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EQS_{sed} – Proposal by the Ecotox Centre for:

Perfluorooctane Sulfonate (PFOS)

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Summary

SQC (EQS_{sed}): 2.7 µg/kg d.w.

$SQC_{sec.pois.}$ ($EQS_{sed, sec.pois.}$): 1.85 µg/kg d.w.

In the framework of the Module Sediment, which is intended to help cantons in sediment quality assessment, the Ecotox Centre develops proposals for Environmental Quality Criteria for sediment (SQC). SQC are derived applying the methodology described in the EU-Technical Guidance (TGD) for Deriving Environmental Quality Standards (EQS). In order to ensure that the dossiers are internationally comparable, the English terminology of the TGD will be used in the remainder of the dossier. These criteria provide a first screening tool to evaluate sediment chemical quality and the potential risk for the aquatic ecosystem. Based on the scientific literature available at present a preliminary SQC for perfluorooctane sulfonate (PFOS) of 2.7 µg/kg d.w. is proposed for standard sediments with 1 % OC to protect benthic organisms from direct toxicity. When the objective of protection are top predators from secondary poisoning, a preliminary $SQC_{sec.pois.}$ of 1.85 µg/kg d.w. is proposed.

Zusammenfassung

SQK (EQS_{sed}): 2.7 µg/kg TS

$SQK_{sec.pois.}$ ($EQS_{sed, sec.pois.}$): 1.85 µg/kg d.w.

Im Rahmen des Sedimentmoduls, das den Kantonen bei der Bewertung der Sedimentqualität helfen soll, entwickelt das Oekotoxzentrum Vorschläge für Umweltqualitätskriterien für Sedimente (SQK). Diese Kriterien dienen als Methode für ein erstes Screening zur Bewertung der chemischen Sedimentqualität und des potenziellen Risikos für aquatische Ökosysteme. Auf der Basis von Literaturdaten für die Wirkung von Perfluoroktansulfonat (PFOS) und unter Verwendung der Methode, die in der Technischen Richtlinie der EU zur Ableitung von Umweltqualitätsnormen beschriebenen wird, schlägt das Oekotoxzentrum einen vorläufiger SQK für PFOS von 2.7 µg/kg TS für Standardsedimente mit 1 % OC vor. Wenn es das Ziel ist, Spitzenräuber vor einer Sekundärvergiftung zu schützen, wird ein vorläufiger $SQK_{sec.pois.}$ von 1.85 µg/kg d.w. vorgeschlagen.

Résumé

CQS (EQS_{sed}): 2,7 µg/kg p.s.

$CQS_{sec.pois.}$ ($EQS_{sed, sec.pois.}$): 1,85 µg/kg p.s.

Dans le cadre du module Sédiments qui devrait aider les cantons à évaluer la qualité des sédiments, le Centre Ecotox élabore des propositions de critères de qualité environnementale pour les sédiments (CQS). Les CQS sont dérivés en appliquant la méthodologie décrite dans le Guide Technique de l'UE (TGD) pour la Dérivation des Normes de Qualité Environnementale (EQS). Afin que les dossiers soient comparables au niveau international, la terminologie anglaise du TGD est utilisée ci-dessous. Ces critères fournissent un premier outil de dépistage pour évaluer la qualité chimique des sédiments et le risque potentiel pour l'écosystème aquatique. Sur la base des données sur les effets existants dans la littérature un CQS préliminaire pour le perfluorooctane sulfonate de 2,7 µg/kg p.s. est proposé pour les sédiments standards avec 1 % CO. Lorsque l'objectif de protection sont les prédateurs, une $CQS_{sec.pois.}$ provisoire de 1,85 µg/kg p.s. est proposé.

Sommario

CQS: 2,7 µg/kg p.s.

$CQS_{sec.pois.}$ ($EQS_{sed, sec.pois.}$): 1,85 µg/kg p.s.

Nell'ambito del modulo Sedimenti, che è finalizzato ad aiutare i Cantoni nella valutazione della qualità dei sedimenti, il Centro Ecotox sviluppa proposte per i criteri di qualità ambientale per i sedimenti (CQS). I CQS sono derivati applicando la metodologia descritta nella Guida Tecnica dell'UE (TGD) per la Derivazione degli Standard di Qualità Ambientale (EQS). Per garantire che i dossier siano comparabili a livello internazionale, viene utilizzata la terminologia inglese del TGD. Questi criteri forniscono un primo strumento di screening per valutare la qualità chimica dei sedimenti e il potenziale rischio per l'ecosistema acquatico. Sulla base della letteratura scientifica disponibile allo stato attuale un CQS preliminare per il perfluorottano solfonato (PFOS) di 2,7 µg/kg p.s. è proposto per sedimenti standard con 1 % CO. Quando l'obiettivo di protezione sono i predatori, un $CQS_{sed,sec.pois.}$ provvisorio di 1,85 µg/kg p.s. è proposto.

Table of content

1 General Information

Selected information on Perfluorooctane Sulfonate (PFOS) relevant for sediment is presented in this chapter. Registration information and risk assessments referred to are:

- EC (2011a). PFOS EQS dossier 2011.
- Moermond CTA, Verbruggen EMJ, Smit CE. (2010). Environmental risk limits for PFOS: A proposal for water quality standards in accordance with the Water Framework Directive. RIVN Report 601714013/2010.
- Heads of EPA Australia and New Zealand (HEPA). 2020. PFAS National Environmental Management Plan Version 2.0.
- Organisation for Economic Co-operation and Development (OECD). 2018. Toward a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs)
- Organisation for Economic Co-operation and Development (OECD). Environment Directorate. 2002. Hazard Assessment of Perfluorooctane Sulfonate (PFOS) and its Salts.
- United Nations Environment Programme (UNEP). 2006. “Risk Profile on Perfluorooctane Sulfonate.” Stockholm Convention on Persistent Organic Pollutants Review Committee. Geneva, 6 -10 November 2006.
- Environment Canada (2006). Ecological Screening Assessment Report on Perfluorooctane Sulfonate, Its Salts and Its Precursors that Contain the C8F17SO2 or C8F17SO3, or C8F17SO2N Moiety.

1.1 Identity and physico-chemical properties

Per- and polyfluoroalkyl substances (PFAS) are a family of anthropogenic chemicals that contain one or more C atoms on which all the H substituents have been replaced by F atoms, in such a manner that they contain the perfluoroalkyl moiety (C_nF_{2n+1}–) (Buck et al. 2011). The replacement of hydrogen atoms by fluorine atoms provides unique chemical properties that enabled this group of chemicals to be used for a range of uses. According to the most recent review by OECD (2018), PFAS include in total 4730 PFAS-related CAS numbers, including several new groups of PFASs that fulfil the common definition of PFAS (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFAS.

The family of Perfluoroalkyl acids (PFAAs) include perfluoroalkyl carboxylic, sulfonic, sulfinic, phosphonic, and phosphinic acids. PFAAs are important both because they are highly persistent substances and very stable, resisting physical, chemical and biological degradation and have been directly emitted to the environment or are formed indirectly from the environmental degradation or metabolism of precursor substances, and because they (or their salts) are or have been used in a wide variety of industrial and consumer applications. Depending on their acid strength (pK_a value), PFAAs will dissociate to a greater or lesser extent to their anions in aqueous environmental media, soils, or sediments. The protonated and anionic forms have different physicochemical properties (Buck et al. 2011).

PFOS is the acronym for perfluorooctane sulfonic acid and perfluorooctane sulphonate anion[1], which is commercially available in the form of salts, derivatives (PFOS-substances) and polymers (PFOS-

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[1] According to Buck et al. (2011), all PFASs containing an acid functionality can be referred to as *acids* “regardless of whether or not they are likely to be highly or completely ionized in environmental or human matrices”.

polymers), each with a specific CAS Number[2]. PFOS belong to the perfluoroalkane sulfonic acid (PFSAs) family, containing a perfluoroalkyl moiety with eight carbons and therefore considered a long-chain PFAS. Theoretically, 89 congeners are possible, although PFOS is routinely present in many environmental samples as a mixture of the linear isomer and 10 branched isomers (Riddell et al. 2009).

According to the EC TGD EQS (EC 2018), the general criteria for triggering an effects assessment for sediments include log K_{OC} and log K_{OW} properties, toxicity to benthic organisms and evidence of accumulation in sediment.

PFOS is hydrophobic and lipophobic at the same time, it tends to form three immiscible layers when added to an octanol-water system. Thus, it is impossible to directly determine its K_{OW} value using ‘regular’ methods that are common for organic chemicals. Furthermore, PFOS is fully or partially ionizable in water at conditions that are representative for the environment. Therefore, two kinds of octanol/water partition coefficients should be used to quantify the partitioning of PFOS: one for the neutral species and the other for the ionized molecule.

The log K_{OC} reported for PFOS from experimental studies are in the range of 2.28-5.04 (geomean of 3.55), triggering an effect assessment for sediments.

Table 1 summarizes identity and physico-chemical parameters for PFOS required for EQS derivation according to the TGD (EC 2018). Where available, experimentally collected data is identified as (exp.) and estimated data as (est.). When not identified, no indication is available in the cited literature.

Table 1 Information required for EQS derivation according to the TGD (EC 2018). All information refer to perfluorooctane sulfonic acid (CAS 1763-23-1), if not stated otherwise.

Characteristics	Values	References
Common name	Perfluorooctane Sulfonate (PFOS) 1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro- 1-Octanesulfonic acid, heptadecafluoro- (6CI) 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Heptadecafluoro-1-octanesulfonic acid 1-Perfluorooctanesulfonic acid EF 101 Eftop EF 101 Heptadecafluoro-1-octanesulfonic acid Heptadecafluorooctanesulfonic acid Perfluoro-n-octanesulfonic acid Perfluorooctanesulfonic acid Perfluorooctylsulfonic acid	OECD (2018)
IUPAC name	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	OECD (2018)
Chemical group	Perfluoroalkane sulfonic acids (PFSAs), their salts and esters	Buck et al. (2011)

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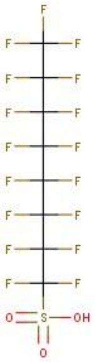
[2] Perfluorooctane sulfonic acid: acronym (PFOS), formula ($C_8F_{17}SO_3H$), CAS N° (1763-23-1)
Perfluorooctane sulfonate anion: acronym (PFOS), formula ($C_8F_{17}SO_3^-$), CAS N° (45298-90-6)
Ammonium perfluorooctane sulfonate: acronym (NH_4- PFOS), formula (NH_4^+ $C_8F_{17}SO_3^-$), CAS N° (29081-56-9)
Sodium perfluorooctane sulfonate: acronym (Na^+-PFOS), formula (Na^+ $C_8F_{17}SO_3^-$), CAS N° (4021-47-0)
Potassium perfluorooctane sulfonate: acronym (K-PFOS), formula (K^+ $C_8F_{17}SO_3^-$), CAS N° (2795-39-3)
Lithium perfluorooctane sulfonate: acronym (Li-PFOS), formula (Li^+ $C_8F_{17}SO_3^-$), CAS N° (29457-72-5)
Tetraethylammonium perfluorooctane sulfonate: acronym (NEt_4-PFOS), formula ($N(C_2H_5)_4^+$ $C_8F_{17}SO_3^-$), CAS N° (56773-42-3)

Characteristics	**Values**	**References**
Structural formula		ECHA (2019)
Molecular formula	C8 H F17 O3 S	ECHA (2019)
CAS	1763-23-1	ECHA (2019)
EC Number	217-179-8	ECHA (2019)
SMILES code	OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F) C(F)(F)C(F)(F)C(F)(F)F	ECHA (2019)
Molecular weight [g/mol]	500 (acid)	Environmental Agency (2004)
Melting point [°C]	>400°C	Environmental Agency (2004)
Boiling point [°C]	In view of the high melting point, no attempts made to measure the boiling point	Environmental Agency (2004)
Vapour pressure [Pa]	3.31x10^{-4} (exp., OECD 104, for potassium salt) 1.9x10^{-9} (est., MPBPVPWIN, for potassium salt) 3.1x10^{-11} (est. for diethanolamine salt) 0.85 (calculated for the acid)	Environment Agency (2004)
Henry's law constant [Pa·m^3/mol]	3.19x10^{-4} from vapour pressure/ solubility ratio	Environment Agency (2004)
Water solubility [mg/L]	[1] 570 in pure water [2] 519 at 20°C in pure water [3] 370 in freshwater [4] 680 at 24-25°C in pure water, with additional centrifugation before sampling and analysis [5] 12.4 at 22-23°C in natural seawater [6] 20.0 for 3.5% salinity (NaCl)	[1] 3M (1999) cited in Environment Agency (2004) [2] 3M (2003) cited and used in Environment Agency (2004) [3] OECD (2002) [4-6] 3M (2003) cited in Environment Agency (2004)
Dissociation constant (pK_a)	[1] -3.27 (est.) Considered a strong acid. PFOS will be present in the environment completely in the ionised form, all determination of properties that involve the substance in solution relate to the anionic form.	[1] Environment Agency (2004) [2] Arp et al. (2006) cited in Ding and Peijnenburg (2013)
Octanol-water partition coefficient (log K_{OW})	[1] Not possible to measure/calculate [2] 6.43 (est. using Wang et al. 2011 model) [3] 5.26 (est. SPARC general partitioning model or calculated by ChemAxon)	[1] Environment Agency (2004) [2] Chen et al. (2019)

Characteristics	Values	References
	[4] 2.45 (exp. ion-transfer cyclic voltammetry)	[3] Arp et al. 2006 cited in Deng et al. (2012) [4] Jing et al. (2009) cited in Ding and Peijnenburg (2013)
Membrane-water partitioning coefficient (log K_{MW})	4.88 (exp. batch sorption test with solid supported lipid membranes)	Droge et al. (2019)
Sediment/soil-water partition coefficient (log K_{OC}) [a]	[1] 4.76 (exp. OECD 106, river sediment OC 1.3% clay 19% pH 7.7) [2] 2.68 (exp. Batch equilibrium, slope Kd vs OC (n=4), freshwater sediments) [3]2.68, 2.97 (exp. Batch equilibrium, Freshwater sediments) [4] 3.26 (exp. Batch equilibrium, freshwater sediment) [5] 2.28-4.61 (exp. field studies, freshwater sediment) [6] 3.00 brached-PFOS, 3.40 linear-PFOS (exp. field studies, freshwater sediment N=129) [7] 5.04 (exp. field studies, average N=18, freshwater suspended matter) [8] 2.57-3.1 [9] 2.43-3.04 (exp. Batch equilibrium, studies, soils, N=15)	[1] OECD (2002) [2] Higgins and Luthy (2006) [3] Zhao et al. (2012) [4] Chen et al. (2016b) [5] See Appendix 1 for individual references [6] Munoz et al. (2015) [7] Li et al. (2020) [8] 3M (2000) cited in Brusseau et al. (2019) [9] Mejia-Avendano et al. (2020)
Sediment adsorption coefficient (K_d [L/kg])	[1] 6.0-223.9 (exp. Batch equilibrium studies, N=4, freshwater sediment) [2] 45.7 (exp. Batch equilibrium study, freshwater sediment) [3] 135 (exp. field study, freshwater sediments N=18); 7 586 (exp. field study, freshwater suspended matter pH in surface water 6.7-9.3 N=86) [4] 79 branched-PFOS, 200 linear-PFOS (exp. field studies, freshwater sediment N=129) [5] 20-760 (field studies, freshwater sediments)	[1] Higgins and Luthy (2006) [2] Chen et al. (2016) [3] Chen et al. (2019) [4] Munoz et al. (2015) [5] See Appendix 1 for individual references
Aqueous hydrolysis DT_{50}	No hydrolysis (exp. for potassium salt of PFOS; estimated half-life of >41 years at 25°C based on limit of quantification)	3M (2003) cited in Environment Agency (2004)
Aqueous photolysis DT_{50}	No evidence of photolysis (exp. for potassium salt of PFOS, estimated half-life of >3.7 years based on limit of quantification)	3M (2003) cited in Environment Agency (2004)
Biodegradation in aqueous environment DT_{50} [d]	None of the available studies showed biodegradation of PFOS in the aquatic environment under either aerobic or anaerobic conditions	Environment Agency (2004)

Characteristics	Values	References
Biodegradation in sediment DT_{50} [d]	None of the available studies showed biodegradation of PFOS in the aquatic environment under either aerobic or anaerobic conditions	Environment Agency (2004) and Sáez et al. (2008)

[a] Data in grey font not used for EQS derivation.

1.2 Regulatory context and environmental limits

Table 2 summarizes existing regulation in Switzerland, Europe and elsewhere for PFOS.

Concerns about the potential environmental and toxicological impact of long-chain PFSAs and PFCAs have led to the phase-out of production of PFOS (and perfluorohexane sulfonic acid (PFHxS), perfluorodecane sulfonic acid (PFDS)) and its precursors by their major global manufacturer (3M Company) in 2000 to 2002 (USEPA 2000). A European Union Marketing and Use Directive restricting the use of ‘‘perfluorooctane sulfonates’’ in the European Union was signed in 2006 (EC 2006). A stewardship agreement between the US Environmental Protection Agency (USEPA) and leading global companies also concluded to reduce emissions and product content of PFOA and related chemicals by 95% by 2010 and to work toward their elimination by 2015 (USEPA 2006) and a similar agreement was signed between the Canadian environmental and health authorities and 5 companies to restrict PFCAs in products (Environment Canada 2010).

PFOS has been classified as a persistent (P), bioaccumulative (B), and toxic substance (T) (OECD 2002, 2013) and was added to Annex B (requiring use restrictions) of the Stockholm Convention list of persistent organic pollutants (UNEP 2009). PFOS and related compounds were the subject of EU Commission Regulation No 757/2010 of 24 August 2010 prohibiting/restricting its use, production, import, and export, complementing provisions of international agreements on POPs.

In Switzerland, PFOS is regulated by the Ordinance on the Reduction of Risks relating to the Use of Certain Particularly Dangerous Substances, Preparations and Articles (Chemical Risk Reduction Ordinance, ORRChem) of 18 May 2005 (Status as of 1 January 2020). From 1 August 2011, it is prohibited to manufacture, place on the market or use PFOS, and any substances or preparations containing more than 0.001 % PFOS. New articles may not be placed on the market if the components treated with PFOS contain more than 0.1 % PFOS. For textiles and other coated materials, the specified limit is 1 µg/m^2 of the coated material. Exemptions apply for applications where no substitutes for PFOS are available at present. Fire-fighting foams placed on the market before the prohibition entered into force may still be used during a transitional period. Under the POPs Convention, notification requirements apply for applications where use remains permissible.

Table 2 Existing regulation for PFOS in Switzerland and Europe.

Europe	
EU Priority substance list	Priority Hazardous Substance
POPs Stockholm Convention	**Annex B:** **Production:** In accordance with part III of Annex B, production of other chemicals to be used solely for the uses in part III of Annex B, and production for uses in part III of Annex B **Use:** Acceptable purposes and specific exemptions in accordance with Part III of Annex B

PBT Substance	Yes
EU Commission Regulation No 757/2010 of 24 August 2010	PFOS prohibited/restricted in its use, production, import, and export, complementing provisions of international agreements on POPs
Switzerland	
Ordinance on the Reduction of Risks relating to the Use of Certain Particularly Dangerous Substances, Preparations and Articles (Chemical Risk Reduction Ordinance, ORRChem) of 18 May 2005 (Status as of 1 January 2020)	From 1 August 2011, it is prohibited to manufacture, place on the market or use PFOS, and any substances or preparations containing more than 0.001 % PFOS. New articles may not be placed on the market if the components treated with PFOS contain more than 0.1% PFOS. For textiles and other coated materials, the specified limit is 1 µg/m^2 of the coated material. Exemptions apply for applications where no substitutes for PFOS are available at present. Fire-fighting foams placed on the market before the prohibition entered into force may still be used during a transitional period. Under the POPs Convention, notification requirements apply for applications where use remains permissible.

Table 3 presents existing environmental quality standards and limit value available for PFOS.

No specific quality standard is set for PFOS under the Swiss Water Protection Ordinance. The Drinking Water Ordinance (TBDV) set a limit value of 300 ng/L for PFOS.

As a Priority Hazardous Substance, Directive 2013/39/EU of the European Parliament and of the Council of 12 August 2013 amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy sets in Annex II an annual average EQS (AA-EQS) for inland surface waters of 0.65 ng/L. The AA-EQS was based on the quality standard for biota for protecting human health ($QS_{biota,hh}$), which sets the EQS_{biota} at 9.1 µg/kg w.w. (EC 2013). Additionally, a maximum allowable concentration (MAC-EQS) applicable to short-term pollution peaks in continuous discharges for PFOS is set at 36 µg/L.

Non-regulatory proposals for quality standards (QS), predicted no effect concentrations (PNEC) and environmental risk limits have been proposed by several national and international agencies within different contexts and following different derivation methods. Specifically for sediments, the EQS sheet for the WFD did not derive a QS_{sed} due to the insufficient data available for confirming the need for a QS_{sed} and for its derivation (EC 2011a). INERIS has a proposal at 67 µg/kg d.w. derived using the EqP, while Norway has established an $EQS_{freshwater}$ at 2.3 µg/kg d.w. (method for derivation unknown, Miljødirectoratet 2016). Additional values are available for sediment management in Norway, as reported in Bakke et al. (2007) and Bakke et al. (2010), with a background concentration for marine sediments estimated at 0.17 µg/kg d.w., a no effect threshold equivalent to a QS_{sed} of 220 µg/kg d.w., a chronic toxicity range of 220- 630 µg/kg d.w., and an acute short-term effects range of 630-3100 µg/kg d.w. While the EC (2003) TGD is referred to for derivation, the exact approach used is not reported.

The EU technical guidance document for EQS derivation does not foresee converting a biota standard into an equivalent sediment concentration (EC 2018). However, the protection of humans against adverse health effects from consuming contaminated fisheries is often the driver for remediation of contaminated sediments, and a $QS_{sed,hh\ food}$ is needed in early tiers when assessing biomagnifying substances. Babut (2018) converted this EQS$_{biota}$ into a QS$_{sed,hh\ food}$ of 0.51 µg/kg d.w. using published Biota-Sediment Accumulation Factors and Trophic Magnification Factors for PFOS. Alternatively, the same BSAF-TMF approach results in a QS$_{sed,sec.pois.}$ of 1.85 µg/kg d.w. from the biota QS$_{biota,sec.pois.,fw}$ to protect wildlife from secondary poisoning of 33 µg/kg w.w. (EC 2011a). This value is close to the lowest sediment NOAEL (no-observed adverse effect level)-based risk-based screening level (RBSL) for wildlife of 1.43 µg/kg, derived using foodweb models (Zodrow et al. 2020).

For general toxicity in surface waters, the most recent Federal Water Quality Guideline (FWQG) derived by Environment Canada in 2017 through statistical extrapolation was set at 6.8 µg/L, based on the HC5 with no additional assessment factor (AF) according to the SSD based on no effect concentrations, EC$_{10}$, IC$_{10}$, MATC and LOEC values. The AA-QS$_{eco,\ freshwater}$ derived using the EU TGD methodology was set at 0.23 µg/L (EC 2011b and Moermond et al. 2010), while higher PNECs of 25 and 0.465 µg/L were derived for risk assessments based on different effect concentrations and AF (Environment Canada 2006, Environment Agency 2004).

Additionally, a QS$_{sec.pois.freshwater}$ intended to protect organisms of higher trophic levels against secondary poisoning of 0.002 µg/L was derived following the EU TGD in the EU EQS dossier (EC 2011a,b) from a QS$_{biota}$ of 33 µg/kg w.w. in whole fish, value that was also proposed by the Ecotox Centre (2011).

Table 3 Existing environmental limit values and quality guidelines for PFOS.

Description	Value	Development method	References
Sediment [µg/kg d.w.]			
Direct toxicity			
QS$_{sed}$	--	EU TGD (EC 2011b): Insufficient data to confirm the need for a QS$_{sed}$ and insufficient data for derivation.	EC (2011a)
PNEC / QS$_{sed}$	67	EU TGD (EC 2011b): derived using the EqP.	INERIS (2018)
EQS$_{freshwater}$	2.3	EU TGD (EC 2011b): exact methodology not reported. For 1% OC.	Miljødirectoratet (2016) (M608)
Boundary Class II-III	220	EC (2003): concentration above which long-term exposure may cause effects on sufficient number of species to damage community structure and function. Equivalent to PNEC chronic and QS$_{sed}$, approached used for derivation (AF or EqP not known).	Bakke et al. (2007); Bakke et al. (2010)
Secondary poisoning for top predators			
NOAEL-based RBSL	1.43	US EPA (2005): foodweb modeling. Lowest value among different values calculated for different birds and mammals	Zodrow et al. (2020)
Secondary poisoning for human health			
NQE$_{sediment}$[a]	0.51	Adapted EU TGD (EC 2011b): derived from a QS$_{biota}$ of 9.1 µg/kg w.w. to protect human health from fish consumption	Babut (2018)
Water [µg/L]			
Direct toxicity			
AA-QS$_{eco}$ freshwater	0.23	EU TGD (EC 2011b): Based on NOEC for *Chironomus riparius* emergence (<23 µg/L) and AF of 10.	EC (2011a) and Moermond et al. (2010)

Description	Value	Development method	References
Chronic RWQ RBSL[b]	51	US EPA (2012): Based on statistical extrapolation	Zodrow et al. (2020)
FWQG[c]	6.8	Based on statistical extrapolation (SSD HC_5 = 6.8 µg/L), no additional AF.	Environment Canada (2017)
ENEV[d]	0.491	Based on 10-d NOEC for *Chironomus riparius* (49.1 µg/L) and AF of 100.	Environment Canada (2006)
PNEC	25	Based on NOEC for *Americamysis bahia* (250 µg/L) and AF of 10.	Environmental Agency (2004)
Secondary poisoning for top predators			
$QS_{secpois.\ freshwater}$	0.002	EU TGD (EC 2011b): Derived from a QS_{biota} of 33 µg/kg w.w.	EC (2011a)
$MPC_{secpois.\ freshwater}$[e]	0.0026	EU TGD (EC 2011b): Derived from a QS_{biota} of 37 µg/kg w.w.	Moermond et al. (2010)
NOAEL-based RBSLs	0.075	US EPA (2005): foodweb modeling. Lowest value among different values calculated for different birds and mammals	Zodrow et al. (2020)

[a] French acronym for Environmental Quality Standard; [b] Chronic Recommended Water Quality Risk-Based Screening Level; [c] Federal Water Quality Guideline; [d] Estimated No Effects Value; [e] Maximum Permissible Concentration.

1.3 Use and emissions

PFOS has been used in a wide range of industrial processes and products due to their unique physico-chemical properties. In the EU, PFOS and PFOS derivatives were historically used in carpets, leather (apparel), textiles and upholstery, paper and packaging, coatings and coating additives, industrial and household cleaning products, and pesticides and insecticides. POSF[3]-based substances are used or have been used in metal plating, POSF-based firefighting foams, in the photographic industry, in semiconductors and in photolithography, and in hydraulic fluids for the aviation (RPA 2004 cited in Buser and Morf 2009).

The total historical worldwide production of POSF was estimated to be 96 000 t (122 500 t including unusable wastes) between 1970 and 2002 (Paul et al. 2009 cited in Buser and Morf 2009), with an estimated global release of 45 250 t to air and water during these years (Paul et al. 2009). The major producer 3M stopped POSF-based substances production in 2003, then the Italian Miteni became the world's largest producer of PFAS while China's annual output started to grow as from 2005 to satisfy overseas' demand of PFOS' application (MEP 2008 cited in Buser and Morf 2009).

According to Buser and Morf (2009), a reliable quantitative assessment of PFOS production, direct and indirect emissions[4], and environmental inventory is lacking.

The use of PFOS in Switzerland is not allowed since 2011, with phase out periods for various use categories. The last phase out period, concerning fire-fighting foams, ended November 2018. According to OECD survey in 2000, no domestic production of PFOS was reported in Switzerland although no detailed information on the use of PFOS or POSF-based substances use was reported (Buser and Morf 2009). The stop of domestic manufacture of these substances was confirmed in the 2006 OECD survey, but again no detailed information on import volumes of PFOS and PFOA was provided and only one company reported importing PFOS potassium salt and ammonium perfluorooctanoate (APFO) in the low kg range for industrial use.

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[3] Perfluorooctanelsulfonyl fluoride –POSF- is chemical intermediate in the synthesis of PFOS as well as perfluorooctanesulfonamide –FOSA- and perfluorooctane sulfonamido ethanol –FOSE- derivatives.

[4] Direct emission sources of PFASs are defined as emissions throughout their product cycle, and indirect emission sources are defined as emissions from transformation of their precursors (Buck et al. 2011).

The presence of PFOS, PFOA, and similar substances in the environment originates from the industrial use and environmental release of these substances, from use and disposal of consumer products that may contain them as an impurity, and from the abiotic or biotic degradation of larger functional derivatives and polymers that contain a perfluoroalkyl moiety and degrade in the environment to form PFOS, PFOA, and similar substances (Paul et al. 2009; Prevedouros et al. 2006). The total (direct and indirect) historic emissions of POSF-based substances are estimated to be 6 800 to 45 300 t (1972–2002), whereas total emissions of PFCAs range from 3200 t to 7300 t (1951– 2004) (Paul et al. 2009; Prevedouros et al. 2006). The majority of these emissions (>95 %) are directly released into the aquatic environment, whereas emissions through the atmosphere are considered to be rather small (<5 %) (Paul et al. 2009; Prevedouros et al. 2006). Waste water is the main source of PFOS to the aquatic environment (Becker et al. 2008) but also diffuse inputs can play a significant role (Müller 2011; Paul et al. 2012). PFOS concentrations levels in freshwater have been linked to population density in Europe (Pistocchi and Loos 2009), presumably discharged from WWTPs after consumer cleaning of treated fabrics. Pistocchi and Loos (2009) gave a value of 27 mg/day per capita as a European average; Becker et al. (2008) reported 40 mg/day per capita for a German WWTP, while Schultz et al. (2005) and Huset et al. (2008) gave values of 42 and 57 mg/day per capita for outflows from US and Swiss WWTPs, respectively.

According to a substance flow analysis of PFOS and PFOA commissioned by the Federal Office of the Environment (Buser and Morf 2009), PFOS consumption in Switzerland for 2007 occurred mainly for metal plating, while products and processes for photography and photolithography were much smaller. Stocked fire-fighting foams were by that time still used and contributed significantly to the use of PFOS. Simulated total emissions of PFOS to the Swiss environment were estimated at 500 kg/year, with over 90 % directly to the hydrosphere mostly through the wastewater pathway. Measurements in WWTP effluents showed no other apparent source of PFOS in a highly populated section of the Glatt, with an estimated per-capita discharge of 57 µg/day/person (Huset et al. 2008). Assuming a similar discharge per person all over Switzerland, the total release to surface waters would be approximately 160 kg/year (using 2007 estimates). Although the presence of metal plating industries and recycling plants as well as major fire incidents have a high impact on the occurrence of PFOS, the order of magnitude of this estimate was in good agreement with the total emission estimated to the hydrosphere of ca. 500 kg/year (Buser and Morf 2009). As the compound is phased out, emissions have reduced over time. In the river Glatt, PFOS concentrations noticeably declined (2-3 fold) from 2006 to 2009 (Müller et al. 2011). Stock build up from historical consumption of PFOS in other application areas constitutes a potential long-term emission source such as in the service life and in landfills.

1.4 Mode of action and relative sensitivity of taxonomic groups

PFOS has a harmonized classification as toxic to reproduction and suspected to be carcinogenic (ECHA 2019), but was not genotoxic in a variety of assay systems (OECD 2002).

According to the hazard profile completed by OECD (2002), PFOS is persistent, bioaccumulative and toxic to mammalian species. Elimination half-life of PFOS ranges from 100 days in rats, 200 days in monkeys, to years in humans but the toxicity profile of PFOS is similar among rats and monkeys. Repeated exposure results in hepatotoxicity and mortality, with a very steep dose-response curve for mortality for animals of all ages although neonates may be more sensitive (OECD 2002). Rats exposed to PFOS in a 2-year bioassay presented thyroid follicular cell adenomas and hepatocellular adenomas that apparently not relate to peroxisome proliferation. In addition, PFOS exposure was associated with the incidence of bladder cancer in epidemiologic studies.

According to EC (2011a), available data indicates that PFOS has the potential to induce adverse effects on the endocrine system of animals, including rats and fish. However, the data suggest that endocrine effects occur at concentrations higher than those causing effects on growth, reproduction and mortality in standard toxicity tests (Environment Agency 2008). Four different estrogen receptor (ESR) assays reported activation following PFOS treatment, all of which were Estrogen Receptor 1- (ESR1-) related (US EPA 2016). Endocrine modulation effects on the estrogen receptor and thyroid receptor occurred in zebrafish (Du et al. 2013). In a recent study of Chen et al. (2016a), a 5-month exposure of zebrafish to 250 µg/L caused significant alterations in the expression of key genes involved in hormone pathways and induced male and female gonadal structural alterations (e.g. incomplete seminiferous lobule structures, ruptured basilar membranes, cytoplasmic vacuolization, diminished mitochondrial cristae).

According to Environment Canada (2017), the modes of action of PFOS are not entirely understood but they are diverse, including activation of the nuclear peroxisome proliferator activated receptor-alpha (PPAR-α) (Berthiaume and Wallace 2002; Hickey et al 2009, Rosen et al. 2010). Activation of this receptor alters gene expression related to a broad spectrum of action, including fatty acid metabolism and transport, cholesterol transport (Feige et al. 2006), glucose metabolism, inflammation response, and development. Toxic effects have been also demonstrated that do not involve peroxisome proliferator activated receptor mechanisms (O'Brien et al. 2009).

PFOS is also believed to interfere at the mitochondrial level through the uncoupling of oxidative phosphorylation, causing a reduction in the production of ATP and thereby reducing energy stores (Environment Canada 2017). Other modes of action that have been hypothesized include inflammation-independent leakage of liver cell membranes in fish, which leads to cell necrosis (Hoff et al. 2003), interference with the homeostasis of DNA metabolism (Hoff et al. 2003), inhibition of glycogen synthesis and increased glycogen breakdown (Hagenaars et al. 2008), and the inhibition of intercellular communication processes involving gap junctions (Hu et al. 2002). Altered neurochemistry from a single dose of PFOS to neonatal mice resulted in developmental neurotoxicity (Johansson et al. 2008).

PFOS shows moderate acute toxicity to aquatic organisms, with sensitivities overlapping among taxa (most recent review in Environment Canada 2017). The lowest effect concentration for fish is a 14-d LOEC (growth) of 10 µg/L for Japanese medaka (*Oryzias latipes*) (Ji et al. 2008). For aquatic invertebrates, MacDonald et al. (2004) recorded considerable effects on emergence of *Chironomus tentans* at a PFOS concentration of 2.3 µg/L, and Bots et al. (2010) derived a NOEC < 10 µg/L for metamorphosis of *Enallagma cyathigerum.* 21-d EC$_{10}$ (survival) for water flea range from 6 000 µg/L (*Daphnia pulicaria;* Sanderson et al. 2004) to 12 000 µg/L (*D. magna;* geometric mean Boudreau et al. 2003 and Sanderson et al. 2004). The lowest effect concentration for amphibians is a 67-d NOEC (survival) for the African clawed frog (*Xenopus laevis*) of 100 µg/L (Cheng et al. 2011).

For primary producers, the most sensitive plant species is watermilfoil (*Myriophyllum sibiricum*) with a 42-d EC$_{10}$ (growth) of 100 µg/L (Hanson et al. 2005) while the most sensitive microalga is *Chlorella vulgaris* with a 96-h EC$_{10}$ (cell density) of 8 200 µg/L (Boudreau et al. 2003).

PFOS does not appear to be toxic to sewage sludge microorganisms, with a 3-h IC$_{50}$ (respiration inhibition test) of >905 mg/L (nominal concentration) (Environment Canada 2017).

While there is broad evidence that linear and branched PFOS isomers have differential environmental distribution and bioaccumulation patters in animals and humans, toxicity studies have traditionally used commercial PFOS standards with relatively constant proportion of branched PFOS (Sigma–Aldrich/Fluka (~20 % branched) or 3M (~30 % branched); Benskin et al. 2010), not differentiating between PFOS isomers. Only in the last years toxicity studies have started to test linear and branched isomers separately (Schulz et al. 2020). The recent review by Schulz et al. (2020) on the distribution and effects of branched versus linear isomers of PFOS, PFOA and PFHxS indicate some studies have found toxicological effects and endpoints for linear but not branched PFOS (and PFOA), or vice versa.

2 Environmental fate

2.1 Stability and degradation products

PFOS does not hydrolyse, photolyze or biodegrade under environmental conditions due to the strength of the carbon-fluorine bond and it is persistent in the environment (OECD 2002).

In several reports and reviews (e.g. Environmental Agency 2004, UNEP 2006, Giesy et al. 2010, Moermond et al. 2010) it is concluded that PFOS is not biodegradable. OECD (2002) and Environmental Agency (2004) report no significant biodegradation of PFOS in 28 days in a MITI-I test (Kurume Laboratory 2002 cited in OECD 2002) as measured by net oxygen demand, loss of total organic carbon, or loss of parent material, concluding that PFOS is not ready biodegradable. No evidence of degradation was found in a 35-day biodegradation test with activated sludge from a municipal waste water treatment plant using PFOS (as the potassium salt) at a concentration of 2.582 mg/L and in an additional 18 days study performed at similar experimental conditions except that the activated sludge was allowed to settle for five weeks rather than two days after collection as reported in OECD (2002) and Environmental Agency (2004). Additional biodegradation experiments reported by Giesy et al. (2010) (Lange 2001, Gledhill and Markley 2000a,b,c) also found no loss or biotransformation of PFOS over a 20-week period under aerobic conditions, nor were there any losses observed in a study conducted for 56 d with activated sludge under anaerobic conditions. In addition, no losses of PFOS were observed in a biodegradation study conducted with soil under aerobic conditions.

Another biodegradation experiment based on the OECD guideline 301D (closed bottle test with slight modifications, OECD 1992) where municipal sewage sludge was spiked with a mixture of PFOS, PFHxA, PFOA and PFNA at initial nominal concentrations of 2 to 4 mg/L showed no significant decrease of PFOS concentrations for 15 weeks under aerobic or anaerobic conditions (Saez et al. 2008). Saez et al. (2008) report that similar experiments with sediment contaminated with PFAS also showed no evidence for biodegradation of any of the PFAS tested but these data are not shown and could not be located.

In the analytical study reported by Schröder (2003) and Meesters and Schröder (2004) where wastewater samples from German WWTPs were spiked with PFOS and PFOA and incubated under aerobic and anaerobic conditions, PFOS and PFOA were not eliminated by metabolic (primary degradation), mineralization processes or by adsorption under aerobic conditions. In the anaerobic treatment (redox potential below – 300 mV) there was a rapid decrease of PFOS concentrations (within 2 d) while PFOA remained stable during breakdown of PFOS. After the disappearance of PFOS, the degradation continued and after 25 days PFOA could no longer be detected. Against the background that no laboratory data exist that demonstrates that PFOS undergoes significant biodegradation under environmental conditions (see above) and the fact that no metabolites or increases in fluoride ion concentration were detected, the results of the studies of Schröder (2003) and Meesters and Schröder (2004) on anaerobic degradation of PFOS should be treated with caution and deserve further assessment.

2.2 Sorption/desorption processes

According to the hydrophobic and hydrophilic functionalities of PFAS, this group of chemicals behave differently from traditional non-ionisable organic compounds. At environmental pH values, PFAS usually exist as anionic species due to their low pK_a values. Because of electrostatic attraction, the negatively charged functional head binds the positively charged surfaces of the adsorbents. Oxides provide positively charged surfaces for electrostatic interaction, while the presence of divalent cations act as a bridge between negatively charged surfaces of sorbents and negatively charged functional head of PFAS. Both the mineral phase and organic matter in soils and sediments contribute charged surfaces. In addition, hydrophobic interactions between the C-F chain and the organic matter can also occur during sorption to soil and sediments. Hydrogen bonding, Van der Waals and pi-pi interactions are likely to be insignificant (Du et al. 2014 and literature therein).

Available literature indicates that organic carbon (OC) plays a role in sorption of anionic PFAS with a perfluoroalkyl carbon chain length ≥6 carbon atoms (Mejia-Avendaño et al. 2020 and references therein). Several studies have found statistically significant relationships between sorption of PFOS and OC, although they have mostly been conducted in a small number of sediments and constant pH (Ahrens et al. 2011, Chen et al. 2012, Li et al. 2018). Others have found no correlation (Becker et al. 2008), weak correlation (Pan and You 2010), or strongly skewed correlations by one single sediment with a high OC content (Higgins and Luthy 2006, You et al. 2010, Milinovic et al. 2015). A critical review completed by Li et al. (2018) found that the relationship between peer-reviewed literature K_d values for PFOS and OC was significant ($P < 0.05$, $N = 178$) but with $R^2 = 0.05$, thus only 5 % of the variation in sorption is explained by the model (Li et al. 2018).

Experimental K_d values from the literature from batch equilibrium studies using freshwater sediments range from 6.0 to 223.9 L/kg (corresponding to log K_d of 0.78-2.35) (Higgins and Luthy 2006; Chen et al. 2016b). Experimental K_d values calculated from field studies for freshwater sediments tend to be higher than those from batch equilibrium studies, ranging from 20 to 760 L/kg (log K_d of 1.30-2.88) (Table 1 and Appendix 1).

OECD (2002) reports a K_{OC} value of 57 100 L/kg (log K_{OC} = 4.76) in the hazard assessment of PFOS obtained in a batch equilibrium study (OECD 106) with river sediment of 1.3 % OC and 19 % clay, pH of 7.7. Experimental K_{OC} values obtained in batch equilibrium studies with freshwater sediments range from 478.6 to 1819.7 L/kg (log K_{OC} of 2.68-3.26) (Zhao et al. 2012, Chen et al. 2016b), in good agreement with the K_{OC} value derived from the slope between K_d and OC for 4 freshwater sediments with OC ranging from 1.02 to 9.66 %, pH 5.7-7.6 and clay content 5-53 %. (Higgins and Luthy 2006). Experimental K_{OC} values obtained in batch equilibrium studies for soils of different properties also fall within the same range as those for freshwater sediments, ranging from 272.2 to 1 100 L/kg (Mejia-Avendaño et al. 2020). Although experimental K_{OC} from field studies tend to be higher than K_{OC} from batch experiments, they cover a wider range from 191 to 11 801 L/kg. According to results from Li et al. (2020), K_{OC} values estimated from field studies for freshwater suspended matter tend to be higher than those for sediments.

PFOS is an acidic chemical and the proportion of anionic molecule increases with increasing pH, resulting in decreased sorption. Changes in pH also affect surface properties of the sorbent, thus changes in pH or ionic strength are expected to affect sorption of PFOS. Several studies have shown a decrease of PFOS sorption to sediment at increasing pH (e.g. Higgins and Luthy 2006, see above), although the relationship between peer-reviewed literature K_d values for PFOS and pH was not significant ($R^2 = 0.06$, $P > 0.05$, $N = 27$; Li et al. 2018). The unsuccessful estimation of K_{OC} values for PFOS as a function of pKa, pH and OC suggests that pH and OC together are also not sufficient to explain the sorption of PFAS (Li et al. 2018).

Cations in solution also affect PFAS sorption to sediments. Increasing concentrations of Ca^{2+}, Mg^{2+} and Na^{+} have been associated with increased PFOS sorption to sediments, although contradictory results are reported in the literature resulting in a non-significant relationship between peer-reviewed collated K_d values and Ca^{2+} ($R^2 = 0.11$, $N = 32$) and Na^{2+} ($R^2 = 0.05$, $N = 23$) (Li et al. 2018 and literature therein). According to the variation of solution ionic composition, PFOS in seawater has shown higher sorption to sediment than in freshwater (ten times higher at relatively constant OC and clay content, pH 7.1-7.6), in accordance with the importance of electrostatic interaction expected in seawater (Chen et al. 2012). K_d values derived from marine sediments are therefore considered not relevant in sediment EQS derivation for Switzerland and are not used here.

Because PFASs exist as anionic compounds at environmental pH values an inverse relationship with Cation Exchange Capacity (CEC) would be expected, but no significant relationship between soil CEC and PFOS sorption to soil was identified (Li et al. 2018). Clay content, indicator of potential binding sites for electrostatic interaction, also showed no significant relationship with K_d (Li et al. 2018).

Once adsorbed to these matrices, PFOS does not readily desorb. Giesy et al. (2010) reports an average desorption coefficient (Kdes) for soils of less than 1 L/kg. In soil, sediment and sludge adsorption and desorption equilibria is achieved in less than 24 hours, and approximately after 1 min of contact with the test adsorbents for more than 50 % of cases suggesting that PFOS exhibits little mobility and no expected migration. The shape of the adsorption isotherm (H-type) indicates a very strong chemical/adsorption interaction for PFOS (Giesy et al. 2010).

2.3 Bioavailability

Bioavailability is a complex process which depends on many factors including the sorption capacity of the sediment considered (e.g. OC content), the hydrophobicity of the compound, and the physiology, feeding behaviour and burrowing activity of the benthic organism considered (Warren et al. 2003). However, the particular physico-chemical properties of PFOS and PFAS in general challenge the use of traditional bioavailability paradigms for this group of substances.

According to available information on PFOS sorption/desorption to sediments and soils and evidence indicating reduced bioaccumulation at increasing TOC content (Higgins and Luthy 2006, Higgins et al. 2007, Wen et al. 2015) it is assumed that TOC is an important factor driving PFOS bioavailability and this factor will be considered for normalization of effect data in EQS derivation. Nevertheless, other factors such as pH or clay content that are shown to describe PFOS sorption may be also important drivers of PFOS bioavailability although the absence of simple models for normalization prevents accounting for these factors in EQS derivation.

2.4 Bioaccumulation and biomagnification

The available bioaccumulation and biomagnification data for PFOS has been collated and discussed in previous reports from several agencies (e.g. OECD 2002, Environment Agency 2004, UNEP 2006, Moermond et al. 2010, Babut 2018). A non-exhaustive summary is provided in Table 4.

PFOS has been shown to bioconcentrate in fish in laboratories studies, with bioconcentration factors (BCF) ranging from 720 to 5 400 and a BCF of 2796 chosen for fish in the voluntary risk assessment (Environment Agency 2004; EC 2011). Steady-state BCF[5] for bluegill sunfish (*Lepomis macrochirus)* in an OECD 305 study were of 1 124 (edible tissue), 4 013 (non-edible), and 2 796 (whole fish tissues)[6] (OECD 2002). PFOS depurated slowly, with estimated time to reach 50 % clearance of 86, 116, and 112 days for edible, nonedible, and whole fish tissues respectively. Exposure to 0.87 mg/L PFOS caused excessive mortality and resulted in steady-state BCF after 35 d of 136, 386 and 270 for edible, non-edible and whole fish, respectively.

BCF for carp (*Cyprinus carpio*) were 720 for 20 µg/L and 200-1 500 for 2 µg/L in a 58 days uptake study (Kurume Laboratory 2001 cited in OECD 2002). In combination with other perfluorinated acids (both carboxylates and sulphonates), Martin et al (2003a) calculated kinetic BCF values for rainbow trout (*Oncorhynchus mykiss*) exposed for 12 days in a flow-through system to 0.35 µg/L PFOS of 1 100, 4 300

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[5] BCF and BAF are derived from wet weight and not lipid normalized if not otherwise stated.

[6] Calculated as tissue concentrations at apparent steady-state divided by the mean water concentration as of 484 (edible tissue), 1 124 (non-edible), and 859 (whole fish tissues).

and 5 400 for carcass, blood and liver respectively[7]. Liver and blood are protein-rich tissues that tend to accumulate PFAS at concentrations orders of magnitude higher than concentrations in other biological compartments in agreement with the *proteophilic* nature of these substances. As noted in the risk assessment profile for PFOS (UNEP 2006), PFOS does not follow the classical pattern of partitioning into fatty tissues followed by accumulation typical of many persistent organic pollutants. PFOS is both hydrophobic and lipophobic and binds preferentially to proteins in the plasma and in the liver. According to the levels of PFOS concentrations in wildlife, including marine mammals, and the high levels in top predators it was concluded that the BCF may not adequately represent the bioaccumulation (and biomagnification) potential of PFOS (see reviews in UNEP 2006, OECD 2002).

Concerning the risk of benthic invertebrates to transfer toxic and bioaccumulative substances to higher trophic levels, the EFSA scientific opinion for sediment risk assessment proposes to perform spiked sediment bioaccumulation tests with benthic invertebrates for substances that show significant bioaccumulation in fish (BCF ≥ 2000) when the substance is (1) persistent in sediment (DT_{50} >120 d in water-sediment fate studies) and log K_{OW} >3; or (2) non-persistent in sediment, log K_{OW} >3 and >10 % of the substance found in the sediment in a water-sediment fate study (EFSA 2015). The bioaccumulation criterion and persistence suggest studying bioaccumulation from sediments, and an exhaustive review of BSAFs was completed recently by Babut (2018).

Bioaccumulation of PFOS in spiked sediment bioaccumulation studies have been completed for the freshwater oligochaete *Lumbriculus variegatus* (Higgins et al. 2007). In semi-static 28 d batch experiments with spiked sediment at concentrations of 160-400 µg/kg-OC d.w. (4 % OC) steady-state was not achieved at the end of exposure, kinetic Biota-Sediment Accumulation Factors (BSAF) from uptake and loss constants were estimated at 1.22 expressed as wet weight, not lipid normalized but normalized for the sediment organic carbon content. BSAF derived at the end of exposure to two naturally contaminated sediments were 0.83 and 0.98, slightly lower than BSAF from spiked sediments either because steady state was not achieved or because of the lower bioavailability of naturally contaminated sediments. Small elimination constants indicated that PFOS is not excreted effectively by oligochaetes, and at lower rate than other organic substances. N-EtFOSAA, a PFOS precursor was accumulated and underwent biotransformation to PFOS and precursors. N-EtFOSAA is often accumulated in sediments at concentrations higher than those for PFOS, therefore it was concluded that N-EtFOSAA may contribute substantially to the body burden of PFOS in oligochaetes.

Lower BSAF were reported by Lasier et al. (2011) for *L. variegatus* exposed to naturally contaminated sediments, with an average for 24 naturally contaminated sediments of 0.49 (with OC ranging from 0.4 to 2.6 %). An additional study from Prosser et al. (2016) reported BSAF from 28 days bioaccumulation studies with *L. variegatus* of 0.3-1.1 when exposed in the laboratory to naturally contaminated sediments (N=5) with PFOS concentrations 0.15-4.80 µg/kg d.w. and OC 2.4-4.8 %. The studies from Higgins et al. (2007) and Lasier et al. (2011) suggested that accumulation of PFAS in aquatic oligochaetes appeared to be primarily related to sediment concentrations, with patterns among concentrations virtually the same for sediments and tissues representing the contaminated sites and showing highly significant positive correlations.

Prosser et al. (2016) also reported BSAF for *Hexagenia* sp. of 1.05. Additional BSAFs are available for chironomids, ranging from 0.01 to 0.02 for the species *Chironomus riparius* (Bertin et al. 2014, 2018) in 4 days laboratory exposures to a naturally contaminated sediment with 0.24-0.29 µg/kg d.w. PFOS and 4.3 % OC, and 0.39 (steady-state) and 0.38 (kinetic) for *C. plumosus* in 10 days laboratory exposures to spiked sediments with 100 µg/kg d.w. (nominal) PFOS and 2.18 % OC (Xia et al. 2012). BSAF for

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[7] Accumulation ratios at end of uptake (12 days) were 690, 3 100 and 2 900

amphipods are slightly higher, ranging from 4.76 for the freshwater amphipod *Gammarus* sp. after 21 d of exposure to the same naturally contaminated sediment as in Bertin et al. (2014; 2016) and 6.3 to 9.12 (reported as log BSAF of 0.80 to 0.96) for field-collected amphipods *Monoporeia affinis* from a relatively clean pond in Sweden (Jacobson et al. 2010).

Bioaccumulation of PFOS in field-collected organisms is also well described in the literature. In the review from Conder et al. (2008), a geometric mean bioaccumulation factor BAF of 1 800 (range 18-11 000) from field data measurements in Houde et al. (2006), Morikawa et al. (2006) and Kannan et al. (2005) is provided. BAF reported for invertebrates from the Great Lakes area (590 for zebra mussel, 830 for amphipods and 920-1 200 for crayfish) are in the low range of BAF for different fish species from the same area (710 for smallmouth bass to 4 700 for round gobies; Kannan et al. 2005). Houde et al. (2006) also reported BAF for fish species ranging from 1 600 in pinfish to 9 800 in spotted seatrout.

Two studies have reported increased PFOS concentrations in organisms from areas with high PFAS release. Bhavsar et al. (2016) reported BAF for different fish species (N=100) from a former firefighting training area in Canada ranging from 251 to 50 119 (average 2 512) and BSAF from 5.0 to 794 (average 50.1). Kwadijk et al. (2014) reported BAF of 1 148 and 234.4 for eel, 2 291 and 6 310 for perch and 1 549 for pike few weeks and three years after an accidental release of aqueous film forming foam at Schiphol Amsterdam airport. BSAF not normalized for lipid and organic matter in the study of Kwadijk et al. (2014) were 9.3 and 11.5 for eel, 74.1 and 49.0 for perch and 53.7 for pike, also in good agreement with those reported by Bhavsar et al. (2016).

de Vos et al. (2008) studied the accumulation of PFOS in the food chain of the Western Scheldt estuary. Although comparison of results from freshwater and marine studies should be made with care, the results appear in good agreement, with derived BSAF ranging from 3.9 for a detritivore marine polychaete (*Arenicola marina*, trophic level 2), 14 for primary carnivores (geomean of *Crangon crangon, Sprattus sprattus, Ammodytes* sp, trophic level 3), 57 for primary-secondary carnivores (geomean of *Carcinus maenas, Solea solea, Pleuronectes platessa, Trisopterus lucus, Anguilla anguilla, Dicentrarchus labrax*, trophic level 3.5) and 34 for secondary carnivores (*Sterna hirundo*, trophic level 4).

Biomagnification of PFOS can be considered by means of Trophic Magnification Factors, which represents the average value of the prey-to-predator magnification factor over a whole food chain or a segment thereof. According to the critical review from Franklin (2016) and Babut (2018), a geometric mean TMF of 3.0 for PFOS is obtained from studies for freshwater (plus one estuarine) trophic chains from temperate climates. TMF for different rivers in France range from 2.4 to 4.1 (Convention Onema-Irstea 2012-2016, action n°38, cited in Babut 2018). TMF for temperate lakes range from 2.9 for a food chain including bird species, carnivorous fish, omnivorous fish, herbivorous fish, zooplankton, phytoplankton, zoobenthos and white shrimp from Tahiu Lake in China, an area subject to anthropogenic pressures but not highly contaminated with PFAS (Xu et al. 2014), to 5.9 for a food chain in Lake Ontario including predator fish, lake trout, three forage fish, fish feeding primarily on invertebrate benthic insects, fish feeding on benthic prey (e.g. amphipods, mysids and crangonids), and two invertebrates (Diporeia and Mysis) (Martin et al. 2004). The study from Lake Ontario showed the highest mean body burdens in the benthic macroinvertebrate Diporeia, which occupies the lowest trophic level of all organisms analyzed, with concentrations up to 10-fold higher than in Mysis, a predominantly pelagic feeder, suggesting that a major source of PFAS to this food web was the sediment, not the water (Martin et al. 2004).

Table 4 Overview of bioconcentration and bioaccumulation factors (BCF and BAF) and biota-sediment accumulation factors (BSAF) for PFOS (non-exhaustive review). BCF and BAF are derived from wet weight and not lipid normalized if not otherwise stated.

Species	BCF/BAF/BSAF	Comments	Reference
Bioconcentration Factors (BCF) from laboratory exposures			
Bluegill sunfish (*Lepomis macrochirus*)	86 µg/L Edible: 484 (1124)[a] Non-edible: 1124 (4013) Whole fish: 859 (2796)	Standard test protocol: OECD 305, OPPTS 850.1730 Duration: 62 d uptake 56 d depuration	OECD (2002)
Carp (*Cyprinus carpio*)	2 µg/L: 200-1500 (1300 at end uptake) 20 µg/L: 720	58 d uptake 37 d depuration	Kurume Laboratory 2001 cited in OECD (2002)
Rainbow trout (*Oncorhynchus mykiss*)	0.35 µg/L Carcass: 1 100 (690)[c] Blood: 4 300 (3 100) Liver: 5 400 (2 900)	12 d uptake 33 d depuration Exposure to perfluorinated acids (carboxylates and sulphonates)	OECD (2002)
Biota-Sediment Accumulation Factors (BSAF) from laboratory exposures			
Lumbriculus variegatus	1.22 (spiked sediment); 0.83 and 0.98 (field contaminated sediment)[d]	28 d uptake, then transfer to clean sediment Exposure to several perfluorinated compound at 7-17 µg/kg d.w.; 4 % OC spiked sediment and 0.4 % OC field contaminated sediment	Higgins et al. (2007)
Lumbriculus variegatus	0.49 (average, N= 24)	28 d uptake Field contaminated sediments, <0.149-20.18 µg/kg d.w.; 0.4 to 2.6 % OC	Lasier et al. (2011)
Lumbriculus variegatus *Hexagenia* sp.	0.3-1.1 (N=5) 1.05	28 d uptake Field contaminated sediments, 0.15-4.80 µg/kg d.w.; 2.4-4.8 % OC	Prosser et al. (2016)
Chironomus riparius	0.01 to 0.02	4 d uptake Field contaminated sediments, 0.24-0.29 µg/kg d.w.; 4.3 % OC	Bertin et al. (2014, 2018)
Chironomus plumosus	0.39 (steady-state), 0.38 (kinetic)	10 d uptake Spiked sediments, 100 µg/kg d.w. (nominal) PFOS and 2.18 % OC	Xia et al. (2012)
Gammarus sp.	4.76	21 d uptake Field contaminated sediments, 0.24-0.29 µg/kg d.w.; 4.3 % OC	Bertin et al. (2016)
Bioaccumulation Factors (BAF) from field organisms			
Carp (*Cyprinus carpio*)	6300 – 125 000	Fish collected at firefighting foam spill	Environmental Agency (2004)
Fish	Pinfish: 1 600 Spotted seatrout: 9 800		Houde et al. (2006) cited in Conder et al. (2008)
Invertebrates Fish	Zebra mussel: 590 Amphipods: 830 Crayfish: 920-1 200 Smallmouth bass: 710 Round gobies: 4 700	Great Lakes	Kannan et al. (2005) cited in Conder et al. (2008)

Species	BCF/BAF/BSAF	Comments	Reference
Fish	251 to 50 119 (average 2 512; N=100) 5.0 to 794 BSAF (average 50.1)	Former firefighting training area in Canada	Bhavsar et al. (2016)
Fish	Eel: 1 148, 234.4 (BSAF[e] 9.3, 11.5) Perch: 2 291, 6 310 (BSAF 74.1, 49.0) Pike: 1 549 (BSAF 53.7)	Few weeks and three years after an accidental release of aqueous film forming foam at Schiphol Amsterdam airport	Kwadijk et al. (2014)

[a] Steady-state BCF, robust kinetic BCF calculated at apparent steady-state divided by the mean water concentration in parenthesis.

[b] Uptake duration at 0.87 mg/L was 35 days due to excessive mortality.

[c] Steady-state BCF, accumulation ratios in parenthesis.

[d] Kinetic, wet weight, not lipid normalized, OC-normalized.

[e] Not normalized for lipid and organic matter.

3 Analysis

3.1 Methods for analysis and quantification limit

Different types of chromatographic techniques have being employed for PFAS analysis, such as liquid chromatography (LC) including high performance liquid chromatography (HPLC), ultra-high-performance liquid chromatography/or ultra performance liquid chromatography (UHPLC/UPLC). To enhance selectivity, sensitivity and clean-up of target analysts from the sample background, sample preparation and/or pre-treatment process is typically required including extraction techniques such as solid phase extraction (SPE) and solid–liquid extraction (SLE). Table 5 summarizes different methods reported in the literature for the determination of several PFAS including PFOS in sediments, leading to different limit of detection/quantification (LOD/Q). Further information can be found in the critical reviews recently published by Ami et al. (2020) and HEPA (2020).

For the sensitive and selective detection of PFAS using LC (usually coupled with mass spectrometry (MS) detector, LC/MS), EPA 537, EPA 537.1 and ASTM D7979-17, ASTM D7968-17a have been developed by the United States Environmental Protection Agency (US EPA) and the American Society for Testing and Materials (ASTM), respectively with additional methodological adaptations for specific environmental media (either developed or under development).

Higgins et al. (2005) and Chen et al. (2011) implemented LC-MS/MS with negative electrospray ionisation (-ESI) to detect 12 PFAS including PFOS in sediment in the ranges of 0.04–0.246 µg/kg d.w., for PFOS 0.1 to 0.5 µg/kg d.w. Analytes were extracted by solid–liquid extraction (SLE) in ultra-sonication with methanol: water (9:1) and 0.1 % acetic acid. Extracts were then purified by SPE using C18 sorbent. Recoveries reached more than 80 %.

Bao et al. (2010) implemented HPLC-MS/MS with negative electrospray ionisation (-ESI) for the analysis of eight PFAS including PFOS in river sediments after extraction by tetrabutylammonium hydrogensulfate (TBAHS) and sodium carbonate (Na_2CO_3) (1:5). This method reached LOD of 0.03-0.13 µg/kg d.w. and LOQ of 0.08-0.17 µg/kg d.w. with recoveries of 81 to 108 %. Similar LOD and LOQ are achieved for PFOS with Ultra Performance Liquid Chromatography UPLC/ESI-MS/MS after extraction of dry sediments by ultra-sonication in methanol (Li et al. 2017). This method allowed quantifying PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnA, PFDoA and 8:2 FTUCA in addition to PFOS.

Mazzoni et al. (2016) determined PFAS by liquid chromatography tandem mass spectrometry (HPLC-MS/MS) coupled to an on-line turbulent flow chromatography (TFC) for on-line purification of the extracts after extraction of freeze-dried sediment by sonication with an ACN/H_2O mixture enhanced by salting out and acidification. This method allows quantifying PFHpA, PFHxS, PFOA, PFNA, PFDA, PFUnDA, FOSA, PFDoDA, PFTrDA, PFTeDA in addition to branch PFOS and linear PFOS at LOQ of 0.01, and 0.02 µg/kg d.w. Similar detection limit is reported to PFOS and additional 39 PFAS using UPLC coupled to a triple quadrupole mass spectrometer, with PFOS, PFOA and PFOSA isomers further separated and quantified by UPLC-MS/MS with electrospray ionization in negative LC-MS/MS operation conditions after extraction by ultra sonication with methanol and followed by cartridge purification (Li et al. 2020).

PFAS analysis on sediments have been also recently included in a global interlaboratory assessment carried out in the framework of the Stockholm convention (Fiedler et al. 2020). The interlaboratory coefficient of variation for PFOS was 15 % for linear PFOS anion in a first round testing a marine sediment from the Netherlands with average concentration of 7.99 µg/kg d.w. (N=18), with a percentage of inclusion rate of results excluding outliers of 71 %. In a second round testing a freshwater sediment from the Elbe River, Germany was tested with average concentration of 0.65 µg/kg d.w. (N=16) and inclusion rate of results (excluding outliers) was 63 %. Measurements of branched PFOS resulted in a Coefficient of Variation (CV) of 17 % (average concentration of 0.12 µg/kg d.w.) but only 52 % (N=10) of the measurements were included in the statistical evaluation of the data (i.e. 48 % were considered not valid as being outliers). While CV of 25 % are considered satisfactory, the high percentage of outliers shows difficulties in reporting satisfactory results for PFOS. Overall, the CV is better for sediments than for water samples (Fiedler et al. 2020).

Table 5 Methods for PFOS analysis in sediments and corresponding limits of detection (LOD) and limits of quantification (LOQ) (µg/kg d.w.). -- means not reported. See text for details.

LOD	LOQ	Analytical method	Additional PFAS identified	Reference
0.109	0.246	LC/(-)ESI-MS/MS	PFHxS, PFDS, FOSAA, N-MeFOSAA, N-EtFOSAA, PFOA, PFNA, PFDA, PFUnA, PFDoA, PFTA	Higgins et al. (2005)
0.1	0.5	LC/(-)ESI-MS/MS	PFOA, PFBA, PFPeA, PFHxA, PFHpA, PFNA, PFDA, PFUnA, PFDoA, PFTDA, PFTeDA, PFBS, PFHxS, PFDS	Chen et al. (2011)
0.03-0.13[a]	0.08-0.17[a]	LC/(-)ESI-MS/MS	PFBS, PFHxS, PFOA, PFNA, PFDA, PFDoA, PFTA	Bao et al. (2010)
0.04	0.13	UPLC/ESI-MS/MS	PFHxA, PFHpA, PFOA, PFNA, PFDA, PFUnA, PFDoA and 8:2 FTUCA	Li et al. (2017)
--	0.01-0.02	TFC-HPLC-MS/MS	PFHpA, PFHxS, PFOA, PFNA, PFDA, PFUnDA, FOSA, PFDoDA, PFTrDA, PFTeDA	Mazzoni et al. (2016)
<0.01[b]	--	UPLC-MS/MS	PFBA, PFPeA, PFHxA, PFHpA, *n*-PFOA, *iso*-PFOA, 4*m*-PFOA, 5*m*-PFOA, PFNA, PFDA, PFUnA, PFDoA, PFTrA, PFTeA, PFBS, PFHxS, *n*-PFOS, *iso*-PFOS, 1*m*-PFOS, 3+5*m*-PFOS, 4*m*-PFOS, PFDS, PFOSA, iso-PFOSA, 1*m*-PFOSA, 2*m*-PFOSA, 3*m*-PFOSA, 4*m*-PFOSA, 5*m*-PFOSA, 4:2 FTS, 6:2 FTS, 8:2 FTS, 6:2 Cl-PFESA, 8:2 Cl-PFESA, HFPO-DA, HFPO-TA, ADONA, PFECHS, 6:2 diPAP	Li et al. (2020)

[a] LOD and LOQ for the individual compounds not included.

[b] Method detection limit, depending on the PFOS isomer and matrix (sediment or suspended matter).

3.2 Environmental concentrations

Measured environmental concentrations (MEC) of PFOS in sediments are summarized in Table 6. Measured concentrations in sediments from Swiss small streams range from 0.02 (limit of quantification) to 2.34 µg/kg d.w. in sediments sieved at 2 mm, while the concentrations range from 0.252 to 20.1 µg/kg d.w. when the fraction for analysis is < 63 µm. A sampling campaign in Austria at Lake Constance and the Danube reported maximum concentrations of ca. 1 µg/kg d.w. in sediment <63 µm. While PFOS concentrations were not directly related to anthropogenic pressures in Lake Constance, higher concentrations in the upstream region of the Danube were related to industrial activities. At remote Alpine lakes, where wet deposition is the major source, PFOS was not detected while other PFAS were detected and quantified at higher concentrations than PFOS (Clara et al. 2009).

A monitoring campaign performed at 18 sites across Canada also found maximum concentrations in the urbanized Lake Ontario (geomean = 10 µg/kg d.w.) but relatively low concentrations in open waters of the Great Lakes. However, similarly low concentrations were reported in other heavily developed lakes such as Lake Eire and in harbour areas, therefore PFOS levels were not always associated with human population (Environment Canada 2013).

A nationwide campaign carried out in 2012 in France detected PFOS (linear) in 74 % of the water bodies studied including rivers and lakes (N=128), with maximum concentration of 17 µg/kg d.w. in sediments < 2 mm (Munoz et al. 2015). A recent study performed in Australia (Saldiña et al. 2019) detected the highest concentrations of PFOS in residential and industrial areas at concentrations up to 4 µg/kg d.w. (no information on grain size thus concentrations are assumed to be for bulk sediment). The high detection limit decreases relevance of detection frequency in the Saldiña et al. (2019) study. Maximum concentrations of PFOS (up to 64 µg/kg d.w.) have been reported in sediments close to firefighting training areas in Sweden, the Netherlands and Canada (Mussabek et al. 2019). Maximum concentrations in the range of few µg/kg d.w. have been also reported in freshwater sediments from Malta (Sammut et al. 2019), in sediments over the watershed of the river Ebro and Guadalquivir in Spain (Lorenzo et al. 2016) and river and lake sediments from South Korea (Lee et al. 2020).

Table 6 Measured environmental concentrations (MEC) of PFOS in Switzerland and elsewhere. All concentrations expressed as µg/kg d.w. for sediment if not indicated. n.d. not detected and not reported.

Country	MEC (min-max)	No. of sites	Comments	Reference
Switzerland	Sediment < 2 mm: 0.417 (mean) (<0.02-2.34) Sediments < 63 µm: 1.801 (mean) (0.252-20.2)	18	Small streams sampled in August 2018. Different levels and sources of pollution. Detection frequency ca. 100 %	Centre Ecotox, unpubl. data
	Lake Geneva: mean 1.95 (0.64-2.98)	5	Whole sediment	Loizeau et al. (2017)
Austria	Lake Constance: n.d.-<0.94	5	Sediments < 63 µm Sediments from shallow waters and harbour areas, no direct relationship of MECs with anthropogenic activities	Clara et al. (2009)
	Remote Alpin Lakes: n.d.	6	Sediments < 63 µm	

Country	MEC (min-max)	No. of sites	Comments	Reference
			MECs for other PFAS higher than PFOS, wet deposition	
	Danube: n.d.-0.91	8	Sediments < 63 µm Bank sediments from upstream industrial areas and downstream with more population density	
France	Linear: < 0.01-17 Brached: < 0.04-2.7	129	Sediments < 2 mm. Nationwide sampling campaign in 2012. Detection frequency: 74 % linear and 41 % branch	Munoz et al. (2015)
Malta	< 0.04-5.91	24	Sediments sampled in 2015 from valleys used for water collection, different types of water bodies. Detection frequency: 95 %	Sammut et al. (2019)
Australia	<2-4	25	Detected in residential and industrial areas. Low detection frequency due to high method detection limits	Saldiña et al. (2019)
Spain	Mean: 0.3 (0.01-2.0)	22	Large rivers (Guadalquivir, Ebro). Detection frequency 59 %	Lorenzo et al. (2016)
South Korea	0.04-4.4	47	Lake sediments collected in 2017 and 2018. Detection frequency 100 %. Influence of seawater due to water level regulation, salinity positively correlated with sediment concentrations	Lee et al. (2020)
Canada	Lake Ontario: 10 (geomean; max among sites) Lake Ontario Harbours: 1.9 (max) Open waters of Great Lakes: 0.89, 2.2 and 1.4	65	Lake sediments sampled in 2008 at 18 sites	Environment Canada (2013)
Sweden	<0.5-64	2	Sediments from canal and pond close to firefighting training area	Mussabek et al. (2019)

4 Effect data (spiked sediment toxicity tests)

A non-filtered bibliographic search was performed for Perfluorooctanesulfonic acid in the US EPA Ecotoxicity Data Base (U.S. EPA 2020) which did not yield data on sediment organisms. A key word search was performed on Web of Science and PubMed (Perfluorooctanesulfonic acid OR PFOS OR Perfluorooctane sulfonate) AND (sediment OR benthic OR benthos, no restriction regarding publication date) which resulted in 471 publications, with duplicates removed. Of the 471 publications, 11 were identified as potentially relevant based on an initial screen of abstracts. An additional search was also performed on Web of Science and PubMed (Perfluorooctanesulfonic acid OR PFOS OR Perfluorooctane sulfonate) AND (mesocosm OR microcosm, no restriction regarding publication date) which resulted in 35 publications, with duplicates removed. Of the 35 publications, three were identified as potentially relevant based on an initial screen of abstracts.

Table 7 Sediment effect data collection for PFOS in mg/kg d.w. Data were evaluated for relevance and reliability according to the CRED criteria for sediments (Casado-Martinez et al. 2017). Data assessed as not relevant or not reliable is in grey font.

Group	**Species**	**Test compound**	**Exposure**	**Equilibration time**	**Endpoint**	**Test duration**	**Effect concentration**	**Value [mg/kg d.w.]**	**Sediment type**	**Normalized value [mg/kg d.w., 1 % OC]**	**Normalized value [mg/kg d.w., 5 % OC]**	**Chem. analysis**	**Note**	**Validity**	**References**
Acute toxicity data in freshwater															
No data available															
Acute toxicity data in marine water															
No data available															
Chronic toxicity data in freshwater															
Amphibian	*Rana pipiens* tadpoles[a]	PFOS (> 96 % purity)	Static (outdoor mesocosm)	15 d	Dopamine in brain	30 d	NOEC	0.06735	Field Sediment OM = 5.7% 34% sand ; 52% silt ; 14% clay	0.0204	0.1020	Measured	Average measured concentration OC = OM/1.72 = 3.3%	R3/C3	Foguth et al. (2019)
					Dopamine turnover			0.5975		0.181	0.905			R3/C3	
					DOPAC, HVA, NE, 5-HT, 5-HIAA, 5-HT turnover[b]			>0.5975		> 0.181	> 0.905			R3/C3	
Amphibian	*Rana pipiens* tadpoles[a]	PFOS (> 96 % purity)	Static (outdoor mesocosm)	15 d	Survival	30 d	NOEC	>0.5975	Field Sediment OM = 5.7% 34% sand; 52% silt; 14% clay	> 0.181	> 0.905	Measured	Average measured concentration OC = OM/1.72 = 3.3%	R3/C2	Wesley Flynn et al. (2020)
					Larval Development			<0.00691		< 0.0021	< 0.011			R3/C2	
					Snout–vent length			>0.5975		> 0.181	> 0.905			R3/C2	
					Body mass			>0.5975		> 0.181	> 0.905			R3/C2	
Chronic toxicity data in marine water															
Amphipod	*Monoporeia affinis*[c]	PFOS	Semi-static	1 d	Survival	22 d	NOEC	1.3	Field Sediment Grain size: Sand 0.5%, Silt 30%, Clay 70%. OM: 8.2%	0.27	1.35	Measured	Measured concentration at end of exposure. PFOS spiked to water. OC = OM/1.72 = 4.8%	R2/C2	Jacobson et al. (2010)
					Body mass			>4.2		>0.875	>4.375			R2/C2	
					Male sexual maturation			1.3		0.27	1.35			R2/C2	
Amphipod	*Monoporeia affinis*[c]	PFOS	Semi-static	1 d	Survival	5 weeks	NOEC	< 1.35	Field Sediment Sand 0.8%, Silt 31%, Clay 68% OM: 7.6%	<0.306	<1.534	Measured	Measured concentration. PFOS spiked to water. OC = OM/1.72 = 4.4%	R2/C2	Jacobson et al. (2010)

[a] From field collected egg mass, uncontaminated area. [b] DOPAC: 3,4-dihydroxyphenylacetic acid, HVA: homovanillic acid, NE: norepinephrine, 5-HT: serotonin, 5-HIAA: 5-hydroxyindoleacetic acid. [c] Field collected individuals, uncontaminated area with measured levels of PFOS.

4.1 Graphic representation of effect data

As there are only two reliable and relevant studies in the sediment dataset for PFOS, no graphical representation of the data has been generated.

4.2 Comparison between marine and freshwater species

There is only one reliable and relevant freshwater study, and one reliable and relevant marine study in the sediment database for PFOS.

4.3 Overview of reliable and relevant long-term studies

According to the EC EQS TGD (EC (2018) p. 25): "*All available data for any taxonomic group or species should be considered, provided the data meet quality requirements for relevance and reliability*".

The chronic effect data for the marine amphipod *Monoporeia affinis* (survival), has been evaluated as R2/C2 based on the available information in the published paper Jacobson et al. (2010). It is classified as reliable with restrictions according to the presence of PFOS concentrations in sediments from the field where the individuals were collected and relevant with restrictions because PFOS was spiked to waters instead of sediments, although sediment concentrations were measured and reported and therefore effect concentrations could be expressed as sediment concentration at the end of exposure.

Chronic freshwater effect data (development) are available for tadpoles of the Leopard Frog, *Rana pipiens* from Wesley Flynn et al. (2020) and the companion paper by Foguth et al. (2019). This study is assessed as not reliable due to a number of limitations, but mainly due to the large variability in water quality parameters in particular temperature. It is recognized that tadpoles were exposed to PFOS via spiked sediment in outdoor mesocosms this large variability reflects natural conditions, but it also may have had a critical impact on the observed toxic effects. A further limitation of this study is that only three concentrations were tested and significant developmental effects were observed at the lowest PFOS exposure concentration (measured as 6.91 µg/kg d.w.), similar to the observed effects at the two other concentrations tested concentrations. The LOEC and NOEC for this study are therefore 6.91 and < 6.91 µg/kg, respectively and are retained as supportive information.

Tadpoles are not generally considered to be benthic organisms, and indeed the WFD EQS TGD (EC 2018) highlights that only data from studies with benthic invertebrates and rooted macrophytes should be applied to derive sediment EQS. Nevertheless, the tadpoles of many frog species live and feed at the sediment surface and may be exposed to substances bound to, or released from, sediments. In this sense, the effect data are considered relevant for sediment EQS derivation.

5 Derivation of QS_{sed}

According to the EC TGD for EQS, sediment toxicity tests, aquatic toxicity tests in conjunction with equilibrium partitioning (EqP) and field/mesocosm studies are used as several lines of evidence to derive QS_{sed} (EC 2018). Thus, in the following, the appropriateness of the deterministic approach (AF-Method), the probabilistic approach (SSD method) and the EqP approach were examined.

5.1 Derivation of $QS_{sed, AF}$ using the Assessment Factor (AF) method

The derivation of $QS_{sed, AF}$ is determined using assessment factors (AFs) applied to the lowest credible datum from long-term toxicity tests.

Reliable long-term effect data are available for PFOS for one species, with additional supportive information for another species. The lowest NOEC is 1.3 mg/kg d.w. (Table 7 and Table 8) for *Monoporeia affinis* survival.

Table 8 Most sensitive relevant and reliable chronic data summarized from Table 7.

Species	**Exposure duration [d]**	**Endpoint**	**NOEC/EC_{10} [µg/kg d.w.]**	**OC [%]**
Monoporeia affinis	22 d	Survival	1300	4.8

In case of long term tests (NOEC or EC_{10}) being available for one species, the TGD recommends the application of an assessment factor of 100 on the critical datum (Table 11 in EC (2018)). This results in a $QS_{sed,AF}$ = 13 µg/kg, which corresponds to a lowest value of 13.5 µg/kg d.w. for a sediment with 5 % OC, or 2.7 µg/kg d.w. for a sediment with 1 % OC representing a worst case scenario in Switzerland.

5.2 Derivation of $QS_{sed,SSD}$ using the species sensitivity distribution (SSD) method

The minimum data requirements recommended for the application of the SSD approach for EQS water derivation is preferably more than 15, but at least 10 NOECs/EC_{10}s, from different species covering at least eight taxonomic groups (EC (2018), p. 43). In this case, not enough data from spiked sediment toxicity tests are available for applying the SSD approach.

6 Derivation of $QS_{sed,EqP}$ using the Equilibrium Partitioning approach

If no reliable sediment toxicity data are available, the Equilibrium Partitioning (EqP) can be used to estimate the $EQS_{sed,EqP}$. The applicability of the EqP, which was developed for non-ionic substances, was assessed in the context of PNEC derivation for soil and sediment by OECD (2002) because there was at the time no effect data from soil or sediment toxicity tests. OECD (2002) concluded that, on the basis of the available data for PFOS at the time of the assessment, the equilibrium partitioning theory could not be applied because:

- the nature of the adsorption process could not be assumed to be linearly dependent upon concentration;
- the adsorption was likely to be highly dependent upon soil/sediment composition and particularly the inorganic component; and
- the rate at which equilibrium might be achieved was unknown.

However, it was also noted that available scientific literature on the environmental fate and behavior properties of substances with similar chemistry and properties to PFOS relevant to the consideration of EqP as a suitable model for PFOS environmental fate did not preclude the possibility of applying equilibrium partitioning to PFOS but did highlight the technical difficulties that might be encountered.

The EqP is therefore used here for comparison purposes given the small data base of sediment toxicity studies (Conder et al. 2020). Uncertainties in the use of this approach are further discussed below.

6.1 Selection of QS for water

Several environmental risk limits and quality standards are available for PFOS in water (section 1.2). For the derivation of the $EQS_{sed,EqP}$, a PNEC for the aquatic freshwater environment derived with a methodology similar to the procedure described in the TGD for deriving the AA-EQS for freshwater (e.g. with regard to the AF) should be used. With this premise, the AA-EQS of 0.23 µg/L (EC 2011 and Moermond et al. 2010) is used to protect from pelagic organisms.

A $QS_{secpois.freshwater}$ of 0.002 µg/L is used to derive a $QS_{sed,EqP}$ to protect top predators from secondary poisoning, for harmonization within environmental compartments at the national level (Ecotox Centre 2011).

6.2 Selection of partition coefficient

One of the main factors influencing the application of the EqP model is the choice of the partition coefficient. It is stipulated in the ECHA 2017 guideline (p. 143, ECHA (2017)) that "To increase the reliability of PNEC sediment screen derived using the EqP, it is imperative that a conservative but realistic partitioning coefficient (e.g. K_d, K_{OC}, K_{OW}) is chosen. A clear justification must be given for the chosen coefficient and any uncertainty should be described in a transparent way." The EC EQS TGD requires deriving a geometric mean of all available K_{OC} values including one derived from a log K_{OW} value (EC 2018).

Although for non-ionic substances the distribution between water and sediment is estimated through the K_{OC}, assuming that only the organic components of sediments are important in establishing equilibrium between water and sediment, for anionic surfactants such as PFOS the use of K_d values may be more appropriate because organic carbon alone does not explain sorption to sediments (even if K_d values are significantly correlated with OC, see section 2.2). This is similar to the recommendtions for applying the EqP for metals, in which measured K_d values for sediment/suspended solids can be used, with preference to values derived from field measurements.

K_d values for PFOS are available for 17 freshwater sediments and one suspended matter from 11 studies (Appendix I), giving an average (geometric mean) K_d value of 136 L/ kg (log K_d 2.13).

In addition, 62 values for K_{OC} from 16 studies (Appendix II) covering freshwater sediments, suspended matter and soil are available. Taking forward only the 47 values for freshwater sediment/suspended matter, an average (geometric mean) K_{OC} of 3 549 (log K_{OC} 3.55) is derived.

The equivalent K_{OC} values calculated from empirical K_d values are relatively consistent with the K_{OC} values reported for empirical partitioning studies. Using the relationship between K_d and the organic carbon content of the sediments from the partition coefficient studies ($\log K_d = 0.2071\ \%\ OC + 0.9393$; $r^2 = 0.62$; N=8) results in a K_d value of 14.0 L/kg being predicted for a sediment with 1 % organic carbon ($\log K_d = 1.15$), and a value of 94.4 L/kg for a sediment with 5 % organic carbon ($\log K_d = 1.97$). These K_d values are broadly consistent with those calculated from the average (geomean of empirical) K_{OC} value above of 3 549, which would be translated in a Kp_{sed} of 35.5 L/kg for 1% OC and 177.5 L/Kg for 5 % OC. The average (geomean) of empirical K_{OC} values are therefore used for EQS sediment derivation separately to enable a comparison against the K_d values.

6.3 Selection of OC content for a reference sediment

To account for the influence of OC content on $QS_{sed,EqP}$ development, calculations have been performed for a standard sediment according to the EU TGD with 5 % OC (EC 2018). As 5 % OC might not be representative for sediment in Switzerland, calculation was made as well for a worst-case scenario considering measurement on total sediment with 1 % OC (approx. 10th percentile of OC content in Swiss Rivers).

6.4 Derivation of $QS_{sed,EqP}$

The Equilibrium Partitioning was used to derive a sediment $QS_{sed,EqP}$ as proposed in the EU TGD (EC 2018), using the average (geomean) empirical K_d. $QS_{sed,EqP}$ are also derived using K_d values estimated for 1 % OC and 5 % OC from the empirical relationship of available K_d-OC data pairs (see §6.2 and Appendix I). Calculated $QS_{sed,EqP}$ from empirical K_{OC} values (Appendix II) following the Di Toro et al. (1991) approach for 1 % and 5 % OC content are provided in Appendix III for comparison purposes.

An additional AF of 10 should be applied to the resulting $QS_{sed,EqP}$ for substances with log K_{OW} >5 to account for exposure through food. An equivalent K_{OC} value has been derived for PFOS from the results of multiple empirical partitioning studies, and this value could be used to estimate an equivalent log K_{OW} value that would be typical of a non-ionisable organic substance that exhibited the same degree of partitioning to sediment based on the QSAR for non-hydrophobics. Following this approach an equivalent log K_{OW} value of 4.86 would be calculated for PFOS, as this is below the cut-off of a log K_{OW} value of 5 indicated by the guidance the additional assessment factor is not warranted as the level of partitioning is lower than that of a substance that would just meet the criteria.

Direct toxicity ($QS_{sed,EqP}$):

The $QS_{sed,EqP}$ calculated using the $K_{sed\text{-}water}$ value calculated from geomean K_d from 17 sediment studies is 31.6 µg/kg d.w. The calculated $QS_{sed,EqP}$ from estimated K_d values for 1 % organic carbon and 5 % organic carbon are 3.6 and 22.1 µg/kg d.w.

These $QS_{sed,EqP}$ are in line with the QS_{sed} available from INERIS (2018) of 67 µg/kg d.w. (5 % TOC) and from Norway of 2.3 µg/kg d.w. (1 % TOC, should be recalculated for site-specific TOC content; Breedveld et al. 2018). The $QS_{sed,EqP}$ derived using the average (geomean) of empirical K_{OC} values are higher but within a factor two than those obtained from K_d values estimated for 1 % and 5 % TOC.

For protecting against secondary poisoning ($QS_{sed,EqP,sec.pois.}$):

The $QS_{sed,EqP,sec.pois.}$ calculated using the $K_{sed\text{-}water}$ value calculated from geomean K_d from 17 sediment studies is 0.275 µg/kg d.w. The calculated $QS_{sed,EqP}$ from estimated K_d values for 1 % organic carbon and 5 % organic carbon are 0.031 and 0.192 µg/kg d.w.

Table 9 Derived $QS_{sed,EqP}$ for a geomean K_d based on Appendix I and the AA-EQS of 0.23 µg/L for toxicity to pelagic organisms (EC 2011s and Moermond et al. 2010) and $QS_{se.cpois.freshwater}$ of 0.002 µg/L for protection of top predators from secondary poisoning (Ecotox Centre 2011). The $QS_{sed,EqP}$ derived from the partition coefficient solid-water sediment (Kp_{sed}) estimated for a sediment with 5 % OC (standard EC TGD sediment) and 1 % TOC (worst case scenario in Switzerland) using the relationship between OC and K_d values in Appendix I are provided for comparison purposes.

	Kp_{sed} [l/kg]	$K_{sed\text{-}water}$ [m^3/m^3]	$PNEC_{water}$ [µg/L]	$QS_{sed,EqP}$ [µg/kg w.w.]	$QS_{sed,EqP}$ [µg/kg d.w.]	Included AF
			Toxicity to pelagic organisms			
Geomean K_d	136	68.8	0.23	12.17	**31.6**	-
1 % OC	14.0	7.8	0.23	1.38	**3.59**	-
5 % OC	94.4	48.0	0.23	8.49	**22.1**	-
			Secondary poisoning			
Geomean K_d	136	68.8	0.002	0.106	**0.275**	-
1 % OC	14.0	7.8	0.002	0.012	**0.031**	-
5 % OC	94.4	48.0	0.002	0.074	**0.192**	-

7 Derivation of QS_{sed} according to mesocosm/field data

No field or mesocosm studies that provide effect concentrations of PFOS in sediment are available, thus, no QS_{sed} based on field data or mesocosm data has been derived.

8 Derivation of $QS_{sed.sec.pois.}$ using BSAF and TMF

Because PFOS tend to bioaccumulate and biomagnify, the protection of sediment-dwelling organisms may not be the key objective for sediment quality assessment and EQS_{sed} may be useful for sediment management and monitoring purposes (EC 2018). For substances meeting the requirements for sediment assessment, QS_{sed} can be derived from QS_{biota} to protect top predators from secondary poisoning ($QS_{sed,sec.pois.}$).

The $QS_{sed,sec.pois.}$ to protect top predators from secondary poisoning through sediment trophic webs were derived following Babut (2018) using BSAF and TMF as:

$$QS_{sed,sec.pois.} = \frac{QS_{inv}}{BSAF}$$

Where:

BSAF: biota-sediment accumulation factor

QS_{inv}: concentration in invertebrate transposed from the QS_{biota} for PFOS as:

$$QS_{inv} = \frac{QS_{biota}}{TMF^{y-2}}$$

Where:

QS_{biota}: quality standard for protecting top predators from secondary poisoning from fish consumption expressed in biota (= 33 µg/kg w.w., EC 2011)

TMF: trophic magnification factor

y: trophic level for fish for the derivation of QS (= 4, EC 2018)

BSAFs and TMFs for PFOS were those used in Babut (2018) and were not further assessed for reliability and relevance due to time constraints. The BSAF database from Babut (2018) contained 11 entries for 5 different species representing 4 different taxons. A single BSAF was retained by taxon. If more than one BSAF was available for a taxon, the 75th percentile was calculated and retained. The BSAF value used in $QS_{sed,sec.pois}$ derivation was 1.98. This value was considered quite uncertain due to the relatively small database available compared to other substances such as PCBs. The TMF database retained for $QS_{sed,sec.pois}$ contained 17 entries for freshwater and one for an estuarine trophic chain. Only those from temperate environments were considered relevant. The TMF value used in $QS_{sed,sec.pois}$ derivation was 3.0 (2.1– 3.3), calculated as the geometric mean of the available TMFs.

The obtained $QS_{sed,sec\text{-}pois.}$ is 1.85 µg/kg.d.w.

9 Toxicity of degradation products

Detailed information on PFOS degradation products was not available for review.

10 Proposed EQS_{sed}

The different QS_{sed} values for protecting benthic species for each derivation method included in the EC EQS TGD 2018 are summarized in Table 10. According to the TGD, the most reliable extrapolation method for each substance should be used (EC 2018). In all cases, data from spiked sediment toxicity tests are preferred over the EqP approach. A tentative EQS_{sed} of 2.7 µg/kg (1 % OC) for PFOS including the application of an AF of 100 is proposed.

Table 10 QS_{sed} derived for protecting benthic organisms from direct toxicity according to the three methodologies stipulated in the EU-TGD and their corresponding AF. All concentrations expressed as µg/kg d.w.

	Sediment 1 % TOC	Sediment 5 % TOC	AF
$QS_{sed,SSD}$	-	-	-
$QS_{sed,EqP}$	3.6	22.1	-
$QS_{sed,AF}$	2.7	13.5	100
Proposed EQS_{sed}	2.7	13.5	100

The different $QS_{sed,sec.pois.}$ values to protect top predators from secondary poisoning obtained from the different approaches are summarized in Table 11. While there is no recommendation in the EU TGD (EC 2018) on the use of the EqP to back-calculate a $QS_{sed,sec.pois.}$ from the $QS_{fw,sec.pois.}$ it is assumed that the resulting QSsed,EqP,sec.pois. is subject to even higher level of uncertainty than the $QS_{sed,EqP}$ to protect from direct toxicity due to the additional back-calculation step. A $QS_{sed,sec.pois.}$ of 1.85 µg/kg d.w. is therefore proposed for this alternative protection objective.

Table 11 QS_{sed} derived for protecting top predators from secondary poisoning. All concentrations expressed as µg/kg d.w.

	Sediment 1 % TOC	Sediment 5 % TOC	AF
$QS_{sed,EqP,sec.pois.}$	0.031	0.192	-
$QS_{sed,sec.pois.}$	1.85		-

10.1 Uncertainty analysis

The EQS_{sed} for protecting benthic organisms is considered preliminary given the conservative AF of 100 applied because of the small number of available effect data. It is important to highlight the tentative label of the EQS_{sed} due to the reliability of the effect database available from spiked sediment toxicity tests.

Uncertainties remain regarding the sensitivity of tadpoles to PFOS in sediments. The study from Wesley Flynn et al. (2020) and the companion paper by Foguth et al. (2019) indicates that tadpoles may be highly sensitive to PFOS in sediments, in particular compared to the effect data available from water-only exposures. Ankley et al. (2004) reported a rough NOEC of 1 mg/L for development of *R. pipiens* in a 60-d study with spiked waters (reported as a MATC of 1732 µg/L in Environment Canada 2017). The relative sensitivities of different taxonomic groups according to the datasets compiled elsewhere for the derivation of EQS for PFOS in surface waters (Moermond et al. 2010, EC 2011 and Environment Canada 2017) indicate that aquatic insects (*E. cyathigerum, C. tentans*) are among the organisms that are most sensitive to chronic PFOS exposure in water-only exposures and considerably more sensitive than *R. pipiens* (based on the study of Ankley et al. 2004). However, the study from Ankley et al. (2004) also had severe limitations, with increased unexplained mortality after 6 weeks in all concentrations including the controls, invalidating the study for quality standards derivation as stated by the own authors. It is also possible that, as argued by Wesley Flynn et al. (2020), the high sensitivity of tadpoles in their study was due to the important contribution of sediment as exposure route to PFOS.

The $QS_{sed,EqP}$ to protect pelagic organisms from general toxicity of 22.1 µg/kg d.w. (5 % TOC) or 3.6 µg/kg d.w. (1 % TOC) should protect insects, the most sensitive group of organisms, and is within the same order of magnitude and in good agreement with the proposed EQS_{sed} based on spiked sediment toxicity tests. There is some remaining uncertainty related to the sensitivity of tadpoles exposed to PFOS in sediments, as the unbounded NOEC (LOEC) is one order of magnitude below the proposed EQS_{sed}. It is therefore highly recommended to address this remaining uncertainty in future studies. Because both the $QS_{sed,AF}$ derived from small toxicity test datasets and the $QS_{sed,EqP}$ entail a high level of uncertainty, in a risk assessment scenario potential risks to benthic invertebrates as identified by comparison with the EQS_{sed} should trigger further sediment toxicity testing (EC 2018).

Based on the evidence of bioaccumulation potential of PFOS and the toxicity to mammals, a $QS_{fw,sec.pois.freshwater}$ of 0.002 µg/L is proposed, which can be further transposed into a $QS_{sed,EqP}$ of 0.031 µg/kg d.w. for 1 % TOC and 0.192 µg/kg d.w. for 5 % TOC. The use of the BSAF-TMF approach results in a $QS_{sed,sec.pois.}$ of 1.85 µg/kg d.w. from the biota $QS_{biota,sec.pois.,fw}$ to protect wildlife from secondary poisoning of 33 µg/kg w.w. (EC 2011a). The EU TGD (2018) highlights the fact that BSAF are highly variable, so its used is more appropriate for local or regional scales. It is noted that the number of BSAF and TMF for PFOS is still relatively small compared to other biomagnifying substances such as PCBs, but we highlight also that it is still more extensive than the effect database for benthic communities. The $QS_{sed,sec.pois.}$ of 1.85 µg/kg d.w. can be used for this alternative protection objective.

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Appendix I. K_d values for PFOS available in the literature

Type		log Kd	Kd (L/kg)	Reference/Source
Batch equilibrium study, freshwater sediment OC 2.48% pH 7.0 clay 53%	exp.	1.43	26.9	Higgins & Luthy (2006)
Batch equilibrium study, freshwater sediment OC 1.02% pH 7.5 clay 26%	exp.	0.78	6.0	Higgins & Luthy (2006)
Batch equilibrium study, freshwater sediment OC 4.34% pH 7.6 clay 31%	exp.	1.29	19.5	Higgins & Luthy (2006)
Batch equilibrium study, freshwater sediment OC 9.66% pH 5.7 clay 5%	exp.	2.35	223.9	Higgins & Luthy (2006)
Batch equilibrium study, freshwater sediment OC 2.52% pH 7.6 clay 35%	exp.	1.66	45.7	Chen et al. (2016)
Field study, average N=18, freshwater sediments OC 1.59-7.47%, clay 13-84%, pH 6.0-7.4	exp.	2.16	134.9	Chen et al. (2019)
Field study, average N=84, freshwater suspended matter pH (surface water) 6.7-9.3	exp.	3.88	134.9	Chen et al. (2019)
Field study, average N=47, freshwater sediment, estimated from Fig. 5	exp.	2.6	398.1	Lee et al. (2020)
Field study, freshwater sediment	exp.	2.15	141.3	Mussabek et al. (2019)
Field study, freshwater sediment OC 6.4%, Clay 1.33%, pH 8.75	exp.	2.88	760.0	Pan and You (2010)
Field study, freshwater sediment OC 7.31%, Clay 5.17%, pH 8.47	exp.	2.70	506.6	Pan and You (2010)
Field study, N=129, freshwater sediment (Br-PFOS)	exp.	1.90	79	Munoz et al. (2015)
Field study, N=129, freshwater sediment (L-PFOS)	exp.	2.30	200	Munoz et al. (2015)
Field study, freshwater sediment OC 4.8% (N=3)	exp.	2.40	251	Labadie and Chevreuil (2011)
Field study, average N=19, freshwater sediment	exp.	2.35	224	Kwadick et al. (2010)
Field study, average N=5, freshwater sediment	exp.	1.30	20	Campo et al. (2015)
Field study, average N=12, freshwater sediment OC 1.74-6.38%	exp.	2.15	141	Pico et al. (2012)
		2.13	**136**	**Geometric mean**

Appendix II. K_{OC} values for PFOS available in the literature

TOC, type		**log K_{OC}**	**K_{OC} (L/kg)**	**Reference/Source**
OECD 106, river sediment OC 1.3% clay 19% pH 7.7	exp.	4.76	57100	OECD (2002)
Batch equilibrium studies, slope Kd vs OC (n=4), freshwater sediments OC 1.02-9.66%, pH 5.7-7.6, clay 5-53%	exp.	2.68	475	Higgins and Luthy (2006)
Batch equilibrium studies, freshwater sediments OC 4.15%, size < 65µm 91.8%	exp.	2.97	933.3	Zhao et al. (2012)
Batch equilibrium studies, freshwater sediments OC 2.41%, size < 65µm 96.0%	exp.	2.68	478.6	Zhao et al. (2012)
Batch equilibrium study, freshwater sediment OC 2.52% pH 7.6 clay 35%	exp.	3.26	1819.7	Chen et al. (2016)
Field study, average N=18, freshwater sediments OC 1.59-7.47%, clay 13-84%, pH 6.0-7.4	exp.	3.46	2884.0	Chen et al. (2019)
Field study, average N=47, freshwater sediment	exp.	3.88	7585.8	Lee et al. (2020)
Field study, average N=21, freshwater sediment	exp.	3.75	5623	Li et al. (2020)
Field study, average N=15, freshwater sediment	exp.	2.82	661	Liu et al. (2019)
Field study, freshwater sediment	exp.	2.28	191	Mussabek et al. (2019)
Field study, freshwater sediment OC 6.4%, Clay 1.33%, pH 8.75	exp.	4.07	11801.0	Pan and You (2010)
Field study, freshwater sediment OC 7.31%, Clay 5.17%, pH 8.47	exp.	3.84	6930.0	Pan and You (2010)
Field study, N=129, freshwater sediment (Br-PFOS)	exp.	3.00	1000	Munoz et al. (2015)
Field study, N=129, freshwater sediment (L-PFOS)	exp.	3.40	2512	Munoz et al. (2015)
Field study, freshwater sediment OC 4.8% (N=3)	exp.	3.70	5012	Labadie and Chevreuil (2011)
Field study, average N=19, freshwater sediment	exp.	3.16	1445	Kwadick et al. (2010)
Field study, average N=12, freshwater sediment OC 1.74-6.38%	exp.	3.58	3802	Pico et al. (2012)
Field study, average N=5, freshwater sediment	exp.	3.26	1820	Campo et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.12	1318	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.01	1023	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.66	4571	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.37	2344	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.35	2239	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.34	2188	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	2.96	912	Chen et al. (2015)

TOC, type		**log K_{OC}**	**K_{OC} (L/kg)**	**Reference/Source**
Field study, sediment from Tihu Lake, China	exp.	3.14	1380	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.85	7079	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.71	5129	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	2.97	933	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.63	4266	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.93	8511	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	4.61	40738	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.57	3715	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.71	5129	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	4.07	11749	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.53	3388	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.76	5754	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	4.4	25119	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.99	9772	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.93	8511	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.51	3236	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.89	7762	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.56	3631	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.67	4677	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.41	2570	Chen et al. (2015)
Field study, sediment from Tihu Lake, China	exp.	3.62	4169	Chen et al. (2015)
Field study, average N=18, freshwater suspended matter	exp.	5.04	109648	Li et al. (2020)
Batch equilibrium study, soil OC 3.4%, clay 24.7%, pH 7.55	exp.	2.67	473	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 3.4%, clay 24.7%, pH 7.55	exp.	2.55	358.8	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 3.4%, clay 24.7%, pH 7.55	exp.	2.43	272.2	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 1.7%, clay 31.3%, pH 8.21	exp.	2.97	932	Mejia-Avendano et al. (2020)

TOC, type		log K_{OC}	K_{OC} (L/kg)	Reference/Source
Batch equilibrium study, soil OC 1.7%, clay 31.3%, pH 8.21	exp.	2.70	500.5	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 1.7%, clay 31.3%, pH 8.21	exp.	2.43	268.8	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 2.9%, clay 30.0%, pH 6.57	exp.	2.74	549	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 2.9%, clay 30.0%, pH 6.57	exp.	2.63	425.9	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 2.9%, clay 30.0%, pH 6.57	exp.	2.52	330.9	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 7.3%, clay 12.6%, pH 4.80	exp.	2.88	760.9	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 7.3%, clay 12.6%, pH 4.80	exp.	2.96	915	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 7.3%, clay 12.6%, pH 4.80	exp.	3.04	1100	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 1.8%, clay 8.6%, pH 5.15	exp.	2.73	537	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 1.8%, clay 8.6%, pH 5.15	exp.	2.72	525	Mejia-Avendano et al. (2020)
Batch equilibrium study, soil OC 1.8%, clay 8.6%, pH 5.15	exp.	2.71	513	Mejia-Avendano et al. (2020)
K_{OC} values for soil are in grey font and are not used in EQS derivation.		**3.55**	**3549**	**Geomean**

Appendix III. Derivation of $QS_{sed,EqP}$ using the Equilibrium Partitioning and empirical K_{OC} values

Derived $QS_{sed,EqP}$ for a geomean K_{OC} based on Appendix II and the $QS_{freshwater}$ as AA-EQS of 0.23 µg/L for toxicity to pelagic organisms (EC 2011 and Moermond et al. 2010) and $QS_{secpois.freshwater}$ of 0.002 µg/L for protection of top predators from secondary poisoning (Ecotox Centre 2011). The $QS_{sed,EqP}$ are derived for a sediment with 5% OC (standard EC TGD sediment) and 1% TOC (worst case scenario in Switzerland).

	K_{OC}	Kp_{sed} [l/kg]	$K_{sed\text{-}water}$ [m³/m³]	$PNEC_{water}$ [µg/L]	$QS_{sed,EqP}$ [µg/kg w.w.]	$QS_{sed,EqP}$ [µg/kg d.w.]	Included AF
Toxicity to pelagic organisms							
1 % OC	3 549	35.5	18.5	0.23	3.28	**8.53**	-
5% OC	3 549	177.5	89.5	0.23	15.8	**41.2**	-
Secondary poisoning							
1 % OC	3 549	35.5	18.5	0.002	0.029	**0.074**	-
5% OC	3 549	177.5	89.5	0.002	0.138	**0.358**	-