Supplemental Information

Surfactant-enhanced coagulation and flocculation improves the removal of perfluoroalkyl substances from surface water

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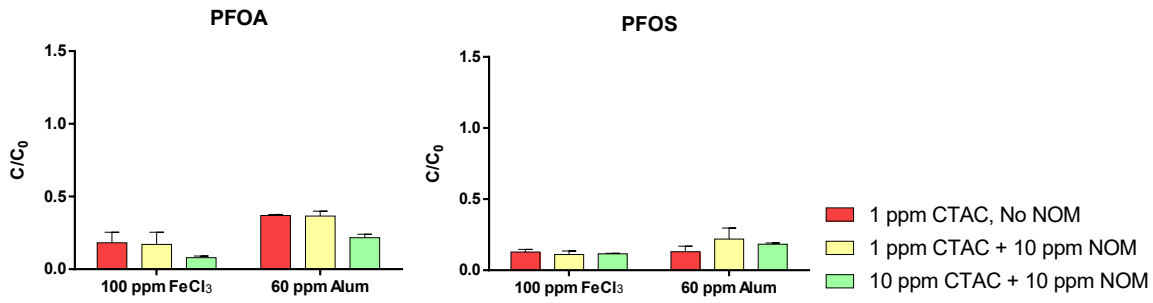

Figure S1. Removal of PFOA and PFOS in the presence increased NOM (10 mg/L) and CTAC (10 mg/L) dosage.

Table S1. Liquid chromatography and mass spectrometry conditions

Parameter	*Value*
LC	Agilent G7120A 1290 Binary Pump Agilent G7116A 1260 Multicolumn Thermostat Agilent G7167A 1260 Multisampler
Analytical column	Agilent ZOBRAX Eclipse Plus C18 3.0 x 50 mm, 1.8 µm
Delayed column	Agilent ZOBRAX Eclipse Plus C18 4.6 x 50 mm, 3.5 µm
Column temperature	50 °C
Injection volume	5 µL
Mobile phase	A) 5 mM Ammonium acetate in water B) 100% MeOH
Flow rate	0.4 mL/min
Gradient	Time (min) %B 0.0 10 0.5 10 2.0 30 14.0 95 14.5 100
Stop time	16.5 minutes
Post time	6 minutes

MS Instrument conditions

Parameter	*Value*
MS	Agilent 6495 Triple Quadrupole MS/MS Agilent Jet Stream ESI source
Gas Temperature	175 °C
Gas flow	17 L/min
Nebulizer	20 psi
Sheath gas temperature	275 °C
Sheath gas flow	11 L/min
Capillary voltage (Neg)	2500 V
Nozzle voltage (Neg)	0 V
iFunnel High pressure RF (Neg) Low pressure RF (Neg)	 90 V 40 V

Table S2. The MRM transitions for PFAS analysts and internal standards (IS) applied.

Analyte		**Precursor Ion (m/z)**	**Product Ion 1 (m/z)**	**Product Ion 2 (m/z)**
PFBS	Perfluorobutanesulfonic acid	299	80	99
PFBA	Perfluorobutanoic acid	213	169	-
PFOA	Perfluorooctanoic acid	413	369	169
PFOS*	Perfluorooctanesulfonic acid	499	80	99
4:2 FTS	4:2 fluorotelomer sulfonic acid	327	81	307
8:2 FTS	8:2 fluorotelomer sulfonic acid	527	81	507
Internal standard		**Precursor Ion (m/z)**	**Product Ion (m/z)**	**Product Ion 2 (m/z)**
$^{13}C_3$-PFBA	Perfluoro-n- [1,2,3,4-$^{13}C_4$] butanoic acid	216	172	-
$^{13}C_3$-PFBS	Perfluoro-1-[2,3,4-$^{13}C_3$] butanesulfonate	302	80	-
$^{13}C_5$-PFHxA	Perfluoro-n-[1,2,3,4,6-$^{13}C_5$] hexanoic acid	318	273	-
$^{13}C_3$-PFHxS	Perfluoro-1-[1,2,3-$^{13}C_3$] hexanesulfonate	402	80	-
$^{13}C_8$-PFOA	Perfluoro-n-[$^{13}C_8$] octanoic acid	421	376	-
$^{13}C_8$-PFOS	Perfluoro-1-[$^{13}C_8$] octanesulfonate	507	80	-

Table S3.Turbidity and pH measured for the batch samples tested under various conditions in Figure 5 before and after coagulation.

Turbidity and pH	Batch-1 (PAC 8mg/L)		Batch-2 (PAC 8mg/L Dup)		Batch-3 (PAC 16 mg/L)		Batch-4 (PAC 16 mg/L Dup)	
	before coagulation							
	Turbidity	pH	Turbidity	pH	Turbidity	pH	Turbidity	pH
Control PFAS	22.97	7.15	23.21	7.11	23.4	7.18	24.5	6.99
	after coagulation							
PAC+ PFAS	23.37	7.3	21.51	7.3	23.4	6.91	21.63	7.21
PAC +$FeCl_3$+ PFAS	0.81	3.75	0.77	3.76	0.72	3.67	2.05	3.52
CTAC+ $FeCl_3$ + PFAS	0.35	3.67	2.6	3.66	0.48	3.65	1.32	3.5
CTAC+ PAC+$FeCl_3$+ PFAS	0.76	3.74	1.33	3.6	1.18	4.22	2.03	3.63
CTAC+ PAC+ PFAS	18.10	6.75	20.4	6.27	21.5	6.13	23.00	7.18
Control PFAS	18.40	7.01	21.4	7.04	27.1	6.71	21.27	7.27