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Accessory publication

Air concentrations and particle–gas partitioning of polyfluoroalkyl compounds at a wastewater treatment plant

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Chemicals

Methanol (LC-MS grade, OmniSolv >99.99%), acetone (OmniSolv 99.84%), petroleum ether (OmniSolv), dichlormethane (OmniSolv >99.96%), iso-octane (2,2,4-Trimethylpentane Omni-Solv >99.97%), water (OmniSolv) and ammonium acetate (min. 97%) were purchased from EMD. Anhydrous sodium sulfate were purchased from Fischer Scientific, supelclean EnviCab from Supelco and glacial acetic acid (99.7+%) from Alfa Aesar. The water (OmniSolv) was cleaned using Oasis WAX cartridges (Waters) to remove possible contaminations. Methane, nitrogen and helium were purchased from Linde.

Table A1. Target compounds with abbreviation, chemical formula, precursor and product ion, supplier, purity and internal standard (IS)

Analyte	Abbreviation	Chemical formula	Precursor/ product ion	Supplier (purity)	IS
Perfluoro hexylethanol	6:2 FTOH	$C_8F_{13}H_4OH$	365/327	Wellington Laboratories (>98%)	^{13}C-6:2 FTOH
Perfluoro octylethanol	8:2 FTOH	$C_{10}F_{17}H_4OH$	465/427	Wellington Laboratories (>98%)	^{13}C-8:2 FTOH
Perfluorodecyl ethanol	10:2 FTOH	$C_{12}F_{21}H_4OH$	565/527	Wellington Laboratories (>98%)	^{13}C-10:2 FTOH
Perfluorooctane sulfonamide	PFOSA	$C_8F_{17}SO_2NH_2$	498/78	Wellington Laboratories (>98%)	$^{13}C_4$-PFOS
N-methyl perfluorooctane sulfonamide	MeFOSA	$C_8F_{17}SO_2NHCH_3$	514	Wellington Laboratories (>98%)	d_3 MeFOSA
N-ethyl perflourooctae sulfonamide	EtFOSA	$C_8F_{17}SO_2NHC_2H_5$	528	Wellington Laboratories (>98%)	d_5 EtFOSA
N-methyl perfluorooctane sulfonamido-ethanol	MeFOSE	$C_8F_{17}SO_2NCH_3C_2H_4OH$	540/558	Wellington Laboratories (>98%)	d_7 MeFOSE
N-ethyl perflourooctane sulfonamido-ethanol	EtFOSE	$C_8F_{17}SO_2NC_2H_5C_2H_4OH$	554/572	Wellington Laboratories (>98%)	d_9 EtFOSE
N-methyl perfluorooctane sulfonamide ethylacrylate	Me PFOSEA	$C_8F_{17}SO_2N(C_2H_4OH)(C_2H_4OCOC_2H_3)$	540	Wellington Laboratories (>98%)	d_7 MeFOSE
Perfluorobutane sulfonate	PFBS	$C_4F_9SO_2O$-	299/80	Wellington Laboratories (>98%)	$^{18}O_2$-PFHxS
Perfluorohexane sulfonate	PFHxS	$C_6F_{13}SO_2O^-$	399/80	Wellington Laboratories (>98%)	$^{18}O_2$-PFHxS
Perfluorooctane sufonate	PFOS	$C_8F_{17}SO_2O^-$	499/80	Aldrich (98%)	$^{13}C_4$-PFOS
Perfluorodecane sulfonate	PFDS	$C_{10}F_{21}SO_2O^-$	599/99	Wellington Laboratories (>98%)	$^{13}C_4$-PFOS
Perfluorobuntanoate	PFBA	$C_3F_7COO^-$	213/169	Wellington Laboratories (>98%)	$^{13}C_4$-PFBA
Perfluoropentanoate	PFPA	$C_4F_9COO^-$	263/219	Wellington Laboratories (>98%)	$^{13}C_2$-PFHxA
Perfluorohexanoate	PFHxA	$C_5F_{11}COO^-$	313/269	Wellington Laboratories (>98%)	$^{13}C_2$-PFHxA
Perfluorohepantoate	PFHpA	$C_6F_{12}COO^-$	363/319	Aldrich (98%)	$^{13}C_4$-PFOA
Perfluorooctanoate	PFOA	$C_7F_{15}COO^-$	413/369	Aldrich (98%)	$^{13}C_4$-PFOA

Analyte	Abbreviation	Chemical formula	Precursor/ product ion	Supplier (purity)	IS
Perfluorononanoate	PFNA	$C_8F_{17}COO^-$	463/419	Aldrich (98%)	$^{13}C_5$-PFNA
Perfluorodecanoate	PFDA	$C_9F_{19}COO^-$	513/469	Aldrich (98%)	$^{13}C_2$-PFDA
Perfluoroundecanoate	PFUnDA	$C_{10}F_{21}COO$-	563/519	Aldrich (98%)	$^{13}C_2$-PFUnDA
Perfluorododecanoate	PFDoDA	$C_{11}F2_3COO^-$	613/569	Aldrich (98%)	$^{13}C_2$-PFDoA
Perfuorotetradecanoate	PFTDA	$C_{13}F_{25}COO^-$	713/669	Aldrich (98%)	$^{13}C_2$-PFDoA

Table A2. Internal standards with abbreviation, chemical formula, precursor and product ion, supplier and purity

Analyte	Abbreviation	Chemical formula	Precursor/ product ion	Supplier (purity)
N, *N*-dimethylperfluoro-1-octanesulfonamide	Me_2FOSA	$C_8F_{17}SO_2N(CH_3)_2$	528	Wellington Laboratories (>98%)
2-perfluorohexyl-($^{13}C_2$)-ethanol	^{13}C-6:2 FTOH	$C_6F_{13}{}^{13}CH_2{}^{13}CD_2OH$	369/331	Wellington Laboratories (>98%)
2-perfluorooctyl-($^{13}C_2$)-ethanol	^{13}C-8:2 FTOH	$C_8F_{17}{}^{13}CH_2{}^{13}CD_2OH$	469/497	Wellington Laboratories (>98%)
2-perfluorodecyl-($^{13}C_2$)-ethanol	^{13}C-10:2 FTOH	$C_{10}F_{21}{}^{13}CH_2{}^{13}CD_2OH$	569/531	Wellington Laboratories (>98%)
Methyl-d_3-perfluorooctane sulfonamide	d_3-MeFOSA	$C_8F_{17}SO_2NHCD_3$	517	Wellington Laboratories (>98%)
Ethyl-d_5-perfluorooctane sulfonamide	d_5-EtFOSA	$C_8F_{17}SO_2NHC_2D_5$	533	Wellington Laboratories (>98%)
Methyl-d_7-perfluorooctane sulfonamido ethanol	d_7-MeFOSE	$C_8F_{17}SO_2NCD_3C_2D_4$	547/565	Wellington Laboratories (>98%)
Ethyl-d_9-perflourooctane sulfonamido ethanol	d_9 EtFOSE	$C_8F_{17}SO_2NC_2D_5\,C_2D_4OH$	581	Wellington Laboratories (>98%)
Perfluoro-1-hexane-($^{18}O_2$) sulfonate	$^{18}O_2$-PFHxS	$C_6F_{13}S[^{18}O_2]O^-$	403/103	Wellington Laboratories (>98%)
Perfluoro-1-($^{13}C_4$)-octane sulfonate	$^{13}C_4$- PFOS	C_4F_9[1,2,3,4-$^{13}C_4$]-$F_8SO_2O^-$	503/99	Wellington Laboratories (>98%)
Perfluoro-*n*-($^{13}C_4$)-butanoate	$^{13}C_4$- PFBA	2,3,4-$^{13}CF_7{}^{13}COO^-$	217/172	Wellington Laboratories (>98%)
Perfluoro-*n*-($^{13}C_4$)-octanoate	$^{13}C_4$-PFOA	C_4F_9[2,3,4-$^{13}C_3$]-$F_6{}^{13}COO^-$	417/372	Wellington Laboratories (>98%)
Perfluoro-*n*-($^{13}C_5$)-nonanoate	$^{13}C_5$-PFNA	C_4F_9[2,3,4,5-$^{13}C_4$]-$F_8{}^{13}COO^-$	468/423	Wellington Laboratories (>98%)
Perfluoro-*n*-($^{13}C_2$)-decanoate	$^{13}C_2$-PFDA	$C_8F_{17}{}^{13}CF_2{}^{13}COO^-$	515/470	Wellington Laboratories (>98%)
Perfluoro-*n*-($^{13}C_2$)-undecanoate	$^{13}C_2$-PFUnDA	$C_9F_{19}{}^{13}CF_2{}^{13}COO^-$	565/520	Wellington Laboratories (>98%)
Perfluoro-*n*-($^{13}C_2$)-dodecanoate	$^{13}C_2$-PFDoA	$C_{10}F_{21}{}^{13}CF_2{}^{13}COO^-$	615/570	Wellington Laboratories (>98%)
Perfluoro-*n*-($^{13}C_2$)-hexanoate	$^{13}C_2$-PFHxA	$C_4F_9{}^{13}CF_2{}^{13}COO^-$	315/270	Wellington Laboratories (>98%)
Perfluoro-1-($^{13}C_4$)-octane sulfonate	$^{13}C_8$-PFOS	C_4F_9[1,2,3,4-$^{13}C_4$]-$F_8SO_2O^-$	507/80	Wellington Laboratories (>98%)
Perfluoro-*n*-($^{13}C_4$)-octanoate	$^{13}C_8$-PFOA	C_4F_9[2,3,4-$^{13}C_3$]-$F_6{}^{13}COO^-$	421/376	Wellington Laboratories (>98%)

Instrumental analysis

Table A3. Temperature program for the GC oven

	Rate ($°C\ min^{-1}$)	Value (°C)	Hold time (min)	Run time (min)
Initial	–	60	2	2.00
Ramp 1	2	70	0	7.00
Ramp 2	8	120	0	13.25
Ramp 3	10	220	0	23.25

Table A4. Eluent gradient for HPLC

Time (min)	H_2O + 10 mM NH_4OAc (%)	MeOH + 10 mM NH_4OAc (%)
0.01	50	50
1.0	45	55
2.0	40	60
3.0	25	75
4.0	20	80
5.0	15	85
10.0	15	85
10.1	5	95
15.0	5	95
15.1	25	75
15.6	50	50
20.0	50	50

Instrumental detection limits

Table A5. Instrument detection limits (IDLs) (expressed as picograms and picograms per cubic metre) were calculated by extrapolating instrument response in blank samples to a concentration that would give a S/N value of 3

Reporting of IDLs in units of picograms per cubic metre was done using an average air volume of 142 pg m^{-3} for PUF/XAD/PUF cartridges and GFFs and compound-specific air volumes for SIP disks

Name	PUF/XAD/PUF IDL		GFFs IDL		SIP disks IDL	
	(pg)	(pg m^{-3})	(pg)	(pg m^{-3})	(pg)	(pg m^{-3})
6:2 FTOH	88	0.61	100	0.73	96	0.60
8:2 FTOH	110	0.77	72	0.51	96	0.60
10:2 FTOH	71	0.50	81	0.57	58	0.36
PFOSA	0.79	0.01	0.55	0.001	1.4	0.01
MeFOSA	59	0.42	17	0.12	110	1.2
EtFOSA	36	0.25	23	0.16	19	0.20
MeFOSE	110	0.74	96	0.67	70	1.3
MePFOSEA	58	0.41	70	0.49	63	1.2
EtFOSE	150	1.1	58	0.41	89	1.8
PFBS	11	0.08	12	0.09	20	0.14
PFHxS	2.2	0.02	0.83	0.01	1.3	0.01
PFOS	7.2	0.05	1.8	0.01	4.3	0.03
PFDS	1.6	0.01	0.89	0.01	2.7	0.02
PFBA	0.79	0.12	9.2	0.06	27	0.19
PFPA	17	0.10	11	0.08	6.8	0.05
PFHxA	15	0.04	3.1	0.02	3.6	0.03
PFHpA	5.8	0.05	8.3	0.06	4.2	0.03
PFOA	6.5	0.01	4.2	0.03	8.6	0.06
PFNA	2.1	0.01	2.2	0.02	2.7	0.02
PFDA	2.0	0.02	2.6	0.02	1.4	0.01
PFUnDA	2.6	0.02	26	0.18	5.7	0.04
PFDoDA	3.0	0.04	3.8	0.03	4.3	0.03
PFTDA	5.9	0.01	2.5	0.02	1.6	0.01

Concentrations in blank samples and limits of detection

Table A6. Mean concentrations ± s.d. and LOD (3 s.d.) (in parentheses) in blank samples for the different air sample media (*n* = 5 for PUF/XAD/PUF cartridges, *n* = 7 for GFFs and *n* = 2 for SIP disks)

Asterisks denote where half of the instrument detection limit (IDL, see Table A5) was used for compounds not detected in blank samples. In these cases LOD could not be calculated and IDL was used instead of LOD

Compound	PUF/XAD/PUF (pg m^{-3})	GFFs (pg m^{-3})	SIP disks (pg m^{-3})
6:2 FTOH	0.3 (0.61)*	0.4 (0.73)*	0.7 ± 0.6 (1.8)
8:2 FTOH	3.1 ± 2.6 (7.8)	0.3 (0.51)*	7.1 ± 0.6 (1.8)
10:2 FTOH	4.9 ± 1.3 (3.9)	1.8 ± 1.1 (3.3)	4.3 ± 0.6 (1.8)
PFOSA	3.9 ± 2.1 (6.3)	4.5 ± 2.4 (7.2)	2.0 ± 0.1 (0.3)
MeFOSA	3.5 ± 0.5 (1.5)	3.1 ± 0.4 (1.2)	3.8 ± 0.8 (2.4)
EtFOSA	0.4 ± 0.2 (0.6)	0.2 ± 0.1 (0.3)	0.1 ± 0.1 (0.3)
MeFOSE	3.7 ± 4.2 (13)	1.6 ± 1.6 (4.8)	0.5 ± 0.4 (1.2)
MePFOSEA	0.2 (0.41)*	0.3 (0.49)	0.5 ± 0.4 (1.2)
EtFOSE	4.4 ± 4.6 (13.8)	0.6 ± 1.1 (3.3)	0.7 ± 0.5 (1.5)
PFBS	0.04 (0.08)*	0.04 (0.09)*	0.07 (0.14)*
PFHxS	1.1 ± 0.47 (1.4)	0.28 ± 0.03 (0.09)	0.30 ± 0.09 (0.27)
PFOS	4.2 ± 1.8 (5.4)	6.4 ± 5.9 (18)	7.04 ± 1.06 (3.2)
PFDS	0.01 (0.01)*	0.03 ± 0.02 (0.06)	0.01 (0.02)*
PFBA	7.1 ± 5.7 (17)	22 ± 42 (125)	14 ± 11 (33)
PFPA	3.4 ± 4.2 (13)	6.7 ± 13 (39)	1.6 ± 1.8 (5.4)
PFHxA	1.2 ± 0.3 (0.9)	0.84 ± 0.3 (0.9)	1.1 ± 0.22 (0.66)
PFHpA	1.4 ± 0.5 (1.5)	2.2 ± 2.8 (8.4)	1.2 ± 0.03 (0.09)
PFOA	5.6 ± 2.0 (6.0)	2.1 ± 0.81 (2.4)	11 ± 2.7 (8.1)
PFNA	0.95 ± 0.46 (1.4)	0.48 ± 0.10 (0.3)	0.65 ± 0.08 (0.24)
PFDA	0.86 ± 0.15 (0.45)	0.95 ± 0.34 (1.0)	0.71 ± 0.01 (0.03)
PFUnDA	1.3 ± 0.27 (0.81)	5.4 ± 9.6 (29)	1.2 ± 0.23 (0.69)
PFDoDA	0.71 ± 0.05 (0.15)	1.2 ± 0.82 (2.5)	0.63 ± 0.03 (0.09)
PFTDA	0.004 (0.01)*	0.13 ± 0.14 (0.43)	0.01 (0.01)*

Recoveries

Table A7. Mean recoveries (%) (±s.d.) of internal standards (IS) in the different air sample media (*n* = 12 for PUF/XAD/PUF cartridges and GFFs, *n* = 4 for SIP disks)

IS	PUF/XAD/PUF Cartridges		GFFs		SIP disks (%)
	Aeration tank (%)	Secondary clarifier (%)	Aeration tank (%)	Secondary clarifier (%)	
^{13}C-6:2 FTOH	18 ± 23	5.9 ± 1.8	9.4 ± 2.8	9.7 ± 2.1	6.4 ± 1.0
^{13}C-8:2 FTOH	75 ± 8.5	67.5 ± 8.7	47 ± 12	49 ± 6.6	66 ± 8.6
^{13}C-10:2 FTOH	98 ± 14	100 ± 18	56 ± 10	58 ± 6.2	110 ± 14
d_3-MeFOSA	72 ± 13	80 ± 21	80 ± 9.2	81 ± 6.3	99 ± 11
D_5-EtFOSA	84 ± 9.4	91 ± 19	85 ± 9.6	85 ± 6.7	100 ± 12
d_7-MeFOSE	220 ± 39	200 ± 47	130 ± 24	130 ± 11	230 ± 46
D_9-EtFOSE	230 ± 37	220 ± 48	150 ± 25	130 ± 15	230 ± 61
$^{18}O_2$-PFHxS	120 ± 37	120 ± 39	62 ± 23	54 ± 14	310 ± 40
$^{13}C_4$-PFOS	78 ± 20	79 ± 20	37 ± 11	38 ± 8.3	75 ± 5.2
$^{13}C_2$-PFBA	150 ± 53	180 ± 96	36 ± 3.9	36 ± 8.5	160 ± 64
$^{13}C_2$-PFHxA	130 ± 240	140 ± 32	63 ± 1	67 ± 16	240 ± 50
$^{13}C_4$-PFOA	83 ± 220	92 ± 17	47 ± 6.9	49 ± 10	73 ± 7.1
$^{13}C_5$-PFNA	66 ± 22	67 ± 15	39 ± 7.3	44 ± 10	34 ± 0.4
$^{13}C_2$-PFDA	59 ± 27	54 ± 14	51 ± 9.0	57 ± 13	27 ± 2.3
$^{13}C_2$-PFUnDA	43 ± 25	38 ± 14	52 ± 11	62 ± 15	25 ± 6.4
$^{13}C_2$-PFDoDA	27 ± 20	21 ± 11	47 ± 9.9	55 ± 15	18 ± 4.0

Atmospheric concentrations

Table A8. Gas-phase concentrations (blank corrected) at the aeration tank

Concentrations are given in picograms per cubic metre. Values that fell below the LOD but above the mean blank are indicated with an asterisk (*). Non-detections and cases where blank correction resulted in a negative value are replaced with ½ LOD value (Table A6) and italicised. Note: in case where more than 25% of samples for a given target chemical are replaced by ½ LOD value, the summary statistics for these compounds are not included in box and whisker plots (due to bias[1]), and only mean values are reported

Name	1	2	3	4	5	6	7
6:2 FTOH	8300	3000	5500	780	3200	1400	6300
8:2 FTOH	3200	1000	1600	3600	11000	16000	5600
10:2 FTOH	600	120	210	590	3100	3100	1100
∑FTOH	12000	4200	7300	4900	17000	33000	13000
MeFOSA	7.6	0.71*	6.5	14	16	36	29
EtFOSA	5.3	0.46*	3.1	5.8	4.8	10	9.6
MeFOSE	27	4.9*	121*	14	24	44	24
EtFOSE	4.1*	*7.0*	*7.0*	*7.0*	*7.0*	*5.4**	*7.0*
PFOSA	*3.1*	4.2*	6.3	3.0*	9.5	5.8*	2.5*
∑FOSA–FOSE	44	17	35	44	61	100	74
PFHxS	*0.70*	0.06*	0.15*	0.63*	0.76*	1.7	0.42*
PFOS	*2.7*	1.1*	1.4*	4.1*	1.5*	41	1.6*
PFDS	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*
∑PFSA	3.4	1.2	1.6	4.7	2.3	42	2.0
PFBA	8.6*	4.1*	6.2*	11*	0.9*	4.9*	10*
PFPA	25	*6.3*	5.9*	7.1*	8.2*	11*	14
PFHxA	7.1	6.6	15	18	22	22	33
PFHpA	0.16*	1.8	3.1	2.5	5.6	5.9	7.3
PFOA	2.1*	4.3*	8.6	9.6	18	18	22
PFNA	*0.69*	0.71*	1.2*	1.1*	1.0*	0.96*	2.0
PFDA	0.28*	0.25*	0.88	0.78	2.1	2.3	1.7
PFUnDA	2.5	0.13*	*0.41*	*0.41*	0.12*	*0.41*	9.0
PFDoDA	*0.09*	*0.09*	0.15*	*0.09*	0.56	0.31	0.20
PFTDA	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*
∑PFCA	46	24	41	51	59	65	99

Table A8. (*Continued*)

Name	8	9	10	11	12	mean	s.d.
6:2 FTOH	11000	7600	4400	2300	2300	5700	3900
8:2 FTOH	6000	4900	1900	930	910	4700	4600
10:2 FTOH	880	900	240	97	72	920	1100
∑FTOH	18000	13000	6500	3400	3300	11000	8600
MeFOSA	16	12	8.5	6.2	4.1	13	10
EtFOSA	7.6	4.5	3.6	2.8	1.4	4.9	3.0
MeFOSE	28	22	16	12*	9.5*	20	11
EtFOSE	6.1*	*7.0*	*7.0*	*7.0*	*7.0*	7.0	1.4
PFOSA	2.6*	2.3*	2.9*	*3.1*	5.8*	3.7	2.7
∑FOSA–FOSE	61	48	38	30	28	48	23
PFHxS	0.95*	0.97*	0.61*	2.05*	0.34*	0.78	0.59
PFOS	3.3*	1.9*	1.9*	6.2	3.1*	5.8	11
PFDS	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*	*0.0*
∑PFSA	4.2	2.9	2.5	8.3	3.4	6.6	11
PFBA	11*	24	9.6*	30	14*	11	8.3
PFPA	7.0*	*6.3*	1.6*	*6.3*	*6.3*	8.7	5.8
PFHxA	50	26	16	14	7.0	20	12
PFHpA	13	5.3	4.7	11	1.3*	5.1	3.8
PFOA	25	17	8.2	21	4.0*	13	7.9
PFNA	3.1	2.7	1.7	9.3	1.7	2.2	2.4
PFDA	2.6	2.8	1.2	1.7	0.68	1.4	0.88
PFUnDA	*0.41*	0.03*	0.27*	0.25*	*0.41*	1.2	2.5
PFDoDA	0.50	0.64	0.10*	*0.09*	*0.09*	0.24	0.21
PFTDA	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*	*0.0*
∑PFCA	110	85	43	93	36	63	28

Table A9. Gas-phase concentrations (blank corrected) at the secondary clarifier

Concentrations are given in picograms per cubic metre. Values that fell below the LOD but above the mean blank are indicated with an asterisk (*). Non-detections and cases where blank correction resulted in a negative value are replaced with ½ LOD value (Table A6) and italicised. Note: in case where more than 25% of samples for a given target chemical are replaced by ½ LOD value, the summary statistics for these compounds are not included in box and whisker plots (due to bias [1]), and only mean values are reported

Name	1	2	3	4	5	6	7
6:2 FTOH	290	330	240	280	350	910	530
8:2 FTOH	180	83	110	170	240	670	420
10:2 FTOH	46	6.2	16	29	62	113	60
∑FTOH	510	420	360	470	650	1700	1000
MeFOSA	2.9	0.23*	0.93*	0.84*	6.1	6.7	0.58*
EtFOSA	3.4	0.45*	0.63	1.0	1.9	2.5	0.72
MeFOSE	13	0.57*	*6.3*	*6.3*	*6.3*	2.7*	*6.3*
EtFOSE	8.3*	*7.0*	*7.0*	*7.0*	*7.0*	*7.0*	*7.0*
PFOSA	2.8*	5.0*	1.5*	1.8*	0.94*	2.4*	3.6*
∑FOSA–FOSE	31	13	16	17	22	21	18
PFHxS	0.50*	0.18*	0.12*	0.31*	1.6	1.3*	0.57*
PFOS	1.9*	30	2.6*	2.4*	2.0*	2.3*	1.25*
PFDS	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*
∑PFSA	2.4	30	2.7	2.7	3.6	3.6	1.8
PFBA	9.7*	13*	14*	5.3*	2.1*	17*	16*
PFPA	5.1*	40	23	*6.3*	*6.3*	1.5*	0.42*
PFHxA	1.7	0.98	1.6	1.1	2.2	1.5	2.8
PFHpA	*0.81*	*0.81*	*0.81*	*0.81*	0.68*	0.09*	0.59*
PFOA	1.3*	0.63*	1.2*	2.0*	2.7*	1.8*	3.7*
PFNA	0.69*	0.67*	0.45*	0.59*	0.56*	0.82*	1.1*
PFDA	0.26*	0.42*	0.42*	0.15*	0.50	0.34*	0.39*
PFUnDA	*0.41*	0.06*	*0.41*	0.06*	0.40*	*0.41*	*0.41*
PFDoDA	*0.09*	*0.09*	0.11*	*0.09*	*0.09*	0.10*	0.31
PFTDA	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*
∑PFCA	20	56	42	16	16	23	26

Table A9. (*Continued*)

Name	8	9	10	11	12	mean	s.d.
6:2 FTOH	390	290	230	110	*0.31*	330	230
8:2 FTOH	290	330	100	52	27	220	190
10:2 FTOH	48	74	23	9.9	7.6	41	32
∑FTOH	720	690	350	170	34	590	440
MeFOSA	0.89*	1.3*	0.47*	*0.70*	*0.70*	1.9	2.2
EtFOSA	1.0	1.1	0.77	0.19	*0.29*	1.2	0.96
MeFOSE	0.54*	*6.3*	*6.3*	*6.3*	*6.3*	5.6	3.3
EtFOSE	*7.0*	*7.0*	*7.0*	*7.0*	*7.0*	7.1	0.40
PFOSA	1.6*	0.54*	3.0*	5.3*	11	3.3	2.8
∑FOSA–FOSE	11	16	18	19	25	16	5.3
PFHxS	0.51*	0.49*	0.62*	0.41*	0.42*	0.59	0.43
PFOS	9.51	1.1*	0.94*	1.6*	0.65*	4.7	8.2
PFDS	*0.01*	*0.01*	*0.01*	*0.01*	*0.01*	0.01	0.0
∑PFSA	10	1.6	1.6	2.1	1.1	5.2	8.1
PFBA	23	18	9.1*	25	15*	14	6.6
PFPA	3.6*	2.3*	*6.3*	9.4*	1.7*	8.8	11.4
PFHxA	1.9	1.5	1.6	1.5	0.70*	1.6	0.56
PFHpA	0.04*	*0.81*	0.35*	0.43*	0.22*	0.54	0.30
PFOA	4.9*	3.0*	2.8*	1.9*	1.2*	2.3	1.2
PFNA	0.76*	0.48*	0.52*	1.4	0.67*	0.72	0.27
PFDA	0.65	0.81	0.57	0.14*	0.39*	0.42	0.20
PFUnDA	*0.41*	0.18	*0.41*	*0.41*	*0.41*	0.33	0.14
PFDoDA	*0.09*	*0.09*	0.06*	*0.09*	*0.09*	0.11	0.06
PFTDA	*0.004*	*0.004*	*0.004*	*0.004*	*0.004*	0.004	0.0
∑PFCA	35	27	22	40	20	29	12

Table A10. Particle-phase concentrations (blank corrected) at the aeration tank

Concentrations are given in picograms per cubic metre. Values that fell below the LOD but above the mean blank are indicated with an asterisk (*). Non-detections and cases where blank correction resulted in a negative value are replaced with ½ LOD value (Table A6) and italicised. Note: in case where more than 25% of samples for a given target chemical are replaced by ½ LOD value, the summary statistics for these compounds are not included in box and whisker plots (due to bias[1]), and only mean values are reported

Name	1	2	3	4	5	6	7
6:2 FTOH	*0.36*	32	4.5	*0.36*	34	*0.36*	*0.36*
8:2 FTOH	21	27	5.8	6.8	14	7.3	8.5
10:2 FTOH	17	21	3.0*	2.5*	13	3.6	4.6
∑FTOH	39	79	13	9.7	61	11	14
MeFOSA	0.82*	0.97*	2.5	0.71*	0.81*	0.42*	3.3
EtFOSA	0.72	0.85	0.98	0.43	0.54	0.25*	1.5
MeFOSE	44	8.9	17	20	20	14	20
EtFOSE	24	3.4	6.3	9.2	13	12	14
PFOSA	5.9*	13	45	37	37	95	67
∑FOSA–FOSE	75	27	71	67	72	120	110
PFHxS	5.8	13	21	17	13	43	21
PFOS	830	1700	7200	6000	480	2300	6900
PFDS	*0.04*	2.3	18	16	1.1	4.9	15
∑PFSA	830	1700	7300	6000	500	2300	6900
PFBA	*63*	20*	9.3*	*63*	*63*	*63*	10*
PFPA	*19*	0.99*	1.3*	1.9*	73	44	31*
PFHxA	5.7	15	57	63	66	110	110
PFHpA	2.5*	5.5*	10	20	29	40	32
PFOA	12	23	60	64	76	150	110
PFNA	3.0	8.0	48	40	8.6	23	44
PFDA	4.0	15	110	93	9.5	29	110
PFUnDA	4.4*	*15*	1.1*	47	*15*	*15*	4.7*
PFDoDA	*1.2*	0.09*	0.48*	1.2*	0.20*	1.7*	0.58*
PFTDA	*0.21*	0.35*	0.25*	0.03*	0.02*	0.29*	0.13*
∑PFCA	120	100	300	390	340	470	460

Table A10. (*Continued*)

Name	8	9	10	11	12	mean	s.d.
6:2 FTOH	20	*0.36*	*0.36*	*0.36*	*0.36*	7.7	13
8:2 FTOH	9.1	6.7	6.2	9.4	*0.25*	10	7.2
10:2 FTOH	6.6	4.1	4.1	6.0	4.5	7.5	6.1
∑FTOH	35	11	11	16	5.1	25	24
MeFOSA	2.0	2.1	0.66*	1.7	0.27*	1.4	0.94
EtFOSA	1.3	0.89	0.52	0.99	0.74	0.80	0.34
MeFOSE	21	23	12	10	6.6	18	9.8
EtFOSE	14	14	8.8	5.8	4.0	11	5.6
PFOSA	46	29	42	27	12	38	25
∑FOSA–FOSE	85	68	63	45	23	69	28
PFHxS	16	6.7	7.8	8.0	3.3	15	11
PFOS	5700	1700	2900	5100	2100	3600	2400
PFDS	9.7	3.1	4.1	11	2.7	7.4	6.4
∑PFSA	5700	1700	3000	5100	2100	3600	2500
PFBA	38*	16*	*63*	21*	79*	42	26
PFPA	*19*	6.3*	3.7*	19	41	22	22
PFHxA	85	28	34	31	15	52	36
PFHpA	25	12	12	16	12	18	12
PFOA	89	45	44	35	140	71	45
PFNA	32	12	12	16	7.6	21	16
PFDA	85	21	22	39	15	46	40
PFUnDA	0.68*	2.03*	*15*	47	0.59*	14	17
PFDoDA	1.5*	0.20*	*1.2*	0.59*	4.7	1.1	1.2
PFTDA	0.03*	0.14*	0.06*	0.03*	2.2	0.31	0.62
∑PFCA	380	140	210	230	320	290	130

Table A11. Particle-phase concentrations (blank corrected) at the secondary clarifier

Concentrations are given in picograms per cubic metre. Values that fell below the LOD but above the mean blank are indicated with an asterisk (*). Non-detections and cases where blank correction resulted in a negative value are replaced with ½ LOD value (Table A6) and italicised. Note: in case where more than 25% of samples for a given target chemical are replaced by ½ LOD value, the summary statistics for these compounds are not included in box and whisker plots (due to bias[1]), and only mean values are reported

Name	1	2	3	4	5	6	7
6:2 FTOH	*0.36*	*0.36*	*0.36*	*0.36*	*0.36*	*0.36*	*0.36*
8:2 FTOH	*0.25*	*0.25*	*0.25*	*0.25*	*0.25*	*0.25*	*0.25*
10:2 FTOH	4.0	5.2	1.4*	1.0*	1.7*	0.82*	1.3*
∑FTOH	4.6	5.8	2.0	1.6	2.3	1.4	2.0
MeFOSA	0.31*	0.13*	0.10*	*0.66*	0.10*	*0.66*	0.10*
EtFOSA	0.32*	0.29*	0.24*	0.10*	0.23*	0.30*	0.17*
MeFOSE	12	2.6*	2.5*	2.8*	3.6*	2.3*	3.5*
EtFOSE	13	0.82*	1.4*	1.0*	1.5*	1.6*	0.94*
PFOSA	5.7*	1.7*	2.3*	0.97*	8.0	12	3.8*
∑FOSA–FOSE	31	5.5	6.6	5.6	13	17	8.5
PFHxS	14	7.7	7.2	5.8	41	35	15
PFOS	770	840	800	620	760	1100	1500
PFDS	1.6	1.2	0.88	0.95	1.8	2.6	1.4
∑PFSA	790	850	810	630	800	1200	1600
PFBA	*63*	3.7*	9.0*	*63*	*63*	*63*	7.8*
PFPA	*19*	*19*	*19*	*19*	*19*	*19*	*19*
PFHxA	8.5	5.5	6.9	6.4	45	26	12
PFHpA	8.8	1.1*	0.66*	4.3*	7.7*	5.5*	3.8*
PFOA	19	12	13	16	57	44	18
PFNA	5.4	4.4	4.5	3.7	12	12	6.8
PFDA	6.7	6.3	6.8	4.5	9.8	15	11
PFUnDA	1.94*	*15*	*15*	*15*	*15*	*15*	*15*
PFDoDA	*1.2*	*1.2*	*1.2*	*1.2*	0.08*	0.41*	*1.2*
PFTDA	0.16*	0.09*	*0.21*	0.03*	0.13*	0.36*	0.05*
∑PFCA	130	68	76	130	230	200	95

Table A11. (*Continued*)

Name	8	9	10	11	12	mean	s.d.
6:2 FTOH	*0.36*	*0.36*	*0.36*	*0.36*	*0.36*	*0.36*	*0.0*
8:2 FTOH	*0.25*	*0.25*	*0.25*	*0.25*	*0.25*	*0.25*	*0.0*
10:2 FTOH	1.8*	1.7*	1.6*	1.2*	0.84*	1.9	1.3
∑FTOH	2.4	2.3	2.2	1.8	1.5	2.5	1.3
MeFOSA	*0.66*	0.17*	*0.66*	*0.66*	*0.66*	0.41	0.27
EtFOSA	0.25*	0.18*	0.27*	*0.19*	0.20*	0.23	0.06
MeFOSE	4.7	5.0	2.6*	0.77*	1.7*	3.7	2.8
EtFOSE	1.7*	1.3*	0.81*	0.94*	0.94*	2.1	3.5
PFOSA	1.5	3.1*	4.9*	2.3*	1.9*	4.0	3.2
∑FOSA–FOSE	8.7	9.8	9.2	4.9	5.5	11	7.5
PFHxS	12	13	16	9.7	10	15	11
PFOS	1100	1400	1600	1100	860	1000	320
PFDS	1.2	1.6	1.8	1.2	0.84	1.4	0.55
∑PFSA	1100	1400	1600	1100	880	1100	320
PFBA	17*	9.3*	*63*	11*	1.4*	31	28
PFPA	*19*	*19*	*19*	*19*	*19*	19	0.0
PFHxA	8.9	11	13	8.3	5.0	13	12
PFHpA	2.5*	1.1*	3.1*	3.7*	3.9*	3.8	2.5
PFOA	15	17	21	16	51	24.8	16
PFNA	6.1	7.2	8.2	6.8	4.7	6.8	2.8
PFDA	7.6	9.0	10	7.2	6.5	8.3	2.7
PFUnDA	*15*	*15*	*15*	27	*15*	15	5.4
PFDoDA	2.4*	*1.2*	*1.2*	*1.2*	3.1	1.3	0.77
PFTDA	0.22*	0.05*	*0.21*	*0.21*	0.29*	0.17	0.10
∑PFCA	93	89	150	100	110	120	50

Composition in air samples

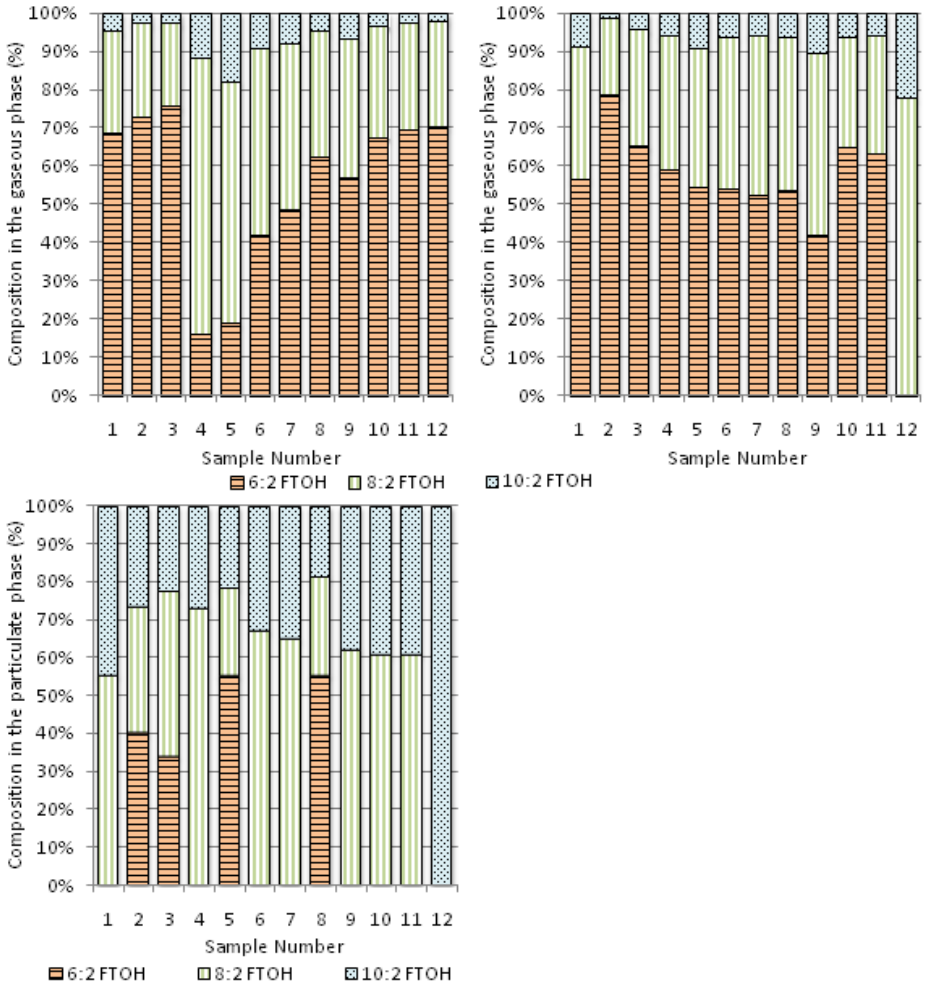

Fig. A1. Composition of FTOHs in the gas phase (top) and the particle phase (bottom) at the aeration tank (left) and the secondary clarifier (right). FTOH concentrations at the secondary clarifier were below the IDL for 6:2 FTOH and 8:2 FTOH.

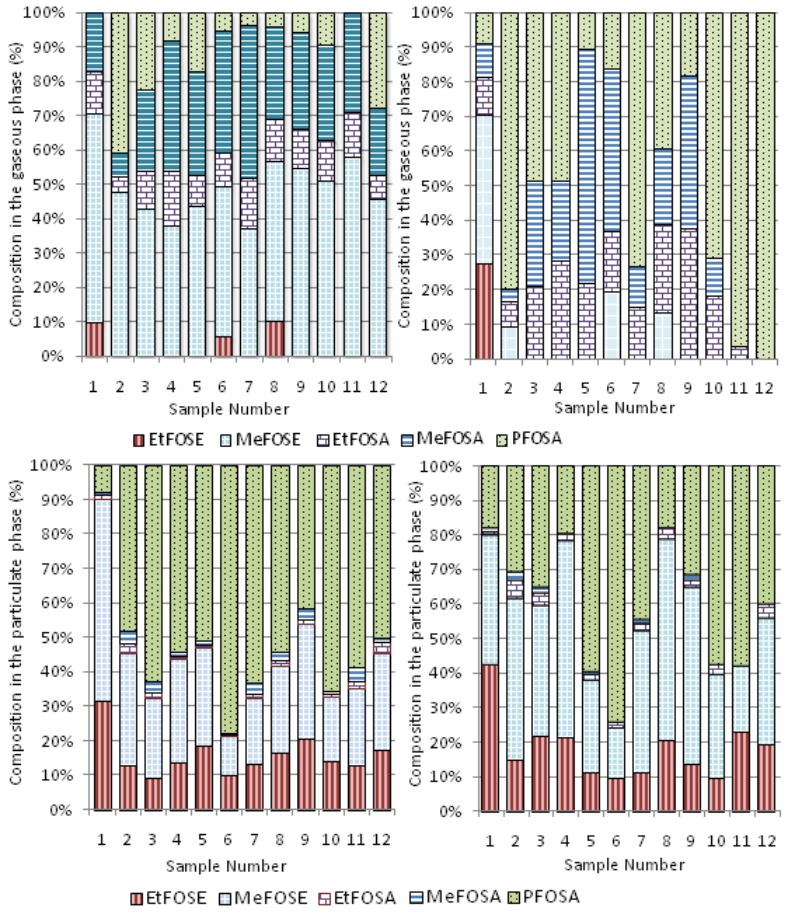

Fig. A2. Composition of FOSAs and FOSEs in the gas phase (top) and the particle phase (bottom) at the aeration tank (left) and the secondary clarifier (right). In the gas phase in sample 12 at the secondary clarifier all compound except of PFOSA were below the IDL.

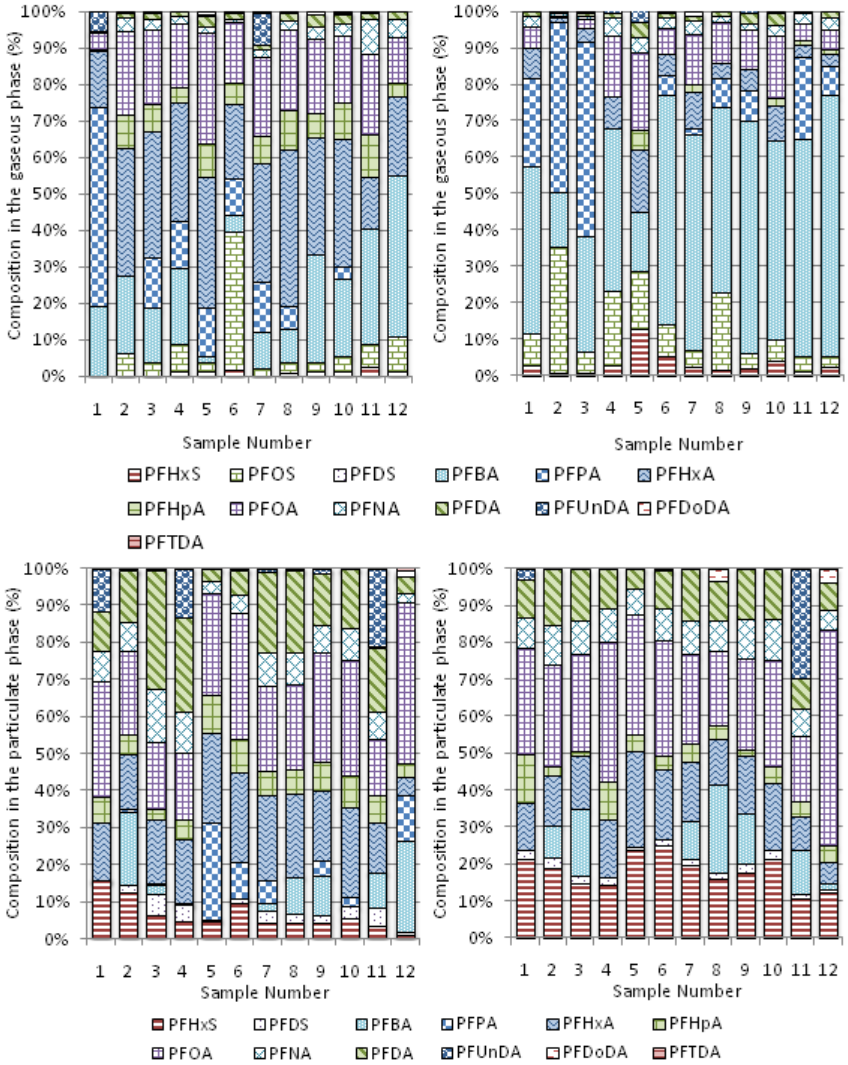

Fig. A3. Composition of PFCAs and PFSAs in the gas phase (top) and the particle phase (bottom) at the aeration tank (left) and the secondary clarifier (right). The particle phase concentrations of PFOS in each sample (~90% in average) are not shown.

References

[1] D. R. Helsel, M. T. Obvious, Better methods for interpreting nondetect data. *Environ. Sci. Technol.* **2005**, *39*, 419A. doi:10.1021/es053368a