Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Distributions and sources of traditional and emerging per- and polyfluoroalkyl substances among multiple environmental media in the Qiantang River watershed, China

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TableS1 The abbreviations and structures of PFASs

Compound name	Abbreviation	Structures	Category
Perfluorobutanoic acid	PFBA	$CF_3(CF_2)_2COOH$	T
Perfluoropentanoic acid	PFPeA	$CF_3(CF_2)_3COOH$	T
Perfluorohexanoic acid	PFHxA	$CF_3(CF_2)_4COOH$	T
Perfluoroheptanoic acid	PFHpA	$CF_3(CF_2)_5COOH$	T
Perfluorooctanoic acid	PFOA	$CF_3(CF_2)_6COOH$	T
Perfluorononanoic acid	PFNA	$CF_3(CF_2)_7COOH$	T
Perfluorodecanoic acid	PFDA	$CF_3(CF_2)_8COOH$	T
Perfluoroundecanoic acid	PFUnA	$CF_3(CF_2)_9COOH$	T
Perfluorododecanoic acid	PFDoA	$CF_3(CF_2)_{10}COOH$	T
Perfluorotridecanoic acid	PFTrA	$CF_3(CF_2)_{11}COOH$	T
Perfluorotetradecanoic acid	PFTeA	$CF_3(CF_2)_{12}COOH$	T
Perfluorobutane sulfonate	PFBS	$CF_3(CF_2)_3SO_3H$	T
Perfluorohexane sulfonate	PFHxS	$CF_3(CF_2)_5SO_3H$	T
Perfluoroheptane sulfonate	PFHpS	$CF_3(CF_2)_6SO_3H$	T
Perfluorooctane sulfonate	PFOS	$CF_3(CF_2)_7SO_3H$	T
Perfluorodecane sulfonate	PFDS	$CF_3(CF_2)_9SO_3H$	T
N-methylperfluoro octanesulfonamidoacetic acid	N-MeFOSAA	$CF_3(CF_2)_7SO_2N(CH_3)CH_2CO_2H$	T
N-ethylperfluorooctane sulfonamidoacetic acid	N-EtFOSAA	$CF_3(CF_2)_7SO_2N(CH_2CH_3)CH_2CO_2H$	T
Hexafluoropropylene oxide-dimer acid	HFPO-DA	$CF_3(CF_2)_2$ $OCF(CF_3)COOH$	E
Sodium 4,8-dioxa-3H-perfluorononanoate	ADONA	$CF_3O(CF_2)_3OCFCF_2COONa$	E
6:2 Chlorinated polyfluorinated ether sulfonate	6:2Cl-PFESA	$Cl(CF_2)_6O(CF_2)_2SO_3^-$	E
8:2 Chlorinated perfluoroether ether sulfonate	8:2Cl-PFESA	$Cl(CF_2)_8O(CF_2)_2SO_3^-$	E
Perfluoro-methoxypropionic acid	PFMPA	$CF_3O(CF_2)_2COOH$	E

Compound name	Abbreviation	Structures	Category
Perfluoro-4-methoxybutanoic acid	PFMBA	$CF_3O(CF_2)_3COOH$	E
Perfluoro-3,6-dioxaheptanoic acid	NFDHA	$CF_3O(CF_2)_2OCF_2COOH$	E
Perfluoro-2-ethoxyethane sulfonate	PFEESA	$CF_3CF_2O(CF_2)_2SO_3^-$	E

Compounds were categorized as traditional (T) or emerging (E) using data presented in Xiao [1] and Wang et al. [2]

TableS2 Detection limit, quantitation limit and recovery of PFASs in different matrix

Compound	Water（n=6）			Soil/Sediment（n=6）			$PM_{2.5}$（n=6）		
	LLOD	LLOQ	Recovery	LLOD	LLOQ	Recovery	LLOD	LLOQ	Recovery
	ng/L	ng/L	%	ng/L	ng/L	%	ng/L	ng/L	%
PFBA	0.2	0.8	95.4±23.4	0.03	0.12	112.5±29.6	2.2	8.8	95.0±21.4
PFPeA	0.2	0.8	114.5±19.2	0.03	0.12	89.7±5.4	2.2	8.8	112.7±18
PFHxA	0.02	0.08	102.7±15.6	0.003	0.01	127.2±10.6	0.2	0.8	108.7±18
PFHpA	0.02	0.08	94.3±24.0	0.003	0.01	85.7±16.6	0.2	0.8	78.2±20.4
PFOA	0.02	0.08	131.5±35.2	0.003	0.01	97.9±28.6	0.2	0.8	130.3±34
PFNA	0.02	0.08	108.8±29.6	0.003	0.01	96±27.8	0.2	0.8	111.8±26.4
PFDA	0.04	0.2	84.9±20.2	0.004	0.02	98.4±4.6	0.3	1.2	81.0±30.0
PFUnA	0.03	0.2	102.7±22.4	0.004	0.02	75.4±18.8	0.3	1.2	94.4±30.0
PFDoA	0.03	0.2	91.7±18.6	0.004	0.02	72.4±29.6	0.3	1.2	105.8±0.6
PFTrA	0.03	0.2	102.6±38.2	0.004	0.02	104.9±1.0	0.3	1.2	81.6±28.2
PFTeA	0.03	0.2	80.3±34.2	0.004	0.02	108.2±25.2	0.3	1.2	111.0±1.0
PFBS	0.09	0.4	88.3±11.0	0.01	0.04	119.2±15.8	0.9	3.6	116.2±18.8
PFHxS	0.02	0.08	107.4±5.6	0.003	0.01	126.5±2.4	0.2	0.8	67.9±29.8
PFHpS	0.01	0.04	97.8±4.2	0.001	0.004	98.5±37.6	0.09	0.4	71.3±20.2
PFOS	0.01	0.04	108.6±11.6	0.001	0.004	99.9±26.4	0.09	0.4	106.5±7.8
PFDS	0.01	0.04	62.7±10.2	0.001	0.004	60.0±18.8	0.09	0.4	126.1±2.6
N-MeFOSAA	0.02	0.08	98±13.8	0.003	0.01	98.5±17.0	0.2	0.8	103.6±14.8
N-EtFOSAA	0.02	0.08	95.7±6.8	0.003	0.01	81.5±35.6	0.2	0.8	62.0±6.8
HFPO-DA	0.2	0.8	85±22.8	0.03	0.12	98.6±29.6	2.2	8.8	74.0±20.0
ADONA	0.005	0.02	120.6±10.0	0.001	0.004	121.2±18.2	0.04	0.2	116.5±8.8
6:2Cl-PFESA	0.004	0.02	75±37.2	0.001	0.004	63.7±20.2	0.04	0.2	104.7±3.8
8:2Cl-PFESA	0.005	0.02	110.3±19.4	0.001	0.004	112.0±14.4	0.04	0.2	82.6±34.0

Compound	Water（n=6）			Soil/Sediment（n=6）			$PM_{2.5}$（n=6）		
	LLOD ng/L	LLOQ ng/L	Recovery %	LLOD ng/L	LLOQ ng/L	Recovery %	LLOD ng/L	LLOQ ng/L	Recovery %
PFMPA	0.01	0.04	86.3±10.4	0.001	0.004	85.7±18.0	0.09	0.4	67.6±33.4
PFMBA	0.01	0.04	113.3±22.8	0.001	0.004	101.1±15.6	0.09	0.4	64.8±37.4
NFDHA	0.2	0.8	106.7±17.6	0.02	0.08	95.7±22.4	1.3	5.2	66.9±39.2
PFEESA	0.004	0.02	105.5±17.4	0.001	0.004	73.6±24.2	0.04	0.2	104.8±0.6

LLOD means detection limit; LLOQ means quantitation limit.

Table S3 Concentrations of 26 PFASs in the environment of Qiantang River watershed

Compound	Water (ng/L)			$PM_{2.5}$ (pg/m^3)			Soil (ng/g)			Sediment (ng/g)		
	Mean	Range	DF(%)	Mean	Range	DF(%)	Mean	Range	DF(%)	Mean	Range	DF(%)
PFBA	0.28	<LLOD~1.02	9.4	1.14	<LLOD~4.07	29	<LLOD	<LLOD	/	<LLOD	<LLOD	/
PFPeA	1.66	<LLOD~16.5	97	53.7	17.0~110.7	100	<LLOD	<LLOD	/	<LLOD	<LLOD	/
PFHxA	14.7	0.3~170	100	3.09	0.56~9.13	100	0.07	<LLOD~0.94	7.1	0.17	<LLOD~0.87	7.1
PFHpA	2.74	<LLOD~21.4	97	4.35	<LLOD~10.2	71	<LLOD	<LLOD	/	<LLOD	<LLOD	/
PFOA	96.7	3.01~525	100	50.4	9.01~216	100	1.05	0.71~2.8	100	1.18	0.72~3.00	100
PFNA	1.20	<LLOD~9.27	100	2.03	<LLOD~7.10	57	0.21	<LLOD~0.97	21	0.20	<LLOD~0.99	21
PFDA	2.21	<LLOD~4.98	94	1.59	<LLOD~7.66	71	0.61	<LLOD~1.22	50	0.26	<LLOD~1.29	50
PFUnA	0.23	<LLOD~3.16	59	2.30	<LLOD~10.3	71	0.38	<LLOD~1.33	29	0.53	<LLOD~1.35	29
PFDoA	0.46	<LLOD~1.46	41	3.91	<LLOD~13.7	29	<LLOD	<LLOD	7.1	<LLOD	<LLOD	/
PFTrA	0.06	<LLOD~0.84	19	5.85	<LLOD~19.9	86	<LLOD	<LLOD	/	<LLOD	<LLOD	/
PFTeA	0.04	<LLOD~0.51	16	6.26	<LLOD~19.7	71	0.12	<LLOD~1.68	/	<LLOD	<LLOD	7.1
PFBS	0.61	0.13~2.53	100	14.6	<LLOD~43.2	57	<LLOD	<LLOD	/	<LLOD	<LLOD	/
PFHxS	7.27	<LLOD~65.8	88	0.06	<LLOD~0.40	14	0.06	<LLOD~0.83	7.1	0.37	<LLOD~1.01	7.1
PFHpS	0.02	<LLOD~0.22	9.4	<LLOD	<LLOD	<LLOD	<LLOD	<LLOD	/	<LLOD	<LLOD	/
PFOS	2.31	<LLOD~12.3	97	6.30	2.90~17.0	100	0.57	<LLOD~1.05	57	0.60	<LLOD~1.02	57
PFDS	0.02	<LLOD~0.1	3.1	<LLOD	<LLOD	<LLOD	<LLOD	<LLOD	/	<LLOD	<LLOD	/
N-MeFOSAA	0.21	<LLOD~0.11	3.1	36.0	33.0~39.0	14	0.24	<LLOD~1.96	14	<LLOD	<LLOD	14
N-EtFOSAA	<LLOD	<LLOD	/	<LLOD	<LLOD	14	0.59	<LLOD~3.15	21	<LLOD	<LLOD	21
HFPO-DA	3.54	<LLOD~47.1	72	0.04	<LLOD~0.29	<LLOD	<LLOD	<LLOD	/	<LLOD	<LLOD	/
ADONA	0.09	<LLOD~1.27	28	0.07	<LLOD~0.48	43	<LLOD	<LLOD	/	<LLOD	<LLOD	/
6:2Cl-PFESA	34.1	<LLOD~4.61	91	<LLOD	<LLOD	57	0.57	<LLOD~1.16	50	0.68	<LLOD~1.14	50
8:2Cl-PFESA	2.16	<LLOD~0.34	16	0.04	<LLOD~0.24	<LLOD	0.23	<LLOD~1.63	14	0.33	<LLOD~1.63	14

Compound	Water (ng/L)			$PM_{2.5}$ (pg/m^3)			Soil (ng/g)			Sediment (ng/g)		
	Mean	Range	DF(%)	Mean	Range	DF(%)	Mean	Range	DF(%)	Mean	Range	DF(%)
NFDHA	1.13	<LLOD~5.07	78	0.59	<LLOD~2.73	<LLOD	<LLOD	<LLOD	/	<LLOD	<LLOD	/
PFEESA	0.03	<LLOD~0.49	9.4	<LLOD	<LLOD	<LLOD	<LLOD	<LLOD	/	<LLOD	<LLOD	/
PFMBA	0.03	<LLOD~0.46	13	<LLOD	<LLOD	<LLOD	<LLOD	<LLOD	/	<LLOD	<LLOD	/
Emerging PFASs	143	3.58~735	88	156	93.6~255	100	3.90	<LLOD	56	3.31	0.73~8.48	56
Traditional PFASs	6.08	<LLOD~51.4	100	0.63	<LLOD~2.77	25	0.81	0.72~11.1	25	1.00	<LLOD~2.76	25
ΣPFASs	149	3.58~786	100	156	93.9~255.2	77	4.70	<LLOD~2.79	46	4.31	0.73~8.48	46

LLOD means detection limit; DF means detection frequencies.

Table S4 The lgKd of PFASs between water and sediment / (ng/kg)

Compound	lgK_d
PFHxA	0.71
PFOA	1.16
PFNA	2.46
PFDA	2.85
PFUnA	4.02
PFHxS	2.36
PFOS	2.81
6:2Cl-PFESA	3.04
8:2Cl-PFESA	4.00

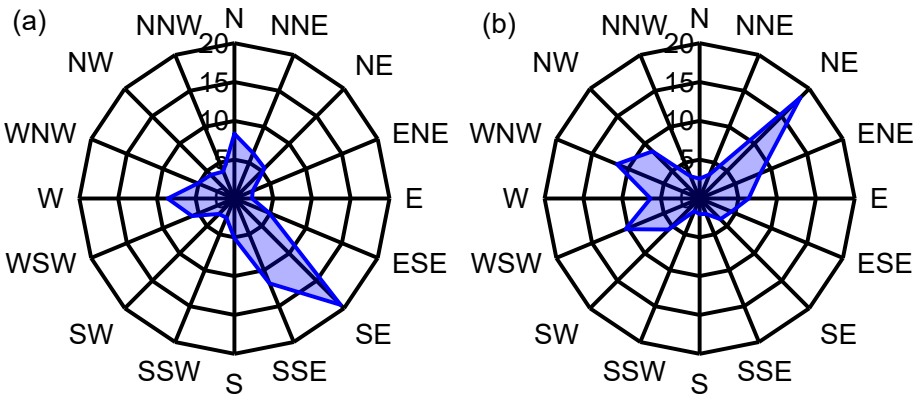

Fig. S1 The windrose diagram of (a) site 39 and (b) site 38

Reference

[1] F. Xiao, *Water Res*. 2017, 124, 482-495.

[2] Z. Y. Wang, I. T. Cousins, M. Scheringer, K. Hungerbuhler. *Environ Int*. 2013,60, 242-248.