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NEW YORK STATE
- AQUATIC FACT SHEET -

Ambient Water Quality Value
For Protection of Aquatic Life

SUBSTANCE: Perfluorooctane sulfonic acid (PFOS)

CAS REGISTRY NUMBER: 1763-23-1

		Ambient Water Quality Value, µg/L	
TYPE:	**BASIS:**	**FRESHWATER**	**SALTWATER**
Chronic	Propagation	160 µg/L	41 µg/L
Acute	Survival	710 µg/L	190 µg/L

INTRODUCTION

These values apply to the water column and are derived to protect aquatic life from the effects of waterborne contaminants. Values for the protection of propagation of aquatic life are referred to as Aquatic (Chronic) *or* A(C) values. Values for the protection of survival of aquatic life are referred to as Aquatic (Acute) *or* A(A) values. The procedures for deriving Tier I and Tier II acute and chronic values for the protection of aquatic life in both fresh and salt water are described in 6NYCRR Part 706.1.

CHEMICAL BACKGROUND

Perfluorooctane sulfonic acid (PFOS) has the molecular formula $C_8HF_{17}O_3S$. Its molecular weight is 500.13, and it exists as a liquid at ambient temperatures with a boiling point of 133ºC. The solubility of PFOS decreases with increased salt content. The potassium salt of PFOS has a solubility of 370 mg/l in fresh water and 124 mg/l in sea water. Because it is a surface-active anion in water, it does not have a measurable *n*-octanol water partition coefficient (HSDB 2003); however, by comparing the solubility of PFOS in water to the solubility of PFOS in *n*-octane independently, the log K_{ow} was estimated to be -1.08, indicating that PFOS is clearly not lipophilic (MPCA 2007).

PFOS is a powerful surfactant. It and related chemicals have been produced since the 1950s as additives in commercial and industrial products, including fire-fighting foams, shampoo, insecticides and corrosion inhibitors. It was the main active ingredient of the stain repellant "Scotchguard." However, the primary manufacturer, 3M, voluntarily phased out production of all perfluorinated sulfonates by the end of 2003 because of the pervasiveness and persistence of the compounds (Sanderson, et al. 2002).

PFOS is extremely resistant to almost any kind of environmental degradation. Because the carbon-fluorine bond is one of the strongest in nature, its cleavage requires large amounts of energy. Chemical and physical processes occurring in the environment lack the required energy, and as a result, PFOS resists most forms of abiotic and microbial degradation. Absorption-desorption studies have shown that PFOS will bind to sediment, but it does not strongly bind to organic matter and is considered mobile in the environment (MPCA 2007). Because it is persistent in aquatic environments and does not strongly bind to organic matter, biota is the sink rather than sediment or soil (Sanderson, et al. 2002). Bioconcentration factors generally fall within the 1,000 – 3,000 range. PFOS does not appear to biomagnify strongly, although greater amounts appear to be bioaccumulated from diet rather than taken up from water (MPCA 2007).

SUMMARY OF INFORMATION AND DERIVATION OF VALUES

The primary source of aquatic toxicity data for PFOS was (OECD 2002). (MPCA 2007) documented the derivation of a Tier II ambient water quality value for PFOS for Minnesota. However, data from this document were not used to derive Tier II values for PFOS in New York. MPCA (2007) does not specifically identify the individual studies used, so they cannot be independently reviewed or cited. A database search was also conducted in the EPA ECOTOXicology knowledgebase (ECOTOX) for available toxicity data on PFOS. A total of 46 studies on toxicity in freshwater organisms and 28 studies on toxicity in saltwater organisms published between 2000-2018 were reviewed. Most of these studies are peer-reviewed open literature studies. Many of them, particularly the sub-chronic and chronic studies, included advanced molecular and genetic endpoints. Although these endpoints are considered more sensitive than the physiological and morphological endpoints, their implications on ecological impacts are not well defined. The results on standard endpoints reported in the open literature studies were generally in agreement with the studies evaluated in the OECD 2002 review.

Most of the studies referenced in both (OECD 2002) and (MCPA 2007) appear to be proprietary studies done for or by 3M Corporation. However unlike (MPCA 2007), (OECD 2002) provides very detailed reviews and summaries of the individual studies, although (OECD 2002) also documents fewer toxicity studies and species than does (MPCA 2007). To derive aquatic life values for New York, only studies from (OECD 2002) with a Klimisch Reliability ranking of 1 or 2 (Klimisch, et al. 1997) were used to derive the Tier II values for PFOS. Studies with a Klimisch ranking of 2 were only used if a study with a Klimisch ranking of 1 was not available for the same species. Open literature studies that were conducted in accordance with OECD toxicity testing guidelines were given preference over non-guideline studies. For PFOS, Tier II acute and chronic values were derived for the protection of aquatic life in both fresh and salt water.

DERIVATION OF ACUTE VALUES

A Tier I aquatic life value is a value derived using acute toxicity data from all eight minimum data requirements (MDRs) listed in 6 NYCRR Part 706.1 (III). A Tier II aquatic life value is derived when less than eight MDRs are satisfied.

The procedure to derive a Tier II water quality value is as follows: the lowest genus mean acute value (GMAV) of all acceptable studies is first identified. Then, the Secondary Acute Value

(SAV) is calculated by dividing the lowest GMAV by a secondary acute factor (SAF), which is based on the number of MDRs satisfied (see Table 1 of 6 NYCRR Part 706.1 (XII)). Lastly, the Tier II acute value (A(A)) for the protection of aquatic life is calculated by dividing the SAV by two.

6 NYCRR Part 706.1 (XII) does not provide SAF values for saltwater. The saltwater SAF values needed to derive a Tier II value were obtained from (Host, et al. 1995) as allowed under 702.9 (g) (1).

Freshwater

The freshwater acute toxicity data used to derive the PFOS acute value for freshwater are listed in Table 1. With only six MDRs available, Tier II aquatic life value was derived. The lowest GMAV was 7,416 µg/L. An SAF of 5.2 was used to derive the SAV: 7416 µg/L ÷ 5.2 = 1426.154 µg/L. To derive the Tier II freshwater acute aquatic life value (A(A)), the SAV was divided by two and rounded to two significant digits: 1426.154 ÷ 2 = 713.077 ≈ 710 µg/L.

Saltwater

The acute toxicity data used for deriving saltwater aquatic life value for PFOS are listed in Table 2. Because only three MDRs were satisfied, the Tier II value was derived. The lowest GMAV was 3,600 µg/L. Three MDRs were satisfied, including data for a species from either the family Mysidae or Penaeidae. No data were available for a species in the genus Menidia, so a SAF of 9.5 was selected from Host, et al. (1995) to derive a SAV: 3,600 µg/L ÷ 9.5 = 378.947. To derive the Tier II saltwater acute aquatic life value (A(A)) for PFOS the SAV was divided by two and rounded to two significant digits: 378.947 ÷ 2 = 189.474 ≈ 190 µg/L.

DERIVATION OF CHRONIC VALUES

A Tier I Final Chronic Value (FCV) is derived either using chronic toxicity data for all eight MDRs listed in 6 NYCRR Part 706.1 (III) or by using measured acute to chronic ratios (ACRs) for at least three species. A Tier II Secondary Chronic Value (SCV) is derived when less than three measured ACRs are available. An ACR is the ratio between the EC_{50}/LC_{50} from an acute test and the endpoint from a chronic test, which is usually the Maximum Acceptable Toxicant Concentration (MATC). The MATC is geometric mean of the NOEC (No Observed Effects Concentration) and the LOEC (Lowest Observed Effects Concentration)[1].

If ACRs for three or more species are available for the chemical, a Final ACR (FACR) is determined by calculating their geometric mean. For freshwater FACR calculation, at least one ACR for an acutely sensitive freshwater species is required. Saltwater ACRs can be used for the other two ACRs if no other freshwater ACRs are available. Similarly, for saltwater FACR, at least one ACR for an acutely sensitive saltwater species is required; the freshwater ACRs can be used for the remaining two ACRs. The Tier I FCV is determined by dividing the Tier I FAV by the FACR. If fewer than three ACRs are available for the chemical, a Secondary ACR (SACR) is

[1] Synonymous terms are the no observed effects level (NOEL) and lowest observed effects level (LOEL), respectively.

determined by using enough assumed ACRs so that the total number of ACRs equals three. An assumed ACR of 18 should be used for deriving freshwater SACR while and assumed ACR of 14 should be used when deriving a saltwater SACR (Host, et al. 1995). The SACR is then calculated as the geometric mean of the measured and assumed ACRs. If no measured ACRs are available, the corresponding assumed ACR value will be assigned as SACR. The Tier II SCV is determined by dividing the Tier II FAV by the FACR, or by dividing either the Tier I FAV or the Tier II SAV by the SACR.

Because Tier I FAV could not be derived for either freshwater or saltwater, chronic values for both freshwater and saltwater were derived as Tier II SCVs.

The Tier II chronic value (A(C)) is the lower of the SCV or the Final Plant Value (FPV).

Freshwater

The chronic toxicity data used for deriving the freshwater FCV for PFOS are listed in Table 3. Chronic studies on two freshwater species and one saltwater species were conducted by the same laboratory during the same year as the corresponding acute studies. A 21-day full life cycle test was conducted with *Daphnia magna,* a 47-day early life stage (ELS) test was conducted with fathead minnow (*Pimephales promelas*), and a 35-day ELS test, was conducted with opossum shrimp (*Mysidopsis bahia*). An FACR was calculated as the geometric mean of the three measured ACRs and the result is 9.2. To calculate the freshwater SCV, the freshwater SAV is divided by the FACR: 1426.154 µg/L ÷ 9.2 = 155.017 µg/L.

Saltwater

The same FACR of 9.2 was used to calculate the saltwater secondary chronic value, the saltwater SAV is divided by the FACR: 378.947 µg/L ÷ 9.2 = 41.190 µg/L.

Final Plant Value

The Final Plant Value (FPV) is the lowest plant value that was obtained with an important aquatic plant species in an acceptable toxicity test. Plant toxicity data for PFOS are described in Table 4. The FPV is 22,100 µg/L for freshwater and > 3,200 µg/L for saltwater.

Selection of the A(C) Value

The A(C) value is the lowest of either the FPV or the SCV. The SCVs are lower than the FPVs, so the SCVs rounded to two significant digits are selected as the Tier II chronic aquatic life values. The A(C) value for freshwater = 155.017 ≈ 160 µg/L, and 41.190 ≈ 41 µg/L for saltwater.

Table 1. Freshwater toxicity data used to derive the PFOS acute value. Data categories are listed in order they appear in 6 NYCRR 706.1 (III) (B) (1) (a-h) NDA - No Data Available

Data Requirement	Species (Common name - Family)	Endpoint Conc. µg/L	SMAV µg/L	GMAV µg/L	Reference
Family Salmonidae	*Oncorhynchus mykiss* (rainbow trout – Salmonidae)	22,000	7,416	7,416	OECD 2002
		2,500			Sharpe et al 2010
A second family in the Class Osteichthyes	*Pimephales promelas* (fathead minnow – Cyprinidae)	9,500	9,500	9,500	OECD 2002
A third family from the phylum Chordata	Xenopus laevis (African clawed frog - Pipidae)	12,100	12,100	12,100	OECD 2002
A planktonic crustacean	*Daphnia magna* (waterflea – Daphnidae)	61,000	61,000	61,000	OECD 2002
A benthic crustacean	NDA				
An insect	NDA				
A family in a phylum other than Arthropoda or Chordata	*Unio complamatus* (freshwater mussel – Unionidae)	59,000	59,000	59,000	OECD 2002
A family in any order of insect or any other phylum not already represented	*Danio rerio* (zebrafish - Cyprinidae)	22,200	22,200	22,200	Sharpe et al 2010

Table 2. Saltwater toxicity data used to derive the PFOS acute value. Data categories are listed in order they appear in 6 NYCRR 706.1 (III) (C) (1) (a-e) NDA - No Data Available

Data Requirement	**Species (Common name-Family)**	**Endpoint Conc. µg/L**	**SMAV µg/L**	**GMAV µg/L**	**Reference**
A family from the phylum Chordata	*Cyprinodon variegatus* (sheepshead minnow – Cyprinodontidae)	>15,000	>15,000	>15,000	OECD 2002
A second family from the phylum Chordata	NDA				
A family in a phylum other than Arthropoda or Chordata	*Crassostrea virginica* (Eastern Oyster – Ostreidae)	>3,000	>3,000	>3,000	OECD 2002
Either the Mysidae or Penaeidae family	*Mysidopsis bahia* (opossum shrimp – Mysidae)	3,600	3,600	3,600	OECD 2002
A family not in the family Chordata; may include Mysidae or Penaeidae, which ever was not used above	NDA				
A family not in the family Chordata; may include Mysidae or Penaeidae, which ever was not used above	NDA				
A family not in the family Chordata; may include Mysidae or Penaeidae, which ever was not used above	NDA				
Any other family	NDA				

Table 3. Chronic toxicity data used to derive the PFOS secondary acute to chronic ratio (FACR).

Species (Common name - Family)	**Habitat**	**acute endpoint (µg/L)**	**chronic endpoint (µg/L)**	**Acute:Chronic Ratios (ACR)**	**Reference**
Daphnia magna (waterflea – Daphnidae)	FW	48 hr EC_{50} = 61,000	NOEC = 12,000 LOEC = 24,000 MATC = 16,971	3.6	OECD 2002
Pimephales promelas (fathead minnow – Cyprinidae)	FW	96 hr LC_{50} = 9,500	NOEC = 300 LOEC = 600 MATC = 424.3	22.4	OECD 2002
Mysidopsis bahia (opossum shrimp – Mysidae)	SW	96 hr LC_{50} = 3,600	NOEC = 250 LOEC = 550 MATC = 371	9.7	OECD 2002
			Freshwater and saltwater final ACR	9.2	

Table 4. Freshwater plant toxicity data used to derive the PFOS final plant value (FPV).

Species (common name)	**Habitat**	**Test and endpoint**	**Measured effect concentration, µg/L**	**Measured No-effect concentration, µg/L**	**Reference**
Lemna gibba (duckweed)	Freshwater	7 day IC_{10} for growth inhibition	22,100	15,100	OECD 2002
Selenastrum capricornutum (green algae) a.k.a. *Pseudokirchneriella subcapitata*	freshwater	96 hour EC_{10} for cell density (growth)	49,000	44,000	OECD 2002
Navicula pellicosa (diatom)	Freshwater	96 hour EC_{10} for cell density (growth)	<62,300	150,000	OECD 2002
Anabaena flos-aquae (blue-green algae)	freshwater	96 hour EC_{10} for cell density (growth)	82,000	NR	OECD, 2002
Skeletonema costatum (diatom)	saltwater	96 hour EC_{10} for cell density (growth)	>3,200	3,200	OECD 2002
			Final Plant Value (FPV) freshwater, µg/L =	22,100	
			Final Plant Value (FPV) saltwater, µg/L =	>3,200	

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