Supporting Information

Effect of chain length, electrolyte composition and aerosolization on the removal of per- and polyfluoroalkyl substances during electrochemical oxidation process

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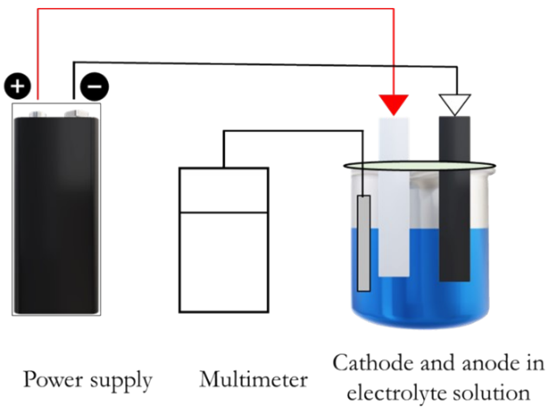

Figure S1: Schematic of the two-electrode electrochemical oxidation system

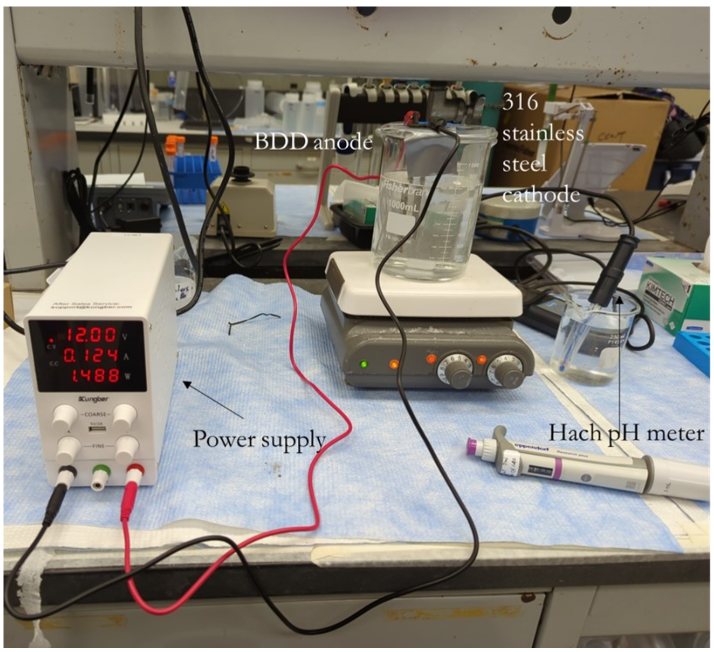

Figure S2: Actual picture of the two-electrode electrochemical oxidation system

Table S1. Variation of anodic voltage in solutions containing different electrolytes with varying applied voltage. Note: Solution conductivity maintained at 1000 μS/cm

Applied voltage	**Anodic voltage vs Ag/AgCl in**		
	Na_2SO_4	NaCl	$NaNO_3$
5	3.6	3.5	3.5
7.5	5.6	5.5	5.5
10	7.6	7.5	7.5
12	9.2	9.1	9.1
15	11.6	11.5	11.5
20	15.7	15.5	15.5
28	22.3	22.1	22.1

Table S2. MRM transitions for all compounds studied

Analyte	**Full name**	**Internal standard**	**Precursor (m/z)**	**Product 1 (m/z)***	**Product 2 (m/z)***
PFBA	Perfluorobutanoic acid	^{13}C4-PFBA	213	169	-
PFPeA	Perfluoropentanoic acid	^{13}C5-PFHxA	263	219	-
PFBS	Perfluorobutanesulfonic acid	^{13}C3-PFBS	299	80	99
PFHxA	Perfluorohexanoic acid	^{13}C5-PFHxA	313	269	119
PFHpA	Perfluoroheptanoic acid	^{13}C8-PFOA	363	319	169
PFHxS	Perfluorohexanesulfonic acid	^{13}C3-PFHxS	399	80	99
PFOA	Perfluorooctanoic acid	^{13}C8-PFOA	413	369	169
6:2FTS	1H,1H, 2H, 2H-Perfluorooctane sulfonic acid	^{13}C8-PFOS	427	407	81
PFNA	Perfluorononanoic acid	^{13}C8-PFOA	463	419	169
PFOS	Perfluorooctanesulfonic acid	^{13}C8-PFOS	499	80	99

*Products 1 and 2 serve as quantifier and qualifier, respectively.

Table S3. LC-MS/MS conditions

LC Instrument 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 micron
Delayed column	Agilent ZOBRAX Eclipse Plus C18 4.6 x 50 mm, 3.5 micron
Column temperature	50 °C
Injection volume	5 µL
Mobile phase	A) 5 mM Ammonium acetate in water B) Methanol
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
Drying gas temperature	175 °C
Drying 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 S4. Correlation between k_{obs} and physicochemical parameters for tested PFAS. Parameter values obtained from EPA's CompTox dashboard (predicted average values utilized).[1]

PFAS tested	**Parameter**	**Correlation factor with k_{obs}**
PFBS, PFOS, PFOA,PFNA, PFHxS, 6:2 FTS	Log K_{ow}	0.8
	Henry's law constant	0.19
	Polarizability	0.79
	Surface tension	-0.55
	Vapor pressure	-0.20
	Water solubility	-0.59
	Log K_{oa}	0.19
	Log K_{oc}	0.53

References

1. U. S. E. P. Agency, CompTox Chemicals Dashboard, https://comptox.epa.gov/dashboard/, (accessed November 2023).