE, Ovesen NB, Blicher-Mathiesen G, Kjeldgaard A. 2021. Vandløb 2020. NOVANA. Aarhus Universitet, DCE – Nationalt Center for Miljø og Energi, 82 s. - Videnskabelig rapport nr. 473
http://dce2.au.dk/pub/SR473.pdf

UNEP. 2006. Report of the Persistent Organic Pollutants Review Committee on the work of its second meeting. Addendum: Risk profile on perfluorooctane sulfonate. UNEP/POPS/POPRC.2/17/Add.5

UNEP. 2019. Perfluorohexane sulfonic acid (PFHxS), its salts and PFHxS-related compounds. Decision POPRC-15/1. Persistent Organic Pollutants Review Committee.

Vorkamp, K.; Castaño, A.; Antignac, J.-P.; Boada, L.D.; Cequier, E.; Covaci, A.; Esteban López, M.; Haug, L.S.; Kasper-Sonnenberg, M.; Koch, H.M.; Luzardo, O.P.; Osīte, A.; Rambaud, L.; Pinorini, M.-T.; Sabbioni, G.; Thomsen, C. 2021. Biomarkers, matrices and analytical methods targeting human exposure to chemicals selected for a European human biomonitoring initiative. Environ. Int. 146, 106082.

Wackett LP. 2021. Nothing lasts forever: understanding microbial biodegradation of polyfluorinated compounds and perfluorinated alkyl substances. Microbial Biotechnology 15: 773– 792.

Weidemann E, Lämmer R, Stahl T, Göckener B, Bücking M, Breuer J, Kowalczyk J, Just H, Boeddinghaus RS, Gassmann M. 2022. Leaching and Transformation of Perfluoroalkyl Acids and Polyfluoroalkyl Phosphate Diesters in Unsaturated Soil Column Studies. Environ Toxicol Chem. 41(9):2065-2077. doi: 10.1002/etc.5417.

Xu B, Liu S, Zhou JL, Zheng C, Weifeng J, Chen B, Zhang T, Qiu W. 2021. PFAS and their substitutes in groundwater: Occurrence, transformation and remediation. J Hazard Mater. 412:125159. doi: 10.1016/j.jhazmat.2021.125159.

Zareitalabad P, Siemens J, Hamer M, Amelung W. 2013. Perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) in surface waters, sediments, soils and wastewater – A review on concentrations and distribution coefficients. Chemosphere 91: 725-732. doi: 10.1016/j.chemosphere.2013.02.024.

Zhang W, Pang S, Lin Z, Mishra S, Bhatt P, Chen S. 2021. Biotransformation of perfluoroalkyl acid precursors from various environmental systems: advances and perspectives. Environmental Pollution 272:115908. https://doi.org/10.1016/j.envpol.2020.115908.

Zhang Q, Cao H, Liang Y. 2021. Plant uptake and soil fractionation of five ether-PFAS in plant-soil systems. Science of The Total Environment 771: 144805, https://doi.org/10.1016/j.scitotenv.2020.144805.

Zhang Z, Sarkar D, Biswas JK, Datta R. 2022. Biodegradation of per- and polyfluoroalkyl substances (PFAS): A review. Bioresource Technology 344, Part B, 126223, https://doi.org/10.1016/j.biortech.2021.126223.

Zhu X, Song X, Schwarzbauer J. 2021. First insights into the formation and long-term dynamic behaviors of nonextractable perfluorooctanesulfonate and its alternative 6:2 chlorinated

polyfluorinated ether sulfonate residues in a silty clay soil. Sci Total Environ761:143230. doi: 10.1016/j.scitotenv.2020.143230.

Appendix A
Chemical-Physical properties of PFAS

It is beyond the scope and resources of this report to review all published literature on the chemical and physical properties of PFAS. It has therefore been decided to refer to the very exhaustive compilation of data presented and compiled by the US Interstate Technology and Regulatory Council (ITRC) online. The document includes the resources that the ITRC PFAS Team has developed since it began work in 2017. More information can be found at: https://pfas-1.itrcweb.org/

The ITRC PFAS Technical and Regulatory Guidance Document contains Tables for chemical and physical properties at web page: https://pfas-1.itrcweb.org/4-physical-and-chemical-properties/

Please also see ITRC Disclaimer https://pfas-1.itrcweb.org/about-itrc/#disclaimer

Molecular Weight

From ITRC the following molecular weights (g/mol) are collected

PFOA: 414.1
PFOS: 500.1
PFNA: 464.1
PFHxS: 400.1

Vapour Pressure
ITRC reviews the vapour pressure for PFAS and reported values for PFOS and PFOA in the range of <0,01-16,98 and 0.03-1333 Pa, respectively. Much of the data on PFAS is extrapolated or modeled. If secondary sources are omitted the ranges come out as 2.0-1700 and 16.98 Pa, respectively.

The EU dossier for PFOS stabling EQS values (EU 2011) reports a vapour pressure of $3.31x10^{-4}$ Pa (measured for the potassium salt), but it is stressed that the result may be associated uncertainties, as it is suggested that this result may be due to volatile impurities in the substance. The ECHA report on PFOA (ECHA 2013) summarized the vapour pressure for PFOA and found values between 2.3 and 128 Pa.

As a conservative approach, a low vapour pressure of 0.01 Pa for all PFAS is chosen as a worst-case consideration, which basically neglects evaporation as a dissipation process.

Solubility
ITRC reviews the solubility of PFAS and concludes that currently experimentally measured data for the solubility of PFAS in water are available for just a few of the more studied compounds. Most cited values are based on predicted or modeled values and the input values to these calculations may themselves be estimates. Further, because PFAS can form micelles and hemi-micelles, the reported water solubilities may include microdispersions of micelles in addition to truly solubilized molecules. ITRC reviews the solubility for PFOA and PFOS in the range of <0.01-9524 and <0.01-910 mg/L, respectively. If secondary sources are omitted, the ranges come out as 64-9524 and 7.7-910 mg/L. The EU dossier for PFOS (EU 2011), establishing EQS values reports a solubility of 370 mg/L I freshwaters. The ECHA report on PFOA

(ECHA 2013) lists two studies covering solubility of 9500 and 4140 mg/L.

For calculations related to leaching (ground water and freshwater), solubility of 9500 mg/L for PFOA and 370 mg/L for PFOS are selected as input values. For worst-case calculations for the soil environment, solubility of 64 mg/L for PFOA and 7.7 mg/L for PFOS are selected as input values.

For PFNA and PFHxS, far less experimental data is available. ECHA (2015) reports a lack of data on solubility for PFNA, whereas ITCR lists an extrapolated solubility of 12 mg/L originating from Kim et al. (2015), who - with the help of improved quantitative structure–property relationship (QSPR) - predicted the solubility of PFNA. On the Hazardous Substances Data Bank[13] (part of PubChem, which is an open chemistry database at the National Institutes of Health, US), the solubility is listed as 0.0625 mg/L at 25 C and reported as calculated by EPI Suite.

ECHA (2017) reports a solubility of 2.3 mg/L of PFHxS. ITRC reported modelled solubility between 0.62 and 6.0 mg/L for PFHxS using the EPI Suite.

This report will use a solubility of 0.0625 mg/L for PFNA and 2.3 mg/L for PFHxS.

Organic Carbon Normalized Sorption Coefficient (K_{oc})

K_{oc} is a metric commonly used to quantify the potential of a given dissolved compound to associate with or sorb to organic matter occurring in soil. Shorter chained PFAS are more soluble in water, while the longer chained PFAS adsorb and partition more into (organic) soils. Where no measured Koc value is available, estimation can be used based on correlation with the Kow or water solubility.

For common PFAS, like PFOA and PFOS, studies have suggested K_{oc} can be appropriately defined as a distribution coefficient (K_d) normalized to organic carbon content, thus implying Koc represents a singular process of hydrophobic interaction. However, broader reviews highlight the complexity and variability of processes that may contribute to the sorption of PFAS. Due to the uncertainty regarding K_{oc}, it may be appropriate to evaluate mobility and transport of an individual PFAS using a range of partitioning coefficients to account for uncertainties in this parameter.

Zareitalabad et al. (2013) reviewed the distribution coefficients of PFOS and PFOA in soils and sediments and concluded based upon sorption experiments that PFAS sorption can be described reasonably well as a partitioning-like process. They calculated an average and median log Koc of approximately 2.1 and 2.1 for PFOA and 3.0 and 2.8 for PFOS. They also suggest that effective log Koc distribution coefficients for the field situation may be close to 3.7 for PFOA and 4.2 for PFOS, suggesting that field-based distribution coefficients may be larger than lab-based coefficients. Hence, applying lab-based log Koc distribution coefficients can result in a serious overestimation of PFAS concentrations in water and in turn to an underestimation of the residence time of PFOA and PFOS in contaminated soils. In this report, limited information from field studies has been available for the majority of PFAS, which is why lab-based Koc values generally have been used.

ITRC reviews the reported log K_{oc} of PFAS and finds log K_{oc} for PFOA in the range of 0.041-5.0 and for PFOS in the range of 1.2-5.2. The PFOS dossier from EU suggested a Koc of 66 L/kg. However, this seems very low, and the report also list the value having “low reliability”

[13] https://pubchem.ncbi.nlm.nih.gov/source/hsdb/8040

and no reference to original literature is given.

To establish a K_{oc} value for PFOS, Pettersson et al. (2015) compiled measured Koc values for PFOS from five previous studies covering 13 soils (see Table A2). Based on the data from 13 soils, the mean, median, 10th and 90th percentiles were calculated as 1935, 987, 685 and 3638, respectively.

In a number of batch experiments, Campos Pereira et al. (2018) investigated the effect of solution pH and calculated soil organic matter (SOM) on the sorption of 14 PFASs onto a soil as a function of pH and added concentrations of Al^{3+}, Ca^{2+} and Na^{+}. The results are presented below in Table A1, and data are used for all PFAS other than PFOS.

Nguyen et al. (2020) assessed the soil−water partitioning behavior of a wider range of PFAS and soil types. The PFAS studied include perfluoroalkyl carboxylates (PFCAs), perfluoroalkane sulfonates (PFSAs), fluorotelomer sulfonates (FTSs), nonionic perfluoroalkane sulfonamides (FASAs), cyclic PFAS (PFEtCHxS), per- and polyfluoroalkyl ether acids, and three AFFF-related zwitterionic PFASs (AmPr-FHxSA, TAmPr-FHxSA, 6:2 FTSA-PrB). Log K_d values ranged from <0 to approx. 3 and were chain length- and molecular weight-dependent. Across all soils, the K_d values of all short-chain PFASs were similar and varied less compared to long-chain PFAS. Solution pH could change both PFAS speciation and soil chemistry affecting surface complexation and electrostatic processes. The K_d values of all PFASs increased when solution pH decreased from approximately eight to three. Short-chain PFASs were less sensitive to solution pH than long-chain PFASs.

Below is listed the compiled Koc and K_d values**.** Table 2.4 contains a summary of data.

TABLE A.1. Compiled K_{oc} for PFAS used in model calculations

PFBS							
Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median:			pH3,4			1,8000	
N:						58,0000	
S1	0,7	3,4	0,66	94,2857	-0,1805	1,9744	Nguyen et al. 2020
S2	0,37	3,4	0,54	145,9459	-0,2676	2,1642	Nguyen et al. 2020
S3	0,08	3,4	0,36	450,0000	-0,4437	2,6532	Nguyen et al. 2020
S4	0,25	3,4	0,31	124,0000	-0,5086	2,0934	Nguyen et al. 2020
S5	2,23	3,4	0,48	21,5247	-0,3188	1,3329	Nguyen et al. 2020
S6	4,9	3,4	1,08	22,0408	0,0334	1,3432	Nguyen et al. 2020
S7	0,13	3,4	0,36	276,9231	-0,4437	2,4424	Nguyen et al. 2020
S8	0,4	3,4	0,22	55,0000	-0,6576	1,7404	Nguyen et al. 2020
S9	1,19	3,4	0,54	45,3782	-0,2676	1,6568	Nguyen et al. 2020
S10	0,17	3,4	0,47	276,4706	-0,3279	2,4416	Nguyen et al. 2020
S1	0,7	5,2	0,48	68,5714	-0,3188	1,8361	Nguyen et al. 2020
S2	0,37	5,2	0,43	116,2162	-0,3665	2,0653	Nguyen et al. 2020
S3	0,08	5,2	0,28	350,0000	-0,5528	2,5441	Nguyen et al. 2020
S4	0,25	5,2	0,25	100,0000	-0,6021	2,0000	Nguyen et al. 2020
S5	2,23	5,2	0,37	16,5919	-0,4318	1,2199	Nguyen et al. 2020
S6	4,9	5,2	0,87	17,7551	-0,0605	1,2493	Nguyen et al. 2020
S7	0,13	5,2	0,31	238,4615	-0,5086	2,3774	Nguyen et al. 2020
S8	0,4	5,2	0,07	17,5000	-1,1549	1,2430	Nguyen et al. 2020
S9	1,19	5,2	0,25	21,0084	-0,6021	1,3224	Nguyen et al. 2020
S10	0,17	5,2	0,36	211,7647	-0,4437	2,3259	Nguyen et al. 2020
S1	0,7	7,2	0,41	58,5714	-0,3872	1,7677	Nguyen et al. 2020
S2	0,37	7,2	0,36	97,2973	-0,4437	1,9881	Nguyen et al. 2020
S3	0,08	7,2	0,25	312,5000	-0,6021	2,4949	Nguyen et al. 2020
S4	0,25	7,2	0,17	68,0000	-0,7696	1,8325	Nguyen et al. 2020

S5	2,23	7,2	0,34	15,2466	-0,4685	1,1832	Nguyen et al. 2020
S6	4,9	7,2	0,5	10,2041	-0,3010	1,0088	Nguyen et al. 2020
S7	0,13	7,2	0,2	153,8462	-0,6990	2,1871	Nguyen et al. 2020
S8	0,4	7,2	0,05	12,5000	-1,3010	1,0969	Nguyen et al. 2020
S9	1,19	7,2	0,24	20,1681	-0,6198	1,3047	Nguyen et al. 2020
S10	0,17	7,2	0,31	182,3529	-0,5086	2,2609	Nguyen et al. 2020
S1	0,7	8,3	0,5	71,4286	-0,3010	1,8539	Nguyen et al. 2020
S2	0,37	8,3	0,39	105,4054	-0,4089	2,0229	Nguyen et al. 2020
S3	0,08	8,3	0,23	287,5000	-0,6383	2,4586	Nguyen et al. 2020
S4	0,25	8,3	0,19	76,0000	-0,7212	1,8808	Nguyen et al. 2020
S5	2,23	8,3	0,35	15,6951	-0,4559	1,1958	Nguyen et al 2020
S6	4,9	8,3	0,53	10,8163	-0,2757	1,0341	Nguyen et al. 2020
S7	0,13	8,3	0,19	146,1538	-0,7212	2,1648	Nguyen et al. 2020
S8	0,4	8,3	0,08	20,0000	-1,0969	1,3010	Nguyen et al. 2020
S9	1,19	8,3	0,23	19,3277	-0,6383	1,2862	Nguyen et al. 2020
S10	0,17	8,3	0,29	170,5882	-0,5376	2,2319	Nguyen et al. 2020
Al pH 3		2,8				−0,1	Campos Periera et al. 2018
Al pH 4		4				1,8000	Campos Periera et al. 2018
Al pH 5		4,8				2,2000	Campos Periera et al. 2018
Al pH 6		5,7				1,9000	Campos Periera et al. 2018
Al pH 3		2,8				−0,7	Campos Periera et al. 2018
Al pH 4		4				1,9000	Campos Periera et al. 2018
Al pH 5		4,7				2,0000	Campos Periera et al. 2018
Al pH 6		5,7				1,9000	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9					Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5					Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				1,3000	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9					Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,6					Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				0,8000	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9					Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9				1,1000	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,9					Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6				0,9000	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9				1,1000	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9					Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,8				0,7000	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6				0,8000	Campos Periera et al. 2018
Na pH 3		3,1					Campos Periera et al. 2018
Na pH 4		4,2					Campos Periera et al. 2018
Na pH 5		4,9				0,5000	Campos Periera et al. 2018
Na pH 6		5,8				1,4000	Campos Periera et al. 2018
Na pH 3		3,1					Campos Periera et al. 2018
Na pH 4		4,2					Campos Periera et al. 2018
Na pH 5		4,9					Campos Periera et al. 2018
Na pH 6		5,8				1,9000	Campos Periera et al. 2018
Jyndevad	1	6,1	0,41	41,0000		1,6128	Enevoldsen, Juhler 2010
Sj. Odde	0,42	7,6	0,007	1,6667		0,2218	Enevoldsen, Juhler 2010

PFPS

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						1,853872	
N						40	
S1	0,7	3,4	0,66	94,2857	-0,1805	1,9744	Nguyen et al. 2020
S2	0,37	3,4	0,54	145,9459	-0,2676	2,1642	Nguyen et al. 2020
S3	0,08	3,4	0,36	450,0000	-0,4437	2,6532	Nguyen et al. 2020
S4	0,25	3,4	0,31	124,0000	-0,5086	2,0934	Nguyen et al. 2020
S5	2,23	3,4	0,48	21,5247	-0,3188	1,3329	Nguyen et al. 2020
S6	4,9	3,4	1,08	22,0408	0,0334	1,3432	Nguyen et al. 2020
S7	0,13	3,4	0,36	276,9231	-0,4437	2,4424	Nguyen et al. 2020
S8	0,4	3,4	0,22	55,0000	-0,6576	1,7404	Nguyen et al. 2020
S9	1,19	3,4	0,54	45,3782	-0,2676	1,6568	Nguyen et al. 2020
S10	0,17	3,4	0,47	276,4706	-0,3279	2,4416	Nguyen et al. 2020
S1	0,7	5,2	0,48	68,5714	-0,3188	1,8361	Nguyen et al. 2020
S2	0,37	5,2	0,43	116,2162	-0,3665	2,0653	Nguyen et al. 2020
S3	0,08	5,2	0,28	350,0000	-0,5528	2,5441	Nguyen et al. 2020
S4	0,25	5,2	0,25	100,0000	-0,6021	2,0000	Nguyen et al. 2020
S5	2,23	5,2	0,37	16,5919	-0,4318	1,2199	Nguyen et al. 2020
S6	4,9	5,2	0,87	17,7551	-0,0605	1,2493	Nguyen et al. 2020
S7	0,13	5,2	0,31	238,4615	-0,5086	2,3774	Nguyen et al. 2020
S8	0,4	5,2	0,07	17,5000	-1,1549	1,2430	Nguyen et al. 2020
S9	1,19	5,2	0,25	21,0084	-0,6021	1,3224	Nguyen et al. 2020
S10	0,17	5,2	0,36	211,7647	-0,4437	2,3259	Nguyen et al. 2020
S1	0,7	7,2	0,41	58,5714	-0,3872	1,7677	Nguyen et al. 2020
S2	0,37	7,2	0,36	97,2973	-0,4437	1,9881	Nguyen et al. 2020
S3	0,08	7,2	0,25	312,5000	-0,6021	2,4949	Nguyen et al. 2020
S4	0,25	7,2	0,17	68,0000	-0,7696	1,8325	Nguyen et al. 2020
S5	2,23	7,2	0,34	15,2466	-0,4685	1,1832	Nguyen et al. 2020
S6	4,9	7,2	0,5	10,2041	-0,3010	1,0088	Nguyen et al. 2020
S7	0,13	7,2	0,2	153,8462	-0,6990	2,1871	Nguyen et al. 2020
S8	0,4	7,2	0,05	12,5000	-1,3010	1,0969	Nguyen et al. 2020
S9	1,19	7,2	0,24	20,1681	-0,6198	1,3047	Nguyen et al. 2020
S10	0,17	7,2	0,31	182,3529	-0,5086	2,2609	Nguyen et al. 2020
S1	0,7	8,3	0,5	71,4286	-0,3010	1,8539	Nguyen et al. 2020
S2	0,37	8,3	0,39	105,4054	-0,4089	2,0229	Nguyen et al. 2020
S3	0,08	8,3	0,23	287,5000	-0,6383	2,4586	Nguyen et al. 2020
S4	0,25	8,3	0,19	76,0000	-0,7212	1,8808	Nguyen et al. 2020
S5	2,23	8,3	0,35	15,6951	-0,4559	1,1958	Nguyen et al. 2020
S6	4,9	8,3	0,53	10,8163	-0,2757	1,0341	Nguyen et al. 2020
S7	0,13	8,3	0,19	146,1538	-0,7212	2,1648	Nguyen et al. 2020
S8	0,4	8,3	0,08	20,0000	-1,0969	1,3010	Nguyen et al. 2020
S9	1,19	8,3	0,23	19,3277	-0,6383	1,2862	Nguyen et al. 2020
S10	0,17	8,3	0,29	170,5882	-0,5376	2,2319	Nguyen et al. 2020

PFHxS

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						2,311946	
N						71	
S1	0,7	3,4	2,29	327,1429	0,3598	2,5147	Nguyen et al. 2020
S2	0,37	3,4	2,32	627,0270	0,3655	2,7973	Nguyen et al. 2020
S3	0,08	3,4	1,14	1425,0000	0,0569	3,1538	Nguyen et al. 2020
S4	0,25	3,4	0,75	300,0000	-0,1249	2,4771	Nguyen et al. 2020
S5	2,23	3,4	1,3	58,2960	0,1139	1,7656	Nguyen et al. 2020
S6	4,9	3,4	7,77	158,5714	0,8904	2,2002	Nguyen et al. 2020
S7	0,13	3,4	0,82	630,7692	-0,0862	2,7999	Nguyen et al. 2020
S8	0,4	3,4	2,05	512,5000	0,3118	2,7097	Nguyen et al. 2020
S9	1,19	3,4	4,11	345,3782	0,6138	2,5383	Nguyen et al. 2020
S10	0,17	3,4	1,03	605,8824	0,0128	2,7824	Nguyen et al. 2020
S1	0,7	5,2	1,36	194,2857	0,1335	2,2884	Nguyen et al. 2020
S2	0,37	5,2	0,97	262,1622	-0,0132	2,4186	Nguyen et al. 2020
S3	0,08	5,2	0,67	837,5000	-0,1739	2,9230	Nguyen et al. 2020
S4	0,25	5,2	0,62	248,0000	-0,2076	2,3945	Nguyen et al. 2020
S5	2,23	5,2	0,69	30,9417	-0,1612	1,4905	Nguyen et al. 2020
S6	4,9	5,2	6,45	131,6327	0,8096	2,1194	Nguyen et al. 2020
S7	0,13	5,2	0,83	638,4615	-0,0809	2,8051	Nguyen et al. 2020
S8	0,4	5,2	0,41	102,5000	-0,3872	2,0107	Nguyen et al. 2020
S9	1,19	5,2	0,87	73,1092	-0,0605	1,8640	Nguyen et al. 2020
S10	0,17	5,2	0,74	435,2941	-0,1308	2,6388	Nguyen et al. 2020
S1	0,7	7,2	0,77	110,0000	-0,1135	2,0414	Nguyen et al. 2020
S2	0,37	7,2	0,69	186,4865	-0,1612	2,2706	Nguyen et al. 2020
S3	0,08	7,2	0,4	500,0000	-0,3979	2,6990	Nguyen et al. 2020
S4	0,25	7,2	0,45	180,0000	-0,3468	2,2553	Nguyen et al. 2020
S5	2,23	7,2	0,52	23,3184	-0,2840	1,3677	Nguyen et al. 2020
S6	4,9	7,2	2,12	43,2653	0,3263	1,6361	Nguyen et al. 2020
S7	0,13	7,2	0,39	300,0000	-0,4089	2,4771	Nguyen et al. 2020
S8	0,4	7,2	0,28	70,0000	-0,5528	1,8451	Nguyen et al. 2020
S9	1,19	7,2	0,57	47,8992	-0,2441	1,6803	Nguyen et al. 2020
S10	0,17	7,2	0,63	370,5882	-0,2007	2,5689	Nguyen et al. 2020
S1	0,7	8,3	0,71	101,4286	-0,1487	2,0062	Nguyen et al. 2020
S2	0,37	8,3	0,78	210,8108	-0,1079	2,3239	Nguyen et al. 2020
S3	0,08	8,3	0,35	437,5000	-0,4559	2,6410	Nguyen et al. 2020
S4	0,25	8,3	0,34	136,0000	-0,4685	2,1335	Nguyen et al. 2020
S5	2,23	8,3	0,58	26,0090	-0,2366	1,4151	Nguyen et al. 2020
S6	4,9	8,3	2,41	49,1837	0,3820	1,6918	Nguyen et al. 2020
S7	0,13	8,3	0,35	269,2308	-0,4559	2,4301	Nguyen et al. 2020
S8	0,4	8,3	0,24	60,0000	-0,6198	1,7782	Nguyen et al. 2020
S9	1,19	8,3	0,57	47,8992	-0,2441	1,6803	Nguyen et al. 2020
S10	0,17	8,3	0,5	294,1176	-0,3010	2,4685	Nguyen et al. 2020
Al pH 3		2,8				2,9000	Campos Periera et al. 2018
Al pH 4		4				4,1000	Campos Periera et al. 2018
Al pH 5		4,8				3,9000	Campos Periera et al. 2018
Al pH 6		5,7				2,8000	Campos Periera et al. 2018
Al pH 3		2,8				3,5000	Campos Periera et al. 2018
Al pH 4		4				3,8000	Campos Periera et al. 2018
Al pH 5		4,7				3,4000	Campos Periera et al. 2018
Al pH 6		5,7				3,1000	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				2,4000	Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				2,3000	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				2,3000	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				2,4000	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				2,4000	Campos Periera et al. 2018

Ca pH 5 [5 mM]	4,6	2,3000	Campos Periera et al. 2018
Ca pH 6 [5 mM]	5,2	2,3000	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	2,4000	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	2,1000	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,9	1,9000	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	1,9000	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	2,4000	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	2,0000	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,8	2,0000	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	2,0000	Campos Periera et al. 2018
Na pH 3	3,1	2,4000	Campos Periera et al. 2018
Na pH 4	4,2	2,0000	Campos Periera et al. 2018
Na pH 5	4,9	1,8000	Campos Periera et al. 2018
Na pH 6	5,8	1,7000	Campos Periera et al. 2018
Na pH 3	3,1	2,5000	Campos Periera et al. 2018
Na pH 4	4,2	1,9000	Campos Periera et al. 2018
Na pH 5	4,9	1,8000	Campos Periera et al. 2018
Na pH 6	5,8	2,8000	Campos Periera et al. 2018

PFHpS

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						2,762212	
N						40	
S1	0,7	3,4	6,63	947,1429	0,8215	2,9764	Nguyen et al. 2020
S2	0,37	3,4	3,31	894,5946	0,5198	2,9516	Nguyen et al. 2020
S3	0,08	3,4	2,25	2812,5000	0,3522	3,4491	Nguyen et al. 2020
S4	0,25	3,4	2,08	832,0000	0,3181	2,9201	Nguyen et al. 2020
S5	2,23	3,4	3,56	159,6413	0,5514	2,2031	Nguyen et al. 2020
S6	4,9	3,4	26,66	544,0816	1,4259	2,7357	Nguyen et al. 2020
S7	0,13	3,4	2,45	1884,6154	0,3892	3,2752	Nguyen et al. 2020
S8	0,4	3,4	4,88	1220,0000	0,6884	3,0864	Nguyen et al. 2020
S9	1,19	3,4	11,38	956,3025	1,0561	2,9806	Nguyen et al. 2020
S10	0,17	3,4	2,76	1623,5294	0,4409	3,2105	Nguyen et al. 2020
S1	0,7	5,2	3,71	530,0000	0,5694	2,7243	Nguyen et al. 2020
S2	0,37	5,2	3,77	1018,9189	0,5763	3,0081	Nguyen et al. 2020
S3	0,08	5,2	1,2	1500,0000	0,0792	3,1761	Nguyen et al. 2020
S4	0,25	5,2	1,9	760,0000	0,2788	2,8808	Nguyen et al. 2020
S5	2,23	5,2	1,75	78,4753	0,2430	1,8947	Nguyen et al. 2020
S6	4,9	5,2	20,83	425,1020	1,3187	2,6285	Nguyen et al. 2020
S7	0,13	5,2	2,43	1869,2308	0,3856	3,2717	Nguyen et al. 2020
S8	0,4	5,2	1,3	325,0000	0,1139	2,5119	Nguyen et al. 2020
S9	1,19	5,2	2,44	205,0420	0,3874	2,3118	Nguyen et al. 2020
S10	0,17	5,2	1,55	911,7647	0,1903	2,9599	Nguyen et al. 2020
S1	0,7	7,2	2,02	288,5714	0,3054	2,4603	Nguyen et al. 2020
S2	0,37	7,2	1,89	510,8108	0,2765	2,7083	Nguyen et al. 2020
S3	0,08	7,2	0,84	1050,0000	-0,0757	3,0212	Nguyen et al. 2020
S4	0,25	7,2	1,53	612,0000	0,1847	2,7868	Nguyen et al. 2020
S5	2,23	7,2	1,08	48,4305	0,0334	1,6851	Nguyen et al. 2020
S6	4,9	7,2	7,48	152,6531	0,8739	2,1837	Nguyen et al. 2020
S7	0,13	7,2	1,14	876,9231	0,0569	2,9430	Nguyen et al. 2020
S8	0,4	7,2	0,95	237,5000	-0,0223	2,3757	Nguyen et al. 2020
S9	1,19	7,2	1,88	157,9832	0,2742	2,1986	Nguyen et al. 2020
S10	0,17	7,2	2,73	1605,8824	0,4362	3,2057	Nguyen et al. 2020
S1	0,7	8,3	2,05	292,8571	0,3118	2,4667	Nguyen et al. 2020
S2	0,37	8,3	2,14	578,3784	0,3304	2,7622	Nguyen et al. 2020
S3	0,08	8,3	0,8	1000,0000	-0,0969	3,0000	Nguyen et al. 2020
S4	0,25	8,3	1,08	432,0000	0,0334	2,6355	Nguyen et al. 2020
S5	2,23	8,3	1,02	45,7399	0,0086	1,6603	Nguyen et al. 2020
S6	4,9	8,3	8,68	177,1429	0,9385	2,2483	Nguyen et al. 2020
S7	0,13	8,3	1,04	800,0000	0,0170	2,9031	Nguyen et al. 2020
S8	0,4	8,3	0,74	185,0000	-0,1308	2,2672	Nguyen et al. 2020
S9	1,19	8,3	1,89	158,8235	0,2765	2,2009	Nguyen et al. 2020
S10	0,17	8,3	1,23	723,5294	0,0899	2,8595	Nguyen et al. 2020

PFOS

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						3,5952206	
N						87	
S1	0,7	3,4	19,2	2742,8571	1,2833	3,4382	Nguyen et al. 2020
S2	0,37	3,4	14,95	4040,5405	1,1746	3,6064	Nguyen et al. 2020
S3	0,08	3,4	6,49	8112,5000	0,8122	3,9092	Nguyen et al. 2020
S4	0,25	3,4	12,78	5112,0000	1,1065	3,7086	Nguyen et al. 2020
S5	2,23	3,4	10,93	490,1345	1,0386	2,6903	Nguyen et al. 2020
S6	4,9	3,4	103,62	2114,6939	2,0154	3,3252	Nguyen et al. 2020
S7	0,13	3,4	8,01	6161,5385	0,9036	3,7897	Nguyen et al. 2020
S8	0,4	3,4	10,89	2722,5000	1,0370	3,4350	Nguyen et al. 2020
S9	1,19	3,4	29,97	2518,4874	1,4767	3,4011	Nguyen et al. 2020
S10	0,17	3,4	9,6	5647,0588	0,9823	3,7518	Nguyen et al. 2020
S1	0,7	5,2	9,96	1422,8571	0,9983	3,1532	Nguyen et al. 2020
S2	0,37	5,2	3,95	1067,5676	0,5966	3,0284	Nguyen et al. 2020
S3	0,08	5,2	4,27	5337,5000	0,6304	3,7273	Nguyen et al. 2020
S4	0,25	5,2	10,05	4020,0000	1,0022	3,6042	Nguyen et al. 2020
S5	2,23	5,2	5,67	254,2601	0,7536	2,4053	Nguyen et al. 2020
S6	4,9	5,2	70,31	1434,8980	1,8470	3,1568	Nguyen et al. 2020
S7	0,13	5,2	8,3	6384,6154	0,9191	3,8051	Nguyen et al. 2020
S8	0,4	5,2	4,96	1240,0000	0,6955	3,0934	Nguyen et al. 2020
S9	1,19	5,2	8,18	687,3950	0,9128	2,8372	Nguyen et al. 2020
S10	0,17	5,2	4,98	2929,4118	0,6972	3,4668	Nguyen et al. 2020
S1	0,7	7,2	5,92	845,7143	0,7723	2,9272	Nguyen et al. 2020
S2	0,37	7,2	3,45	932,4324	0,5378	2,9696	Nguyen et al. 2020
S3	0,08	7,2	3,15	3937,5000	0,4983	3,5952	Nguyen et al. 2020
S4	0,25	7,2	4,18	1672,0000	0,6212	3,2232	Nguyen et al. 2020
S5	2,23	7,2	3,71	166,3677	0,5694	2,2211	Nguyen et al. 2020
S6	4,9	7,2	34,3	700,0000	1,5353	2,8451	Nguyen et al. 2020
S7	0,13	7,2	3,52	2707,6923	0,5465	3,4326	Nguyen et al. 2020
S8	0,4	7,2	3,22	805,0000	0,5079	2,9058	Nguyen et al. 2020
S9	1,19	7,2	8,78	737,8151	0,9435	2,8679	Nguyen et al. 2020
S10	0,17	7,2	5,66	3329,4118	0,7528	3,5224	Nguyen et al. 2020
S1	0,7	8,3	5,79	827,1429	0,7627	2,9176	Nguyen et al. 2020
S2	0,37	8,3	7,15	1932,4324	0,8543	3,2861	Nguyen et al. 2020
S3	0,08	8,3	4,02	5025,0000	0,6042	3,7011	Nguyen et al. 2020
S4	0,25	8,3	3,48	1392,0000	0,5416	3,1436	Nguyen et al. 2020
S5	2,23	8,3	2,98	133,6323	0,4742	2,1259	Nguyen et al. 2020
S6	4,9	8,3	31,19	636,5306	1,4940	2,8038	Nguyen et al. 2020
S7	0,13	8,3	3,15	2423,0769	0,4983	3,3844	Nguyen et al. 2020
S8	0,4	8,3	3,29	822,5000	0,5172	2,9151	Nguyen et al. 2020
S9	1,19	8,3	6,19	520,1681	0,7917	2,7161	Nguyen et al. 2020
S10	0,17	8,3	4,33	2547,0588	0,6365	3,4060	Nguyen et al. 2020
Al pH 3		2,8				4,6	Campos Periera et al. 2018
Al pH 4		4				4,8	Campos Periera et al. 2018
Al pH 5		4,8				4,4	Campos Periera et al. 2018
Al pH 6		5,7				4,3	Campos Periera et al. 2018
Al pH 3		2,8				4,6	Campos Periera et al. 2018
Al pH 4		4				4,7	Campos Periera et al. 2018
Al pH 5		4,7				4,1	Campos Periera et al. 2018
Al pH 6		5,7				4,3	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				5,1	Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5					Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				4,3	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				4,8	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				5	Campos Periera et al. 2018

Ca pH 5 [5 mM]		4,6				4,4	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				4,6	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9				5,3	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9				4,9	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,9				4,5	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6				4	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9				4,8	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9				4,6	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,8				4,3	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6				4,4	Campos Periera et al. 2018
Na pH 3		3,1				3,9	Campos Periera et al. 2018
Na pH 4		4,2				4,3	Campos Periera et al. 2018
Na pH 5		4,9				4,4	Campos Periera et al. 2018
Na pH 6		5,8				4,3	Campos Periera et al. 2018
Na pH 3		3,1				4,7	Campos Periera et al. 2018
Na pH 4		4,2				4,3	Campos Periera et al. 2018
Na pH 5		4,9				4,3	Campos Periera et al. 2018
Na pH 6		5,8				4,4	Campos Periera et al. 2018
1	0,52			1400		3,15	Petterson et al. 2015
2	2,1			676		2,83	Petterson et al. 2015
3	2,5			644		2,81	Petterson et al. 2015
4	5,2			775		2,89	Petterson et al. 2015
5	16			718,75		2,86	Petterson et al. 2015
6	0,2	8		9500		3,98	Petterson et al. 2015
7	1,6	5,9		2000		3,30	Petterson et al. 2015
8	3,9	6,3		974		2,99	Petterson et al. 2015
9	7,7	7,9		987		2,99	Petterson et al. 2015
10	9,4	4,6		1170		3,07	Petterson et al. 2015
11	39	5,3		756		2,88	Petterson et al. 2015
Jyndevad	1	6,1	15	1500		3,18	Enevoldsen, Juhler 2010
Sj. Odde	0,42	7,6	17	4048		3,61	Enevoldsen, Juhler 2010

10%	2,84
50%	3,60
95%	4,80
N=	83

PFNS

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						3,763245	
N						40	
S1	0,7	3,4	51,98	7425,7143	1,7158	3,8707	Nguyen et al. 2020
S2	0,37	3,4	181,25	48986,4865	2,2583	4,6901	Nguyen et al. 2020
S3	0,08	3,4	24,9	31125,0000	1,3962	4,4931	Nguyen et al. 2020
S4	0,25	3,4	63,96	25584,0000	1,8059	4,4080	Nguyen et al. 2020
S5	2,23	3,4	65,73	2947,5336	1,8178	3,4695	Nguyen et al. 2020
S6	4,9	3,4	364,58	7440,4082	2,5618	3,8716	Nguyen et al. 2020
S7	0,13	3,4	33,82	26015,3846	1,5292	4,4152	Nguyen et al. 2020
S8	0,4	3,4	23,18	5795,0000	1,3651	3,7631	Nguyen et al. 2020
S9	1,19	3,4	121,3	10193,2773	2,0839	4,0083	Nguyen et al. 2020
S10	0,17	3,4	48,95	28794,1176	1,6898	4,4593	Nguyen et al. 2020
S1	0,7	5,2	22,37	3195,7143	1,3497	3,5046	Nguyen et al. 2020
S2	0,37	5,2	46,15	12472,9730	1,6642	4,0960	Nguyen et al. 2020
S3	0,08	5,2	12,98	16225,0000	1,1133	4,2102	Nguyen et al. 2020
S4	0,25	5,2	35,72	14288,0000	1,5529	4,1550	Nguyen et al. 2020
S5	2,23	5,2	26,1	1170,4036	1,4166	3,0683	Nguyen et al. 2020
S6	4,9	5,2	284,08	5797,5510	2,4534	3,7632	Nguyen et al. 2020
S7	0,13	5,2	24,88	19138,4615	1,3959	4,2819	Nguyen et al. 2020
S8	0,4	5,2	9,02	2255,0000	0,9552	3,3531	Nguyen et al. 2020
S9	1,19	5,2	25,97	2182,3529	1,4145	3,3389	Nguyen et al. 2020
S10	0,17	5,2	19,6	11529,4118	1,2923	4,0618	Nguyen et al. 2020
S1	0,7	7,2	15,54	2220,0000	1,1915	3,3464	Nguyen et al. 2020
S2	0,37	7,2	25,22	6816,2162	1,4017	3,8335	Nguyen et al. 2020
S3	0,08	7,2	12,2	15250,0000	1,0864	4,1833	Nguyen et al. 2020
S4	0,25	7,2	5,88	2352,0000	0,7694	3,3714	Nguyen et al. 2020
S5	2,23	7,2	13,73	615,6951	1,1377	2,7894	Nguyen et al. 2020
S6	4,9	7,2	119,76	2444,0816	2,0783	3,3881	Nguyen et al. 2020
S7	0,13	7,2	9,46	7276,9231	0,9759	3,8619	Nguyen et al. 2020
S8	0,4	7,2	6,26	1565,0000	0,7966	3,1945	Nguyen et al. 2020
S9	1,19	7,2	21,39	1797,4790	1,3302	3,2547	Nguyen et al. 2020
S10	0,17	7,2	9,57	5629,4118	0,9809	3,7505	Nguyen et al. 2020
S1	0,7	8,3	14,18	2025,7143	1,1517	3,3066	Nguyen et al. 2020
S2	0,37	8,3	25,34	6848,6486	1,4038	3,8356	Nguyen et al. 2020
S3	0,08	8,3	14,21	17762,5000	1,1526	4,2495	Nguyen et al. 2020
S4	0,25	8,3	8,13	3252,0000	0,9101	3,5122	Nguyen et al. 2020
S5	2,23	8,3	9,72	435,8744	0,9877	2,6394	Nguyen et al. 2020
S6	4,9	8,3	102,08	2083,2653	2,0089	3,3187	Nguyen et al. 2020
S7	0,13	8,3	8,65	6653,8462	0,9370	3,8231	Nguyen et al. 2020
S8	0,4	8,3	10,1	2525,0000	1,0043	3,4023	Nguyen et al. 2020
S9	1,19	8,3	23,19	1948,7395	1,3653	3,2898	Nguyen et al. 2020
S10	0,17	8,3	13,57	7982,3529	1,1326	3,9021	Nguyen et al. 2020

PFDS

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						4,23393842	
N						40	
S1	0,7	3,4	176,15	25164,2857	2,2459	4,4008	Nguyen et al. 2020
S2	0,37	3,4	1284,3	347108,1081	3,1087	5,5405	Nguyen et al. 2020
S3	0,08	3,4	176,99	221237,5000	2,2479	5,3449	Nguyen et al. 2020
S4	0,25	3,4	401,01	160404,0000	2,6032	5,2052	Nguyen et al. 2020
S5	2,23	3,4	349,28	15662,7803	2,5432	4,1949	Nguyen et al. 2020
S6	4,9	3,4	827,97	16897,3469	2,9180	4,2278	Nguyen et al. 2020
S7	0,13	3,4	302,88	232984,6154	2,4813	5,3673	Nguyen et al. 2020
S8	0,4	3,4	71,61	17902,5000	1,8550	4,2529	Nguyen et al. 2020
S9	1,19	3,4	607,43	51044,5378	2,7835	4,7079	Nguyen et al. 2020
S10	0,17	3,4	347,41	204358,8235	2,5408	5,3104	Nguyen et al. 2020
S1	0,7	5,2	119,96	17137,1429	2,0790	4,2339	Nguyen et al. 2020
S2	0,37	5,2	194,42	52545,9459	2,2887	4,7205	Nguyen et al. 2020
S3	0,08	5,2	78,64	98300,0000	1,8956	4,9926	Nguyen et al. 2020
S4	0,25	5,2	182,36	72944,0000	2,2609	4,8630	Nguyen et al. 2020
S5	2,23	5,2	142,47	6388,7892	2,1537	3,8054	Nguyen et al. 2020
S6	4,9	5,2	679,91	13875,7143	2,8325	4,1423	Nguyen et al. 2020
S7	0,13	5,2	123,24	94800,0000	2,0908	4,9768	Nguyen et al. 2020
S8	0,4	5,2	29,12	7280,0000	1,4642	3,8621	Nguyen et al. 2020
S9	1,19	5,2	124,8	10487,3950	2,0962	4,0207	Nguyen et al. 2020
S10	0,17	5,2	101,64	59788,2353	2,0071	4,7766	Nguyen et al. 2020
S1	0,7	7,2	41,98	5997,1429	1,6230	3,7779	Nguyen et al. 2020
S2	0,37	7,2	124,51	33651,3514	2,0952	4,5270	Nguyen et al. 2020
S3	0,08	7,2	65,23	81537,5000	1,8144	4,9114	Nguyen et al. 2020
S4	0,25	7,2	10,36	4144,0000	1,0154	3,6174	Nguyen et al. 2020
S5	2,23	7,2	66,5	2982,0628	1,8228	3,4745	Nguyen et al. 2020
S6	4,9	7,2	324,98	6632,2449	2,5119	3,8217	Nguyen et al. 2020
S7	0,13	7,2	28,93	22253,8462	1,4613	4,3474	Nguyen et al. 2020
S8	0,4	7,2	27,34	6835,0000	1,4368	3,8347	Nguyen et al. 2020
S9	1,19	7,2	76,74	6448,7395	1,8850	3,8095	Nguyen et al. 2020
S10	0,17	7,2	16,31	9594,1176	1,2125	3,9820	Nguyen et al. 2020
S1	0,7	8,3	54,11	7730,0000	1,7333	3,8882	Nguyen et al. 2020
S2	0,37	8,3	92,4	24972,9730	1,9657	4,3975	Nguyen et al. 2020
S3	0,08	8,3	101,33	126662,5000	2,0057	5,1026	Nguyen et al. 2020
S4	0,25	8,3	35,01	14004,0000	1,5442	4,1463	Nguyen et al. 2020
S5	2,23	8,3	53,92	2417,9372	1,7317	3,3834	Nguyen et al. 2020
S6	4,9	8,3	286,32	5843,2653	2,4569	3,7667	Nguyen et al. 2020
S7	0,13	8,3	24,94	19184,6154	1,3969	4,2830	Nguyen et al. 2020
S8	0,4	8,3	44,78	11195,0000	1,6511	4,0490	Nguyen et al. 2020
S9	1,19	8,3	86,61	7278,1513	1,9376	3,8620	Nguyen et al. 2020
S10	0,17	8,3	49,8	29294,1176	1,6972	4,4668	Nguyen et al. 2020

(P)FOSA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						4,358222	
N						71	
S1	0,7	3,4	71,75	10250,0000	1,8558	4,0107	Nguyen et al. 2020
S2	0,37	3,4	124,63	33683,7838	2,0956	4,5274	Nguyen et al. 2020
S3	0,08	3,4	19,36	24200,0000	1,2869	4,3838	Nguyen et al. 2020
S4	0,25	3,4	73,53	29412,0000	1,8665	4,4685	Nguyen et al. 2020
S5	2,23	3,4	63,97	2868,6099	1,8060	3,4577	Nguyen et al. 2020
S6	4,9	3,4	311,06	6348,1633	2,4928	3,8026	Nguyen et al. 2020
S7	0,13	3,4	29,81	22930,7692	1,4744	4,3604	Nguyen et al. 2020
S8	0,4	3,4	55,55	13887,5000	1,7447	4,1426	Nguyen et al. 2020
S9	1,19	3,4	80,82	6791,5966	1,9075	3,8320	Nguyen et al. 2020
S10	0,17	3,4	43,98	25870,5882	1,6433	4,4128	Nguyen et al. 2020
S1	0,7	5,2	42,63	6090,0000	1,6297	3,7846	Nguyen et al. 2020
S2	0,37	5,2	152,45	41202,7027	2,1831	4,6149	Nguyen et al. 2020
S3	0,08	5,2	15,16	18950,0000	1,1807	4,2776	Nguyen et al. 2020
S4	0,25	5,2	49,76	19904,0000	1,6969	4,2989	Nguyen et al. 2020
S5	2,23	5,2	13,96	626,0090	1,1449	2,7966	Nguyen et al. 2020
S6	4,9	5,2	178,13	3635,3061	2,2507	3,5605	Nguyen et al. 2020
S7	0,13	5,2	16,89	12992,3077	1,2276	4,1137	Nguyen et al. 2020
S8	0,4	5,2	40,27	10067,5000	1,6050	4,0029	Nguyen et al. 2020
S9	1,19	5,2	70,68	5939,4958	1,8493	3,7737	Nguyen et al. 2020
S10	0,17	5,2	22,5	13235,2941	1,3522	4,1217	Nguyen et al. 2020
S1	0,7	7,2	7,42	1060,0000	0,8704	3,0253	Nguyen et al. 2020
S2	0,37	7,2	6,64	1794,5946	0,8222	3,2540	Nguyen et al. 2020
S3	0,08	7,2	18,16	22700,0000	1,2591	4,3560	Nguyen et al. 2020
S4	0,25	7,2	4,18	1672,0000	0,6212	3,2232	Nguyen et al. 2020
S5	2,23	7,2	3,14	140,8072	0,4969	2,1486	Nguyen et al. 2020
S6	4,9	7,2	47,29	965,1020	1,6748	2,9846	Nguyen et al. 2020
S7	0,13	7,2	2,22	1707,6923	0,3464	3,2324	Nguyen et al. 2020
S8	0,4	7,2	15,58	3895,0000	1,1926	3,5905	Nguyen et al. 2020
S9	1,19	7,2	8,49	713,4454	0,9289	2,8534	Nguyen et al. 2020
S10	0,17	7,2	12,82	7541,1765	1,1079	3,8774	Nguyen et al. 2020
S1	0,7	8,3	4,36	622,8571	0,6395	2,7944	Nguyen et al. 2020
S2	0,37	8,3	3,38	913,5135	0,5289	2,9607	Nguyen et al. 2020
S3	0,08	8,3	2,03	2537,5000	0,3075	3,4044	Nguyen et al. 2020
S4	0,25	8,3	4,06	1624,0000	0,6085	3,2106	Nguyen et al. 2020
S5	2,23	8,3	1,81	81,1659	0,2577	1,9094	Nguyen et al. 2020
S6	4,9	8,3	34,02	694,2857	1,5317	2,8415	Nguyen et al. 2020
S7	0,13	8,3	1,61	1238,4615	0,2068	3,0929	Nguyen et al. 2020
S8	0,4	8,3	3,74	935,0000	0,5729	2,9708	Nguyen et al. 2020
S9	1,19	8,3	5,91	496,6387	0,7716	2,6960	Nguyen et al. 2020
S10	0,17	8,3	3,88	2282,3529	0,5888	3,3584	Nguyen et al. 2020
Al pH 3		2,8				5,9	Campos Periera et al. 2018
Al pH 4		4				5,6	Campos Periera et al. 2018
Al pH 5		4,8				4,6	Campos Periera et al. 2018
Al pH 6		5,7				4,4	Campos Periera et al. 2018
Al pH 3		2,8				6	Campos Periera et al. 2018
Al pH 4		4				5,7	Campos Periera et al. 2018
Al pH 5		4,7				4,4	Campos Periera et al. 2018
Al pH 6		5,7				4,3	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				5,4	Campos Periera et al. 2018
Ca pH 4 [5mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				5,5	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				4,5	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				5,6	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				5,4	Campos Periera et al. 2018

Ca pH 5 [5 mM]	4,6	4,8	Campos Periera et al. 2018
Ca pH 6 [5 mM]	5,2	4,6	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	5,8	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	5,2	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,9	4,8	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	4,3	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	5,3	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	4,8	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,8	5	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	4,6	Campos Periera et al. 2018
Na pH 3	3,1	5,4	Campos Periera et al. 2018
Na pH 4	4,2	5	Campos Periera et al. 2018
Na pH 5	4,9	4,8	Campos Periera et al. 2018
Na pH 6	5,8	4,4	Campos Periera et al. 2018
Na pH 3	3,1	6	Campos Periera et al. 2018
Na pH 4	4,2	5,1	Campos Periera et al. 2018
Na pH 5	4,9	4,7	Campos Periera et al. 2018
Na pH 6	5,8	4,5	Campos Periera et al. 2018

6.2 FTS

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						2,283301	
N						40	
S1	0,7	3,4	1,57	224,2857	0,1959	2,3508	Nguyen et al. 2020
S2	0,37	3,4	1,52	410,8108	0,1818	2,6136	Nguyen et al. 2020
S3	0,08	3,4	1,17	1462,5000	0,0682	3,1651	Nguyen et al. 2020
S4	0,25	3,4	1,51	604,0000	0,1790	2,7810	Nguyen et al. 2020
S5	2,23	3,4	1,04	46,6368	0,0170	1,6687	Nguyen et al. 2020
S6	4,9	3,4	5,55	113,2653	0,7443	2,0541	Nguyen et al. 2020
S7	0,13	3,4	1,53	1176,9231	0,1847	3,0707	Nguyen et al. 2020
S8	0,4	3,4	1,16	290,0000	0,0645	2,4624	Nguyen et al. 2020
S9	1,19	3,4	2,38	200,0000	0,3766	2,3010	Nguyen et al. 2020
S10	0,17	3,4	1,45	852,9412	0,1614	2,9309	Nguyen et al. 2020
S1	0,7	5,2	1,23	175,7143	0,0899	2,2448	Nguyen et al. 2020
S2	0,37	5,2	0,9	243,2432	-0,0458	2,3860	Nguyen et al. 2020
S3	0,08	5,2	0,73	912,5000	-0,1367	2,9602	Nguyen et al. 2020
S4	0,25	5,2	1,8	720,0000	0,2553	2,8573	Nguyen et al. 2020
S5	2,23	5,2	0,81	36,3229	-0,0915	1,5602	Nguyen et al. 2020
S6	4,9	5,2	4,81	98,1633	0,6821	1,9919	Nguyen et al. 2020
S7	0,13	5,2	1,35	1038,4615	0,1303	3,0164	Nguyen et al. 2020
S8	0,4	5,2	0,27	67,5000	-0,5686	1,8293	Nguyen et al. 2020
S9	1,19	5,2	0,71	59,6639	-0,1487	1,7757	Nguyen et al. 2020
S10	0,17	5,2	0,84	494,1176	-0,0757	2,6938	Nguyen et al. 2020
S1	0,7	7,2	0,87	124,2857	-0,0605	2,0944	Nguyen et al. 2020
S2	0,37	7,2	0,61	164,8649	-0,2147	2,2171	Nguyen et al. 2020
S3	0,08	7,2	0,51	637,5000	-0,2924	2,8045	Nguyen et al. 2020
S4	0,25	7,2	0,48	192,0000	-0,3188	2,2833	Nguyen et al. 2020
S5	2,23	7,2	0,47	21,0762	-0,3279	1,3238	Nguyen et al. 2020
S6	4,9	7,2	1,77	36,1224	0,2480	1,5578	Nguyen et al. 2020
S7	0,13	7,2	0,64	492,3077	-0,1938	2,6922	Nguyen et al. 2020
S8	0,4	7,2	0,19	47,5000	-0,7212	1,6767	Nguyen et al. 2020
S9	1,19	7,2	0,64	53,7815	-0,1938	1,7306	Nguyen et al. 2020
S10	0,17	7,2	0,87	511,7647	-0,0605	2,7091	Nguyen et al. 2020
S1	0,7	8,3	0,8	114,2857	-0,0969	2,0580	Nguyen et al. 2020
S2	0,37	8,3	0,74	200,0000	-0,1308	2,3010	Nguyen et al. 2020
S3	0,08	8,3	0,64	800,0000	-0,1938	2,9031	Nguyen et al. 2020
S4	0,25	8,3	0,45	180,0000	-0,3468	2,2553	Nguyen et al. 2020
S5	2,23	8,3	0,49	21,9731	-0,3098	1,3419	Nguyen et al. 2020
S6	4,9	8,3	1,68	34,2857	0,2253	1,5351	Nguyen et al. 2020
S7	0,13	8,3	0,49	376,9231	-0,3098	2,5763	Nguyen et al. 2020
S8	0,4	8,3	0,19	47,5000	-0,7212	1,6767	Nguyen et al. 2020
S9	1,19	8,3	0,48	40,3361	-0,3188	1,6057	Nguyen et al. 2020
S10	0,17	8,3	0,76	447,0588	-0,1192	2,6504	Nguyen et al. 2020

PFBA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						1,90309	
N						40	
S1	0,7	3,4	0,56	80,0000	-0,2518	1,9031	Nguyen et al. 2020
S2	0,37	3,4	0,55	148,6486	-0,2596	2,1722	Nguyen et al. 2020
S3	0,08	3,4	0,52	650,0000	-0,2840	2,8129	Nguyen et al. 2020
S4	0,25	3,4	0,44	176,0000	-0,3565	2,2455	Nguyen et al. 2020
S5	2,23	3,4	0,51	22,8700	-0,2924	1,3593	Nguyen et al. 2020
S6	4,9	3,4	0,68	13,8776	-0,1675	1,1423	Nguyen et al. 2020
S7	0,13	3,4	0,47	361,5385	-0,3279	2,5582	Nguyen et al. 2020
S8	0,4	3,4	0,14	35,0000	-0,8539	1,5441	Nguyen et al. 2020
S9	1,19	3,4	0,3	25,2101	-0,5229	1,4016	Nguyen et al. 2020
S10	0,17	3,4	0,44	258,8235	-0,3565	2,4130	Nguyen et al. 2020
S1	0,7	5,2	0,48	68,5714	-0,3188	1,8361	Nguyen et al. 2020
S2	0,37	5,2	0,43	116,2162	-0,3665	2,0653	Nguyen et al. 2020
S3	0,08	5,2	0,37	462,5000	-0,4318	2,6651	Nguyen et al. 2020
S4	0,25	5,2	0,37	148,0000	-0,4318	2,1703	Nguyen et al. 2020
S5	2,23	5,2	0,5	22,4215	-0,3010	1,3507	Nguyen et al. 2020
S6	4,9	5,2	0,6	12,2449	-0,2218	1,0880	Nguyen et al. 2020
S7	0,13	5,2	0,4	307,6923	-0,3979	2,4881	Nguyen et al. 2020
S8	0,4	5,2	0,11	27,5000	-0,9586	1,4393	Nguyen et al. 2020
S9	1,19	5,2	0,21	17,6471	-0,6778	1,2467	Nguyen et al. 2020
S10	0,17	5,2	0,37	217,6471	-0,4318	2,3378	Nguyen et al. 2020
S1	0,7	7,2	0,44	62,8571	-0,3565	1,7984	Nguyen et al. 2020
S2	0,37	7,2	0,41	110,8108	-0,3872	2,0446	Nguyen et al. 2020
S3	0,08	7,2	0,32	400,0000	-0,4949	2,6021	Nguyen et al. 2020
S4	0,25	7,2	0,2	80,0000	-0,6990	1,9031	Nguyen et al. 2020
S5	2,23	7,2	0,31	13,9013	-0,5086	1,1431	Nguyen et al. 2020
S6	4,9	7,2	0,47	9,5918	-0,3279	0,9819	Nguyen et al. 2020
S7	0,13	7,2	0,22	169,2308	-0,6576	2,2285	Nguyen et al. 2020
S8	0,4	7,2	0,06	15,0000	-1,2218	1,1761	Nguyen et al. 2020
S9	1,19	7,2	0,23	19,3277	-0,6383	1,2862	Nguyen et al. 2020
S10	0,17	7,2	0,3	176,4706	-0,5229	2,2467	Nguyen et al. 2020
S1	0,7	8,3	0,47	67,1429	-0,3279	1,8270	Nguyen et al. 2020
S2	0,37	8,3	0,5	135,1351	-0,3010	2,1308	Nguyen et al. 2020
S3	0,08	8,3	0,31	387,5000	-0,5086	2,5883	Nguyen et al. 2020
S4	0,25	8,3	0,21	84,0000	-0,6778	1,9243	Nguyen et al. 2020
S5	2,23	8,3	0,36	16,1435	-0,4437	1,2080	Nguyen et al. 2020
S6	4,9	8,3	0,45	9,1837	-0,3468	0,9630	Nguyen et al. 2020
S7	0,13	8,3	0,17	130,7692	-0,7696	2,1165	Nguyen et al. 2020
S8	0,4	8,3	0,1	25,0000	-1,0000	1,3979	Nguyen et al. 2020
S9	1,19	8,3	0,25	21,0084	-0,6021	1,3224	Nguyen et al. 2020
S10	0,17	8,3	0,32	188,2353	-0,4949	2,2747	Nguyen et al. 2020

PFPeA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median			pH3,4			1,3786	
N						55	
S1	0,7	3,4	0,56	80,0000	-0,2518	1,9031	Nguyen et al. 2020
S2	0,37	3,4	0,55	148,6486	-0,2596	2,1722	Nguyen et al. 2020
S3	0,08	3,4	0,52	650,0000	-0,2840	2,8129	Nguyen et al. 2020
S4	0,25	3,4	0,44	176,0000	-0,3565	2,2455	Nguyen et al. 2020
S5	2,23	3,4	0,51	22,8700	-0,2924	1,3593	Nguyen et al. 2020
S6	4,9	3,4	0,68	13,8776	-0,1675	1,1423	Nguyen et al. 2020
S7	0,13	3,4	0,47	361,5385	-0,3279	2,5582	Nguyen et al. 2020
S8	0,4	3,4	0,14	35,0000	-0,8539	1,5441	Nguyen et al. 2020
S9	1,19	3,4	0,3	25,2101	-0,5229	1,4016	Nguyen et al. 2020
S10	0,17	3,4	0,44	258,8235	-0,3565	2,4130	Nguyen et al. 2020
S1	0,7	5,2	0,48	68,5714	-0,3188	1,8361	Nguyen et al. 2020
S2	0,37	5,2	0,43	116,2162	-0,3665	2,0653	Nguyen et al. 2020
S3	0,08	5,2	0,37	462,5000	-0,4318	2,6651	Nguyen et al. 2020
S4	0,25	5,2	0,37	148,0000	-0,4318	2,1703	Nguyen et al. 2020
S5	2,23	5,2	0,5	22,4215	-0,3010	1,3507	Nguyen et al. 2020
S6	4,9	5,2	0,6	12,2449	-0,2218	1,0880	Nguyen et al. 2020
S7	0,13	5,2	0,4	307,6923	-0,3979	2,4881	Nguyen et al. 2020
S8	0,4	5,2	0,11	27,5000	-0,9586	1,4393	Nguyen et al. 2020
S9	1,19	5,2	0,21	17,6471	-0,6778	1,2467	Nguyen et al. 2020
S10	0,17	5,2	0,37	217,6471	-0,4318	2,3378	Nguyen et al. 2020
S1	0,7	7,2	0,44	62,8571	-0,3565	1,7984	Nguyen et al. 2020
S2	0,37	7,2	0,41	110,8108	-0,3872	2,0446	Nguyen et al. 2020
S3	0,08	7,2	0,32	400,0000	-0,4949	2,6021	Nguyen et al. 2020
S4	0,25	7,2	0,2	80,0000	-0,6990	1,9031	Nguyen et al. 2020
S5	2,23	7,2	0,31	13,9013	-0,5086	1,1431	Nguyen et al. 2020
S6	4,9	7,2	0,47	9,5918	-0,3279	0,9819	Nguyen et al. 2020
S7	0,13	7,2	0,22	169,2308	-0,6576	2,2285	Nguyen et al. 2020
S8	0,4	7,2	0,06	15,0000	-1,2218	1,1761	Nguyen et al. 2020
S9	1,19	7,2	0,23	19,3277	-0,6383	1,2862	Nguyen et al. 2020
S10	0,17	7,2	0,3	176,4706	-0,5229	2,2467	Nguyen et al. 2020
S1	0,7	8,3	0,47	67,1429	-0,3279	1,8270	Nguyen et al. 2020
S2	0,37	8,3	0,5	135,1351	-0,3010	2,1308	Nguyen et al. 2020
S3	0,08	8,3	0,31	387,5000	-0,5086	2,5883	Nguyen et al. 2020
S4	0,25	8,3	0,21	84,0000	-0,6778	1,9243	Nguyen et al. 2020
S5	2,23	8,3	0,36	16,1435	-0,4437	1,2080	Nguyen et al. 2020
S6	4,9	8,3	0,45	9,1837	-0,3468	0,9630	Nguyen et al. 2020
S7	0,13	8,3	0,17	130,7692	-0,7696	2,1165	Nguyen et al. 2020
S8	0,4	8,3	0,1	25,0000	-1,0000	1,3979	Nguyen et al. 2020
S9	1,19	8,3	0,25	21,0084	-0,6021	1,3224	Nguyen et al. 2020
S10	0,17	8,3	0,32	188,2353	-0,4949	2,2747	Nguyen et al. 2020
Al pH 3		2,8				1,3	Campos Periera et al. 2018
Al pH 4		4				1,3	Campos Periera et al. 2018
Al pH 5		4,8				1,2	Campos Periera et al. 2018
Al pH 6		5,7				1,2	Campos Periera et al. 2018
Al pH 3		2,8				1,1	Campos Periera et al. 2018
Al pH 4		4				1,1	Campos Periera et al. 2018
Al pH 5		4,7				1,2	Campos Periera et al. 2018
Al pH 6		5,7				1,1	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				1	Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				−0,2	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				0,8	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				−0,8	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8					Campos Periera et al. 2018

Ca pH 5 [5 mM]	4,6		Campos Periera et al. 2018
Ca pH 6 [5 mM]	5,2		Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	0,8	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	1	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,9		Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6		Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	0,5	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	−0,1	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,8		Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6		Campos Periera et al. 2018
Na pH 3	3,1	0,7	Campos Periera et al. 2018
Na pH 4	4,2	0,5	Campos Periera et al. 2018
Na pH 5	4,9	−0,6	Campos Periera et al. 2018
Na pH 6	5,8		Campos Periera et al. 2018
Na pH 3	3,1		Campos Periera et al. 2018
Na pH 4	4,2		Campos Periera et al. 2018
Na pH 5	4,9		Campos Periera et al. 2018
Na pH 6	5,8		Campos Periera et al. 2018

PFHxA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						1,5	
N						71	
S1	0,7	3,4	0,69	98,5714	-0,1612	1,9938	Nguyen et al. 2020
S2	0,37	3,4	0,56	151,3514	-0,2518	2,1800	Nguyen et al. 2020
S3	0,08	3,4	0,46	575,0000	-0,3372	2,7597	Nguyen et al. 2020
S4	0,25	3,4	0,34	136,0000	-0,4685	2,1335	Nguyen et al. 2020
S5	2,23	3,4	0,5	22,4215	-0,3010	1,3507	Nguyen et al. 2020
S6	4,9	3,4	1	20,4082	0,0000	1,3098	Nguyen et al. 2020
S7	0,13	3,4	0,38	292,3077	-0,4202	2,4658	Nguyen et al. 2020
S8	0,4	3,4	0,34	85,0000	-0,4685	1,9294	Nguyen et al. 2020
S9	1,19	3,4	0,68	57,1429	-0,1675	1,7570	Nguyen et al. 2020
S10	0,17	3,4	0,48	282,3529	-0,3188	2,4508	Nguyen et al. 2020
S1	0,7	5,2	0,48	68,5714	-0,3188	1,8361	Nguyen et al. 2020
S2	0,37	5,2	0,43	116,2162	-0,3665	2,0653	Nguyen et al. 2020
S3	0,08	5,2	0,27	337,5000	-0,5686	2,5283	Nguyen et al. 2020
S4	0,25	5,2	0,28	112,0000	-0,5528	2,0492	Nguyen et al. 2020
S5	2,23	5,2	0,38	17,0404	-0,4202	1,2315	Nguyen et al. 2020
S6	4,9	5,2	0,88	17,9592	-0,0555	1,2543	Nguyen et al. 2020
S7	0,13	5,2	0,33	253,8462	-0,4815	2,4046	Nguyen et al. 2020
S8	0,4	5,2	0,11	27,5000	-0,9586	1,4393	Nguyen et al. 2020
S9	1,19	5,2	0,27	22,6891	-0,5686	1,3558	Nguyen et al. 2020
S10	0,17	5,2	0,38	223,5294	-0,4202	2,3493	Nguyen et al. 2020
S1	0,7	7,2	0,39	55,7143	-0,4089	1,7460	Nguyen et al. 2020
S2	0,37	7,2	0,35	94,5946	-0,4559	1,9759	Nguyen et al. 2020
S3	0,08	7,2	0,24	300,0000	-0,6198	2,4771	Nguyen et al. 2020
S4	0,25	7,2	0,17	68,0000	-0,7696	1,8325	Nguyen et al. 2020
S5	2,23	7,2	0,31	13,9013	-0,5086	1,1431	Nguyen et al. 2020
S6	4,9	7,2	0,52	10,6122	-0,2840	1,0258	Nguyen et al. 2020
S7	0,13	7,2	0,21	161,5385	-0,6778	2,2083	Nguyen et al. 2020
S8	0,4	7,2	0,05	12,5000	-1,3010	1,0969	Nguyen et al. 2020
S9	1,19	7,2	0,22	18,4874	-0,6576	1,2669	Nguyen et al. 2020
S10	0,17	7,2	0,29	170,5882	-0,5376	2,2319	Nguyen et al. 2020
S1	0,7	8,3	0,45	64,2857	-0,3468	1,8081	Nguyen et al. 2020
S2	0,37	8,3	0,41	110,8108	-0,3872	2,0446	Nguyen et al. 2020
S3	0,08	8,3	0,22	275,0000	-0,6576	2,4393	Nguyen et al. 2020
S4	0,25	8,3	0,2	80,0000	-0,6990	1,9031	Nguyen et al. 2020
S5	2,23	8,3	0,34	15,2466	-0,4685	1,1832	Nguyen et al. 2020
S6	4,9	8,3	0,51	10,4082	-0,2924	1,0174	Nguyen et al. 2020
S7	0,13	8,3	0,19	146,1538	-0,7212	2,1648	Nguyen et al. 2020
S8	0,4	8,3	0,08	20,0000	-1,0969	1,3010	Nguyen et al. 2020
S9	1,19	8,3	0,23	19,3277	-0,6383	1,2862	Nguyen et al. 2020
S10	0,17	8,3	0,24	141,1765	-0,6198	2,1498	Nguyen et al. 2020
Al pH 3		2,8				1,8	Campos Periera et al. 2018
Al pH 4		4				1,7	Campos Periera et al. 2018
Al pH 5		4,8				1,6	Campos Periera et al. 2018
Al pH 6		5,7				1,4	Campos Periera et al. 2018
Al pH 3		2,8				1,8	Campos Periera et al. 2018
Al pH 4		4				1,6	Campos Periera et al. 2018
Al pH 5		4,7				1,6	Campos Periera et al. 2018
Al pH 6		5,7				1,5	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				1,6	Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				1,2	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				1,3	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				1,5	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				1,2	Campos Periera et al. 2018

Ca pH 5 [5 mM]	4,6	1,2	Campos Periera et al. 2018
Ca pH 6 [5 mM]	5,2	1,1	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	1,6	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	1,2	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,9	1	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	0,7	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	1,6	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	1	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,8	0,9	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	0,5	Campos Periera et al. 2018
Na pH 3	3,1	1,5	Campos Periera et al. 2018
Na pH 4	4,2	1,3	Campos Periera et al. 2018
Na pH 5	4,9	1	Campos Periera et al. 2018
Na pH 6	5,8	1,1	Campos Periera et al. 2018
Na pH 3	3,1	1,4	Campos Periera et al. 2018
Na pH 4	4,2	0,2	Campos Periera et al. 2018
Na pH 5	4,9	1	Campos Periera et al. 2018
Na pH 6	5,8	1,1	Campos Periera et al. 2018

PFHpA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						1,90823	
N						73	
S1	0,7	3,4	1,29	184,2857	0,1106	2,2655	Nguyen et al. 2020
S2	0,37	3,4	1,28	345,9459	0,1072	2,5390	Nguyen et al. 2020
S3	0,08	3,4	1,18	1475,0000	0,0719	3,1688	Nguyen et al. 2020
S4	0,25	3,4	0,64	256,0000	-0,1938	2,4082	Nguyen et al. 2020
S5	2,23	3,4	0,91	40,8072	-0,0410	1,6107	Nguyen et al. 2020
S6	4,9	3,4	3,34	68,1633	0,5237	1,8336	Nguyen et al. 2020
S7	0,13	3,4	0,9	692,3077	-0,0458	2,8403	Nguyen et al. 2020
S8	0,4	3,4	1,53	382,5000	0,1847	2,5826	Nguyen et al. 2020
S9	1,19	3,4	6	504,2017	0,7782	2,7026	Nguyen et al. 2020
S10	0,17	3,4	0,97	570,5882	-0,0132	2,7563	Nguyen et al. 2020
S1	0,7	5,2	0,96	137,1429	-0,0177	2,1372	Nguyen et al. 2020
S2	0,37	5,2	0,6	162,1622	-0,2218	2,2099	Nguyen et al. 2020
S3	0,08	5,2	0,48	600,0000	-0,3188	2,7782	Nguyen et al. 2020
S4	0,25	5,2	0,82	328,0000	-0,0862	2,5159	Nguyen et al. 2020
S5	2,23	5,2	0,54	24,2152	-0,2676	1,3841	Nguyen et al. 2020
S6	4,9	5,2	2,5	51,0204	0,3979	1,7077	Nguyen et al. 2020
S7	0,13	5,2	0,83	638,4615	-0,0809	2,8051	Nguyen et al. 2020
S8	0,4	5,2	0,33	82,5000	-0,4815	1,9165	Nguyen et al. 2020
S9	1,19	5,2	0,8	67,2269	-0,0969	1,8275	Nguyen et al. 2020
S10	0,17	5,2	0,88	517,6471	-0,0555	2,7140	Nguyen et al. 2020
S1	0,7	7,2	0,55	78,5714	-0,2596	1,8953	Nguyen et al. 2020
S2	0,37	7,2	0,61	164,8649	-0,2147	2,2171	Nguyen et al. 2020
S3	0,08	7,2	0,5	625,0000	-0,3010	2,7959	Nguyen et al. 2020
S4	0,25	7,2	0,46	184,0000	-0,3372	2,2648	Nguyen et al. 2020
S5	2,23	7,2	0,55	24,6637	-0,2596	1,3921	Nguyen et al. 2020
S6	4,9	7,2	1,41	28,7755	0,1492	1,4590	Nguyen et al. 2020
S7	0,13	7,2	0,47	361,5385	-0,3279	2,5582	Nguyen et al. 2020
S8	0,4	7,2	0,3	75,0000	-0,5229	1,8751	Nguyen et al. 2020
S9	1,19	7,2	1,92	161,3445	0,2833	2,2078	Nguyen et al. 2020
S10	0,17	7,2	0,84	494,1176	-0,0757	2,6938	Nguyen et al. 2020
S1	0,7	8,3	0,79	112,8571	-0,1024	2,0525	Nguyen et al. 2020
S2	0,37	8,3	0,84	227,0270	-0,0757	2,3561	Nguyen et al. 2020
S3	0,08	8,3	0,42	525,0000	-0,3768	2,7202	Nguyen et al. 2020
S4	0,25	8,3	0,52	208,0000	-0,2840	2,3181	Nguyen et al. 2020
S5	2,23	8,3	0,5	22,4215	-0,3010	1,3507	Nguyen et al. 2020
S6	4,9	8,3	1,51	30,8163	0,1790	1,4888	Nguyen et al. 2020
S7	0,13	8,3	0,46	353,8462	-0,3372	2,5488	Nguyen et al. 2020
S8	0,4	8,3	0,36	90,0000	-0,4437	1,9542	Nguyen et al. 2020
S9	1,19	8,3	0,65	54,6218	-0,1871	1,7374	Nguyen et al. 2020
S10	0,17	8,3	0,76	447,0588	-0,1192	2,6504	Nguyen et al. 2020
Al pH 3		2,8				2,1	Campos Periera et al. 2018
Al pH 4		4				2	Campos Periera et al. 2018
Al pH 5		4,8				1,9	Campos Periera et al. 2018
Al pH 6		5,7				1,7	Campos Periera et al. 2018
Al pH 3		2,8				2,1	Campos Periera et al. 2018
Al pH 4		4				1,9	Campos Periera et al. 2018
Al pH 5		4,7				1,8	Campos Periera et al. 2018
Al pH 6		5,7				1,8	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				2	Campos Periera et al. 2018
Ca pH4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				1,7	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				1,7	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				2	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				1,6	Campos Periera et al. 2018

Ca pH 5 [5 mM]		4,6			1,6	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2			1,6	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9			2	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9			1,6	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,9			1,1	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6			1,3	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9			2,1	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9			1,6	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,8			1,4	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6			1,3	Campos Periera et al. 2018
Na pH 3		3,1			2	Campos Periera et al. 2018
Na pH 4		4,2			1,6	Campos Periera et al. 2018
Na pH 5		4,9			1,5	Campos Periera et al. 2018
Na pH 6		5,8			1,5	Campos Periera et al. 2018
Na pH 3		3,1			1,9	Campos Periera et al. 2018
Na pH 4		4,2			1,4	Campos Periera et al. 2018
Na pH 5		4,9			1,4	Campos Periera et al. 2018
Na pH 6		5,8			1,5	Campos Periera et al. 2018
Jyndevad	1	6,1	0,63	63	1,80	Enevoldsen, Juhler 2010
Sj. Odde	0,42	7,6	0,63	150	2,18	Enevoldsen, Juhler 2010

PFOA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						2,3	
N						77	
S1	0,7	3,4	2,82	402,8571	0,4502	2,6052	Nguyen et al. 2020
S2	0,37	3,4	2,21	597,2973	0,3444	2,7762	Nguyen et al. 2020
S3	0,08	3,4	2,48	3100,0000	0,3945	3,4914	Nguyen et al. 2020
S4	0,25	3,4	1,41	564,0000	0,1492	2,7513	Nguyen et al. 2020
S5	2,23	3,4	2,53	113,4529	0,4031	2,0548	Nguyen et al. 2020
S6	4,9	3,4	9,23	188,3673	0,9652	2,2750	Nguyen et al. 2020
S7	0,13	3,4	1,3	1000,0000	0,1139	3,0000	Nguyen et al. 2020
S8	0,4	3,4	4,12	1030,0000	0,6149	3,0128	Nguyen et al. 2020
S9	1,19	3,4	8,22	690,7563	0,9149	2,8393	Nguyen et al. 2020
S10	0,17	3,4	1,89	1111,7647	0,2765	3,0460	Nguyen et al. 2020
S1	0,7	5,2	1,72	245,7143	0,2355	2,3904	Nguyen et al. 2020
S2	0,37	5,2	0,47	127,0270	-0,328	2,1039	Nguyen et al. 2020
S3	0,08	5,2	0,89	1112,5000	-0,051	3,0463	Nguyen et al. 2020
S4	0,25	5,2	1,41	564,0000	0,1492	2,7513	Nguyen et al. 2020
S5	2,23	5,2	0,94	42,1525	-0,027	1,6248	Nguyen et al. 2020
S6	4,9	5,2	6,91	141,0204	0,8395	2,1493	Nguyen et al. 2020
S7	0,13	5,2	1,41	1084,6154	0,1492	3,0353	Nguyen et al. 2020
S8	0,4	5,2	0,83	207,5000	-0,081	2,3170	Nguyen et al. 2020
S9	1,19	5,2	1,16	97,4790	0,0645	1,9889	Nguyen et al. 2020
S10	0,17	5,2	1,01	594,1176	0,0043	2,7739	Nguyen et al. 2020
S1	0,7	7,2	1,04	148,5714	0,0170	2,1719	Nguyen et al. 2020
S2	0,37	7,2	0,68	183,7838	-0,168	2,2643	Nguyen et al. 2020
S3	0,08	7,2	0,81	1012,5000	-0,092	3,0054	Nguyen et al. 2020
S4	0,25	7,2	0,64	256,0000	-0,194	2,4082	Nguyen et al. 2020
S5	2,23	7,2	0,74	33,1839	-0,131	1,5209	Nguyen et al. 2020
S6	4,9	7,2	2,84	57,9592	0,4533	1,7631	Nguyen et al. 2020
S7	0,13	7,2	1,42	1092,3077	0,1523	3,0383	Nguyen et al. 2020
S8	0,4	7,2	0,53	132,5000	-0,276	2,1222	Nguyen et al. 2020
S9	1,19	7,2	1,18	99,1597	0,0719	1,9963	Nguyen et al. 2020
S10	0,17	7,2	0,86	505,8824	-0,066	2,7040	Nguyen et al. 2020
S1	0,7	8,3	1,13	161,4286	0,0531	2,2080	Nguyen et al. 2020
S2	0,37	8,3	2,94	794,5946	0,4683	2,9001	Nguyen et al. 2020
S3	0,08	8,3	0,85	1062,5000	-0,071	3,0263	Nguyen et al. 2020
S4	0,25	8,3	0,59	236,0000	-0,229	2,3729	Nguyen et al. 2020
S5	2,23	8,3	0,63	28,2511	-0,201	1,4510	Nguyen et al. 2020
S6	4,9	8,3	2,72	55,5102	0,4346	1,7444	Nguyen et al. 2020
S7	0,13	8,3	0,56	430,7692	-0,251	2,6342	Nguyen et al. 2020
S8	0,4	8,3	0,59	147,5000	-0,229	2,1688	Nguyen et al. 2020
S9	1,19	8,3	0,83	69,7479	-0,081	1,8435	Nguyen et al. 2020
S10	0,17	8,3	0,82	482,3529	-0,086	2,6834	Nguyen et al. 2020
Al pH 3		2,8				2,8	Campos Periera et al. 2018
Al pH 4		4				2,7	Campos Periera et al. 2018
Al pH 5		4,8				2,5	Campos Periera et al. 2018
Al pH 6		5,7				2,1	Campos Periera et al. 2018
Al pH 3		2,8				2,9	Campos Periera et al. 2018
Al pH 4		4				2,6	Campos Periera et al. 2018
Al pH 5		4,7				2,4	Campos Periera et al. 2018
Al pH 6		5,7				2,2	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				2,6	Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				2,1	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				2,1	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				2,6	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				2,3	Campos Periera et al. 2018

Ca pH 5 [5 mM]		4,6				2,1	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				2,1	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9				2,6	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9				2,1	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,9				1,9	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6				1,7	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9				2,6	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9				2,1	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,8				1,9	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6				1,7	Campos Periera et al. 2018
Na pH 3		3,1				2,5	Campos Periera et al. 2018
Na pH 4		4,2				2	Campos Periera et al. 2018
Na pH 5		4,9				1,8	Campos Periera et al. 2018
Na pH 6		5,8				1,7	Campos Periera et al. 2018
Na pH 3		3,1				2,5	Campos Periera et al. 2018
Na pH 4		4,2				2	Campos Periera et al. 2018
Na pH 5		4,9				1,8	Campos Periera et al. 2018
Na pH 6		5,8				1,9	Campos Periera et al. 2018
Jyndevad	1	6,1	1,1	110		2,04	Enevoldsen, Juhler 2010
Sj. Odde	0,42	7,6	1,5	357,14286		2,55	Enevoldsen, Juhler 2010

10%	1,77
50%	2,30
90%	3,00
N=	74

PFNA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						2,9	
N						74	
S1	0,7	3,4	7,53	1075,7143	0,8768	3,0317	Nguyen et al. 2020
S2	0,37	3,4	4,88	1318,9189	0,6884	3,1202	Nguyen et al. 2020
S3	0,08	3,4	3,44	4300,0000	0,5366	3,6335	Nguyen et al. 2020
S4	0,25	3,4	5,14	2056,0000	0,7110	3,3130	Nguyen et al. 2020
S5	2,23	3,4	3,87	173,5426	0,5877	2,2394	Nguyen et al. 2020
S6	4,9	3,4	31,79	648,7755	1,5023	2,8121	Nguyen et al. 2020
S7	0,13	3,4	3,6	2769,2308	0,5563	3,4424	Nguyen et al. 2020
S8	0,4	3,4	9,83	2457,5000	0,9926	3,3905	Nguyen et al. 2020
S9	1,19	3,4	17,25	1449,5798	1,2368	3,1612	Nguyen et al. 2020
S10	0,17	3,4	5,04	2964,7059	0,7024	3,4720	Nguyen et al. 2020
S1	0,7	5,2	4,32	617,1429	0,6355	2,7904	Nguyen et al. 2020
S2	0,37	5,2	2,3	621,6216	0,3617	2,7935	Nguyen et al. 2020
S3	0,08	5,2	1,98	2475,0000	0,2967	3,3936	Nguyen et al. 2020
S4	0,25	5,2	6,26	2504,0000	0,7966	3,3986	Nguyen et al. 2020
S5	2,23	5,2	3,24	145,2915	0,5105	2,1622	Nguyen et al. 2020
S6	4,9	5,2	24,29	495,7143	1,3854	2,6952	Nguyen et al. 2020
S7	0,13	5,2	7,38	5676,9231	0,8681	3,7541	Nguyen et al. 2020
S8	0,4	5,2	2,12	530,0000	0,3263	2,7243	Nguyen et al. 2020
S9	1,19	5,2	3,23	271,4286	0,5092	2,4337	Nguyen et al. 2020
S10	0,17	5,2	2,96	1741,1765	0,4713	3,2408	Nguyen et al. 2020
S1	0,7	7,2	2,35	335,7143	0,3711	2,5260	Nguyen et al. 2020
S2	0,37	7,2	1,57	424,3243	0,1959	2,6277	Nguyen et al. 2020
S3	0,08	7,2	1,31	1637,5000	0,1173	3,2142	Nguyen et al. 2020
S4	0,25	7,2	2	800,0000	0,3010	2,9031	Nguyen et al. 2020
S5	2,23	7,2	2,1	94,1704	0,3222	1,9739	Nguyen et al. 2020
S6	4,9	7,2	10,69	218,1633	1,0290	2,3388	Nguyen et al. 2020
S7	0,13	7,2	1,77	1361,5385	0,2480	3,1340	Nguyen et al. 2020
S8	0,4	7,2	1,27	317,5000	0,1038	2,5017	Nguyen et al. 2020
S9	1,19	7,2	4,29	360,5042	0,6325	2,5569	Nguyen et al. 2020
S10	0,17	7,2	2,46	1447,0588	0,3909	3,1605	Nguyen et al. 2020
S1	0,7	8,3	2,13	304,2857	0,3284	2,4833	Nguyen et al. 2020
S2	0,37	8,3	2,17	586,4865	0,3365	2,7683	Nguyen et al. 2020
S3	0,08	8,3	1,93	2412,5000	0,2856	3,3825	Nguyen et al. 2020
S4	0,25	8,3	1,65	660,0000	0,2175	2,8195	Nguyen et al. 2020
S5	2,23	8,3	1,19	53,3632	0,0755	1,7272	Nguyen et al. 2020
S6	4,9	8,3	9,38	191,4286	0,9722	2,2820	Nguyen et al. 2020
S7	0,13	8,3	1,24	953,8462	0,0934	2,9795	Nguyen et al. 2020
S8	0,4	8,3	1,3	325,0000	0,1139	2,5119	Nguyen et al. 2020
S9	1,19	8,3	2,65	222,6891	0,4232	2,3477	Nguyen et al. 2020
S10	0,17	8,3	2,19	1288,2353	0,3404	3,1100	Nguyen et al. 2020
Al pH 3		2,8				3,8	Campos Periera et al. 2018
Al pH 4		4				3,7	Campos Periera et al. 2018
Al pH 5		4,8				3,4	Campos Periera et al. 2018
Al pH 6		5,7				2,9	Campos Periera et al. 2018
Al pH 3		2,8				3,9	Campos Periera et al. 2018
Al pH 4		4				3,6	Campos Periera et al. 2018
Al pH 5		4,7				3,3	Campos Periera et al. 2018
Al pH 6		5,7				2,8	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				3,5	Campos Periera et al. 2018
Ca pH 4 [5mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				3,2	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				3,1	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				3,6	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				3,4	Campos Periera et al. 2018

Ca pH 5 [5 mM]		4,6			3,2	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2			3,1	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9			3,6	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9			2,9	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,9			2,7	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6			2,5	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9			3,6	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9			2,9	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,8			2,7	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6			2,6	Campos Periera et al. 2018
Na pH 3		3,1			3,6	Campos Periera et al. 2018
Na pH 4		4,2			2,8	Campos Periera et al. 2018
Na pH 5		4,9			2,5	Campos Periera et al. 2018
Na pH 6		5,8			2,4	Campos Periera et al. 2018
Na pH 3		3,1			3,9	Campos Periera et al. 2018
Na pH 4		4,2			2,8	Campos Periera et al. 2018
Na pH 5		4,9			2,5	Campos Periera et al. 2018
Na pH 6		5,8			2,6	Campos Periera et al. 2018
Jyndevad	1	6,1	4,2	420	2,62	Enevoldsen, Juhler 2010
Sj. Odde	0,42	7,6	n.a			Enevoldsen, Juhler 2010
Jyndevad	1	6,1	5,2	520	2,72	Enevoldsen, Juhler 2010
Sj. Odde	0,42	7,6	7,7	1833,3333	3,26	Enevoldsen, Juhler 2010

PFDA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						3,99702	
N						73	
S1	0,7	3,4	18,04	2577,1429	1,2562	3,4111	Nguyen et al. 2020
S2	0,37	3,4	1,72	464,8649	0,2355	2,6673	Nguyen et al. 2020
S3	0,08	3,4	14,17	17712,5000	1,1514	4,2483	Nguyen et al. 2020
S4	0,25	3,4	33,65	13460,0000	1,5270	4,1290	Nguyen et al. 2020
S5	2,23	3,4	19,1	856,5022	1,2810	2,9327	Nguyen et al. 2020
S6	4,9	3,4	122,98	2509,7959	2,0898	3,3996	Nguyen et al. 2020
S7	0,13	3,4	18,95	14576,9231	1,2776	4,1637	Nguyen et al. 2020
S8	0,4	3,4	30,13	7532,5000	1,4790	3,8769	Nguyen et al. 2020
S9	1,19	3,4	74,28	6242,0168	1,8709	3,7953	Nguyen et al. 2020
S10	0,17	3,4	21,11	12417,6471	1,3245	4,0940	Nguyen et al. 2020
S1	0,7	5,2	17,38	2482,8571	1,2400	3,3950	Nguyen et al. 2020
S2	0,37	5,2	1,01	272,9730	0,0043	2,4361	Nguyen et al. 2020
S3	0,08	5,2	11,6	14500,0000	1,0645	4,1614	Nguyen et al. 2020
S4	0,25	5,2	47,41	18964,0000	1,6759	4,2779	Nguyen et al. 2020
S5	2,23	5,2	20,03	898,2063	1,3017	2,9534	Nguyen et al. 2020
S6	4,9	5,2	73,06	1491,0204	1,8637	3,1735	Nguyen et al. 2020
S7	0,13	5,2	18,93	14561,5385	1,2772	4,1632	Nguyen et al. 2020
S8	0,4	5,2	8,77	2192,5000	0,9430	3,3409	Nguyen et al. 2020
S9	1,19	5,2	12,68	1065,5462	1,1031	3,0276	Nguyen et al. 2020
S10	0,17	5,2	10,81	6358,8235	1,0338	3,8034	Nguyen et al. 2020
S1	0,7	7,2	9,53	1361,4286	0,9791	3,1340	Nguyen et al. 2020
S2	0,37	7,2	0,86	232,4324	-0,0655	2,3663	Nguyen et al. 2020
S3	0,08	7,2	16,87	21087,5000	1,2271	4,3240	Nguyen et al. 2020
S4	0,25	7,2	12,3	4920,0000	1,0899	3,6920	Nguyen et al. 2020
S5	2,23	7,2	8,52	382,0628	0,9304	2,5821	Nguyen et al. 2020
S6	4,9	7,2	45,75	933,6735	1,6604	2,9702	Nguyen et al. 2020
S7	0,13	7,2	7,96	6123,0769	0,9009	3,7870	Nguyen et al. 2020
S8	0,4	7,2	7,53	1882,5000	0,8768	3,2747	Nguyen et al. 2020
S9	1,19	7,2	25,34	2129,4118	1,4038	3,3283	Nguyen et al. 2020
S10	0,17	7,2	11,46	6741,1765	1,0592	3,8287	Nguyen et al. 2020
S1	0,7	8,3	8,94	1277,1429	0,9513	3,1062	Nguyen et al. 2020
S2	0,37	8,3	0,38	102,7027	-0,4202	2,0116	Nguyen et al. 2020
S3	0,08	8,3	16,23	20287,5000	1,2103	4,3072	Nguyen et al. 2020
S4	0,25	8,3	11,98	4792,0000	1,0785	3,6805	Nguyen et al. 2020
S5	2,23	8,3	6,06	271,7489	0,7825	2,4342	Nguyen et al. 2020
S6	4,9	8,3	40,47	825,9184	1,6071	2,9169	Nguyen et al. 2020
S7	0,13	8,3	8,7	6692,3077	0,9395	3,8256	Nguyen et al. 2020
S8	0,4	8,3	9,48	2370,0000	0,9768	3,3747	Nguyen et al. 2020
S9	1,19	8,3	12,1	1016,8067	1,0828	3,0072	Nguyen et al. 2020
S10	0,17	8,3	8,52	5011,7647	0,9304	3,7000	Nguyen et al. 2020
Al pH 3		2,8				5	Campos Periera et al. 2018
Al pH 4		4				4,5	Campos Periera et al. 2018
Al pH 5		4,8				4,5	Campos Periera et al. 2018
Al pH 6		5,7				4,1	Campos Periera et al. 2018
Al pH 3		2,8				5	Campos Periera et al. 2018
Al pH 4		4				4,4	Campos Periera et al. 2018
Al pH 5		4,7				4,1	Campos Periera et al. 2018
Al pH 6		5,7				3,8	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				4,4	Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				5,5	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				4,1	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				5,1	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				5,5	Campos Periera et al. 2018

Ca pH 5 [5 mM]		4,6			4,3	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2			4,4	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9			4,9	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9			4,5	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,9			4,1	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6			3,9	Campos Periera et al. 2018
Ca pH 3 [3 mM]		2,9			4,6	Campos Periera et al. 2018
Ca pH 4 [3 mM]		3,9			4,5	Campos Periera et al. 2018
Ca pH 5 [3 mM]		4,8			4,2	Campos Periera et al. 2018
Ca pH 6 [3 mM]		5,6			4,3	Campos Periera et al. 2018
Na pH 3		3,1			3,9	Campos Periera et al. 2018
Na pH 4		4,2			4,5	Campos Periera et al. 2018
Na pH 5		4,9			4,4	Campos Periera et al. 2018
Na pH 6		5,8			4,2	Campos Periera et al. 2018
Na pH 3		3,1			4,5	Campos Periera et al. 2018
Na pH 4		4,2			4,4	Campos Periera et al. 2018
Na pH 5		4,9			4,3	Campos Periera et al. 2018
Na pH 6		5,8			3,7	Campos Periera et al. 2018
Jyndevad	1	6,1	30	3000	3,48	Enevoldsen, Juhler 2010
Sj. Odde	0,42	7,6	33	7857,14286	3,90	Enevoldsen, Juhler 2010

PFUn(D)A

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						4,3	
N						70	
S1	0,7	3,4	67,44	9634,2857	1,8289	3,9838	Nguyen et al. 2020
S2	0,37	3,4	194,65	52608,1081	2,2893	4,7211	Nguyen et al. 2020
S3	0,08	3,4	78,53	98162,5000	1,8950	4,9919	Nguyen et al. 2020
S4	0,25	3,4	78,61	31444,0000	1,8955	4,4975	Nguyen et al. 2020
S5	2,23	3,4	117,81	5282,9596	2,0712	3,7229	Nguyen et al. 2020
S6	4,9	3,4	186,81	3812,4490	2,2714	3,5812	Nguyen et al. 2020
S7	0,13	3,4	99,3	76384,6154	1,9969	4,8830	Nguyen et al. 2020
S8	0,4	3,4	67,82	16955,0000	1,8314	4,2293	Nguyen et al. 2020
S9	1,19	3,4	100,57	8451,2605	2,0025	3,9269	Nguyen et al. 2020
S10	0,17	3,4	137,04	80611,7647	2,1368	4,9064	Nguyen et al. 2020
S1	0,7	5,2	26,74	3820,0000	1,4272	3,5821	Nguyen et al. 2020
S2	0,37	5,2	40,58	10967,5676	1,6083	4,0401	Nguyen et al. 2020
S3	0,08	5,2	24,09	30112,5000	1,3818	4,4787	Nguyen et al. 2020
S4	0,25	5,2	108,74	43496,0000	2,0364	4,6384	Nguyen et al. 2020
S5	2,23	5,2	64,87	2908,9686	1,8120	3,4637	Nguyen et al. 2020
S6	4,9	5,2	248,99	5081,4286	2,3962	3,7060	Nguyen et al. 2020
S7	0,13	5,2	69,85	53730,7692	1,8442	4,7302	Nguyen et al. 2020
S8	0,4	5,2	14,75	3687,5000	1,1688	3,5667	Nguyen et al. 2020
S9	1,19	5,2	50,49	4242,8571	1,7032	3,6277	Nguyen et al. 2020
S10	0,17	5,2	49,42	29070,5882	1,6939	4,4635	Nguyen et al. 2020
S1	0,7	7,2	19,06	2722,8571	1,2801	3,4350	Nguyen et al. 2020
S2	0,37	7,2	32,62	8816,2162	1,5135	3,9453	Nguyen et al. 2020
S3	0,08	7,2	24,15	30187,5000	1,3829	4,4798	Nguyen et al. 2020
S4	0,25	7,2	31,01	12404,0000	1,4915	4,0936	Nguyen et al. 2020
S5	2,23	7,2	20,71	928,6996	1,3162	2,9679	Nguyen et al. 2020
S6	4,9	7,2	131,33	2680,2041	2,1184	3,4282	Nguyen et al. 2020
S7	0,13	7,2	23,32	17938,4615	1,3677	4,2538	Nguyen et al. 2020
S8	0,4	7,2	11,73	2932,5000	1,0693	3,4672	Nguyen et al. 2020
S9	1,19	7,2	68,03	5716,8067	1,8327	3,7572	Nguyen et al. 2020
S10	0,17	7,2	45,09	26523,5294	1,6541	4,4236	Nguyen et al. 2020
S1	0,7	8,3	18,87	2695,7143	1,2758	3,4307	Nguyen et al. 2020
S2	0,37	8,3	30,22	8167,5676	1,4803	3,9121	Nguyen et al. 2020
S3	0,08	8,3	40,46	50575,0000	1,6070	4,7039	Nguyen et al. 2020
S4	0,25	8,3	32,98	13192,0000	1,5183	4,1203	Nguyen et al. 2020
S5	2,23	8,3	19,35	867,7130	1,2867	2,9384	Nguyen et al. 2020
S6	4,9	8,3	139,28	2842,4490	2,1439	3,4537	Nguyen et al. 2020
S7	0,13	8,3	24,87	19130,7692	1,3957	4,2817	Nguyen et al. 2020
S8	0,4	8,3	19,57	4892,5000	1,2916	3,6895	Nguyen et al. 2020
S9	1,19	8,3	53,4	4487,3950	1,7275	3,6520	Nguyen et al. 2020
S10	0,17	8,3	24,81	14594,1176	1,3946	4,1642	Nguyen et al. 2020
Al pH 3		2,8				4,9	Campos Periera et al. 2018
Al pH 4		4				5,1	Campos Periera et al. 2018
Al pH 5		4,8				4,4	Campos Periera et al. 2018
Al pH 6		5,7				4,1	Campos Periera et al. 2018
Al pH 3		2,8				5,8	Campos Periera et al. 2018
Al pH 4		4				5,6	Campos Periera et al. 2018
Al pH 5		4,7				4	Campos Periera et al. 2018
Al pH 6		5,7				4,1	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				5,2	Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				5	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				4,2	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				5,7	Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				5,1	Campos Periera et al. 2018

Ca pH 5 [5 mM]	4,6	4,3	Campos Periera et al. 2018
Ca pH 6 [5 mM]	5,2	4,4	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9		Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	5,2	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,9	4,6	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	3,9	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	5,5	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	4,9	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,8	4,5	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	4,3	Campos Periera et al. 2018
Na pH 3	3,1	3,9	Campos Periera et al. 2018
Na pH 4	4,2	4,7	Campos Periera et al. 2018
Na pH 5	4,9	4,5	Campos Periera et al. 2018
Na pH 6	5,8	4,2	Campos Periera et al. 2018
Na pH 3	3,1	5,7	Campos Periera et al. 2018
Na pH 4	4,2	4,8	Campos Periera et al. 2018
Na pH 5	4,9	4,4	Campos Periera et al. 2018
Na pH 6	5,8	4,3	Campos Periera et al. 2018

PFDoDA

Soil	OC %	pH	Kd	Koc	logKd	logKoc	Reference
Median						4,7657	
N						69	
S1	0,7	3,4	1439,68	205668,5714	3,1583	5,3132	Nguyen et al. 2020
S2	0,37	3,4	1269,68	343156,7568	3,1037	5,5355	Nguyen et al. 2020
S3	0,08	3,4	1331,11	1663887,5000	3,1242	6,2211	Nguyen et al. 2020
S4	0,25	3,4	1620,47	648188,0000	3,2096	5,8117	Nguyen et al. 2020
S5	2,23	3,4	1771,15	79423,7668	3,2483	4,9000	Nguyen et al. 2020
S6	4,9	3,4	2264,71	46218,5714	3,3550	4,6648	Nguyen et al. 2020
S7	0,13	3,4	1606,89	1236069,2308	3,2060	6,0920	Nguyen et al. 2020
S8	0,4	3,4	140,67	35167,5000	2,1482	4,5461	Nguyen et al. 2020
S9	1,19	3,4	1944,78	163426,8908	3,2889	5,2133	Nguyen et al. 2020
S10	0,17	3,4	1255,74	738670,5882	3,0989	5,8685	Nguyen et al. 2020
S1	0,7	5,2	1100,16	157165,7143	3,0415	5,1964	Nguyen et al. 2020
S2	0,37	5,2	214,54	57983,7838	2,3315	4,7633	Nguyen et al. 2020
S3	0,08	5,2	893,23	1116537,5000	2,9510	6,0479	Nguyen et al. 2020
S4	0,25	5,2	1324,96	529984,0000	3,1222	5,7243	Nguyen et al. 2020
S5	2,23	5,2	1344,53	60292,8251	3,1286	4,7803	Nguyen et al. 2020
S6	4,9	5,2	2120,68	43279,1837	3,3265	4,6363	Nguyen et al. 2020
S7	0,13	5,2	1164,62	895861,5385	3,0662	5,9522	Nguyen et al. 2020
S8	0,4	5,2	70,36	17590,0000	1,8473	4,2453	Nguyen et al. 2020
S9	1,19	5,2	1251,04	105129,4118	3,0973	5,0217	Nguyen et al. 2020
S10	0,17	5,2	1160	682352,9412	3,0645	5,8340	Nguyen et al. 2020
S1	0,7	7,2	820,29	117184,2857	2,9140	5,0689	Nguyen et al. 2020
S2	0,37	7,2	293,56	79340,5405	2,4677	4,8995	Nguyen et al. 2020
S3	0,08	7,2	929,03	1161287,5000	2,9680	6,0649	Nguyen et al. 2020
S4	0,25	7,2	1167,41	466964,0000	3,0672	5,6693	Nguyen et al. 2020
S5	2,23	7,2	904,98	40582,0628	2,9566	4,6083	Nguyen et al. 2020
S6	4,9	7,2	1391,13	28390,4082	3,1434	4,4532	Nguyen et al. 2020
S7	0,13	7,2	162,39	124915,3846	2,2106	5,0966	Nguyen et al. 2020
S8	0,4	7,2	93,05	23262,5000	1,9687	4,3667	Nguyen et al. 2020
S9	1,19	7,2	1269,59	106688,2353	3,1037	5,0281	Nguyen et al. 2020
S10	0,17	7,2	187,8	110470,5882	2,2737	5,0432	Nguyen et al. 2020
S1	0,7	8,3	942,72	134674,2857	2,9744	5,1293	Nguyen et al. 2020
S2	0,37	8,3	212,87	57532,4324	2,3281	4,7599	Nguyen et al. 2020
S3	0,08	8,3	1182,21	1477762,5000	3,0727	6,1696	Nguyen et al. 2020
S4	0,25	8,3	1091,06	436424,0000	3,0378	5,6399	Nguyen et al. 2020
S5	2,23	8,3	115,54	5181,1659	2,0627	3,7144	Nguyen et al. 2020
S6	4,9	8,3	1484,54	30296,7347	3,1716	4,4814	Nguyen et al. 2020
S7	0,13	8,3	977,07	751592,3077	2,9899	5,8760	Nguyen et al. 2020
S8	0,4	8,3	102,75	25687,5000	2,0118	4,4097	Nguyen et al. 2020
S9	1,19	8,3	1149	96554,6218	3,0603	4,9848	Nguyen et al. 2020
S10	0,17	8,3	99,65	58617,6471	1,9985	4,7680	Nguyen et al. 2020
Al pH 3		2,8				4,8	Campos Periera et al. 2018
Al pH 4		4				5,1	Campos Periera et al. 2018
Al pH 5		4,8				4,1	Campos Periera et al. 2018
Al pH 6		5,7				3,8	Campos Periera et al. 2018
Al pH 3		2,8					Campos Periera et al. 2018
Al pH 4		4				5,1	Campos Periera et al. 2018
Al pH 5		4,7				3,9	Campos Periera et al. 2018
Al pH 6		5,7				3,8	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9				4,9	Campos Periera et al. 2018
Ca pH 4 [5 mM]*		4					Campos Periera et al. 2018
Ca pH 5 [5 mM]		4,5				4,5	Campos Periera et al. 2018
Ca pH 6 [5 mM]		5,2				3,9	Campos Periera et al. 2018
Ca pH 3 [5 mM]		2,9					Campos Periera et al. 2018
Ca pH 4 [5 mM]		3,8				4,7	Campos Periera et al. 2018

Ca pH 5 [5 mM]	4,6	4,1	Campos Periera et al. 2018
Ca pH 6 [5 mM]	5,2	4	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	5,5	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	4,7	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,9	4,4	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	3,8	Campos Periera et al. 2018
Ca pH 3 [3 mM]	2,9	5	Campos Periera et al. 2018
Ca pH 4 [3 mM]	3,9	4,5	Campos Periera et al. 2018
Ca pH 5 [3 mM]	4,8	4,1	Campos Periera et al. 2018
Ca pH 6 [3 mM]	5,6	3,9	Campos Periera et al. 2018
Na pH 3	3,1	3,9	Campos Periera et al. 2018
Na pH 4	4,2	4,3	Campos Periera et al. 2018
Na pH 5	4,9	4,1	Campos Periera et al. 2018
Na pH 6	5,8	3,8	Campos Periera et al. 2018
Na pH 3	3,1	5	Campos Periera et al. 2018
Na pH 4	4,2	4,3	Campos Periera et al. 2018
Na pH 5	4,9	4,1	Campos Periera et al. 2018
Na pH 6	5,8	3,9	Campos Periera et al. 2018

Data reprinted from from Pettersson et al 2015.

Bilaga A

Sammanställning av publicerade sorptionsdata för PFOS. (-) betyder data saknas.

Substrat	f_{oc} (%)	ler (%)	K_d (L/kgjord)	K_{oc} (L/kgorgC)	PFOS till-satt (µg/kg)	pH	jonmedium	Jämvikts-tid (h)	Referens
Jord K	0,52	-	7,28	1400	1000	-	2 mM NaCl	50	1
Jord L	2,1	-	14,2	676	1000	-	2 mM NaCl	50	1
Jord B	2,5	-	16,1	644	1000	-	2 mM NaCl	50	1
jord D	5,2	-	40,3	775	1000	-	2 mM NaCl	50	1
Jord S	16	-	115	718,75	1000	-	2 mM NaCl	50	1
Jord ASCO	0,2	17,2	19	9500	10000	8	10 mM $CaCl_2$	24	2
Jord ALM	1,6	10,9	32	2000	10000	5,9	10 mM $CaCl_2$	24	2
Jord GOLOSO	3,9	10,4	38	974	10000	6,3	10 mM $CaCl_2$	24	2
Jord DELTA2	7,7	43,6	76	987	10000	7,9	10 mM $CaCl_2$	24	2
Jord OVI01	9,4	23,6	110	1170	10000	4,6	10 mM $CaCl_2$	24	2
Jord Dublin	39	-	295	756	10000	5,3	10 mM $CaCl_2$	24	2
Jord Jynnevad	1	5	15	1500	5	6,1	100 mM $CaCl_2$	96	3
Jord Sj, Odde	0,42	37	17	4048	5	7,6	100 mM $CaCl_2$	96	3
Sediment 1	2,48	53	17,16	692	1000	7	3,5 mM $CaCl_2$	240	4
Sediment 2	1,02	26	1,82	178	1000	7,5	11,8 mM $CaCl_2$	240	4
Sediment 3	4,34	31	14,24	328	1000	7,6	2,2 mM $CaCl_2$	240	4
Sediment 5	9,66	5	45,83	474	1000	5,7	0,5 mM $CaCl_2$	240	4
Sediment 1	0,028	-	6,2	22143	0,2-1,0	-	vatten	48	5
Sediment 2	1,59	-	17	1069	0,2-1,0	-	vatten	48	5
Sediment 3	1,06	-	61,3	5783	0,2-1,0	-	vatten	48	5

1) Chen et al., 2013
2) Milinovic et al., 2015
3) Enevoldsen & Juhler, 2010
4) Higgins & Luthy, 2006
5) Ahrens et al., 2011

References Appendix A:

EU. 2011. PERFLUOROOCTANE SULPHONATE (PFOS). PFOS EQS dossier 2011. EQS dossier was prepared by the Sub-Group on Review of the Priority Substances List under Working Group E of the Common Implementation Strategy for the Water Framework Directive.

ECHA 2013. European Chemical Agency. MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR IDENTIFICATION OF PENTADECAFLUOROOCTANOIC ACID (PFOA) AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS CMR AND PBT PROPERTIES.

ECHA 2017. European Chemical Agency. MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR IDENTIFICATION OF PERFLUOROHEXANE-1-SULPHONIC ACID AND ITS SALTS AS SUBSTANCES OF VERY HIGH CONCERN BECAUSE OF ITS CMR AND PBT PROPERTIES.

ECHA 2015. SUPPORT DOCUMENT FOR IDENTIFICATION OF PERFLUORONONAN-1-OIC ACID AND ITS SODIUM AND AMMONIUM SALTS AS SUBSTANCES OF VERY HIGH CONCERN BECAUSE OF THEIR TOXIC FOR REPRODUCTION AND PBT PROPERTIES.

Zareitalabad P, Siemens J, Hamer M, Amelung W. 2013. Perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) in surface waters, sediments, soils and wastewater – A review on concentrations and distribution coefficients. Chemosphere 91: 725-732. https://doi.org/10.1016/j.

Pettersson, M, Ländell, M, Ohlsson, Y, Berggren Kleja, D, Tiberg, C. 2015. Preliminära riktvärden för högfluorerade ämnen (PFAS) i mark och grundvatten. Statens geotekniska institut, SGI Publikation 21, Linköping. 1.1-1502-0078.

Campos Pereira H, Ullberg M, Kleja DB, Gustafsson JP, Ahrens L. 2018. Sorption of perfluoroalkyl substances (PFASs) to an organic soil horizon - Effect of cation composition and pH. Chemosphere 207:183-191. doi: 10.1016/j.chemosphere.2018.05.012.

Kim M, Li LY, Grace JR, Yue C. Selecting reliable physicochemical properties of perfluoroalkyl and polyfluoroalkyl substances (PFASs) based on molecular descriptors. Environ Pollut. 2015 Jan;196:462-72. doi: 10.1016/j.envpol.2014.11.008.

Appendix B
Terrestrial Ecotoxicity data

Ecotoxicological data presented below is based upon a simple screening of available data basedpon a number of review articles. Data has not been quality assessed, e.g. according to Klimisch or CRED evaluation systems (Klimisch et al. 1997, Moermond et al. 2006).

Ankley et al. (2021) reviewed the existing literature on both aquatic and terrestrial ecotoxicity, including all information found in the USEPA database ECOTOC. Generally, only few toxicological studies with PFAS have been conducted with terrestrial invertebrates. Below, a few of the available ecotoxicological studies with soil organisms are presented in more detail.

Cai et al. (2021) reviewed the ecotoxicological data for terrestrial organisms and concluded that, typically, the addition of PFAS would accelerate the production of reactive oxygen species (ROS) in terrestrial organisms, while the excessive ROS could not be eliminated by the defense system causing potential oxidative damage. The implications of such biomarker responses at population and ecosystem level are not discussed in the review.

Below, a selected set of studies, identified via the two reviews listed above, are described in more detail.

Microorganisms
With regard to the potential of PFAS causing harm to microbial communities, the conclusions from Cai et al. (2021) are not straight forward, as both stimulation and harmful impact on species richness and diversity were observed. For example, in the laboratory conditions, where microbial communities in soil were spiked with four PFAS (PFBS, PFOS, PFHxS, and OBS) to 1 mg/kg for 80 days, Qiao et al. (2018) showed that the treatments increased bacterial richness, but decreased bacterial diversity because PFASs stimulated the growth of some bacteria, but inhibited others. At concentrations of 10 µg/kg 100 µg/kg of PFOS, the promotion action was stronger than the toxic effect on soil bacteria. Conversely, the toxicity was stronger than the promotion action under high concentrations of PFOS (1,000 and 10,000 µg PFOS/kg soil).

It is difficult to establish a NOEC for microorganisms, as tests typically are not performed according to e.g. OECD standards and results often are biased with both negative and positive effects observed. Based upon the available information, it is concluded that a level of 1.0 mg PFAS/kg would be a sound estimate of a NOEC for long-term changes of the microbial community.

Plants
Brooke et al. (2004) published a risk evaluation report for PFOS for the Environment Agency of the UK. Here, they presented the results from an internal non-published study by 3M with several plant species. The text is presented below:

> *The toxicity of PFOS to plants through soil exposure has been investigated using a method based on the OECD 21-day test guideline (3M, 2004). The endpoints examined were emergence, survival, shoot height and shoot weight. These endpoints were measured after 21 days of exposure. Where possible, the plants were allowed to continue growing after this time until they*

produced fruit or sufficient leaf for analysis. The results of these later analyses are included in Section 3.2.6.2.

The seven plant species included in the study were: lettuce (Lactuca sativa); ryegrass (Lolium perenne); tomato (Lycopersicon esculentum); onion (Allium cepa); alfalfa (Medicago sativa); flax (Linum usitatissimum); and soybean (Glycine max). The nominal concentrations used in the tests were 3.91, 15.6, 62.5, 250 and 1000 mg/kg. Concentrations measured in the soil at the beginning of the exposures were all within 70% of the nominal values. Concentrations were also measured at the final termination of the study after 205 days, when the concentrations ranged from 22.8% to 62.8% of nominal. Samples were taken at 21 days, but the results were considered to be artefacts due to the irrigation and sampling methods used. The results presented are based on the nominal concentrations. The lowest no effect concentrations for each endpoint were as follows:

Emergence 62.5 mg/kg onion, ryegrass
Survival 15.6 mg/kg onion, tomato
Shoot height <3.91 mg/kg lettuce (23% reduced compared to control)
Shoot weight <3.91 mg/kg lettuce (35% reduced compared to control)

Unfortunately, it is not possible to establish a NOEC based upon the data presented by Brooks et al. (2004), as significant reductions on lettuce were observed at the lowest test concentration. Li et al. (2022) recently reviewed plant toxicity data with regard to PFAS and concluded that IC50 for growth is much higher than environmentally relevant concentrations of PFAS and that PFAS rarely cause physiological damage in plants at realistic and relevant PFAS concentrations outside extreme hot spots.

Cai et al. (2020) reviewed the phytotoxicity of PFAS and concluded that the performance of plant biomass under PFAS exposure appeared to be affected by plants species, PFAS concentrations and exposure duration. Du et al. (2020) found that PFOA represses plant growth by down-regulating photosynthetic pigments and disturbing the metabolism of carbohydroxides, phenols and amino acids. The biomass of cucumber (*Cucumis sativus*) was inhibited after 60 days of exposure to 0.2 as 5.0 mg PFOA/kg. No significant difference was observed in biomass between the treatments of 0.2 and 5 mg/kg, indicating that rather than dose effect, there are other factors affecting the growth of cucumber, or plants employ strategies to alleviate the toxicity of PFOA. Zhao et al. (2011) investigated phytotoxicity of PFOS (0.1–200 mg/kg) and PFOA (0.1–400mg/kg) by detecting root growth of *Brassica chinensis* in six different Chinese soils for short-term exposure (7 days) and determined the EC50 and EC10 values of PFOA ranged from 107 to 246mg/kg and from 48 to 177mg/kg, respectively. The NOEC values of PFOA varied from 10 to 200 mg/kg. By contrast, the NOECs of PFOS varied from 50 to 150 mg/kg; the values of EC50 ranged from 95 to >200 mg/kg, and the values of EC10 ranged from 40 to 115 mg/kg. The EC10 and EC50 of PFOA in *Sorghum bicolor* root elongation tests were calculated as 5.98 mg/kg and 140.63 mg/kg by Gonzalez-Naranjo and Boltes (2014).

Earthworms

Cai et al. (2020) also reviewed the toxicity of PFAS to earthworms and found that all reported effects were well above 1 mg/kg. Typically, at least one order of magnitude higher. For example, Sindermann et al. (2002, c.f. Beach et al. 2006) performed a standard 14 day toxicity test with *Eisenia fetida* and found the 14-day LC50 estimation for PFOS in an artificial soil substrate to be 373 mg a.i./kg soil, with 95% confidence limits of 316 and 440 mg a.i./kg. Sublethal changes in molecular biomarkers and/or genetic expressions may, however, be seen at lower concentrations.

Zareitalabad et al. (2013) found that both PFOA and PFOS significantly decreased the surviving numbers and dry weight of earthworms (*Aporrectodea caliginosa*) at concentrations of 100 mg kg(-1). No earthworms survived at PFOA and PFOS concentrations of 500 mg/kg. At concentrations of 1 mg/kg, no negative effects were observed.

Yuan et al. (2017) studied effects of PFOA and PFOS on the earthworm *Eisenia fetida*. The LC50 values following 7 and 14 days of exposure to PFOA were 849.82 and 811.42 mg/kg, and to PFOS they were 627.77 and 540.97 mg/kg in the natural field soil test. Also, avoidance behavior was found to be dose dependent. The results indicate significant avoidance behavior at PFOA exposure of 400 mg/kg in soil. Significant avoidance behavior was observed at PFOS concentrations of 160 and 320 mg/kg.

He et al. (2016) studied the toxicity of PFOA towards earthworm and enzymatic activities in soil. In general, PFOA caused inhibition of all the measured microbial processes in a dose-dependent manner, and the inhibition was higher in sandy soil compared to clay soil. EC50 values for the enzymatic assays ranged from 62.35 to 233.75 mg/kg. A minor, but significant, reduction in the potential microbial nitrification activity (nitrite production from soils amended with ammonium sulphate 5 h at 25 °C) was observed in the sandy soil at 1.0 mg/kg with a corresponding NOEC of 0.5 mg/kg. In the clay soil, the LOEC and NOEC were 2.0 and 1.0 mg/kg, respectively. There was no mortality in earthworms exposed up to 100 mg/kg soil in both soils. However, there was a significant weight loss from 25 mg/kg onwards.

Zheng et al. (2016) reported 14 d-LC50 of PFOS and PFOA of 478.0 mg/kg and 759.6 mg/kg, respectively, when exposing the earthworm *Eisenia fetida* to PFAS in soil. Growth was significantly affected, approximately 25% for PFOS and 15-20% for PFOA, at the lowest test concentration of 50 mg/kg.

Karnjanapiboonwong et al. (2018) exposed earthworms to a wider set of PFAS at more environmentally realistic soil concentrations. They concluded that PFAS could be detected in earthworms even in the 0.1 µg/kg soil treatment after 21 days of exposure and that PFAS accumulation in earthworms followed the order: PFNA > PFHxS > PFHpA > PFBS. Generally, no mortality of earthworms was observed in any treatment, including controls after 21-d exposure, except for the highest treatment (100 mg/kg), where a mortality rate of approximately 5% was observed for all PFAS. Earthworm weights generally decreased after 21 days (4.4-29%) of exposure to PFASs in soils, also in the controls as no feeding took place. The highest weight loss (29%) was observed in earthworms exposed to PFNA in the 100 mg/kg treatment.

ETC derivation based upon ecotoxicological data for soil dwelling species

The lowest identified effect level was for a phytoxicity study with cucumber, where a significant adverse effect on biomass was observed at 0.2 mg PFOA/kg (Du et al. 2020). The plants were exposed in soil, and PFOA was mainly found in the leaves with far less in roots and stems. There was no cohenrent dose-response pattern in this study, however, as a comparable effect was observed at 5.0 mg PFOA/kg, it indicates that rather than dose effect, there are other factors affecting the growth of cucumber or the plants employ some strategies to alleviate the toxicity of PFOA.

More than a 20% reduction in growth of lettuce was observed at 3.9 mg PFOS/mg (Brooke et al. 2004).

In none of the studies listed above, a NOEC could be established. As a conservative approach, 0.2 mg PFOA/kg is chosen as LOEC for the PNEC derivation. The Guidance for deriving PNEC provided by ECHA (ECHA 2008 – Part R.10) specifically states:

A LOEC (lowest observed effect concentration) stands for the lowest concentration where an effect is observed. It should therefore not be used as a NOEC. In case only a LOEC is given in the report, it can be used to derive a NOEC with the following procedures: LOEC > 10 and < 20% effect: NOEC can be calculated as LOEC/2. If the effect percentage of the LOEC is unknown, no NOEC can be derived.

In the case of Du et al. (2020), the adverse effect on growth of biomass of stems was larger than 20%, i.e. approximately 50%, at 0.2 mg/kg**,** for which reason the data can be seen more as an EC_{50} value, although no dose-response was present. No guidance on how to extrapolate from an EC_{50} to a NOEC is given in the ECHA R.10 document (ECHA 2008). Hence, a conservative assessment factor of 10 is chosen, resulting in a NOEC of 20 µg/kg. Comparison studies on large aquatic data sets have shown that generally a factor of 10 is sufficient to cover the LC50:NOEC ratio, e.g. Saouter et al. (2019). Such extrapolation typically also accounts for short-term versus long-term exposure and lethal versus sub-lethal endpoints. In the case of Du et al. (2020), the LOEC is based on sub-lethal endpoint (biomass) and long-term exposure (60 days), suggesting a lower assessment factor could have been applied.

ETC_{soil} for the terrestrial ecosystem can be determined by dividing the lowest derived NOEC by an assessment factor of 10, i.e. 20 µg PFOA/kg. /10 = 2.0 µg PFOA/kg.

For the ETC_{soil} derivation for PFOS, a NOEC of 1.0 mg/kg can be selected as the lowest found. This was based upon the study of Zareitalabad et al. (2013), who found that both PFOA and PFOS significantly decreased the surviving numbers and dry weight of earthworms (*Aporrectodea caliginosa*) at concentrations of 100 mg/kg. No earthworms survived at PFOA and PFOS concentrations of 500 mg/kg. At concentrations of 1 mg/kg, however, no negative effects were observed, i.e. NOEC. For PFOS, data is available for three trophic levels (Appendix B), which is why an ETC can be determined as 1.0 mg/kg / 10 = 0.1 mg/kg = 100 µg/kg.

EQS derived by the Norwegian Geotechnical Institute (NGI)

PFOS

NGI (2020) derived Norwegian quality standards for soil biota exposed to PFOS using data from Bodar (2011) supplemented by new data. The quality standards are based on no-observed-effect concentrations (NOEC) or effect concentration for 10% of organisms (EC10) as a chronic endpoint. Results from tests using different plants and soil organisms were assessed. Geometric mean values of studies that were considered of sufficient quality were calculated. The dataset that forms the basis for the derived QS by NGI is presented in Table B.1. below.

Table. B.1. Ecotoxicological data for PFOS included in the QS derived by NGI. Reprinted from NGI (2020).

Taxonomic Group	Species	Criterium	Value (mg/kg dw)
Plants	*Allium cepa*	EC_{10}	2.3
	Brassica rapa chinensis	EC_{10}	72
	Glycine max	EC_{10}	75
	Lactuca sativa	EC_{10}	0.81
	Linum usitatissimum	EC_{10}	28
	Lolium perenne	EC_{10}	0.79
	Medicago sativa	EC_{10}	18
	Lycopersicum esculentem	EC_{10}	3.2
Invertebrates	*Eisenia fetida*	NOEC	3.8
	Folsomia candida	EC_{10}	90
	Oppia nitens		8.6
Geometric Mean			9.1

To derive a QS value that is considered protective for the soil ecosystem, the lowest value in Table B.1 (0.79 mg/kg d.w.) is used and an assessment factor of 50 is applied, as there is no data for microorganisms. This results in a value of 0.016 mg/kg or 16 µg PFOS/kg dw.

PFOA

NGI derived Norwegian quality standards for soil biota exposed to PFOS using data derived by Lijzen et al. (2018). The quality standards are based on no-observed-effect concentrations (NOEC) or effect concentration for 10% of organisms (EC10) as a chronic endpoint, except for soil microorganisms, as no NOEC or EC10 values could be found. The dataset that forms the basis for the derived QS by NGI is presented in the Table B.2 below.

Table B.2. Ecotoxicological data for PFOA included in the QS derived by NGI. Reprinted from NGI (2020).

Taxonomic Group	Species	Criterium	Value (mg/kg dw)
Microorganisms	Dehydrogenase acitivity	EC_{50}	66.2
	Urease acitivity	EC_{50}	87.7
Plants	*Brassica chinensis*	EC_{10}	99.8
	Brassica chinensis	EC_{50}	163
Invertebrates	*Eisenia fetida*	NOEC	25.0
	Eisenia fetida	LC_{50}	872
Geometric Mean for NOEC and EC_{10}			50

To derive a value that is considered protective for the soil ecosystem, the lowest value (25 mg/kg d.w.) is used and an assessment factor of 50 is applied. This results in a value of 0.50 mg/kg or 500 µg/kg d.w., which is considered protective of 95% of soil organisms.

Recommended ETC_{soil} for PFOS and PFOA in this report

Based on the screening of ecotoxicity data presented above and the QS presented by the Norwegian Institute NGI, the following tentative ETC_{soil} is suggested to be used in the assessment presented in this report:

PFOS: 16 µg/kg dw
PFOA: 2.0 µg/kg dw

References for Appendix B.

Ankley, G.T., Cureton, P., Hoke, R.A., Houde, M., Kumar, A., Kurias, J., Lanno, R., McCarthy, C., Newsted, J., Salice, C.J., Sample, B.E., Sepúlveda, M.S., Steevens, J. and Valsecchi, S. 2021. Assessing the Ecological Risks of Per- and Polyfluoroalkyl Substances: Current State-of-the Science and a Proposed Path Forward. Environ Toxicol Chem, 40: 564-605. https://doi.org/10.1002/etc.4869

Bodar CWM, Lijzen JPA, Moermond CTA, Peijnenburg WJGM, Smit CE, Verbruggen EMJ 2011. Advies risicogrenzen grond en grondwater voor PFOS. RIVM rapport 2011. 601050002, RIVM, Bilthoven Nederland.

Beach SA, Newsted JL, Coady K, Giesy JP. 2006. Ecotoxicological Evaluation of Perfluorooctanesulfonate (PFOS). Rev Environ Contam Toxicol 186:133–174.

Brooke D, Footitt A, NwaoguLi TA. 2004. Environmental Risk Evaluation Report: Perfluorooctanesulphate (PFOS). Environment Agency. ISBN: 978-1-84911-124-9**.**

Cai Y, Wang Q, Zhou B, Yuan R, Wang F, Chen Z, Chen H. 2021. A review of responses of terrestrial organisms to perfluorinated compounds. Sci Total Environ. 793:148565. doi: 10.1016/j.scitotenv.2021.148565.

Du W, Liu X, Zhao L, Xu Y, Yin Y, Wu J, Ji R, Sun Y, Guo H. 2020. Response of cucumber (*Cucumis sativus*) to perfluorooctanoic acid in photosynthesis and metabolomics. Science of The Total Environment 724: 138257. ISSN 0048-9697. https://doi.org/10.1016/j.scitotenv.2020.138257.

He W, Megharaj M, Naidu R. 2016. Toxicity of perfluorooctanoic acid towards earthworm and enzymatic activities in soil. Environ Monit Assess188 (7):424. doi: 10.1007/s10661-016-5416-y.

Karnjanapiboonwong A, Deb SK, Subbiah S, Wang D, Anderson TA. 2018. Perfluoroalkylsulfonic and carboxylic acids in earthworms (Eisenia fetida): Accumulation and effects results from spiked soils at PFAS concentrations bracketing environmental relevance. Chemosphere 199: 168-173. ISSN 0045-6535. https://doi.org/10.1016/j.chemosphere.2018.02.027.

Klimisch H-J, Andreae M, Tillmann U. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. Regul Toxicol Pharmacol 25: 1– 5.

Li J, Sun J, Li P. 2022. Exposure routes, bioaccumulation and toxic effects of per- and polyfluoroalkyl substances (PFASs) on plants: A critical review. Environ Int. 158:106891. doi: 10.1016/j.envint.2021.106891.

Lijzen JPA, Wassenaar PNH, Smit CE, Posthuma CJAM, Brand E, Swartjes FA, Verbruggen EMJ, Versteegh JFM. 2018. Risicogrenzen PFOA voor grond en grondwater. Uitwerking voor generiek en gebiedsspecifiek beleid (herziene versie). RIVM rapport 2018-0060, RIVM, Bilthoven, Nederland.

Moermond, C.T., Kase, R., Korkaric, M. and Ågerstrand, M. 2016. CRED: Criteria for reporting and evaluating ecotoxicity data. Environ Toxicol Chem, 35: 1297-1309. https://doi.org/10.1002/etc.3259.

NGI. 2020. Proposal for new Normative Values for PFOS and PFOA in contaminated soil. The Norwegian Geotechnical Institute (NGI). Document no: 20190750-01-R

Sindermann, AB, Porch, JR, Krueger, HO, and Van Hoven, RL. 2002. PFOS: an acute toxicity study with the earthworm in an artificial soil substrate. Project No. 454-111. EPA Docket AR226-1106. Wildlife International Ltd., Easton, MD.

Saouter, E., Wolff, D., Biganzoli, F. and Versteeg, D. 2019. Comparing Options for Deriving Chemical Ecotoxicity Hazard Values for the European Union Environmental Footprint, Part II. Integr Environ Assess Manag, 15: 796-807. https://doi.org/10.1002/ieam.4169

Qiao W, Xie Z, Zhang Y, Liu X, Xie S, Huang J, Yu L. 2018. Perfluoroalkyl substances (PFASs) influence the structure and function of soil bacterial community: Greenhouse experiment. Science of the total environment 642: 1118-1126. ISSN 0048-9697, https://doi.org/10.1016/j.scitotenv.2018.06.113.

Yuan Z, Zhang J, Zhao L, Li J, Liu H. 2017. Effects of perfluorooctanoic acid and perfluorooctane sulfonate on acute toxicity, superoxide dismutase, and cellulase activity in the earthworm Eisenia fetida. Environ Sci Pollut Res 24(22):18188-18194. doi: 10.1007/s11356-017-9477-4.

Zhao H, Chen C, Zhang X, Chen J, Quan X. 2011. Phytotoxicity of PFOS and PFOA to Brassica chinensis in different Chinese soils. Ecotoxicol Environ Saf. 74(5):1343-7. doi: 10.1016/j.ecoenv.2011.03.007.

Zheng X, Shi Y, Lu Y, Xu X. 2016. Growth inhibition and DNA damage in the earthworm (Eiseniafetida) exposed to perfluorooctane sulphonate and perfluorooctanoic acid, Chemistry and Ecology, 32:2, 103-116, DOI: 10.1080/02757540.2015.1116524

Zareitalabad P, Siemens J, Hamer M, Amelung W. 2013. Perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) in surface waters, sediments, soils and wastewater – A review on concentrations and distribution coefficients. Chemosphere 91: 725-732. ISSN 0045-6535. https://doi.org/10.1016/j.chemosphere.2013.02.024.

Appendix C
PFAS concentrations in Danish Sludge

Sludge concentrations of 22 PFAS collected from a wide number of Danish wastewater treatment plants. Numbers in red are concentrations originally reported as lower than the limit of quantification (LoQ). The approximated concentrations listed here are LoQ/2.

µg/kg dw		PFOS	PFOA	PFNA	PFHxS	PFBA	PFBS	PFPeA	PFPeS	PFHxA	PFHpA	PFHpS
		1	2	3	4	5	6	7	8	9	10	11
		4	4	4	4	22	22	22	22	22	22	22
MIN		**0,043**	**0,085**	**0,07**	**0,05**	**0,05**	**0,05**	**0,05**	**0,07**	**0,07**	**0,05**	**0,07**
10P		**2,4**	**0,3**	**0,185**	**0,137**	**0,137**	**0,135**	**0,14**	**0,135**	**0,145**	**0,14**	**0,14**
50P		**4,5**	**0,85**	**0,6**	**0,19**	**0,19**	**0,19**	**0,24**	**0,1825**	**0,48**	**0,235**	**0,185**
90P		**15**	**2,5**	**2,5**	**2,5**	**2,5**	**2,5**	**2,5**	**2,5**	**2,5**	**2,5**	**2,5**
MAX		**55**	**19**	**7,4**	**4,3**	**29**	**3,9**	**2,5**	**4,7**	**9,29**	**3,7**	**7,8**
N Total		**215**	**215**	**215**	**215**	**215**	**215**	**215**	**208**	**215**	**215**	**208**
N > LOQ		**183**	**154**	**99**	**12**	**12**	**10**	**16**	**4**	**57**	**15**	**5**
WWTP#1	Sample#1	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#1	Sample#2	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#1	Sample#3	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#1	Sample#4	4,9	0,36	0,41	0,05	0,05	0,05	0,05	-	0,66	0,05	-
WWTP#1	Sample#5	1,4	0,2	0,3	0,05	0,05	0,05	0,05	-	0,15	0,05	-
WWTP#2	Sample#6	7,4	0,3	6,9	0,15	0,15	0,15	0,15	0,15	0,34	0,15	0,15
WWTP#2	Sample#7	6,8	0,34	7,3	0,15	0,15	0,15	0,15	0,15	0,44	0,15	0,15
WWTP#2	Sample#8	7,3	0,64	0,55	0,14	0,14	0,14	0,14	0,14	0,45	0,14	0,14
WWTP#2	Sample#9	3,2	0,51	0,255	0,255	0,255	0,255	0,255	0,255	0,255	0,255	0,255
WWTP#3	Sample#10	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#3	Sample#11	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#4	Sample#12	4	0,55	0,49	0,165	0,165	0,165	0,165	0,165	0,165	0,165	0,165
WWTP#4	Sample#13	2,5	0,22	0,135	0,135	0,135	0,135	0,135	0,135	0,135	0,135	0,135
WWTP#4	Sample#14	2,4	0,165	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#5	Sample#15	36	0,67	0,185	0,185	0,185	0,185	0,185	0,185	0,185	0,185	0,185
WWTP#5	Sample#16	35	0,52	0,175	0,175	0,175	0,175	0,175	0,175	0,175	0,175	0,175
WWTP#5	Sample#17	31	0,43	0,37	0,19	0,19	0,19	0,19	0,19	0,19	0,19	0,19
WWTP#5	Sample#18	26	0,26	0,135	0,135	0,135	0,135	0,135	0,135	0,135	0,135	0,135
WWTP#5	Sample#19	15	1	2	2	2	2	2	2	2	2	2
WWTP#5	Sample#20	10	1,4	1,45	1,45	1,45	1,45	1,45	1,45	1,45	1,45	1,45
WWTP#5	Sample#21	9,3	1,7	1,05	1,05	1,05	1,05	1,05	1,05	1,05	1,05	1,05
WWTP#5	Sample#22	9,1	0,7	1,35	1,35	1,35	1,35	1,35	1,35	1,35	1,35	1,35
WWTP#5	Sample#23	8,9	1,5	0,7	0,7	0,7	0,7	0,7	0,7	0,7	0,7	0,7
WWTP#5	Sample#24	8,8	1,2	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#25	8	0,83	1	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#26	7,7	1,1	1	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#27	7,6	1,2	0,75	0,75	0,75	0,75	0,75	0,75	0,75	0,75	0,75
WWTP#5	Sample#28	4,4	1,6	1,2	1,2	1,2	1,2	1,2	1,2	1,2	1,2	1,2
WWTP#5	Sample#29	5,8	1,5	0,375	0,375	0,375	0,375	0,375	0,375	0,375	0,375	0,375
WWTP#5	Sample#30	6,4	0,66	0,395	0,395	0,395	0,395	0,395	0,395	0,395	0,395	0,395
WWTP#5	Sample#31	6,4	0,66	0,395	0,395	0,395	0,395	0,395	0,395	0,395	0,395	0,395
WWTP#5	Sample#32	5,1	1,1	0,41	0,41	0,41	0,41	0,41	0,41	0,41	0,41	0,41
WWTP#5	Sample#33	4,7	0,62	1	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6

WWTP#5	Sample#34	5,3	0,58	0,63	0,3	0,3	0,3	0,3	-	0,3	0,3	-
WWTP#5	Sample#35	4,2	0,72	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#36	4	0,75	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#37	3,2	0,3	1	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#38	3,2	0,3	1	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#39	3,8	0,38	0,51	0,17	0,17	0,17	0,17	0,17	0,17	0,17	0,17
WWTP#5	Sample#40	3,3	0,28	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#41	3,6	0,43	0,265	0,265	0,265	0,265	0,265	0,265	0,265	0,265	0,265
WWTP#5	Sample#42	2,9	0,29	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#5	Sample#43	3,5	0,28	0,35	0,11	0,11	0,11	0,11	-	0,11	0,11	-
WWTP#5	Sample#44	2,8	0,26	0,55	0,55	0,55	0,55	0,55	0,55	0,55	0,55	0,55
WWTP#5	Sample#45	1,8	0,14	0,07	0,07	0,07	0,07	0,07	0,07	0,07	0,07	0,07
WWTP#6	Sample#46	18	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#6	Sample#47	7	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#6	Sample#48	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#6	Sample#49	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#7	Sample#50	7,9	0,29	0,44	0,135	0,135	0,135	0,135	0,135	0,48	0,135	0,135
WWTP#7	Sample#51	6,2	0,95	0,81	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#7	Sample#52	5,6	0,87	0,82	0,51	0,155	0,155	0,155	0,155	0,155	0,155	0,155
WWTP#8	Sample#53	8,7	0,71	0,6	0,165	0,165	0,165	0,165	0,165	0,6	0,165	0,165
WWTP#9	Sample#54	12	1,2	0,78	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15
WWTP#9	Sample#55	10	0,85	0,85	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15
WWTP#9	Sample#56	7,9	0,69	0,45	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15
WWTP#10	Sample#57	16	1,3	1,3	0,155	0,155	0,155	0,155	0,155	0,46	0,155	0,155
WWTP#10	Sample#58	14	1	0,88	0,18	0,18	0,18	0,18	0,18	0,18	0,18	0,18
WWTP#10	Sample#59	11	1,8	0,54	0,235	0,235	0,235	0,235	0,235	0,85	0,235	0,235
WWTP#10	Sample#60	11	1,8	0,54	0,235	0,235	0,235	0,235	0,235	0,85	0,235	0,235
WWTP#10	Sample#61	11	1,7	0,305	0,265	0,265	0,265	0,265	0,265	0,52	0,265	0,265
WWTP#10	Sample#62	11	0,85	0,61	0,265	0,265	0,265	0,265	0,265	0,265	0,265	0,265
WWTP#10	Sample#63	7,9	1,1	0,24	0,24	0,24	0,24	0,24	0,24	0,24	0,24	0,24
WWTP#10	Sample#64	7,9	1,1	0,24	0,24	0,24	0,24	0,24	0,24	0,24	0,24	0,24
WWTP#10	Sample#65	3,5	0,42	0,37	0,16	0,16	0,16	0,16	0,16	0,16	0,16	0,16
WWTP#11	Sample#66	55	5,2	0,85	4,1	2,3	0,85	2	2,8	4,9	0,85	4
WWTP#11	Sample#67	5	3,4	0,85	0,85	3,6	3,9	0,85	2,5	2,5	3,7	0,85
WWTP#11	Sample#68	6,2	1	0,82	0,155	0,155	0,155	0,155	0,155	0,46	0,155	0,155
WWTP#11	Sample#69	5,1	0,88	0,88	0,18	0,18	0,18	0,18	0,18	0,41	0,18	0,18
WWTP#12	Sample#70	19	0,33	0,28	0,145	0,145	0,145	0,145	0,145	0,28	0,145	0,145
WWTP#12	Sample#71	15	0,42	0,37	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#12	Sample#72	14	0,55	0,41	0,14	0,14	0,14	0,14	0,14	0,41	0,14	0,14
WWTP#12	Sample#73	13	0,43	0,34	0,13	0,26	0,13	0,13	0,13	0,34	0,13	0,13
WWTP#12	Sample#74	13	0,33	0,33	0,145	0,145	0,145	0,145	0,145	0,28	0,145	0,145
WWTP#12	Sample#75	8,9	0,63	0,47	0,47	0,47	0,47	0,47	0,47	0,47	0,47	0,47
WWTP#13	Sample#76	31	2,2	0,56	0,3	0,155	3,9	0,71	0,155	0,66	0,38	0,155
WWTP#13	Sample#77	31	2,2	0,56	0,3	0,155	3,9	0,71	0,155	0,66	0,38	0,155
WWTP#13	Sample#78	5,9	0,92	1,1	0,165	0,165	0,52	0,76	0,165	0,76	0,165	0,165
WWTP#13	Sample#79	3,4	0,35	0,36	0,16	0,16	0,16	0,16	0,16	0,16	0,16	0,16
WWTP#13	Sample#80	3	0,57	0,185	0,185	0,185	0,42	1,4	0,185	0,41	0,185	0,185
WWTP#14	Sample#81	4,2	0,7	0,4	0,155	0,155	0,155	0,3	0,155	0,95	0,155	0,155
WWTP#14	Sample#82	4	0,48	0,42	0,16	0,16	0,16	0,16	0,16	0,16	0,16	0,16
WWTP#14	Sample#83	4	0,4	0,45	0,155	0,155	0,155	0,155	0,155	0,155	0,155	0,155
WWTP#14	Sample#84	3,5	0,63	0,32	0,32	0,32	0,32	0,32	0,32	0,32	0,32	0,32
WWTP#14	Sample#85	2,8	0,49	0,295	0,295	0,295	0,295	0,295	0,295	0,295	0,295	0,295
WWTP#14	Sample#86	2,4	0,5	0,29	0,125	0,125	0,125	0,125	0,125	0,125	0,125	0,125
WWTP#14	Sample#87	2	0,35	0,31	0,135	0,135	0,135	0,135	0,135	0,135	0,135	0,135
WWTP#15	Sample#88	16	0,88	0,58	0,27	0,135	0,135	0,97	0,135	0,75	0,4	0,135
WWTP#15	Sample#89	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5

WWTP#15	Sample#90	8,3	0,46	0,54	0,125	0,125	0,125	0,125	0,125	0,29	0,125	0,37
WWTP#15	Sample#91	4,1	0,87	0,56	0,155	0,155	0,155	0,155	0,155	0,155	0,155	0,155
WWTP#15	Sample#92	2	0,43	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#15	Sample#93	2	0,43	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#16	Sample#94	5,4	0,33	0,42	0,13	0,13	0,13	0,13	0,13	0,13	0,13	0,13
WWTP#16	Sample#95	4,1	0,78	0,34	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15
WWTP#16	Sample#96	0,043	0,14	0,09	0,09	0,09	0,09	0,09	0,09	0,09	0,09	7,8
WWTP#17	Sample#97	5,5	0,51	0,34	0,17	0,17	0,17	0,17	0,17	0,17	0,17	0,17
WWTP#17	Sample#98	5,5	0,51	0,34	0,17	0,17	0,17	0,17	0,17	0,17	0,17	0,17
WWTP#17	Sample#99	2,6	0,3	0,24	0,09	0,09	0,09	0,09	0,09	0,09	0,09	0,09
WWTP#18	Sample#100	11	0,85	0,85	4,3	4,2	0,85	0,85	0,85	3,8	0,85	0,85
WWTP#18	Sample#101	5,2	2,2	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#102	2,4	0,85	0,85	2,2	1,8	0,85	0,85	4,7	0,85	2,1	2,4
WWTP#18	Sample#103	2,7	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#104	2,6	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#105	2,6	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#106	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#107	2,4	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#108	2,3	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#109	2,1	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#110	2	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#111	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#112	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#113	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#114	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#115	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#116	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#117	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#19	Sample#118	3,7	0,55	0,28	0,14	0,14	0,14	0,14	0,14	0,14	0,14	0,14
WWTP#19	Sample#119	3,1	0,44	0,27	0,135	0,135	0,135	0,135	0,135	0,135	0,135	0,135
WWTP#20	Sample#120	3,3	0,6	0,205	0,205	0,205	0,205	0,205	0,205	0,54	0,205	0,205
WWTP#21	Sample#121	7,2	1,3	0,72	0,155	0,36	1,8	0,155	0,155	0,67	0,155	0,155
WWTP#21	Sample#122	7,8	0,78	0,45	0,17	0,17	1,2	0,17	0,17	0,56	0,17	0,17
WWTP#22	Sample#123	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#23	Sample#124	6,2	0,35	0,27	0,27	0,27	0,27	0,27	0,27	0,27	0,27	1,6
WWTP#24	Sample#125	28	11	1,5	0,46	0,14	0,27	0,55	0,14	3	1,1	0,14
WWTP#24	Sample#126	25	8,2	1,1	0,39	0,39	0,13	0,69	0,13	2,3	1,2	0,13
WWTP#24	Sample#127	23	4,8	0,99	0,24	0,12	0,12	0,28	0,12	0,24	0,71	0,12
WWTP#24	Sample#128	11	0,65	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6	0,6
WWTP#24	Sample#129	8,2	2,1	0,95	0,14	0,32	0,14	0,14	0,14	0,32	0,14	0,14
WWTP#24	Sample#130	7,8	2,3	0,83	0,16	0,16	0,16	0,16	0,16	0,52	0,16	0,16
WWTP#24	Sample#131	7,8	1,7	0,66	0,185	0,185	0,185	0,185	0,185	0,185	0,185	0,185
WWTP#24	Sample#132	7,5	1,8	0,8	0,135	0,135	0,135	0,62	0,135	0,53	0,44	0,135
WWTP#24	Sample#133	6,4	1,9	0,7	0,175	0,175	0,175	0,175	0,175	0,175	0,175	0,175
WWTP#24	Sample#134	6,5	1,5	0,77	0,18	0,18	0,18	0,18	0,18	0,18	0,18	0,18
WWTP#24	Sample#135	4,1	1,4	0,39	0,17	0,17	0,17	0,17	0,17	0,17	0,17	0,17
WWTP#25	Sample#136	6,3	0,85	0,53	0,16	0,16	0,16	0,16	0,16	0,37	0,16	0,16
WWTP#25	Sample#137	4,9	0,95	0,44	0,19	0,19	0,19	0,19	0,19	0,19	0,19	0,19
WWTP#25	Sample#138	3,7	1,3	0,51	0,19	0,19	0,19	0,19	0,19	0,57	0,19	0,19
WWTP#25	Sample#139	3,7	1,3	0,51	0,19	0,19	0,19	0,19	0,19	0,57	0,19	0,19
WWTP#25	Sample#140	3,9	0,65	0,46	0,14	0,14	0,14	0,14	0,14	0,14	0,14	0,14
WWTP#25	Sample#141	1,6	0,19	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#26	Sample#142	4,5	0,85	0,85	0,85	29	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#27	Sample#143	19	1,2	0,85	0,47	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#27	Sample#144	16	0,95	0,7	0,55	0,15	0,15	0,15	0,15	0,15	0,15	0,15
WWTP#27	Sample#145	16	1,2	0,55	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15

WWTP#27	Sample#146	10	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#27	Sample#147	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#27	Sample#148	3,3	0,52	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#27	Sample#149	2,8	0,46	0,46	0,175	0,175	0,175	0,175	0,175	0,175	0,175	0,175
WWTP#27	Sample#150	3	0,52	0,145	0,145	0,145	0,145	0,15	1,29	0,155	2,29	0,16
WWTP#27	Sample#151	2,6	0,44	0,51	0,19	0,19	0,19	0,19	0,19	0,19	0,19	0,19
WWTP#27	Sample#152	2,9	0,15	0,155	0,155	0,155	0,155	0,155	0,155	0,155	0,155	0,155
WWTP#28	Sample#153	5,8	0,79	0,47	0,16	0,16	0,16	0,16	0,16	0,16	0,16	0,16
WWTP#29	Sample#154	3,3	0,38	0,33	0,145	0,145	0,145	0,145	0,145	0,52	0,145	0,145
WWTP#30	Sample#155	3,6	1	0,53	0,16	0,16	0,16	0,16	0,16	1,3	0,16	0,16
WWTP#30	Sample#156	2,6	0,5	0,72	0,17	0,17	0,17	0,17	0,17	0,17	0,17	0,17
WWTP#30	Sample#157	0,38	0,085	0,165	0,165	0,165	0,165	0,165	0,165	0,165	0,165	0,165
WWTP#31	Sample#158	16	0,19	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#31	Sample#159	3,3	0,16	0,125	0,125	0,125	0,125	0,125	0,125	0,125	0,125	0,125
WWTP#31	Sample#160	2,6	0,53	0,45	0,125	0,125	0,29	0,125	0,125	1,3	0,125	0,125
WWTP#31	Sample#161	2,4	0,48	0,36	0,12	0,12	0,12	0,12	0,12	0,64	0,12	0,12
WWTP#32	Sample#162	33	6	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#32	Sample#163	5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#32	Sample#164	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#32	Sample#165	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#32	Sample#166	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#33	Sample#167	27	0,57	0,97	0,175	0,175	0,175	0,175	0,175	0,175	0,175	0,175
WWTP#33	Sample#168	17	0,56	0,88	0,24	0,24	0,24	0,24	0,24	0,24	0,24	0,24
WWTP#33	Sample#169	14	1,1	0,68	0,175	0,175	0,175	0,175	0,175	0,175	0,175	0,175
WWTP#33	Sample#170	7,5	0,67	0,29	0,29	0,29	0,29	0,29	0,29	0,29	0,29	0,29
WWTP#33	Sample#171	5,9	0,64	0,85	0,16	0,16	0,16	0,16	0,16	0,16	0,16	0,16
WWTP#34	Sample#172	7,5	0,7	0,5	0,15	0,15	0,15	0,15	0,15	0,4	0,15	0,15
WWTP#34	Sample#173	6,3	0,85	0,37	0,37	0,37	0,37	0,37	0,37	0,37	0,37	0,37
WWTP#34	Sample#174	5,1	0,43	0,165	0,165	0,165	0,165	0,165	0,165	0,165	0,165	0,165
WWTP#34	Sample#175	4,2	0,49	0,39	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15
WWTP#35	Sample#176	5,6	1,8	0,7	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#35	Sample#177	5,3	1	0,47	0,2	0,2	0,2	0,2	0,2	0,2	0,2	0,2
WWTP#35	Sample#178	3,2	0,61	0,39	0,155	0,155	0,155	0,33	0,155	0,77	0,4	0,155
WWTP#35	Sample#179	2,6	0,27	0,165	0,165	0,165	0,165	0,165	0,165	0,165	0,165	0,165
WWTP#35	Sample#180	2,6	0,28	0,135	0,135	0,135	0,135	0,135	0,135	0,135	0,135	0,135
WWTP#36	Sample#181	14	2,5	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#36	Sample#182	12	0,85	0,85	0,85	2,5	0,85	0,85	0,85	2,5	2,5	0,85
WWTP#36	Sample#183	8,6	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#36	Sample#184	5,7	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#36	Sample#185	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#36	Sample#186	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#36	Sample#187	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#37	Sample#188	9,4	1,2	0,5	0,17	0,17	0,17	0,17	0,17	0,17	0,17	0,17
WWTP#37	Sample#189	7,3	0,78	0,57	0,16	0,16	0,16	0,16	0,16	0,57	0,16	0,16
WWTP#37	Sample#190	6,2	1,5	0,83	0,16	0,41	0,16	0,93	0,16	3,4	0,41	0,16
WWTP#37	Sample#191	5,3	0,86	0,67	0,145	0,145	0,145	0,145	0,145	1,4	0,145	0,145
WWTP#38	Sample#192	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#39	Sample#193	7,43	2,5	2,5	2,5	2,5	2,5	2,5	-	9,29	2,5	-
WWTP#39	Sample#194	5,48	2,5	2,5	2,5	2,5	2,5	2,5	-	2,5	2,5	-
WWTP#40	Sample#195	14	19	7,4	0,16	0,16	0,16	0,42	0,16	1,1	1,7	0,16
WWTP#40	Sample#196	4,3	0,3	0,185	0,185	0,185	0,185	0,185	0,185	0,185	0,185	0,185
WWTP#41	Sample#197	1,9	0,26	0,155	0,155	0,155	0,155	0,155	0,155	0,155	0,155	0,155
WWTP#42	Sample#198	4	0,75	0,47	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#42	Sample#199	3,4	0,77	0,48	0,145	0,145	0,145	0,145	0,145	0,145	0,145	0,145
WWTP#43	Sample#200	5,3	1,2	0,67	0,17	0,17	0,17	0,17	0,17	0,61	0,17	0,17
WWTP#44	Sample#201	5,54	2,5	2,5	2,5	2,5	2,5	2,5	-	2,5	2,5	-

WWTP#45	Sample#202	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#45	Sample#203	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#45	Sample#204	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#45	Sample#205	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#45	Sample#206	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#46	Sample#207	5,2	0,76	0,66	0,145	0,145	0,145	0,145	0,145	0,43	0,145	0,145
WWTP#46	Sample#208	3,7	0,69	0,79	0,14	0,14	0,14	0,14	0,14	0,32	0,14	0,14
WWTP#46	Sample#209	3,4	0,79	0,64	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15
WWTP#47	Sample#210	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#48	Sample#211	4,3	2,6	0,45	0,135	0,135	0,135	1,1	0,135	3,1	0,36	0,135
WWTP#48	Sample#212	2,7	1,8	0,76	0,115	0,68	0,115	2,4	0,115	6,8	0,87	0,115
WWTP#48	Sample#213	2,5	0,88	0,55	0,55	0,55	0,55	0,55	0,55	0,55	0,55	0,55
WWTP#48	Sample#214	2,8	0,39	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15	0,15
WWTP#48	Sample#215	1,2	0,21	0,16	0,16	0,16	0,16	0,16	0,16	0,16	0,16	0,16

µg/kg dw		**6:2 FTS**	**PFOSA**	**PFNS**	**PFDA**	**PFDS**	**PFUnDS**	**PFUnDA**	**PFDoDA**	**PFDoDS**	**PFTrDS**	**PFTrDA**
		12	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**
		22	**22**	**22**	**22**	**22**	**22**	**22**	**22**	**22**	**22**	**22**
MIN		**0,05**	**0,135**	**0,135**	**0,59**	**0,07**	**0,145**	**0,07**	**0,12**	**0,135**	**0,5**	**0,07**
10P		**0,137**	**0,413**	**0,27**	**0,85**	**0,135**	**0,5**	**0,19**	**0,43**	**1**	**0,5**	**0,14**
50P		**0,24**	**0,85**	**0,355**	**2,4**	**0,185**	**1,2**	**0,66**	**0,85**	**1,65**	**1,45**	**0,295**
90P		**2,5**	**2,5**	**5**	**4**	**2,5**	**5**	**2,5**	**2,5**	**5**	**5**	**2,5**
MAX		**6,1**	**3,4**	**7,5**	**18**	**2,55**	**15**	**3,1**	**5**	**20**	**15**	**5**
N Total		**215**	**214**	**206**	**215**	**211**	**209**	**211**	**211**	**205**	**205**	**207**
N > LOQ		**15**	**128**	**2**	**163**	**0**	**4**	**98**	**127**	**0**	**0**	**30**
WWTP#1	Sample#1	2,5	2,5	5	2,5	2,5	5	2,5	2,5	5	5	2,5
WWTP#1	Sample#2	2,5	2,5	5	2,5	2,5	5	2,5	2,5	5	5	2,5
WWTP#1	Sample#3	2,5	2,5	5	2,5	2,5	5	2,5	2,5	5	5	2,5
WWTP#1	Sample#4	0,05	0,51	-	2,5	-	0,5	-	-	-	-	-
WWTP#1	Sample#5	0,05	0,6	-	1,9	-	0,5	-	-	-	-	-
WWTP#2	Sample#6	0,15	1,1	0,3	3,2	0,15	1,5	0,84	1,4	1,5	1,5	0,54
WWTP#2	Sample#7	0,15	0,73	0,295	2,1	0,15	0,68	1,5	0,92	1,5	1,5	0,29
WWTP#2	Sample#8	0,14	0,77	0,275	3,3	0,14	1,4	0,86	1,2	1,4	1,4	0,14
WWTP#2	Sample#9	0,51	0,255	0,55	0,59	0,255	2,55	0,255	0,255	2,55	2,55	0,255
WWTP#3	Sample#10	0,85	0,85	0,85	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#3	Sample#11	0,85	0,85	0,85	2,5	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#4	Sample#12	0,165	0,66	0,33	1,9	1,65	1,65	0,44	0,93	1,65	1,65	0,165
WWTP#4	Sample#13	0,135	1	0,265	2,9	0,135	0,5	0,57	1	1,35	0,5	0,135
WWTP#4	Sample#14	0,145	0,57	0,29	2	0,145	0,5	0,145	0,145	1,45	0,5	0,145
WWTP#5	Sample#15	0,185	0,8	0,37	2,2	0,185	1,85	0,43	0,8	1,85	1,85	0,185
WWTP#5	Sample#16	0,175	0,92	0,35	2,2	0,175	1,75	0,175	0,46	1,75	1,75	0,92
WWTP#5	Sample#17	0,19	1,2	0,75	1,7	0,19	0,5	0,56	1	1,9	0,5	0,19
WWTP#5	Sample#18	0,135	0,66	0,135	1,4	0,135	0,5	0,53	0,53	0,135	0,5	0,135
WWTP#5	Sample#19	2	2	4	4,7	2	0,5	2	2	20	0,5	2
WWTP#5	Sample#20	1,45	1,45	2,9	4,8	1,45	0,5	1,45	1,45	14,5	0,5	1,45
WWTP#5	Sample#21	1,05	1,05	2,1	4,5	1,05	0,5	1,05	2,1	10,5	0,5	1,05
WWTP#5	Sample#22	1,35	1,35	2,65	3	1,35	0,5	1,35	1,35	13,5	0,5	1,35
WWTP#5	Sample#23	0,7	0,7	1,35	3,3	0,7	0,5	0,7	0,7	7	0,5	0,7
WWTP#5	Sample#24	0,6	1,9	1,2	3,9	0,6	0,6	0,6	0,6	6	6	0,6
WWTP#5	Sample#25	0,6	1,6	1,2	3,4	0,6	0,6	0,6	0,6	6	6	0,6
WWTP#5	Sample#26	0,6	0,6	1,2	3	0,6	0,6	0,6	0,6	6	6	0,6
WWTP#5	Sample#27	0,75	0,75	1,5	3,2	0,75	0,5	0,75	0,75	7,5	0,5	0,75
WWTP#5	Sample#28	1,2	1,2	2,4	2,8	1,2	0,5	1,2	1,2	12	0,5	1,2
WWTP#5	Sample#29	0,375	1,6	0,75	3,3	0,5375	0,5	0,88	2,1	3,75	0,5	0,375

WWTP#5	Sample#30	0,395	1,6	0,8	4,9	0,395	0,5	0,395	0,395	3,95	0,5	0,395
WWTP#5	Sample#31	0,395	1,6	0,8	4,9	0,395	0,5	0,395	0,395	3,95	0,5	0,395
WWTP#5	Sample#32	0,41	1,2	0,85	2	0,41	4,1	0,41	0,95	4,1	4,1	0,41
WWTP#5	Sample#33	0,6	0,6	1,2	2,2	0,6	0,6	0,6	0,6	6	6	0,6
WWTP#5	Sample#34	0,3	1,2	-	5,8	-	-	-	-	-	-	-
WWTP#5	Sample#35	0,6	1,2	1,2	2,3	0,6	0,6	0,6	0,6	6	6	0,6
WWTP#5	Sample#36	0,6	0,6	1,2	4,9	0,6	0,6	0,6	0,6	6	6	0,6
WWTP#5	Sample#37	0,6	0,6	2,7	2,7	0,6	0,6	0,6	0,6	6	0,5	0,6
WWTP#5	Sample#38	0,6	0,6	1,2	2,7	0,6	6	0,6	0,6	6	0,5	0,6
WWTP#5	Sample#39	0,45	0,62	0,34	3,6	0,2	0,5	1,2	1,7	1,7	0,5	0,56
WWTP#5	Sample#40	0,6	0,6	1,15	2,4	0,6	0,5	0,6	0,6	6	0,5	0,6
WWTP#5	Sample#41	0,265	1,1	0,55	1,6	0,265	2,65	0,52	0,7	2,65	2,65	0,265
WWTP#5	Sample#42	0,6	0,6	1,2	0,6	0,6	6	0,6	0,6	6	6	0,6
WWTP#5	Sample#43	0,11	-	-	2,4	-	-	-	-	-	-	-
WWTP#5	Sample#44	0,55	0,55	1,05	1,2	0,55	0,5	0,55	0,55	5,5	0,5	0,55
WWTP#5	Sample#45	0,07	0,63	0,14	0,6	0,07	0,7	0,07	0,16	0,7	0,7	0,07
WWTP#6	Sample#46	2,5	2,5	2,5	2,5	2,5	2,5	2,5	4	2,5	4	5
WWTP#6	Sample#47	2,5	2,5	2,5	2,5	2,5	2,5	2,5	4	2,5	2,5	5
WWTP#6	Sample#48	2,5	2,5	2,5	2,5	2,5	2,5	2,5	4	2,5	5	4
WWTP#6	Sample#49	2,5	2,5	2,5	2,5	2,5	2,5	2,5	4	2,5	4	5
WWTP#7	Sample#50	0,3	0,66	0,265	2,6	0,135	0,5	0,62	0,79	1,35	0,5	0,135
WWTP#7	Sample#51	0,145	1,1	0,285	3,3	0,145	1,45	0,71	1,6	1,45	1,45	0,145
WWTP#7	Sample#52	0,155	0,67	0,31	1,7	0,155	0,5	0,51	0,87	1,55	0,5	0,46
WWTP#8	Sample#53	0,165	0,38	0,33	3	0,165	0,5	1,1	1,6	1,65	0,5	0,165
WWTP#9	Sample#54	0,15	1,1	0,295	2,4	0,15	15	0,49	0,88	1,5	15	0,49
WWTP#9	Sample#55	0,15	1,5	0,3	3	0,15	1,5	0,85	1	1,5	1,5	0,15
WWTP#9	Sample#56	0,15	1,7	0,3	2,1	0,15	1,5	0,5	1,3	1,5	1,5	0,54
WWTP#10	Sample#57	0,155	1,3	0,305	5	0,155	1,55	0,86	1,5	1,55	1,55	0,155
WWTP#10	Sample#58	0,18	1,6	0,355	5,2	0,18	1,8	0,88	1,6	1,8	1,8	0,88
WWTP#10	Sample#59	0,235	2,2	0,47	4	0,235	2,35	0,54	1	2,35	2,35	0,235
WWTP#10	Sample#60	0,235	2,2	0,47	4	0,235	2,35	0,54	1	2,35	2,35	0,235
WWTP#10	Sample#61	0,265	2,2	0,55	4	0,265	0,265	0,61	1,6	2,65	2,65	0,265
WWTP#10	Sample#62	0,265	2,2	0,55	4	0,265	2,65	0,61	1,6	2,65	2,65	0,265
WWTP#10	Sample#63	0,24	2,3	0,475	2,4	0,24	2,4	0,47	0,71	2,4	2,445	0,24
WWTP#10	Sample#64	0,24	2,3	0,475	2,4	0,24	2,4	0,47	0,71	2,4	2,4	0,24
WWTP#10	Sample#65	0,16	0,95	0,32	1,9	0,16	1,6	0,16	0,84	1,6	1,6	0,16
WWTP#11	Sample#66	0,85	0,85	5	5	0,85	0,5	0,85	2,55	5	5	0,85
WWTP#11	Sample#67	0,85	1,7	5	4,9	1,7	5	1,7	1,7	5	5	0,85
WWTP#11	Sample#68	0,72	0,67	0,31	3,4	0,155	0,5	1	2	1,55	0,5	0,52
WWTP#11	Sample#69	0,18	0,41	0,355	2	0,18	0,5	0,47	0,76	1,8	0,5	0,18
WWTP#12	Sample#70	0,145	0,84	0,285	2,1	0,145	0,5	0,42	0,61	1,45	0,5	0,145
WWTP#12	Sample#71	0,145	1	0,285	1,9	0,145	0,5	0,47	0,75	0,145	0,5	0,145
WWTP#12	Sample#72	0,14	0,64	0,275	1,7	0,14	1,4	0,32	0,73	1,4	1,4	0,14
WWTP#12	Sample#73	0,13	0,94	0,26	1,4	0,13	0,56	1,3	0,6	1,3	1,3	0,9
WWTP#12	Sample#74	0,145	0,85	0,285	1,4	0,145	0,5	0,38	0,66	1,45	0,5	0,43
WWTP#12	Sample#75	0,47	0,47	0,95	3,8	0,47	0,5	0,47	0,47	4,7	0,5	0,47
WWTP#13	Sample#76	0,66	0,66	0,305	2,4	0,155	0,5	0,34	0,76	1,55	0,5	0,155
WWTP#13	Sample#77	0,66	0,66	0,305	2,4	0,155	0,5	0,34	0,76	1,65	0,5	0,155
WWTP#13	Sample#78	0,165	0,97	0,325	2,8	0,165	0,5	0,97	0,92	1,65	0,5	0,7
WWTP#13	Sample#79	0,16	0,52	0,315	2,5	0,16	0,5	0,39	1,1	1,6	0,5	0,16
WWTP#13	Sample#80	0,185	0,185	0,365	1,7	0,185	0,5	0,53	0,72	1,85	0,5	0,185
WWTP#14	Sample#81	0,155	0,8	0,305	1,5	0,155	0,5	0,55	0,85	1,55	0,5	0,155
WWTP#14	Sample#82	0,16	1,2	0,32	2,3	0,16	0,5	0,74	0,69	1,6	0,5	0,16
WWTP#14	Sample#83	0,155	0,8	0,305	1,5	0,155	1,55	0,55	0,6	1,55	1,55	0,155
WWTP#14	Sample#84	0,32	1,1	0,65	3,5	0,32	0,5	1,1	1,7	3,2	0,5	0,32
WWTP#14	Sample#85	0,295	0,59	0,6	1,6	0,295	2,95	0,295	1,1	2,95	2,95	0,295

WWTP#14	Sample#86	0,125	0,29	0,25	2,1	0,125	1,25	0,33	0,54	1,25	1,25	0,125
WWTP#14	Sample#87	0,135	0,39	0,265	1,4	0,135	1,35	0,26	0,7	1,35	1,35	0,135
WWTP#15	Sample#88	0,135	1,2	0,27	3,7	0,135	0,5	0,66	0,88	1,35	0,5	0,135
WWTP#15	Sample#89	2,5	2,5	5	2,5	2,5	5	2,5	2,5	5	5	2,5
WWTP#15	Sample#90	0,125	0,79	0,25	3,5	0,125	0,5	0,83	1,2	1,25	0,5	0,125
WWTP#15	Sample#91	0,155	0,82	0,31	2,5	0,155	0,5	0,77	0,97	1,55	0,5	0,155
WWTP#15	Sample#92	0,145	0,48	0,29	2,2	1,45	1,45	0,33	0,57	1,45	1,45	0,145
WWTP#15	Sample#93	0,145	0,48	0,29	2,2	0,145	1,45	0,33	0,57	1,45	1,45	0,145
WWTP#16	Sample#94	0,13	0,75	0,255	2	0,13	0,5	0,63	1	1,3	0,5	0,38
WWTP#16	Sample#95	0,15	0,37	0,295	1,1	0,15	0,5	0,64	0,74	1,5	0,5	0,59
WWTP#16	Sample#96	0,09	0,29	0,175	0,74	0,09	0,5	0,17	0,2	0,9	0,5	0,2
WWTP#17	Sample#97	0,17	0,56	0,34	0,96	0,17	0,5	0,17	0,17	1,7	0,5	0,17
WWTP#17	Sample#98	0,17	0,56	0,34	0,96	0,17	0,5	0,17	0,17	1,45	0,5	0,17
WWTP#17	Sample#99	0,09	0,45	0,18	1,5	0,09	0,5	0,36	0,66	0,9	0,5	0,24
WWTP#18	Sample#100	0,85	0,85	-	3	0,85	-	0,85	0,85	-	-	0,85
WWTP#18	Sample#101	0,85	0,85	5	0,85	0,85	5	0,85	0,85	5	5	0,85
WWTP#18	Sample#102	0,85	0,85	-	2	0,85	-	0,85	0,85	-	-	0,85
WWTP#18	Sample#103	0,85	0,85	5	0,85	0,85	5	0,85	0,85	5	5	0,85
WWTP#18	Sample#104	0,85	0,85	5	0,85	0,85	5	0,85	0,85	5	5	0,85
WWTP#18	Sample#105	0,85	0,85	0,85	2,1	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#106	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#107	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#108	0,85	0,85	5	0,85	0,85	5	0,85	2,55	5	5	0,85
WWTP#18	Sample#109	0,85	0,85	5	0,85	0,85	5	0,85	0,85	5	5	0,85
WWTP#18	Sample#110	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#111	0,85	0,85	5	0,85	0,85	5	0,85	1,9	5	5	0,85
WWTP#18	Sample#112	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#113	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#114	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#115	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#116	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#18	Sample#117	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#19	Sample#118	0,14	0,69	0,28	1,7	0,14	1,4	0,32	0,6	1,4	1,4	0,14
WWTP#19	Sample#119	0,135	0,58	0,27	1,7	0,135	0,5	0,58	0,8	0,135	0,5	0,135
WWTP#20	Sample#120	0,205	0,205	0,405	1,6	0,205	2,05	0,74	0,74	2,05	2,05	0,205
WWTP#21	Sample#121	0,51	0,87	0,31	3,6	0,155	0,5	1,2	1,4	1,55	0,5	0,72
WWTP#21	Sample#122	0,89	0,73	0,34	2,8	0,17	0,67	1,7	0,73	1,7	1,7	0,17
WWTP#22	Sample#123	0,85	0,85	0,85	0,85	2,55	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#23	Sample#124	0,27	1,2	0,54	1,9	0,27	2,7	0,27	1	2,7	2,7	0,27
WWTP#24	Sample#125	0,14	1,1	0,275	3	0,14	1,4	0,37	0,68	1,4	1,4	0,14
WWTP#24	Sample#126	0,13	0,91	0,26	1,8	0,13	0,5	0,56	1	1,3	0,5	0,13
WWTP#24	Sample#127	0,12	0,75	0,24	2,3	0,12	1,2	0,12	0,75	1,2	1,2	0,12
WWTP#24	Sample#128	0,6	0,6	1,2	1,5	0,6	6	0,6	0,6	6	6	0,6
WWTP#24	Sample#129	0,14	1	0,275	2,6	0,14	0,5	0,73	1,2	1,4	0,5	0,14
WWTP#24	Sample#130	0,16	1,5	0,315	3,9	0,16	0,5	1	2	1,6	0,5	0,52
WWTP#24	Sample#131	0,185	0,66	0,365	2,5	0,185	1,85	0,42	0,66	1,85	1,85	0,185
WWTP#24	Sample#132	0,135	0,93	0,27	2,7	0,135	1,35	0,71	1,1	1,35	1,35	0,135
WWTP#24	Sample#133	0,175	1,3	0,35	4,5	0,175	1,75	0,7	1,5	1,75	1,75	0,175
WWTP#24	Sample#134	0,18	0,59	0,36	2,8	0,18	1,8	0,47	0,83	1,8	1,8	0,18
WWTP#24	Sample#135	0,17	0,79	0,34	2,6	0,17	1,7	0,51	1	1,7	1,7	0,62
WWTP#25	Sample#136	0,16	0,85	0,32	3,8	0,16	1,6	0,63	0,79	1,6	1,6	0,16
WWTP#25	Sample#137	0,19	1,1	0,38	2,3	0,19	1,9	0,44	0,7	1,9	1,9	0,19
WWTP#25	Sample#138	0,19	0,89	0,38	3,1	0,19	0,5	0,19	1	1,9	0,5	0,19
WWTP#25	Sample#139	0,19	0,89	0,38	3,1	0,19	0,5	0,19	1	1,9	0,5	0,19
WWTP#25	Sample#140	0,14	0,83	0,28	3,1	0,14	1,4	0,6	1,1	1,4	1,4	0,14
WWTP#25	Sample#141	0,145	0,145	0,285	0,66	0,145	0,5	0,145	0,33	1,45	0,5	0,145

WWTP#26	Sample#142	0,85	0,85	5	0,85	0,85	5	0,85	0,85	5	5	0,85
WWTP#27	Sample#143	0,145	0,52	0,285	1,5	0,145	1,45	0,28	0,38	1,45	1,45	0,145
WWTP#27	Sample#144	0,15	0,4	0,3	1,6	0,15	1,5	0,3	0,45	1,5	1,5	0,15
WWTP#27	Sample#145	0,15	0,55	0,3	1,8	0,15	1,5	0,4	0,5	1,5	1,5	0,15
WWTP#27	Sample#146	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#27	Sample#147	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#27	Sample#148	6,1	0,145	0,285	1,3	0,145	1,45	0,145	0,42	1,45	1,45	0,145
WWTP#27	Sample#149	0,175	0,4	0,345	0,97	0,175	1,75	0,34	0,46	1,75	1,75	0,175
WWTP#27	Sample#150	4,4	0,145	0,29	1,2	0,145	0,145	1,45	0,43	1,45	1,45	0,145
WWTP#27	Sample#151	0,19	0,19	0,38	1,3	0,19	0,19	1,9	0,51	1,9	1,9	0,19
WWTP#27	Sample#152	0,155	0,98	0,31	0,62	0,155	1,55	0,155	0,155	1,55	1,55	0,155
WWTP#28	Sample#153	0,16	0,47	0,315	1,9	0,16	0,5	0,73	1,2	1,6	0,5	0,47
WWTP#29	Sample#154	0,57	0,71	0,29	1,5	0,145	0,5	0,33	0,52	1,45	0,5	0,145
WWTP#30	Sample#155	0,16	0,63	0,32	2,4	0,16	1,6	0,58	1,2	1,6	1,6	0,16
WWTP#30	Sample#156	0,17	0,83	0,335	4,2	0,17	1,7	1,4	1,8	1,7	1,7	0,72
WWTP#30	Sample#157	0,165	0,165	0,325	0,59	0,165	0,5	0,165	0,165	1,65	0,5	0,165
WWTP#31	Sample#158	1,1	1,1	0,29	0,62	0,145	1,45	0,145	0,43	1,45	1,45	0,145
WWTP#31	Sample#159	0,45	0,89	0,245	0,61	0,125	0,5	0,33	0,85	1,25	0,5	0,125
WWTP#31	Sample#160	0,125	0,53	0,25	1,6	0,125	0,205	1,25	0,45	1,25	1,25	0,125
WWTP#31	Sample#161	0,12	0,72	0,24	1,8	0,12	0,5	0,36	0,12	1,2	0,5	0,12
WWTP#32	Sample#162	2,5	2,5	5	2,5	2,5	5	2,5	5	2,5	2,5	5
WWTP#32	Sample#163	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#32	Sample#164	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#32	Sample#165	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#32	Sample#166	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#33	Sample#167	0,175	2,8	0,345	8	0,175	1,75	3,1	4,1	1,75	1,75	4,6
WWTP#33	Sample#168	0,24	1,8	0,48	4,7	0,24	2,4	1,1	1,1	2,4	2,4	0,24
WWTP#33	Sample#169	0,175	1,7	0,345	4,3	0,175	1,75	1,7	1	1,75	1,75	1
WWTP#33	Sample#170	0,29	3,4	0,6	3	0,29	0,5	0,29	0,67	2,9	0,5	0,29
WWTP#33	Sample#171	0,16	1,8	0,32	2,7	0,16	0,5	0,8	0,85	1,6	0,5	0,16
WWTP#34	Sample#172	0,15	0,85	0,3	2,9	0,15	1,5	0,55	1,1	1,5	1,5	0,15
WWTP#34	Sample#173	0,37	0,85	0,75	2,2	0,37	3,7	0,37	0,98	3,7	3,7	0,37
WWTP#34	Sample#174	0,165	0,92	0,33	1,8	0,165	1,65	0,71	0,92	1,65	1,65	0,71
WWTP#34	Sample#175	0,15	0,59	0,295	1,4	0,15	1,5	0,29	0,34	1,5	1,5	0,54
WWTP#35	Sample#176	0,145	0,75	0,285	2,4	0,145	0,5	0,75	0,93	1,45	0,5	0,43
WWTP#35	Sample#177	0,73	1	0,4	1,1	0,2	0,5	0,2	0,47	2	0,5	0,2
WWTP#35	Sample#178	0,155	0,33	0,31	1,2	0,155	0,5	0,32	0,61	1,55	0,5	0,155
WWTP#35	Sample#179	0,165	0,38	0,33	1,1	0,165	1,65	0,165	0,38	1,65	1,65	0,165
WWTP#35	Sample#180	0,135	0,135	0,265	0,96	0,135	0,5	0,135	0,83	1,35	0,5	0,135
WWTP#36	Sample#181	0,85	0,85	0,85	0,85	1,7	0,85	0,85	0,85	0,85	0,85	0,85
WWTP#36	Sample#182	0,85	1,7	7,5	2,5	1,7	7,5	1,7	3,4	7,5	7,5	2,5
WWTP#36	Sample#183	0,85	0,85	5	0,85	0,85	5	0,85	1,7	5	5	0,85
WWTP#36	Sample#184	0,85	0,85	5	2,5	0,85	5	0,85	2,55	5	5	0,85
WWTP#36	Sample#185	0,85	0,85	5	0,85	0,85	5	0,85	0,85	5	10	0,85
WWTP#36	Sample#186	0,85	0,85	5	2,5	0,85	5	0,85	2,55	5	5	0,85
WWTP#36	Sample#187	0,85	0,85	5	0,85	0,85	5	0,85	1,7	5	5	0,85
WWTP#37	Sample#188	0,17	0,67	0,335	1,9	0,17	1,7	0,17	0,5	1,7	1,7	0,17
WWTP#37	Sample#189	0,16	0,83	0,315	2	0,16	0,5	0,94	0,83	1,6	0,5	0,16
WWTP#37	Sample#190	0,16	1,3	0,315	3,7	0,16	0,5	0,73	1,2	1,6	0,5	0,16
WWTP#37	Sample#191	0,145	0,81	0,29	3,1	0,145	1,45	0,38	0,77	1,45	1,45	0,145
WWTP#38	Sample#192	0,85	0,85	5	0,85	0,85	5	0,85	0,85	5	5	0,85
WWTP#39	Sample#193	2,5	2,5	-	2,5	2,5	-	2,5	2,5	-	-	-
WWTP#39	Sample#194	2,5	2,5	-	2,5	2,5	-	2,5	2,5	-	-	-
WWTP#40	Sample#195	0,16	0,42	0,32	18	0,16	1,6	2,8	0,47	1,6	1,6	0,16
WWTP#40	Sample#196	0,185	0,185	0,365	1,4	0,185	1,85	0,185	0,185	1,85	1,85	0,185
WWTP#41	Sample#197	0,155	0,31	0,31	1,1	0,155	0,5	0,31	0,36	1,55	0,5	0,155

WWTP#42	Sample#198	0,145	1,3	0,285	1,5	0,145	0,5	0,79	0,93	1,45	0,5	0,56
WWTP#42	Sample#199	0,145	0,67	0,29	1,4	0,145	1,45	0,38	0,67	1,45	1,45	0,145
WWTP#43	Sample#200	0,17	0,5	0,335	1,7	0,17	0,5	0,17	0,78	1,7	0,5	0,17
WWTP#44	Sample#201	2,5	2,5	-	2,5	2,5	0,5	2,5	2,5	-	-	-
WWTP#45	Sample#202	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#45	Sample#203	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5
WWTP#45	Sample#204	2,5	2,5	5	2,5	2,5	0,5	2,5	5	2,5	2,5	5
WWTP#45	Sample#205	2,5	2,5	5	2,5	2,5	5	2,5	5	2,5	2,5	5
WWTP#45	Sample#206	2,5	2,5	2,5	2,5	2,5	2,5	2,5	2,5	5	5	2,5
WWTP#46	Sample#207	0,145	2	0,285	4,3	0,145	1,45	0,76	1,5	1,45	1,45	0,145
WWTP#46	Sample#208	0,14	1,9	0,28	5,1	0,14	0,5	1,1	1,3	0,14	0,5	0,14
WWTP#46	Sample#209	0,15	1,3	0,3	2,8	0,15	1,5	0,54	1	1,5	1,5	0,15
WWTP#47	Sample#210	0,85	0,85	5	0,85	0,85	5	0,85	0,85	5	5	0,85
WWTP#48	Sample#211	0,135	0,63	0,27	2,5	0,135	1,35	0,67	1,1	1,35	1,35	0,135
WWTP#48	Sample#212	0,38	0,61	0,23	2	0,115	0,5	0,3	0,42	1,15	0,5	0,115
WWTP#48	Sample#213	0,55	0,55	1,1	2,1	0,55	5,5	0,55	0,55			
WWTP#48	Sample#214	0,15	0,44	0,3	2,6	0,15	1,5	0,15	0,34	1,5	1,5	0,15
WWTP#48	Sample#215	0,16	0,16	0,32	1,4	0,16	0,5	0,16	0,16	1,6	0,5	0,16

		$PFAS_4$	$PFAS_{22}$	$PFAS_4$: $PFAS_{22}$	PFOS: $PFAS_4$	PFOA: $PFAS_4$	PFNA: $PFAS_4$	PFHxS: $PFAS_4$
		µg/kg	µg/kg	%	%	%	%	%
MIN		**0,36**	**5,35**	**2,89**	**11,85**	**0,98**	**0,49**	**0,39**
10P		**3,40**	**12,48**	**16,53**	**25,00**	**5,02**	**3,37**	**1,11**
50P		**7,49**	**22,94**	**31,60**	**73,53**	**12,14**	**8,42**	**3,81**
90P		**17,83**	**56,35**	**56,63**	**87,63**	**25,00**	**25,00**	**25,00**
MAX		**65,15**	**110,15**	**82,21**	**98,00**	**46,84**	**50,03**	**34,92**
N Total		**215**	**215**	**215**	**215**	**215**	**215**	**215**
N > LOQ		**215**	**215**	**215**	**215**	**215**	**215**	**215**
		30,00						
WWTP#1	Sample#1	10,00	65,00	15,38	25,00	25,00	25,00	25,00
WWTP#1	Sample#2	10,00	65,00	15,38	25,00	25,00	25,00	25,00
WWTP#1	Sample#3	10,00	65,00	15,38	25,00	25,00	25,00	25,00
WWTP#1	Sample#4	5,72	10,14	56,41	85,66	6,29	7,17	0,87
WWTP#1	Sample#5	1,95	5,35	36,45	71,79	10,26	15,38	2,56
WWTP#2	Sample#6	14,75	28,17	52,36	50,17	2,03	46,78	1,02
WWTP#2	Sample#7	14,59	25,75	56,67	46,61	2,33	50,03	1,03
WWTP#2	Sample#8	8,63	20,95	41,20	84,59	7,42	6,37	1,62
WWTP#2	Sample#9	4,22	16,58	25,45	75,83	12,09	6,04	6,04
WWTP#3	Sample#10	5,05	22,00	22,95	49,50	16,83	16,83	16,83
WWTP#3	Sample#11	5,05	22,00	22,95	49,50	16,83	16,83	16,83
WWTP#4	Sample#12	5,21	17,55	29,66	76,85	10,57	9,41	3,17
WWTP#4	Sample#13	2,99	12,43	24,06	83,61	7,36	4,52	4,52
WWTP#4	Sample#14	2,86	9,91	28,82	84,06	5,78	5,08	5,08
WWTP#5	Sample#15	37,04	49,04	75,53	97,19	1,81	0,50	0,50
WWTP#5	Sample#16	35,87	47,72	75,17	97,57	1,45	0,49	0,49
WWTP#5	Sample#17	31,99	42,00	76,17	96,91	1,34	1,16	0,59
WWTP#5	Sample#18	26,53	32,27	82,21	98,00	0,98	0,51	0,51
WWTP#5	Sample#19	20,00	75,70	26,42	75,00	5,00	10,00	10,00
WWTP#5	Sample#20	14,30	56,35	25,38	69,93	9,79	10,14	10,14
WWTP#5	Sample#21	13,10	45,90	28,54	70,99	12,98	8,02	8,02
WWTP#5	Sample#22	12,50	50,20	24,90	72,80	5,60	10,80	10,80
WWTP#5	Sample#23	11,80	33,55	35,17	75,42	12,71	5,93	5,93
WWTP#5	Sample#24	11,20	38,00	29,47	78,57	10,71	5,36	5,36
WWTP#5	Sample#25	10,43	36,43	28,63	76,70	7,96	9,59	5,75
WWTP#5	Sample#26	10,40	35,00	29,71	74,04	10,58	9,62	5,77
WWTP#5	Sample#27	10,30	33,25	30,98	73,79	11,65	7,28	7,28
WWTP#5	Sample#28	8,40	42,20	19,91	52,38	19,05	14,29	14,29
WWTP#5	Sample#29	8,05	25,34	31,76	72,05	18,63	4,66	4,66
WWTP#5	Sample#30	7,85	24,84	31,60	81,53	8,41	5,03	5,03
WWTP#5	Sample#31	7,85	24,84	31,60	81,53	8,41	5,03	5,03
WWTP#5	Sample#32	7,02	28,83	24,35	72,65	15,67	5,84	5,84
WWTP#5	Sample#33	6,92	30,72	22,53	67,92	8,96	14,45	8,67
WWTP#5	Sample#34	6,81	15,61	43,63	77,83	8,52	9,25	4,41
WWTP#5	Sample#35	6,12	30,62	19,99	68,63	11,76	9,80	9,80
WWTP#5	Sample#36	5,95	32,45	18,34	67,23	12,61	10,08	10,08
WWTP#5	Sample#37	5,10	25,40	20,08	62,75	5,88	19,61	11,76
WWTP#5	Sample#38	5,10	29,30	17,41	62,75	5,88	19,61	11,76
WWTP#5	Sample#39	4,86	17,42	27,90	78,19	7,82	10,49	3,50
WWTP#5	Sample#40	4,78	23,13	20,67	69,04	5,86	12,55	12,55
WWTP#5	Sample#41	4,56	19,63	23,23	78,95	9,43	5,81	5,81
WWTP#5	Sample#42	4,39	31,99	13,72	66,06	6,61	13,67	13,67
WWTP#5	Sample#43	4,24	7,30	58,08	82,55	6,60	8,25	2,59
WWTP#5	Sample#44	4,16	20,06	20,74	67,31	6,25	13,22	13,22

WWTP#5	Sample#45	2,08	6,48	32,10	86,54	6,73	3,37	3,37
WWTP#6	Sample#46	25,50	76,00	33,55	70,59	9,80	9,80	9,80
WWTP#6	Sample#47	14,50	63,50	22,83	48,28	17,24	17,24	17,24
WWTP#6	Sample#48	10,00	60,50	16,53	25,00	25,00	25,00	25,00
WWTP#6	Sample#49	10,00	60,50	16,53	25,00	25,00	25,00	25,00
WWTP#7	Sample#50	8,77	17,91	48,94	90,13	3,31	5,02	1,54
WWTP#7	Sample#51	8,11	20,90	38,78	76,50	11,72	9,99	1,79
WWTP#7	Sample#52	7,80	16,27	47,96	71,79	11,15	10,51	6,54
WWTP#8	Sample#53	10,18	21,32	47,73	85,50	6,98	5,90	1,62
WWTP#9	Sample#54	14,13	52,64	26,85	84,93	8,49	5,52	1,06
WWTP#9	Sample#55	11,85	24,50	48,37	84,39	7,17	7,17	1,27
WWTP#9	Sample#56	9,19	21,48	42,78	85,96	7,51	4,90	1,63
WWTP#10	Sample#57	18,76	34,23	54,80	85,31	6,93	6,93	0,83
WWTP#10	Sample#58	16,06	33,60	47,80	87,17	6,23	5,48	1,12
WWTP#10	Sample#59	13,58	31,80	42,69	81,03	13,26	3,98	1,73
WWTP#10	Sample#60	13,58	31,80	42,69	81,03	13,26	3,98	1,73
WWTP#10	Sample#61	13,27	30,70	43,22	82,89	12,81	2,30	2,00
WWTP#10	Sample#62	12,73	32,29	39,41	86,44	6,68	4,79	2,08
WWTP#10	Sample#63	9,48	25,48	37,21	83,33	11,60	2,53	2,53
WWTP#10	Sample#64	9,48	25,44	37,27	83,33	11,60	2,53	2,53
WWTP#10	Sample#65	4,45	15,02	29,63	78,65	9,44	8,31	3,60
WWTP#11	Sample#66	65,15	110,15	59,15	84,42	7,98	1,30	6,29
WWTP#11	Sample#67	10,10	61,40	16,45	49,50	33,66	8,42	8,42
WWTP#11	Sample#68	8,18	20,89	39,13	75,84	12,23	10,03	1,90
WWTP#11	Sample#69	7,04	15,87	44,37	72,44	12,50	12,50	2,56
WWTP#12	Sample#70	19,76	28,05	70,44	96,18	1,67	1,42	0,73
WWTP#12	Sample#71	15,94	22,94	69,48	94,13	2,64	2,32	0,91
WWTP#12	Sample#72	15,10	24,64	61,29	92,72	3,64	2,72	0,93
WWTP#12	Sample#73	13,90	23,97	57,99	93,53	3,09	2,45	0,94
WWTP#12	Sample#74	13,81	21,70	63,62	94,17	2,39	2,39	1,05
WWTP#12	Sample#75	10,47	27,03	38,73	85,00	6,02	4,49	4,49
WWTP#13	Sample#76	34,06	48,16	70,72	91,02	6,46	1,64	0,88
WWTP#13	Sample#77	34,06	48,26	70,58	91,02	6,46	1,64	0,88
WWTP#13	Sample#78	8,09	20,45	39,54	72,97	11,38	13,61	2,04
WWTP#13	Sample#79	4,27	13,30	32,12	79,63	8,20	8,43	3,75
WWTP#13	Sample#80	3,94	13,82	28,52	76,14	14,47	4,70	4,70
WWTP#14	Sample#81	5,46	14,50	37,62	76,99	12,83	7,33	2,84
WWTP#14	Sample#82	5,06	14,51	34,87	79,05	9,49	8,30	3,16
WWTP#14	Sample#83	5,01	14,96	33,46	79,92	7,99	8,99	3,10
WWTP#14	Sample#84	4,77	20,22	23,59	73,38	13,21	6,71	6,71
WWTP#14	Sample#85	3,88	19,87	19,53	72,16	12,63	7,60	7,60
WWTP#14	Sample#86	3,32	11,83	28,03	72,40	15,08	8,75	3,77
WWTP#14	Sample#87	2,80	11,21	24,93	71,56	12,52	11,09	4,83
WWTP#15	Sample#88	17,73	29,86	59,39	90,24	4,96	3,27	1,52
WWTP#15	Sample#89	10,00	65,00	15,38	25,00	25,00	25,00	25,00
WWTP#15	Sample#90	9,43	19,91	47,35	88,06	4,88	5,73	1,33
WWTP#15	Sample#91	5,69	15,16	37,51	72,12	15,30	9,85	2,73
WWTP#15	Sample#92	2,72	13,70	19,86	73,53	15,81	5,33	5,33
WWTP#15	Sample#93	2,72	12,39	21,95	73,53	15,81	5,33	5,33
WWTP#16	Sample#94	6,28	14,77	42,53	85,99	5,25	6,69	2,07
WWTP#16	Sample#95	5,37	12,96	41,45	76,35	14,53	6,33	2,79
WWTP#16	Sample#96	0,36	12,56	2,89	11,85	38,57	24,79	24,79
WWTP#17	Sample#97	6,52	13,12	49,70	84,36	7,82	5,21	2,61
WWTP#17	Sample#98	6,52	12,87	50,66	84,36	7,82	5,21	2,61
WWTP#17	Sample#99	3,23	9,33	34,62	80,50	9,29	7,43	2,79
WWTP#18	Sample#100	17,00	37,35	45,52	64,71	5,00	5,00	25,29

WWTP#18	Sample#101	9,10	41,00	22,20	57,14	24,18	9,34	9,34
WWTP#18	Sample#102	6,30	26,95	23,38	38,10	13,49	13,49	34,92
WWTP#18	Sample#103	5,25	37,15	14,13	51,43	16,19	16,19	16,19
WWTP#18	Sample#104	5,15	37,05	13,90	50,49	16,50	16,50	16,50
WWTP#18	Sample#105	5,15	21,70	23,73	50,49	16,50	16,50	16,50
WWTP#18	Sample#106	5,05	20,35	24,82	49,50	16,83	16,83	16,83
WWTP#18	Sample#107	4,95	20,25	24,44	48,48	17,17	17,17	17,17
WWTP#18	Sample#108	4,85	38,45	12,61	47,42	17,53	17,53	17,53
WWTP#18	Sample#109	4,65	36,55	12,72	45,16	18,28	18,28	18,28
WWTP#18	Sample#110	4,55	19,85	22,92	43,96	18,68	18,68	18,68
WWTP#18	Sample#111	3,40	36,35	9,35	25,00	25,00	25,00	25,00
WWTP#18	Sample#112	3,40	18,70	18,18	25,00	25,00	25,00	25,00
WWTP#18	Sample#113	3,40	18,70	18,18	25,00	25,00	25,00	25,00
WWTP#18	Sample#114	3,40	18,70	18,18	25,00	25,00	25,00	25,00
WWTP#18	Sample#115	3,40	18,70	18,18	25,00	25,00	25,00	25,00
WWTP#18	Sample#116	3,40	18,70	18,18	25,00	25,00	25,00	25,00
WWTP#18	Sample#117	3,40	18,70	18,18	25,00	25,00	25,00	25,00
WWTP#19	Sample#118	4,67	13,86	33,69	79,23	11,78	6,00	3,00
WWTP#19	Sample#119	3,95	10,36	38,08	78,58	11,15	6,84	3,42
WWTP#20	Sample#120	4,31	16,54	26,07	76,57	13,92	4,76	4,76
WWTP#21	Sample#121	9,38	24,14	38,84	76,80	13,87	7,68	1,65
WWTP#21	Sample#122	9,20	23,41	39,30	84,78	8,48	4,89	1,85
WWTP#22	Sample#123	5,05	22,05	22,90	49,50	16,83	16,83	16,83
WWTP#23	Sample#124	7,09	24,13	29,38	87,45	4,94	3,81	3,81
WWTP#24	Sample#125	40,96	56,35	72,70	68,36	26,86	3,66	1,12
WWTP#24	Sample#126	34,69	46,88	74,00	72,07	23,64	3,17	1,12
WWTP#24	Sample#127	29,03	38,86	74,70	79,23	16,53	3,41	0,83
WWTP#24	Sample#128	12,85	41,35	31,08	85,60	5,06	4,67	4,67
WWTP#24	Sample#129	11,39	21,36	53,34	71,99	18,44	8,34	1,23
WWTP#24	Sample#130	11,09	24,73	44,85	70,33	20,74	7,48	1,44
WWTP#24	Sample#131	10,35	22,35	46,29	75,40	16,43	6,38	1,79
WWTP#24	Sample#132	10,24	22,53	45,43	73,28	17,59	7,82	1,32
WWTP#24	Sample#133	9,18	24,53	37,41	69,75	20,71	7,63	1,91
WWTP#24	Sample#134	8,95	21,20	42,22	72,63	16,76	8,60	2,01
WWTP#24	Sample#135	6,06	18,55	32,67	67,66	23,10	6,44	2,81
WWTP#25	Sample#136	7,84	20,84	37,62	80,36	10,84	6,76	2,04
WWTP#25	Sample#137	6,48	19,00	34,11	75,62	14,66	6,79	2,93
WWTP#25	Sample#138	5,70	16,44	34,67	64,91	22,81	8,95	3,33
WWTP#25	Sample#139	5,70	16,44	34,67	64,91	22,81	8,95	3,33
WWTP#25	Sample#140	5,15	16,66	30,91	75,73	12,62	8,93	2,72
WWTP#25	Sample#141	2,08	7,55	27,57	76,92	9,13	6,97	6,97
WWTP#26	Sample#142	7,05	67,10	10,51	63,83	12,06	12,06	12,06
WWTP#27	Sample#143	21,52	30,29	71,06	88,29	5,58	3,95	2,18
WWTP#27	Sample#144	18,20	27,25	66,79	87,91	5,22	3,85	3,02
WWTP#27	Sample#145	17,90	27,45	65,21	89,39	6,70	3,07	0,84
WWTP#27	Sample#146	17,50	62,50	28,00	57,14	14,29	14,29	14,29
WWTP#27	Sample#147	10,00	55,00	18,18	25,00	25,00	25,00	25,00
WWTP#27	Sample#148	4,11	18,16	22,63	80,29	12,65	3,53	3,53
WWTP#27	Sample#149	3,90	13,41	29,05	71,89	11,81	11,81	4,49
WWTP#27	Sample#150	3,81	19,40	19,64	78,74	13,65	3,81	3,81
WWTP#27	Sample#151	3,74	13,91	26,89	69,52	11,76	13,64	5,08
WWTP#27	Sample#152	3,36	11,78	28,52	86,31	4,46	4,61	4,61
WWTP#28	Sample#153	7,22	16,35	44,17	80,33	10,94	6,51	2,22
WWTP#29	Sample#154	4,16	12,21	34,04	79,42	9,15	7,94	3,49
WWTP#30	Sample#155	5,29	17,96	29,45	68,05	18,90	10,02	3,02
WWTP#30	Sample#156	3,99	19,91	20,05	65,16	12,53	18,05	4,26

WWTP#30	Sample#157	0,80	6,51	12,22	47,80	10,69	20,75	20,75
WWTP#31	Sample#158	16,48	25,82	63,83	97,09	1,15	0,88	0,88
WWTP#31	Sample#159	3,71	10,46	35,47	88,95	4,31	3,37	3,37
WWTP#31	Sample#160	3,71	13,08	28,33	70,18	14,30	12,15	3,37
WWTP#31	Sample#161	3,36	10,52	31,94	71,43	14,29	10,71	3,57
WWTP#32	Sample#162	44,00	99,00	44,44	75,00	13,64	5,68	5,68
WWTP#32	Sample#163	12,50	57,50	21,74	40,00	20,00	20,00	20,00
WWTP#32	Sample#164	10,00	55,00	18,18	25,00	25,00	25,00	25,00
WWTP#32	Sample#165	10,00	55,00	18,18	25,00	25,00	25,00	25,00
WWTP#32	Sample#166	10,00	55,00	18,18	25,00	25,00	25,00	25,00
WWTP#33	Sample#167	28,72	58,49	49,10	94,03	1,99	3,38	0,61
WWTP#33	Sample#168	18,68	37,46	49,87	91,01	3,00	4,71	1,28
WWTP#33	Sample#169	15,96	32,83	48,61	87,75	6,89	4,26	1,10
WWTP#33	Sample#170	8,75	23,51	37,22	85,71	7,66	3,31	3,31
WWTP#33	Sample#171	7,55	18,22	41,44	78,15	8,48	11,26	2,12
WWTP#34	Sample#172	8,85	20,80	42,55	84,75	7,91	5,65	1,69
WWTP#34	Sample#173	7,89	27,84	28,34	79,85	10,77	4,69	4,69
WWTP#34	Sample#174	5,86	17,69	33,14	87,03	7,34	2,82	2,82
WWTP#34	Sample#175	5,23	14,54	35,98	80,31	9,37	7,46	2,87
WWTP#35	Sample#176	8,25	17,55	46,99	67,92	21,83	8,49	1,76
WWTP#35	Sample#177	6,97	15,67	44,48	76,04	14,35	6,74	2,87
WWTP#35	Sample#178	4,36	12,26	35,52	73,48	14,01	8,96	3,56
WWTP#35	Sample#179	3,20	12,16	26,33	81,25	8,44	5,16	5,16
WWTP#35	Sample#180	3,15	9,18	34,33	82,54	8,89	4,29	4,29
WWTP#36	Sample#181	19,85	36,00	55,14	70,53	12,59	12,59	4,28
WWTP#36	Sample#182	14,55	69,80	20,85	82,47	5,84	5,84	5,84
WWTP#36	Sample#183	11,15	43,90	25,40	77,13	7,62	7,62	7,62
WWTP#36	Sample#184	8,25	43,50	18,97	69,09	10,30	10,30	10,30
WWTP#36	Sample#185	5,05	41,95	12,04	49,50	16,83	16,83	16,83
WWTP#36	Sample#186	5,05	40,30	12,53	49,50	16,83	16,83	16,83
WWTP#36	Sample#187	5,05	37,80	13,36	49,50	16,83	16,83	16,83
WWTP#37	Sample#188	11,27	21,65	52,07	83,41	10,65	4,44	1,51
WWTP#37	Sample#189	8,81	18,34	48,05	82,86	8,85	6,47	1,82
WWTP#37	Sample#190	8,69	24,65	35,26	71,35	17,26	9,55	1,84
WWTP#37	Sample#191	6,98	19,38	35,99	75,99	12,33	9,61	2,08
WWTP#38	Sample#192	5,05	36,95	13,67	49,50	16,83	16,83	16,83
WWTP#39	Sample#193	14,93	49,22	30,33	49,77	16,74	16,74	16,74
WWTP#39	Sample#194	12,98	40,48	32,07	42,22	19,26	19,26	19,26
WWTP#40	Sample#195	40,56	71,71	56,56	34,52	46,84	18,24	0,39
WWTP#40	Sample#196	4,97	14,69	33,83	86,52	6,04	3,72	3,72
WWTP#41	Sample#197	2,47	8,96	27,57	76,92	10,53	6,28	6,28
WWTP#42	Sample#198	5,37	14,49	37,04	74,56	13,98	8,76	2,70
WWTP#42	Sample#199	4,80	14,01	34,24	70,91	16,06	10,01	3,02
WWTP#43	Sample#200	7,34	15,67	46,86	72,21	16,35	9,13	2,32
WWTP#44	Sample#201	13,04	41,04	31,77	42,48	19,17	19,17	19,17
WWTP#45	Sample#202	10,00	55,00	18,18	25,00	25,00	25,00	25,00
WWTP#45	Sample#203	10,00	55,00	18,18	25,00	25,00	25,00	25,00
WWTP#45	Sample#204	10,00	60,50	16,53	25,00	25,00	25,00	25,00
WWTP#45	Sample#205	10,00	65,00	15,38	25,00	25,00	25,00	25,00
WWTP#45	Sample#206	10,00	60,00	16,67	25,00	25,00	25,00	25,00
WWTP#46	Sample#207	6,77	21,70	31,18	76,87	11,23	9,76	2,14
WWTP#46	Sample#208	5,32	17,72	30,02	69,55	12,97	14,85	2,63
WWTP#46	Sample#209	4,98	16,92	29,43	68,27	15,86	12,85	3,01
WWTP#47	Sample#210	5,05	36,95	13,67	49,50	16,83	16,83	16,83
WWTP#48	Sample#211	7,49	22,21	33,70	57,45	34,74	6,01	1,80
WWTP#48	Sample#212	5,38	22,79	23,58	50,23	33,49	14,14	2,14

WWTP#48	Sample#213	4,48	19,78	22,65	55,80	19,64	12,28	12,28
WWTP#48	Sample#214	3,49	13,32	26,20	80,23	11,17	4,30	4,30
WWTP#48	Sample#215	1,73	8,13	21,28	69,36	12,14	9,25	9,25

Derivation of Cut-off Values for PFAS in Sewage Sludge

This report presents calculation methods and model calculations with an aim to give proposals for cut-off values for PFAS in sewage sludge, which protect the environment and health. In the report, the quantitative aim is to calculate backwards from already existing limit values in the environment to safe cut-off values in sewage sludge. The four exposure routes are set to the soil environment, surface water, groundwater and feed and food.

The calculation methods are based on methods already used in the EU for risk assessment of industrial chemicals, pesticides and pharmaceuticals. The difference is that, they are used backwards to calculate sludge concentrations, which are not expected to pose a risk to the relevant environmental quality criteria. In addition to the calculation methods, several exposure models developed under EU have been used, i.e. FOCUS models PELMO and MACRO, as well as a more simplified newly described so-called box model. However, the models cannot be run backwards like the above calculation methods, which is why they are used with an area-based input of PFAS, which corresponds to the absolute worst possible scenarios. This means that the models calculate the final concentration in e.g. groundwater based on the PFAS load in the field.

It can be concluded that PFAS4 concentrations at the upper end of what is found in Danish sewage sludge are not expected to pose a problem in relation to the environmental quality requirements.

The Danish Environmental
Protection Agency
Tolderlundsvej 5
DK - 5000 Odense C

www.mst.dk