Supporting Information

Detection of poly- and perfluoroalkyl substances (PFASs) in U.S. drinking water linked to industrial sites, military fire training areas and wastewater treatment plants

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Table S1. Acronyms for each poly- and perfluoroalkyl substances (PFASs) included in this study, full name and method reporting limit (MRL) in UCMR3 dataset.

Acronym	Full name	Perfluorinated carbons	Long-chain or short-chain[a]	MRL in UCMR3 (ng/L)
PFBS	perfluorobutane sulfonic acid	4	short-chain	90
PFHxS	perfluorohexane sulfonic acid	6	long-chain	30
PFHpA	perfluoroheptanoic acid	6	short-chain	10
PFOA	perfluorooctanoic acid	7	long-chain	20
PFOS	perfluorooctane sulfonic acid	8	long-chain	40
PFNA	perfluorononanoic acid	8	long-chain	20

[a] For carboxylates, long-chain PFASs are defined as those with 7 or more fluorinated carbons, and for sulfonates, long-chain PFASs include PFHxS as well as those with eight or more fluorinated carbons following the nomenclature recommended by Buck et al.[1]

Table S2. Geographical coordinates of major industrial sites included in this study

Company	State	Coordinates	Company	State	Coordinates
1	WV	39.266469, -81.665904	9	MN	44.788908, -92.911710
2	NJ	39.770261, -75.356080	10	IL	41.751568, -90.289291
3	VA	37.450298, -77.437892	11	NJ	40.660391, -74.107251
4	AL	34.641782, -87.044871	12	NJ	40.452134, -74.330899
5	KY	37.055394, -88.366971	13	NC	34.840297, -78.842319
6	NJ	39.844013, -75.209851	14	MS	30.354016, -88.495710
7	NC	35.294247, -81.007943	15	AR	33.110213, -92.675014
8	AL	31.278142, -87.999580	16	GA	34.145222, -84.828213

Table S3. Sensitivity analysis for the spatial regression models conducted by limiting industrial sites to specific compounds. Results have been transformed to reflect expected changes (%) in drinking water concentrations with each additional source.

Compound	Major industrial sites[a]	MFTAs[b]	AFFF certified airports	WWTPs[c]	λ[d]	R^2
PFOA						
Coefficient[e]	81%	10%	-6%	2%	52%	0.38
p-value[f]	<0.001	0.111	0.353	0.006	<0.001	
PFOS						
Coefficient	44%	34.6%	-5.6%	2.0%	76.2%	0.45
p-value	0.413	<0.001	0.541	0.005	<0.001	

[a] Only the major industrial sites participating in U.S. EPA 2010/2015 PFOA Stewardship Program were included (Table S2).
[b] Military fire training area.
[c] Wastewater treatment plant.
[d] Coefficient for the spatial error term characterizing spatial autocorrelation caused by unobserved variables.
[e] Positive coefficient in the results indicate increasing concentrations with increasing abundance of point sources within the same hydrologic unit.
[f] *p*-values for parameters in spatial error regression model.

Table S4. Detection frequencies for PFASs in different water source types.

	N	All PFASs	Perfluoroalkyl sulfonic acids			Perfluoroalkyl carboxylic acids		
			PFBS	PFHxS	PFOS	PFHpA	PFOA	PFNA
Groundwater[a]	22624	0.62%	0.03%	0.80%	1.0%	0.62%	1.2%	0.08%
Surface water	12733	0.31%	0.09%	0.13%	0.38%	0.68%	0.57%	0.01%
Mixed[b]	792	0.59%	0%	0.76%	1.3%	0.51%	1.0%	0%
All sources	36149	0.51%	0.05%	0.56%	0.79%	0.64%	0.98%	0.05%

[a] Includes both groundwater and groundwater close enough to nearby surface water (e.g., a river or lake) to receive direct surface water recharge.
[b] Any combination of groundwater, groundwater under the direct influence of surface water, and surface water.

Table S5 Detection frequencies for PFASs in drinking water in HUCs with and without point sources.

% PFASs detection	Presence of Point Source		*p*-value[d]
	No	Yes	
Industrial sites[a]	12.2%	46.7%	0.022
MFTA[b]	10.4%	28.2%	<0.001
AFFF certified airports	9.2%	22.2%	<0.001
More than three WWTPs[c]	7.6%	18.3%	<0.001
Overall		12.60%	

[a] Only major industrial sites that are part of the U.S. EPA's 2010/2015 PFOA Stewardship Program were included (Table S2).
[b] MFTA = Military fire training area.
[c] WWTP = Wastewater treatment plant. The median number of WWTPs in HUCs nationally is three. Sites with more than three plants thus have potentially elevated PFAS contributions from this source.
[d] Chi-square test was used to derive *p*-value.

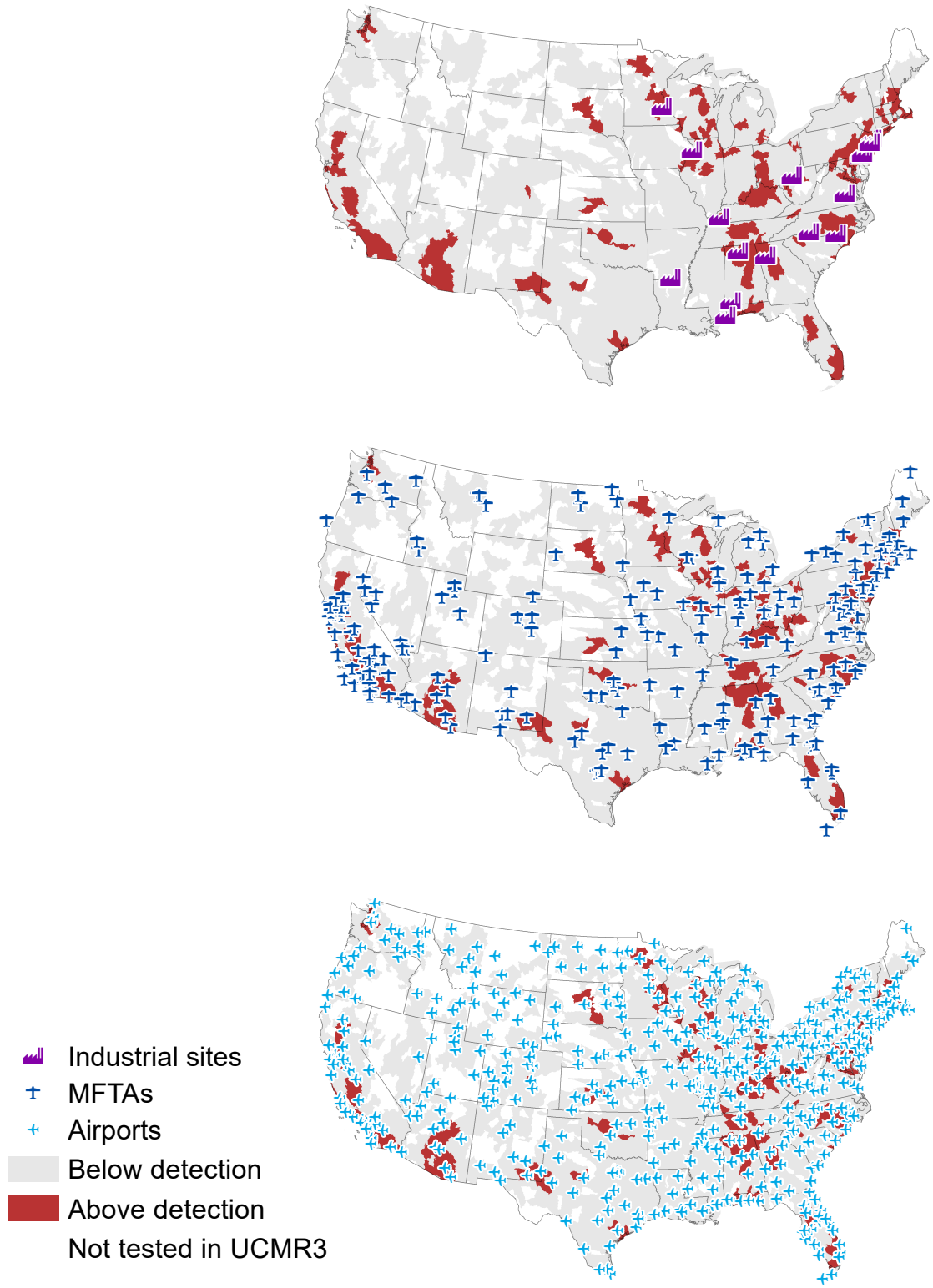

Figure S1. Map of selected point sources considered in this study, wastewater treatment plants are not shown.

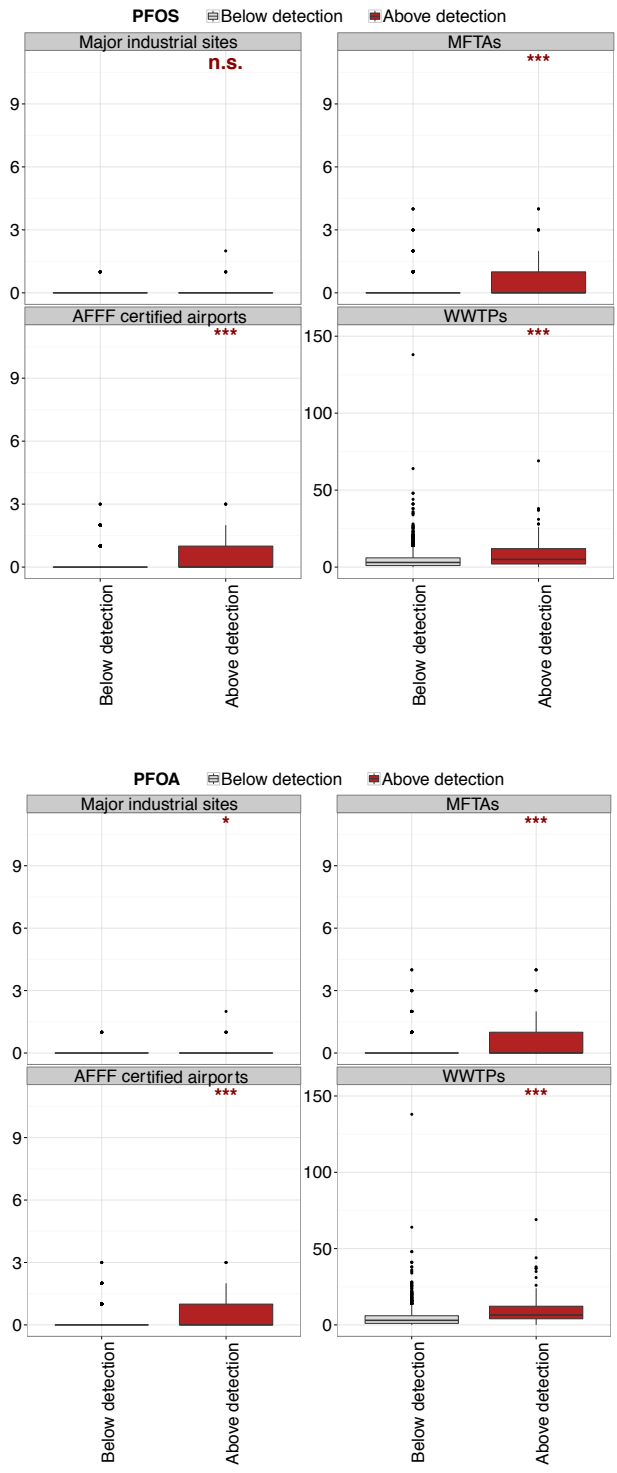

Figure S2. Comparison of the abundance of point sources within 8-digit hydrologic unit codes (HUCs) used a proxy for watersheds with PFOS (or PFOA) in drinking water above and below detection.

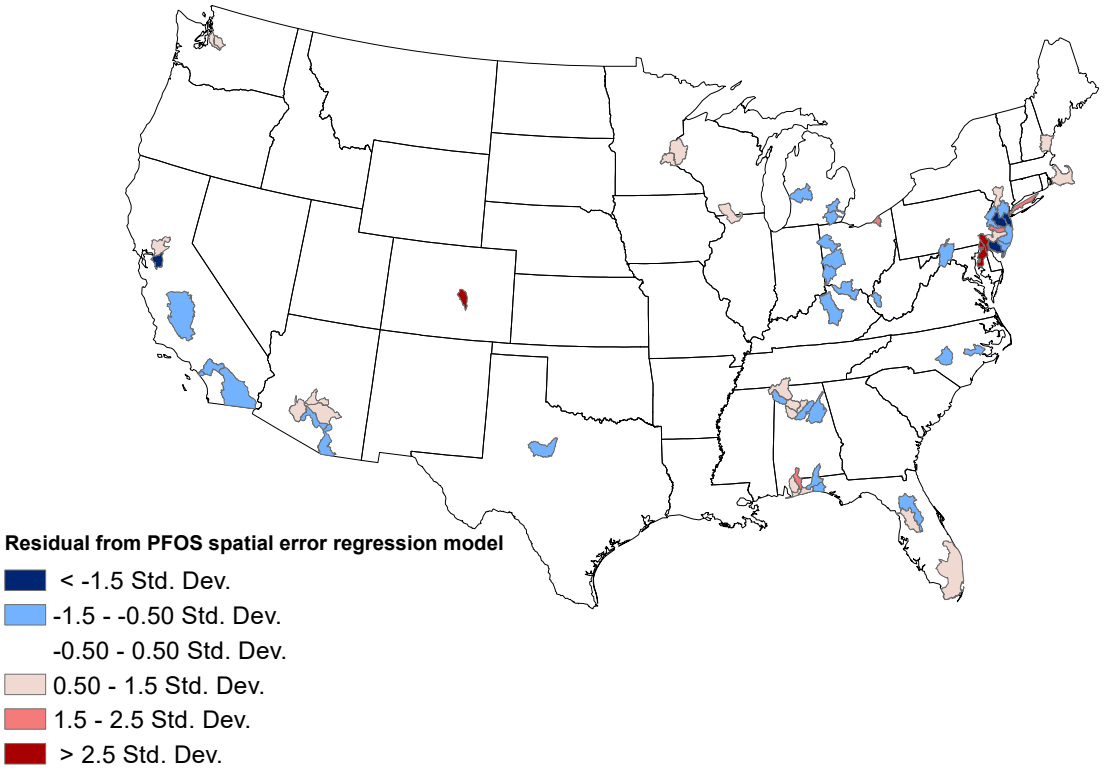

Figure S3. Residual from the spatial error model for concentrations of PFOS in drinking water. Spatial error greater than 1.5 standard deviation indicates that the high observed concentration cannot be explained by current source information. Areas like this such as Colorado Springs, Colorado, Long Island, New York should have high priority in future sampling work.

References Cited

1. Buck, R. C.; Franklin, J.; Berger, U.; Conder, J. M.; Cousins, I. T.; de Voogt, P.; Jensen, A. A.; Kannan, K.; Mabury, S. A.; van Leeuwen, S. P. J., Perfluoroalkyl and Polyfluoroalkyl Substances in the Environment: Terminology, Classification, and Origins. *Integrated Environmental Assessment and Management* **2011,** *7*, (4), 513-541.