Accessory publication

Reconciling measurement and modelling studies of the sources and fate of perfluorinated carboxylates

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Table A1. Definitions of abbreviation of perfluorinated carboxylates (PFCAs) and their precursors

Abbreviation	Name
APFO	Ammonium perfluorooctanoate
APFN	Ammounium perfluorononanoate
PFCA	Perfluorinated carboxylate
TFA	Trifluoroacetate
PFPrA	Perfluoropropanoate
PFBA	Perfluorobutanate
PFPeA	Perfluoropentanoate
PFHxA	Perfluorohexanoate
PFHpA	Perfluoroheptanoate
PFOA	Perfluorooctanoate
PFNA	Perfluorononanoate
PFDA	Perfluorodecanoate
PFUnA	Perfluoroundecanoate
PFDoA	Perfluorododecanoate
PFTrA	Perfluorotridecanoate
PFTA	Perfluorotetradecanoate
PFPeDA	Perfluoropentadecanoate
FTOH	Fluorotelomer alcohol
N-MeFOSE	*N*-Methyl perfluorooctanesulfonamidoethanol
N-EtFOSE	*N*-Ethyl perfluorooctanesulfonamidoethanol
N-MeFOSA	*N*-Methyl perfluorooctanesulfonamide
N-EtFOSA	*N*-Ethyl perfluorooctanesulfonamide
PFOS	Perfluorooctane sulfonate
PFBS	Perfluorobutane sulfonate
POSF	Perfluorooctane sulfonyl fluoride
FTAs	Fluorotelomer acids
FTUAs	Fluorotelomer unsaturated acids

Table A2. Global historical emission estimates (in tonnes) of PFCAs from APFO and APFN manufacture and use[1]

		PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDoA	PFTrA
APFO	1951–1964	1.18	0.74	144.85	0.74	0.00	0.00	0.00	0.00
	1965–1979	3.48	2.18	427.17	2.18	0.00	0.00	0.00	0.00
	1980–1994	10.50	6.56	1288.88	6.56	0.00	0.00	0.00	0.00
	1995–2010	15.92	9.95	1954.18	9.95	0.00	0.00	0.00	0.00
	1951–2010	31.08	19.43	3815.07	19.43	0.00	0.00	0.00	0.00
APFN	1975–1984	0.00	0.32	2.54	233.68	1.27	63.50	0.32	15.88
	1985–1994	0.00	0.51	4.08	375.36	2.04	102.00	0.51	25.50
	1995–2010	0.00	0.62	4.96	456.32	2.48	124.00	0.62	31.00
	1951–2010	0.00	1.45	11.58	1065.36	5.79	289.50	1.45	72.38
Total	1951–2010	31.08	20.87	3826.65	1084.79	5.79	289.50	1.45	72.38

Table A3. Representative reported concentrations (in nanograms per litre) of selected PFCAs in various waters

The representative reported data in various waters was chosen from the critical review by Rayne and Forest.[9] Only data from sites not close to point sources and covering most of the homologues are presented here

Location	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDoA	PFTrA	Ref.
Various rivers, IT	0	1.2	8.3	8.1	5.55	19.05	7.05	0	[2]
Yangtze River, CN	0.47	0.7125	18.25	0.6375	0.22975	0.2395	0	0	[3]
Maggiore Lake, IT	0	0.6	2.35	0.6	0.25	1	1.1	0	[2]
Various lakes, NV, USA	0	4.09	7.2	1.63	1.38	1.45	0	0	[4]
Various Lakes, Northern USA	0.27	1.705	0.555	0.58	0.47	0	0	0	[5]
Various well water, CA, USA	0	8	16.5	2.5	0.2	0	0	0	[6]
Various drinking water, IT	0	0.55	1.95	0.5	0.2	0.25	1.45	0	[2]
Municipal waste water effluent, AT	8.1	4	14	1.3	1.5	1.2	0	0	[7]
Coastal area, JP	14.2	2.06	6.73	47.7	0.199	1.54	0.03	NR	[8]

Table A4. Representative reported concentrations (in nanograms per gram or nanograms per litre) of selected PFCAs in various species

The representative reported data in various species was chosen from the critical review by Houde et al.[14] Only data covering most of the homologues are presented here

Location	Species	Scientific name	PFOA	PFNA	PFDA	PFUnA	PFDoA	PFTrA	Sampling year	Tissue	Ref.
Lake Ontario, Canada	Mysis	*Mysis relicta*	2.5	2.7	1.3	1.3	1.8	1.5	2001	whole	
Lake Ontario, Canada	Alewife	*Alosa pseudoharengus*	1.6	0.8	1.4	1.3	2.1	1.5	2002	whole	
Lake Ontario, Canada	Lake trout	–	1	4.2	6.1	8.3	3.9	4.6	1980–2001	whole	[10]
Lake Ontario, Canada	Rainbow smelt	*Osmerus mordax*	2	6.8	6.1	7	3.9	3.8	2002	whole	
Lake Ontario, Canada	Slimy sculpin	*Cottus cognatus*	44	33	29	39	14	13	2002	whole	
Bering–Chukchi Sea	Polar bear	*Ursus maritimus*	2.4	214	33	27	1.4	1.5	2001	liver	
High Arctic	Polar bear	*Ursus maritimus*	19	182	59	35	1.8	1.6	2002	liver	
Northwest Territories	Polar bear	*Ursus maritimus*	16	405	103	101	3.1	3.9	2001	liver	
South Baffin Island	Polar bear	*Ursus maritimus*	36	182	43	45	2.8	3.3	2002	liver	[11]
East Greenland	Polar bear	*Ursus maritimus*	9	191	72	104	7.9	19	1999–2001	liver	
Greenland	Polar bear	*Ursus maritimus*	10	236	89	114	8	20	1999–2001	liver	
South Hudson Bay	Polar bear	–	25	277	77	114	5	11	2002	liver	
Sanikiluaq, NU, Canada	Polar bear	–	8.6	180	56	63	6.2	11	2002	liver	[12]
Pangnirtung	Ringed seal	–	3.7	8.7	4.5	5.2	2.2	2.8	2002	liver	D. C. G. Muir, et al., unpubl. data, 2004

Table A4. (*Continued*)

Location	Species	Scientific name	PFOA	PFNA	PFDA	PFUnA	PFDoA	PFTrA	Sampling year	Tissue	Ref.
Holman, NT, Canada	Ringed seal	–	<2	5.9	2.1	3.3	0.4	0.6	2001	liver	[12]
Inukjuak, QC, Canada	Gray seal	–	3.2	22	18.3	42.6	6	8.4	2002	liver	D. C. G. Muir, et al., unpubl. data, 2004
Bermuda	Bottlenose dolphin	*Tursiops truncatus*	0.8	17	9.6	45	4.6	7.4	2003	plasma	
Indian River Lagoon, FL, USA	Bottlenose dolphin	–	12	13	18	15	2	1.6	2003	plasma	
New Jersey, USA	Bottlenose dolphin	–	72	326	45	192	5.3	13	2003	plasma	[13]
Sarasota Bay, FL, USA	Bottlenose dolphin	–	6.3	25	22	40	5.2	2.3	2003	plasma	
Charleston, SC, USA	Bottlenose dolphin	–	44	63	159	67	13	2.7	2003	plasma	
Arviat, NU, Canada	Arctic fox	*Alopex lagopus*	<2	22	14	13	1.5	2.2	2001	liver	[12]

Table A5. Concentrations of precursor compounds in air (minimum, maximum and average, pg m^{-3})

BD indicates below detection limit; BQ indicates below quantification limit. Dash indicates not reported. Available data simultaneously covering 6:2, 8:2 and 10:2 FTOH, N-MeFOSE, N-EtFOSE, N-MeFOSA and N-EtFOSA were included

Location	Year	Day	6:2 FTOH			8:2 FTOH			10:2 FTOH			N-MeFOSA			N-EtFOSA			N-MeFOSE			N-EtFOSE			Ref.
Long Point, ON, Canada	2001	28 Mar –3 Apr	16	41	29	25	40	32	15	20	17	–	–	–	–	–	–	34	36	35	68	85	76	[15]
Long Point, Canada	2001	2–15 Nov	–	–	25	–	–	BD	–	–	BD	–	–	–	–	–	10	–	–	10	–	–	25	[16]
Cleves, OH, USA	2001	2–15 Nov	–	–	65	–	–	65	–	–	BQ	–	–	–	–	–	45	–	–	20	–	–	BD	
Waldhof, Germany	2005	19 May –2 Jun	17	125	64	33	112	75	10	32	23	3.8	11	7	1.5	3.4	2.6	1.4	15.7	8.9	1.2	38	16.9	[17]
North Atlantic–Canadian Archipelago	2005	6–27 Jul	–	5.98	2.65	5.23	31.07	14.9	1.74	17.97	7.07	–	–	–	–	–	–		38.6	11.83	–	10.67	2.92	[18]
S2	2005	16–19 Oct	8.4	14	11	21	36	29	6.5	12	9.2	1.7	2	1.9	0.7	0.8	0.8	3	4.8	3.9	–	–	–	
S3	2005	25–28 Oct	–	–	9.4	–	–	15		–	3.3	–	–	1.1	–	–	<0.3	–	–	1.6	–	–	0.9	
S4	2005	28–31 Oct	10	19	14	17	20	18	4.7	4.9	4.8	1.6	1.6	1.6	0.7	0.7	0.7	2.9	3.3	3.1	–	–	–	[19]
S5	2005	31 Oct –3 Nov	19	21	20	35	48	42	7.1	8.3	7.7	2.1	2.4	2.3	0.9	1.3	1.1	7.3	7.5	7.4	1.2	1.7	1.5	
Kjeller, Norway	2005	Nov–Dec	11.5	11.9	11.7	34.4	34.4	34.4	16.5	17.8	17.2	3.1	7.8	5.5	4.3	5.6	5	50.5	54.5	52.5	31.3	34.5	32.9	
Mace Head, Ireland	2006	Mar	1	9.3	4.95	5.8	21.8	11.3	<4.2	8.2	7.8	–	–	<4.9	–	–	<1.6	–	–	<79.6	–	–	<52.4	[20]
Mount Bachelor Observatory, Oregon, USA	2006	3 Apr –12 May	–	–	4.6	–	–	24	–	–	15	–	–	–	BQ	3.2	3.2	BQ	11	11	BQ	3.7	3.7	[21]
Middle Atlantic	2007	12 Apr –2 May	1.9	11.2	5.8	7.3	124.5	25.5	1.7	53.1	9.2	0.9	8.5	3.6	0.4	67.3	6.9	1	10.5	3.8	0.7	5.7	2	[22]
Bermuda	2007	14–30 Jun	1.85	4.9	2.96	7.39	31.65	21.5	7.31	13.35	9.8	BD	1.89	0.79	BD	0.82	0.34	32.92	124.34	62.07	1.15	3.19	1.83	[23]
Sable Island	2007	16 Jun –5 Aug	0.33	10.7	2.85	0.79	42.8	9.78	0.23	17.23	4.23	BD	1.23	0.37	BD	0.7	0.22	4.91	23.4	17.86	0.05	0.43	0.31	

Table A5. (*Continued*)

Location	Year	Day	6:2 FTOH			8:2 FTOH			10:2 FTOH			N-MeFOSA			N-EtFOSA			N-MeFOSE			N-EtFOSE			Ref.
Longyearbyen, Norway–Kiel, Germany	2007	11–19 Aug	12.2	51.2	22.4	10.5	50.5	22	1.9	11.1	4.91	0.9	8.2	2.97	0.4	0.5	0.47	0.9	2.4	1.42	1	3	1.6	
Bremerhaven, Germany–Cape town, South Africa	2007	26 Oct –26 Nov	1.8	35.2	9.2	4	39.5	17.7	1.3	17.1	4.4	0.6	6	2.6	0.8	4.7	2.13	0.8	4.1	1.98	0.8	2.6	1.6	[22]
German Bight Atair 155 3–6	2007	1–05 Nov	3.3	15	7.45	8.2	28	16.3	2.1	6.7	4.5	2.5	13.1	6.9	0.4	9.4	3.85	2	15.2	5.225	0.3	15.3	7	[24]
Rostock, Germany–Tallinn, Estonia–Kiel, Germany	2008	18 Jun –17 Jul	1.8	19.2	7.5	7.5	94.5	28.7	1.4	33.1	9.4	0.8	5.9	2.1	0.5	13.3	1.83	0.6	11	2.3	0.6	1.7	0.95	[22]

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