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Pin the Tail on the PFAS:
Advanced PFAS Fingerprinting for Source Differentiation

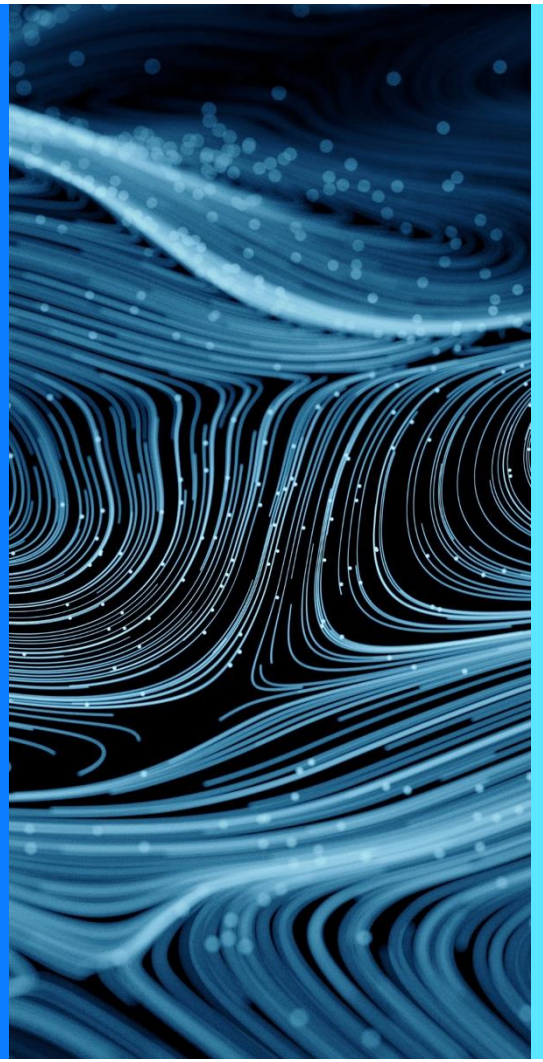


PNWS - 2026

Katie Walker, P.E.

Agenda

- Data Evaluation Techniques
- Case Study in Evaluating PFAS Sources and Transformations
- Translating Contamination to Solutions



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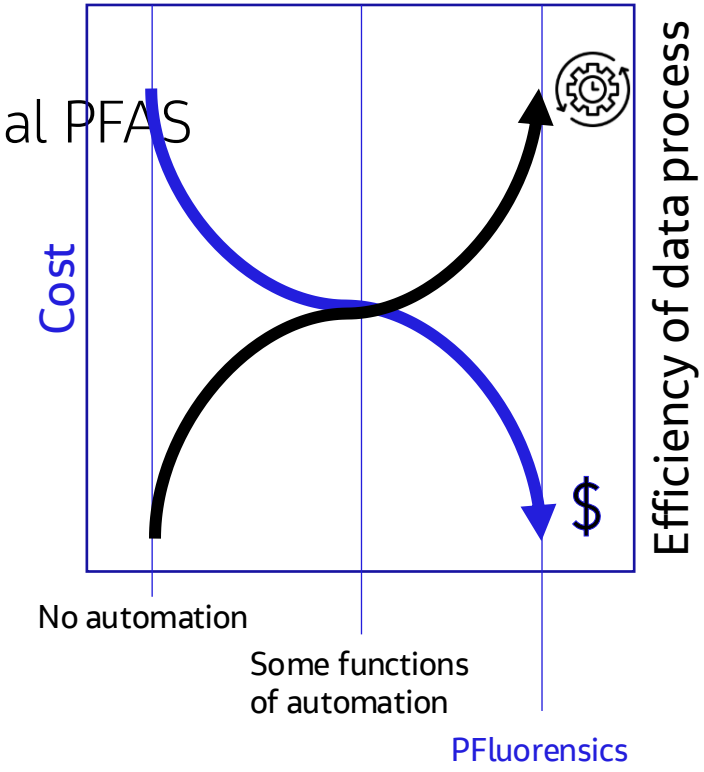


Data Evaluation Techniques

PFAS Data Evaluation Challenge

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- Complexity of PFAS Behavior
  - Variation in mobility, partitioning, and persistence of individual PFAS
  - Co-contaminant interaction and transformation
  - Comingled sources
- Limitations of Traditional Data Analysis Approaches
  - Insufficient for interpreting high-dimensional data
  - Lack of consistency and repeatability
- PFluorensics Facilitates:
  - Automated Exploratory Data Analysis
  - PFAS Fingerprinting
  - Understanding of Biotransformation



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PFluorensics: Data Model

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Data Sources

PFAS Samples

DSSTox1

PubChem[2]

PFAS Properties

Source Material[3]

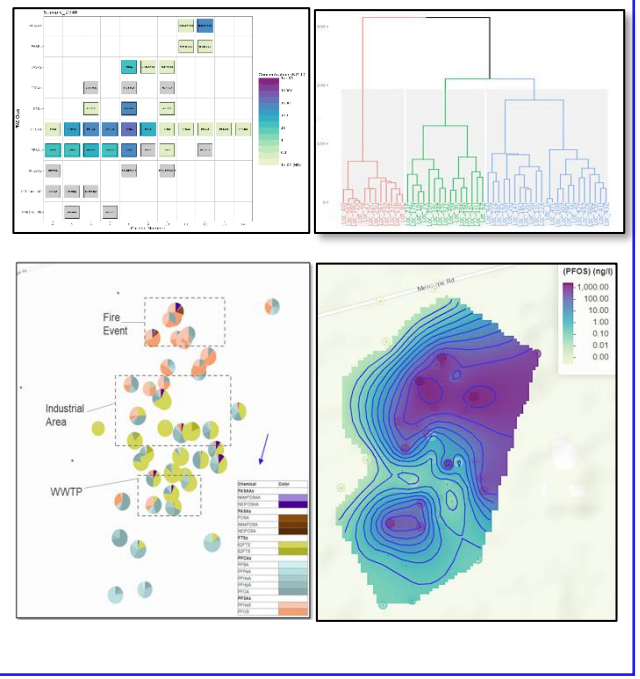
Biotransformation[4]

Cloud Data Storage

Application Process Interface (API)

Web App Analytics

ALLUVIAL SM



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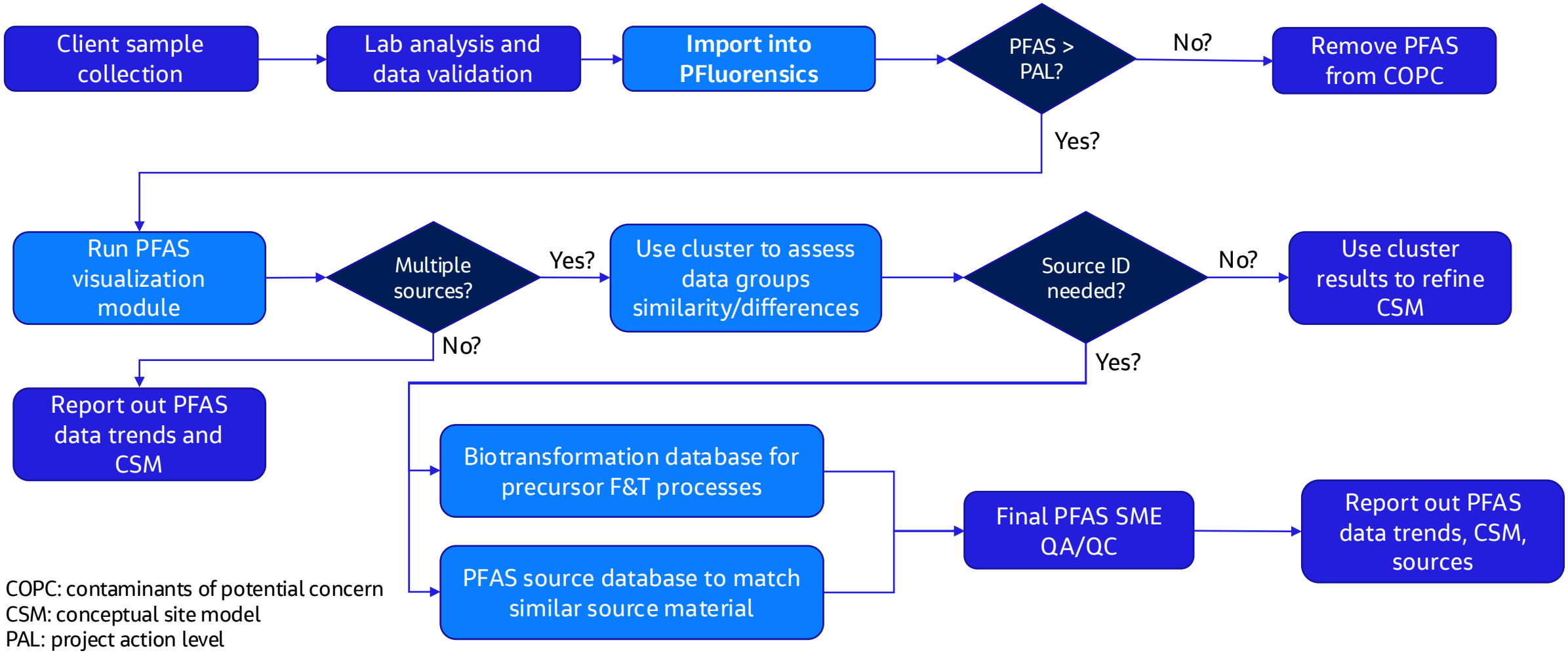
[1]https://www.epa.gov/chemical-research/distributed-structure-searchable-toxicity-dsstox-database
[2]https://pubchem.ncbi.nlm.nih.gov/docs/pug-rest

[3]Peer-reviewed and open-source AFFF, landfill leachate, wastewater, biosolids, textiles, and metal coatings
[4]Peer-reviewed and open-source transformation pathways

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PFluorensics Decision Framework

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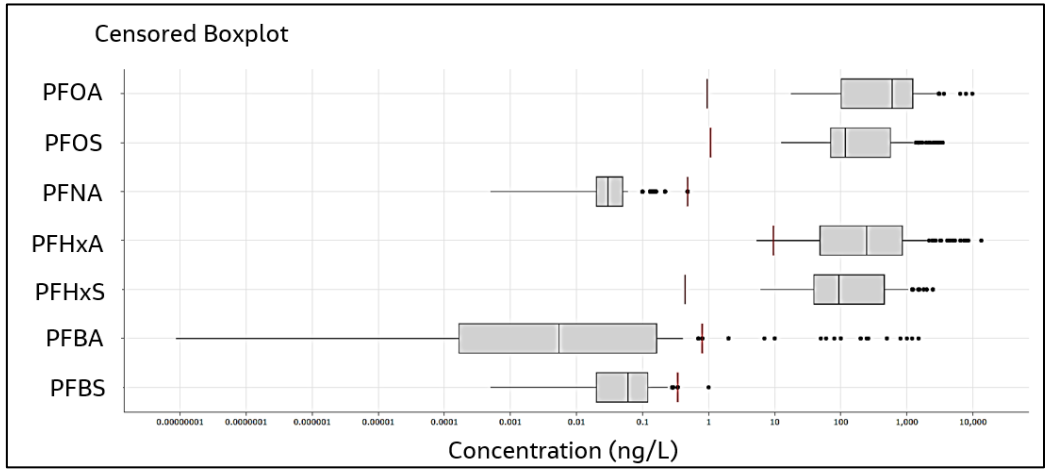


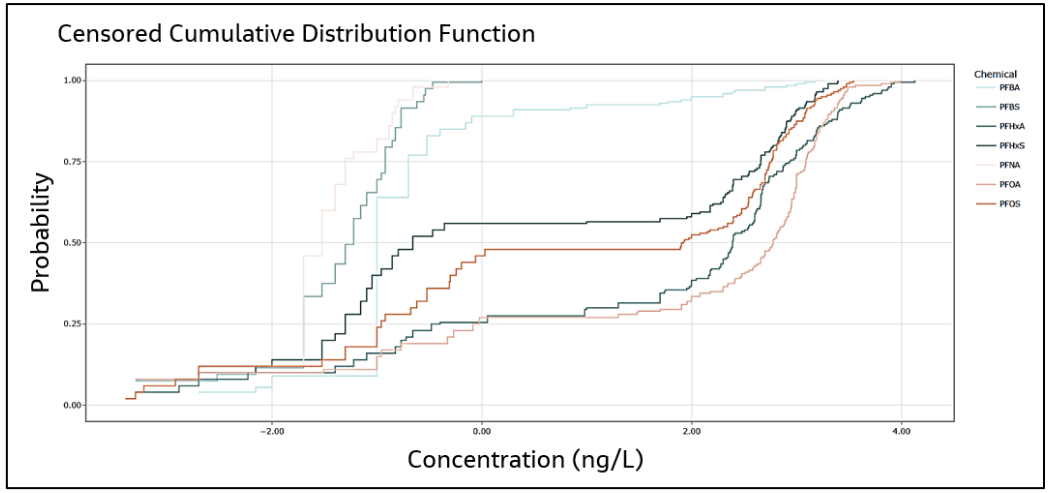
COPC: contaminants of potential concern
CSM: conceptual site model
PAL: project action level
SME: subject matter expert

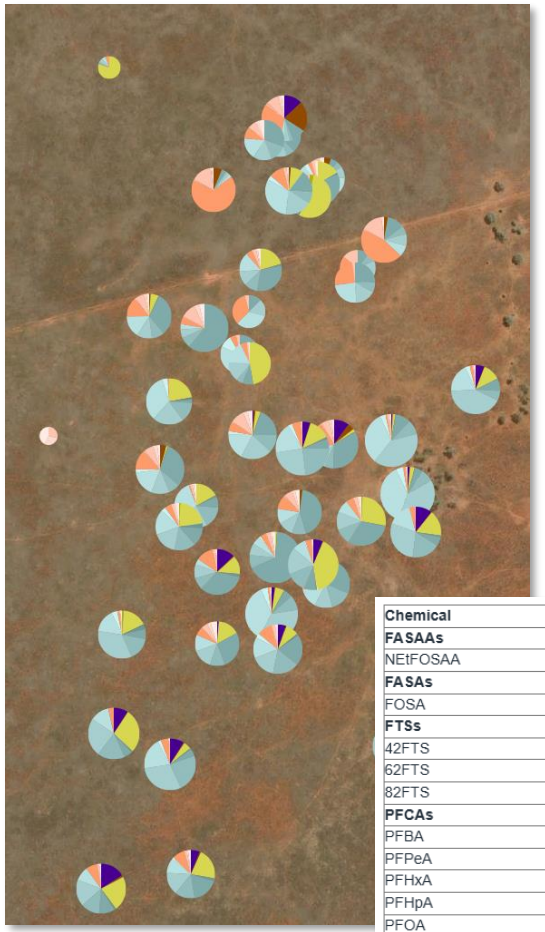
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Sample Distributions

- Sample Distributions
  - Boxplots
  - Empirical Cumulative Distribution Function
- Kaplan-Meier Summary Statistics
- Interactive spatial pie plots
  - Radius is relative to Total PFAS concentration
- Group/filter
  - Location
  - Matrix
  - Sample depth
  - Aquifer unit



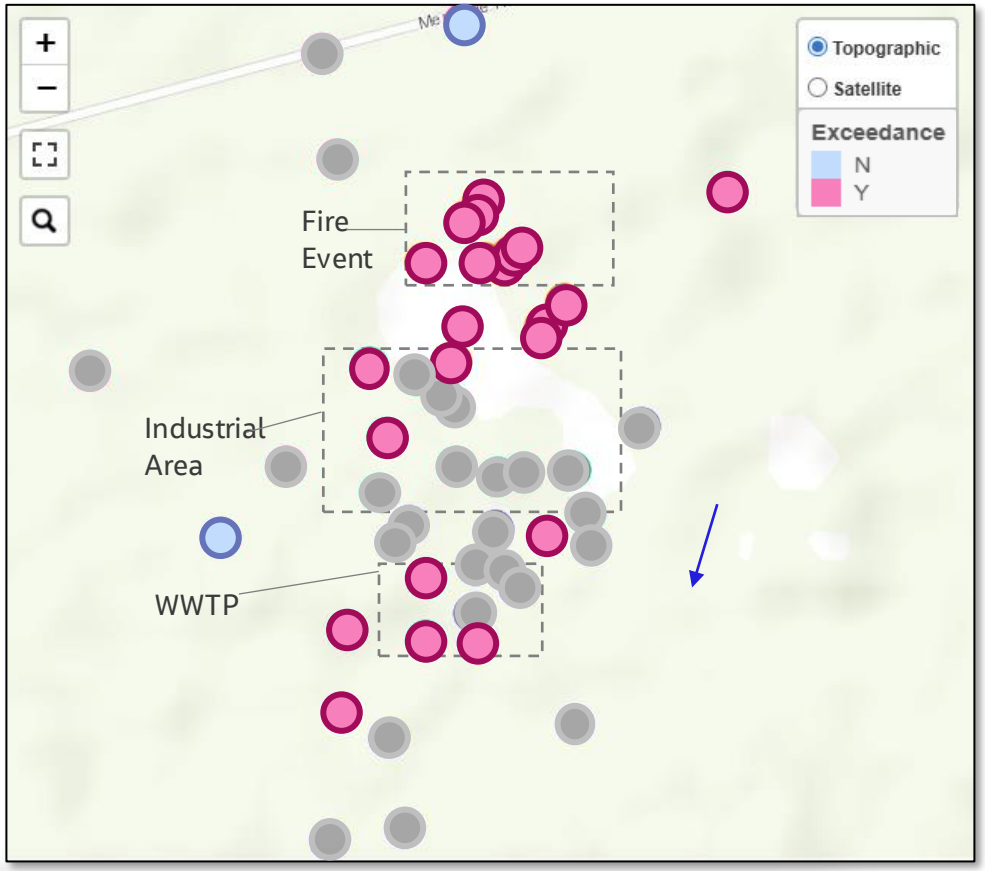




Chemical	Color
FASAAs	
NEtFOSAA	
FASAs	
FOSA	
FTSs	
42FTS	
62FTS	
82FTS	
PFCAs	
PFBA	
PFPeA	
PFHxA	
PFHpA	
PFOA	
PFNA	
PFDA	
PFSAs	
PFBS	
PFPeS	
PFHxS	
PFHpS	
PFOS	

Exceedance Evaluation

- PFAS data are compared against project action levels
- Pink = exceedance of one or more PALs
- Light blue = no exceedance of PALs
- Gray = the specific PFAS was not detected at the location
- View exceedances spatially and tabularly

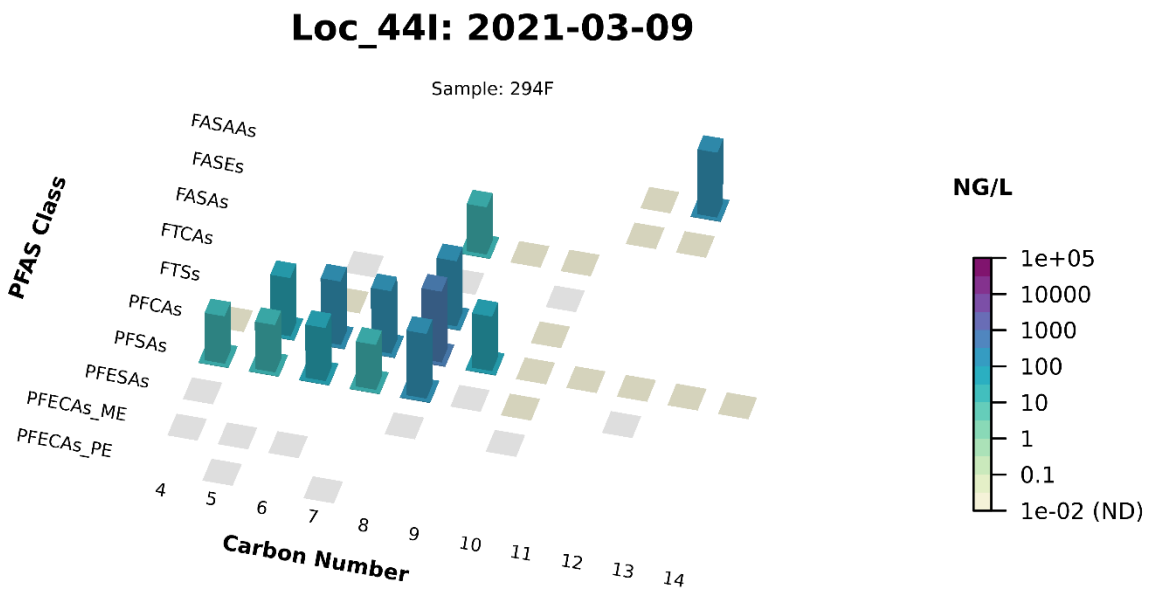


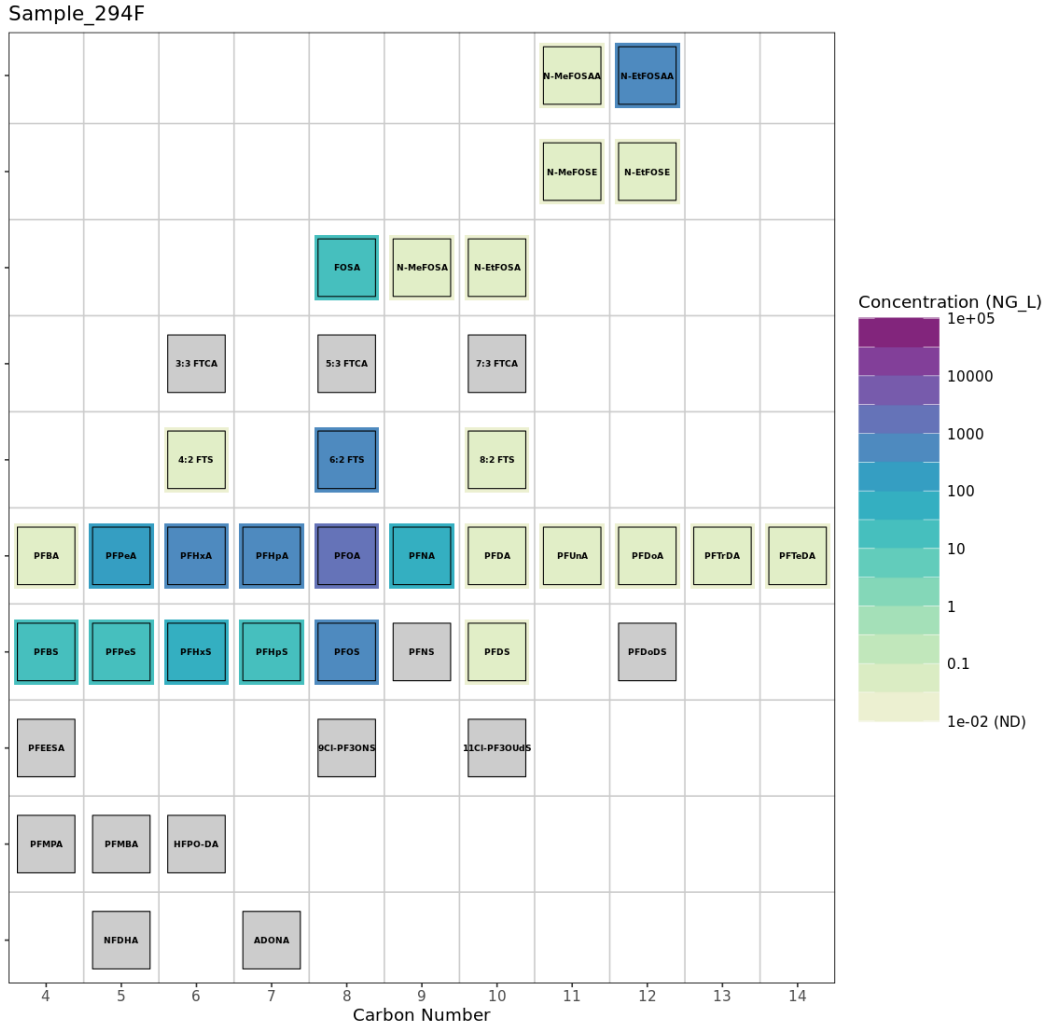
Sample ID	Sample Date	Chemical	CAS	Result	Result Units	Detect Flag	MCL	Exceedance
Loc_21F_2018-03-15	2018-03-12	Perfluorooctane sulfonic acid (PFOS)	1763-23-1	2630	ng/L	Y	4	Y
Loc_2Y_2018-03-09	2018-03-12	Perfluorooctane sulfonic acid (PFOS)	1763-23-1	0.0005	ng/L	N	4	N
Loc_5Q_2018-03-09	2018-03-12	Perfluorooctane sulfonic acid (PFOS)	1763-23-1	0.0006	ng/L	N	4	N

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Sample Matrix Plot

- Plot sample composition structured grid by PFAS Class and Carbon Chain Length
- Evaluate detect and non-detect compounds
- Quickly assess visual patterns in large sample populations





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Plume Extent & Uncertainty

Ordinary Kriging

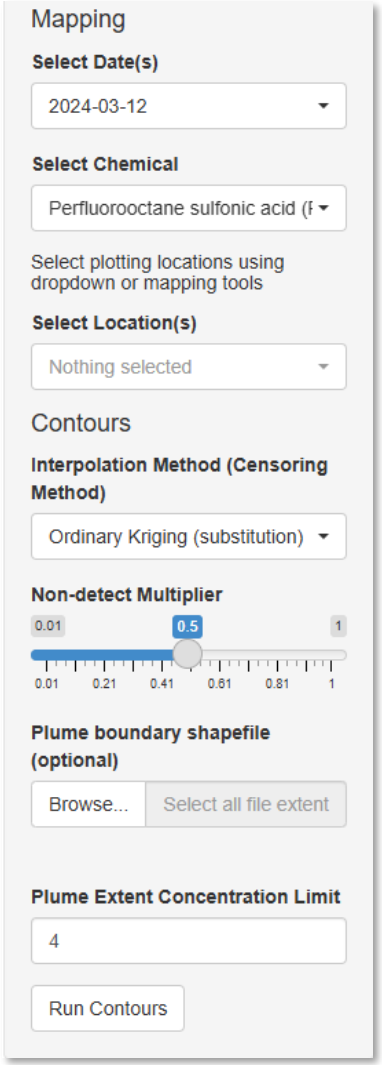
- Substitute non-detects with a fraction of the detection limit. (~0.5*DL)
- May introduce bias

Censored Spatial Regression

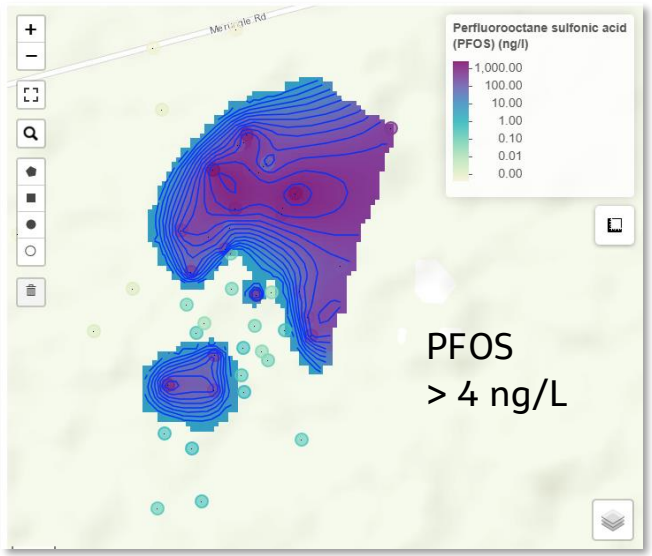
- Treats non-detects as values below detection limits within the maximum likelihood range
- Robust against detection limit > detected concentrations

Uncertainty

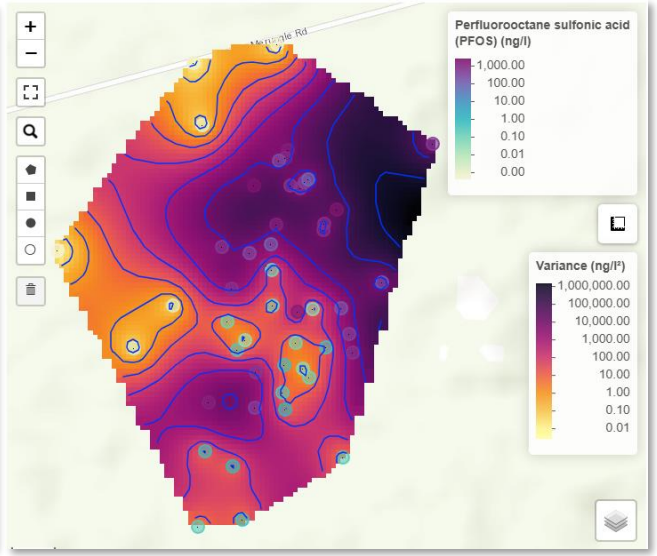
- Spatial variance (high variance = low confidence)
- Leave-one-out cross-validation (RMSE, MAE, R^2) to evaluate predictive accuracy.



Spatial Prediction



Spatial Variance

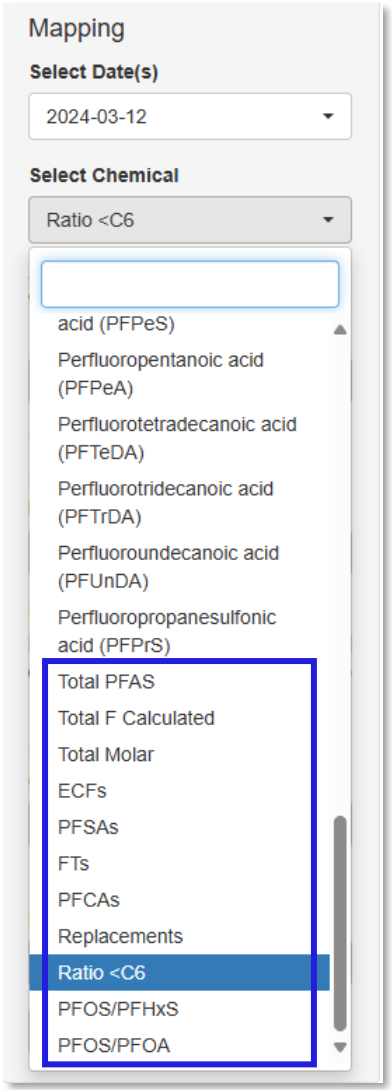


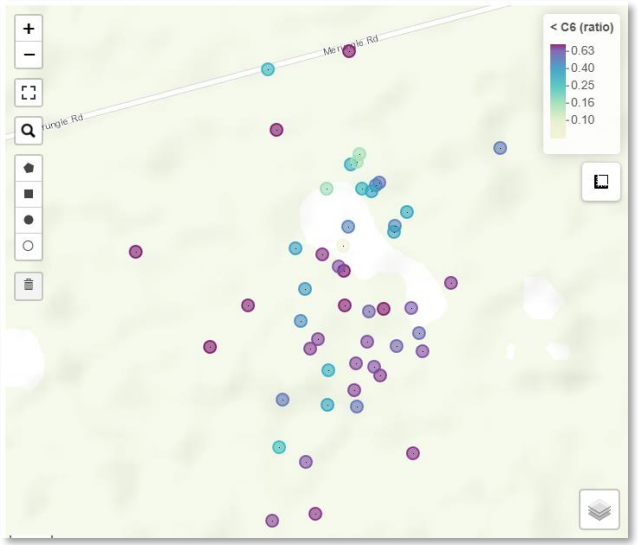
Cross-Validation

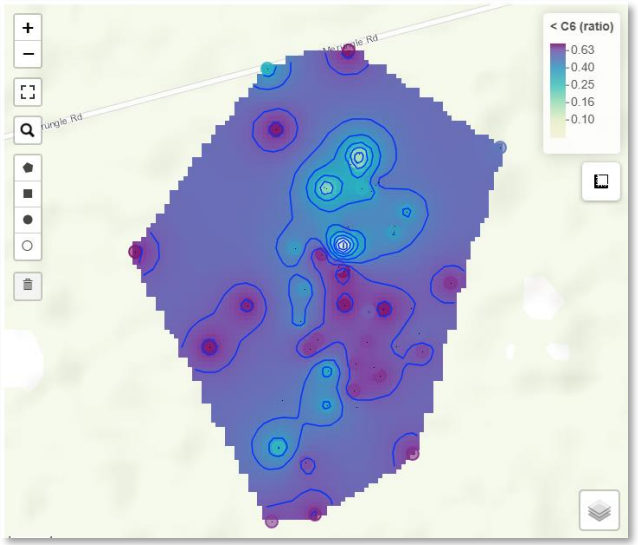
Method	Semivariance Model	RMSE	MAE	R^2
Ordinary Kriging	Spherical	0.46	0.27	0.51
Spatial Regression	Spherical	0.26	0.22	0.63

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Spatial Analysis







Key Metrics

- **Total PFAS:** Sum of all reported PFAS; indicates total mass burden for screening and reporting.
- **Total Fluorine Calculated:** Estimated total fluorine mass from detected PFAS; fluorine-specific loading for mass balance and source strength.
- **Total Molar:** Sum of PFAS on a molar basis; enables chemically meaningful comparisons for mass balance and transformation potential.
- **Diagnostic Ratios:** Ratios of specific PFAS (e.g., PFOS/PFHxS); evaluate sorption effects, proximity to sources, and relative mobility.
- **PFAS Class:** Total molar concentrations for ECFs, PFASs, FTs, PFCAs
- **Precursors:** Total molar concentrations of ECF- and fluorotelomer-derived precursors; distinguishes source types and estimates transformation potential.
- **Ratio <C6:** Proportion of short-chain (≤6 carbon) PFAS to >C6 PFAS; high ratio signals modern C6-based products and/or long-chain degradation.
- **Replacement Compounds:** Identification and quantification of emerging replacement PFAS; assesses recent releases and shifts in usage.

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Ordination & Cluster Analysis

Multidimensional Scaling (MDS) Ordination

- Projects high-dimensional PFAS profiles into 2D space for visualizing similarity, cluster separation, and outliers.

K-means Cluster Analysis

- Groups sampling locations based on PFAS compositional similarity to identify distinct source zones or transport pathways.

Hierarchical Clustering

- Builds a dendrogram showing relationships among samples; cluster cut defines optimal group separation.

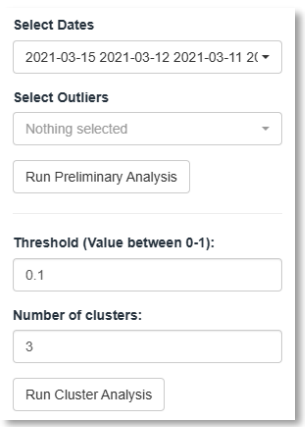
Inferential Statistics

- Uses PERMANOVA, MANOVA, and dispersion tests to quantify cluster distinctness, variance homogeneity, and statistical significance of group separation.

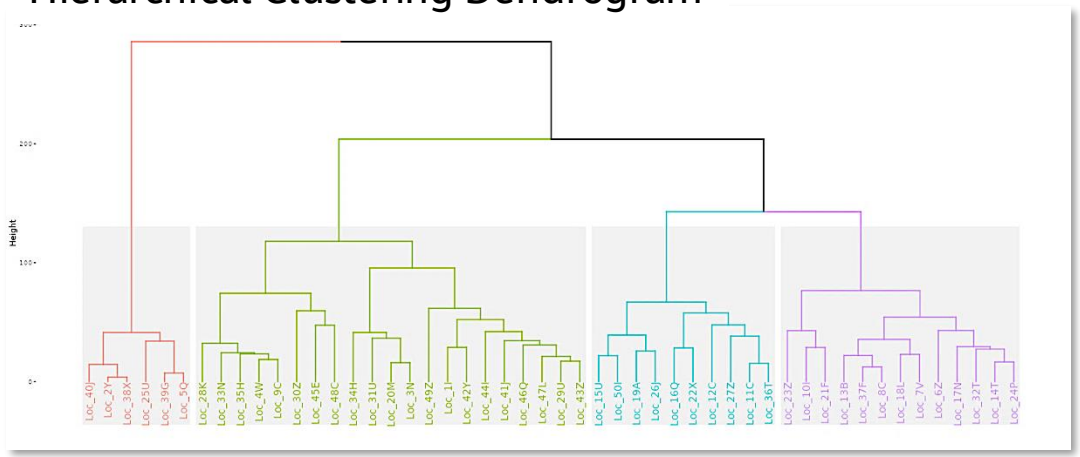
Clustering Method	k	Avg. Silhouette Width				PERMANOVA				
		Obs.	MC p-value	Boot CI L	Boot CI U	R2 Obs.	p-value	MC p-value	Boot CI L	Boot CI U
kmeans	3	0.309	0.000	0.289	0.413	0.366	0.001000	0.000	0.286	0.462
pam	3	0.299	0.000	0.270	0.402	0.202	0.001000	0.000	0.153	0.276

Clustering Method	k	Dispersion				
		F Obs.	p-value	MC p-value	Boot CI L	Boot CI U
kmeans	3	2.925	0.04700	0.04200	0.200	10.438
pam	3	3.926	0.03200	0.02800	0.744	12.141

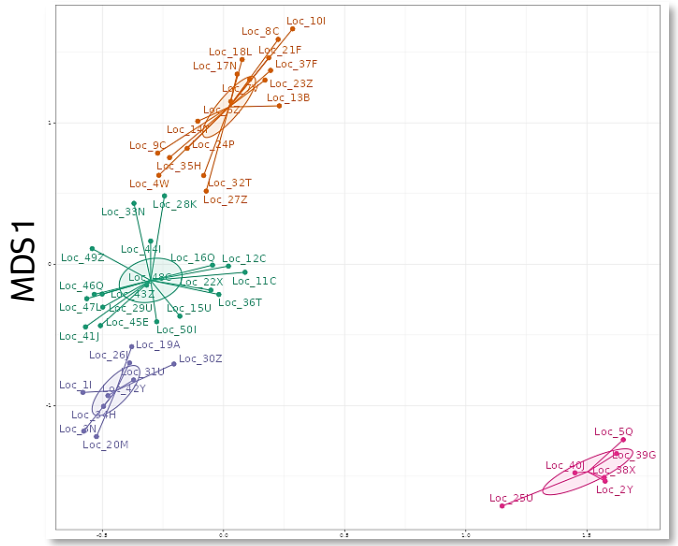
Clustering Method	k	MANOVA on MDS Axes								
		Pillai Obs.	F Obs.	p-value	MC p (Pillai)	MC p (F)	Pillai Boot CI L	Pillai Boot CI U	F Boot CI L	F Boot CI U
kmeans	3	0.692	52.872	0.000	0.000	0.000	0.599	0.796	35.157	91.910
pam	3	0.596	34.699	0.000	0.000	0.000	0.490	0.738	22.535	66.159



Hierarchical Clustering Dendrogram

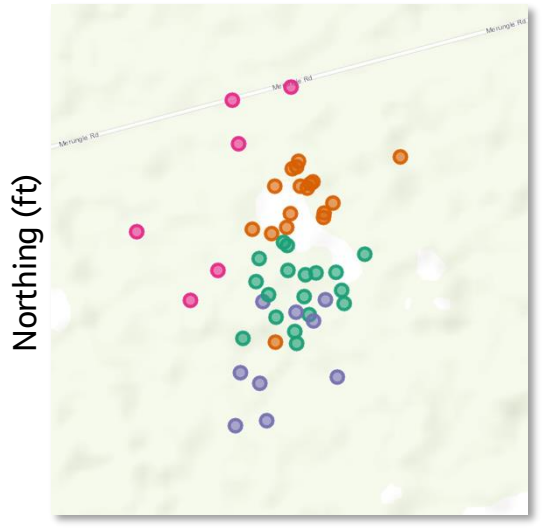


MDS Ordination with Clustering





Spatial Cluster Plot



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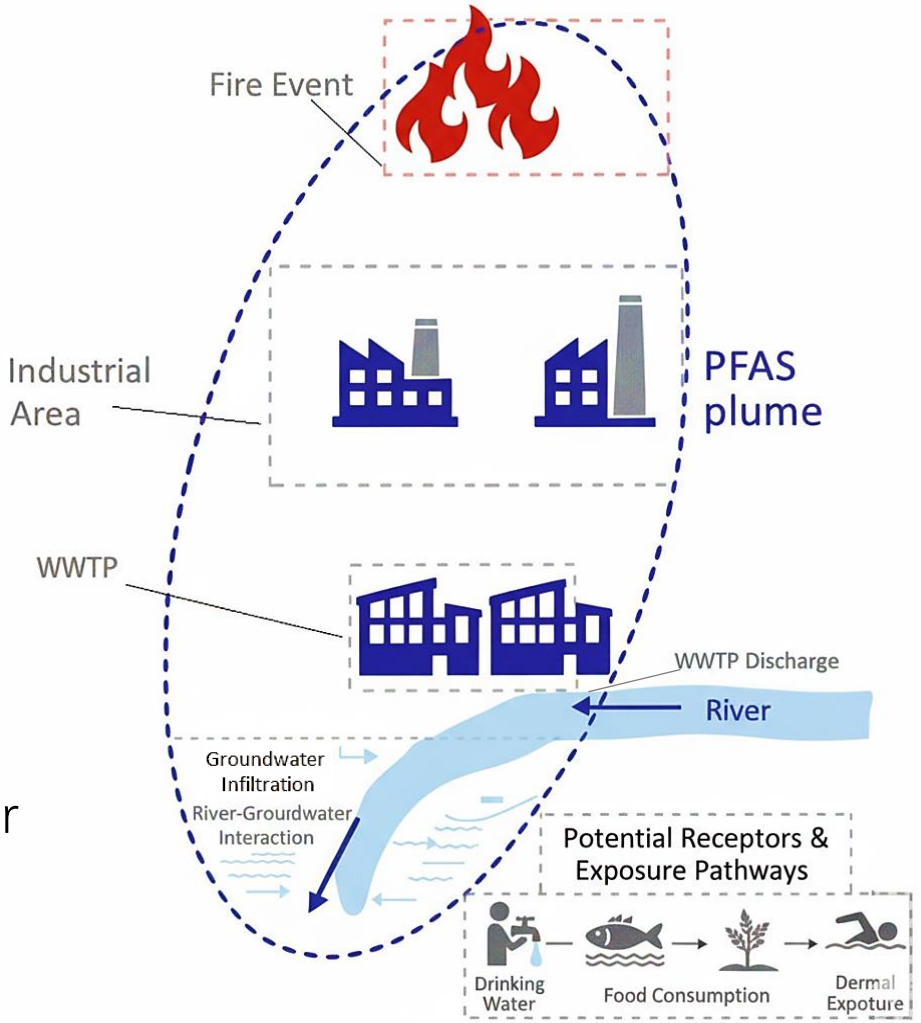
Case Study

Case Study

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Background

- Pre-1990 Fire Event
  - Large storage facility fire in the late 1980s
  - Firefighting foams used for suppression
  - Site remained inactive for several years afterward
- Industrial Manufacturing Area
  - Textile and paper-coating operations since 1970s
  - Produced treated materials for consumer/commercial use
- Onsite Wastewater Treatment Plant (WWTP)
  - Operating since the 1980s to manage industrial wastewater
  - Continues to treat influent from the facility

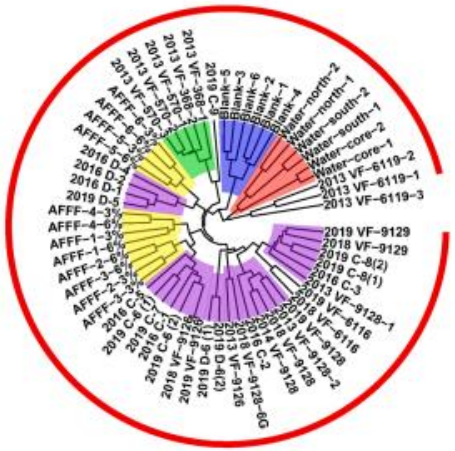


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PFAS Source Identification - Chemical Fingerprints

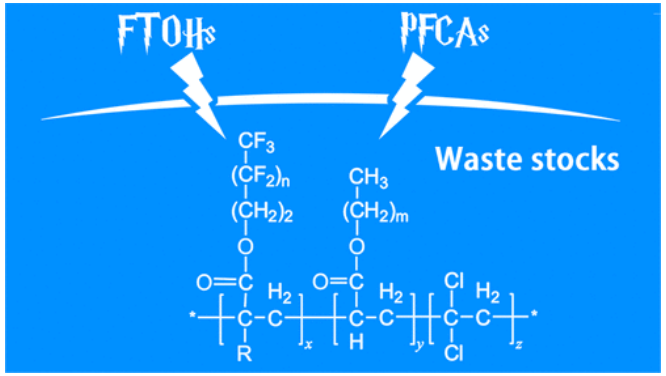
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Characteristics	AFFF	Textile	WWTP
Manufacturing process	ECF vs FT, dictate specific non-polymeric PFAS present	Use side-chain fluorotelomer polymers (SCFP) which can be based on different carbon chains	None
Primary PFAS	Legacy C8 and modern foams with C6 and their precursors	Includes both polymeric and non-polymeric PFAS. SCFP can break down to FT precursors and form different PFCAs	Vary widely depending on the source of PFAS entering WWTP

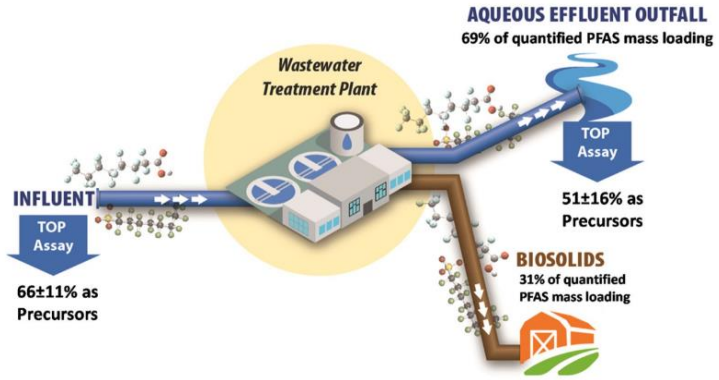


https://doi.org/10.1016/j.envint.2022.107398

Abundant references on AFFF signature identification and comparison



SCFP and other PFAS used in textile are less documented for source tracking



Water Research Volume 233 April 15 2023, 119724

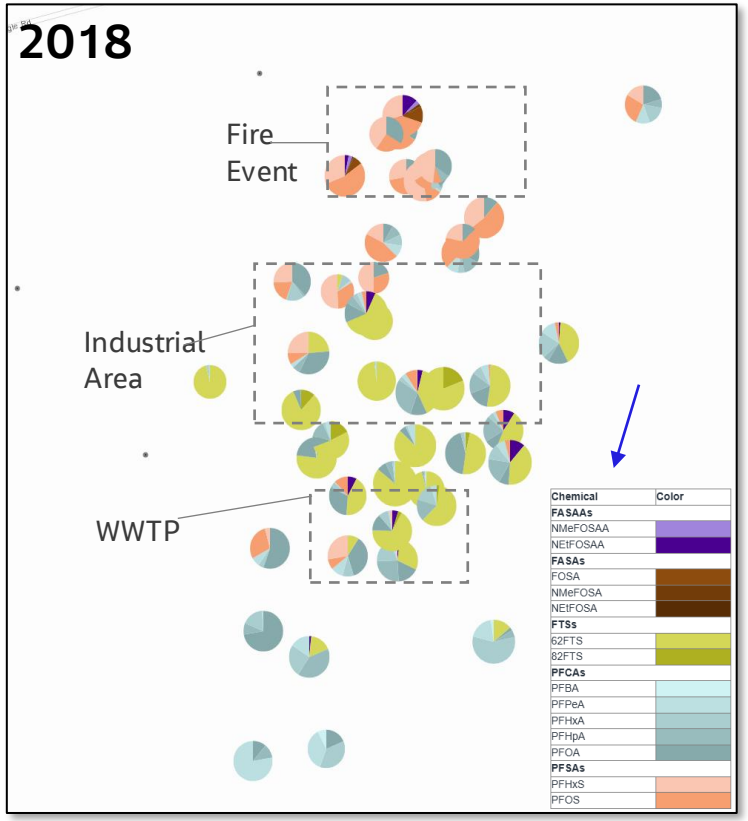
High precursor loading can be possible to WWTP, however, source tracking cannot point to specific PFAS manufacturing processes

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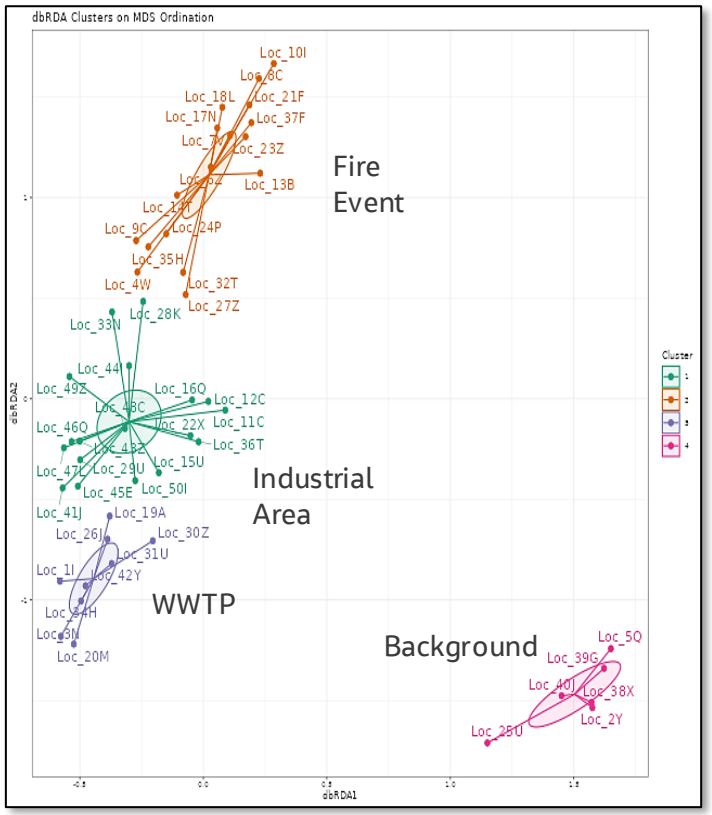
PFAS Distribution Pattern Analysis

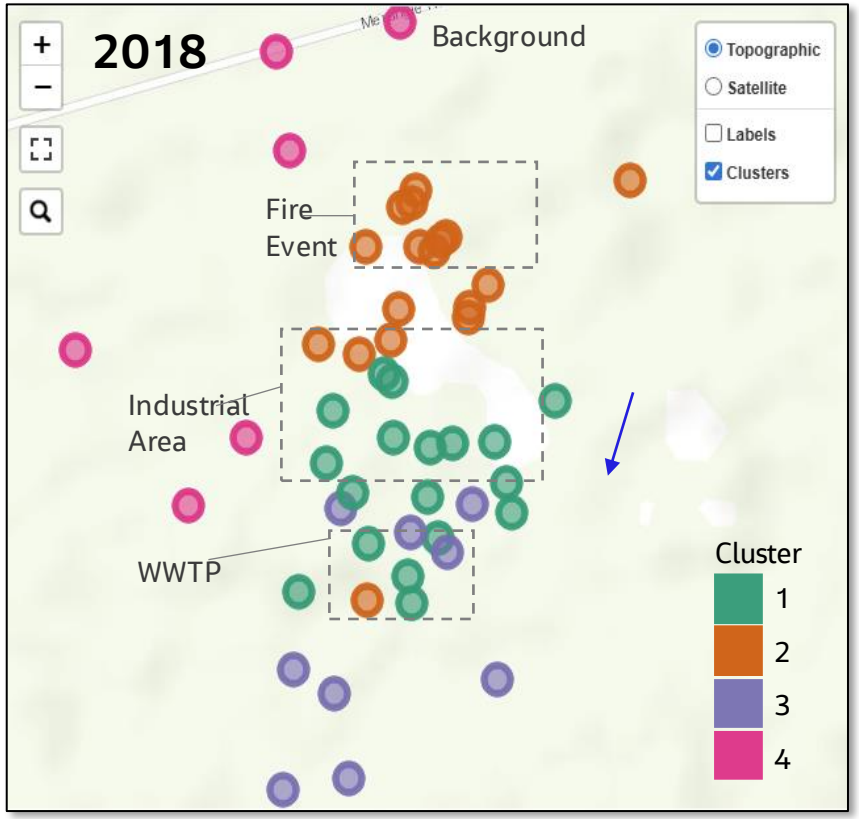
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Cluster analysis shows agreement with compositional differences observed in the pie plot visualization



GW flow direction





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Clusters Analysis Explained

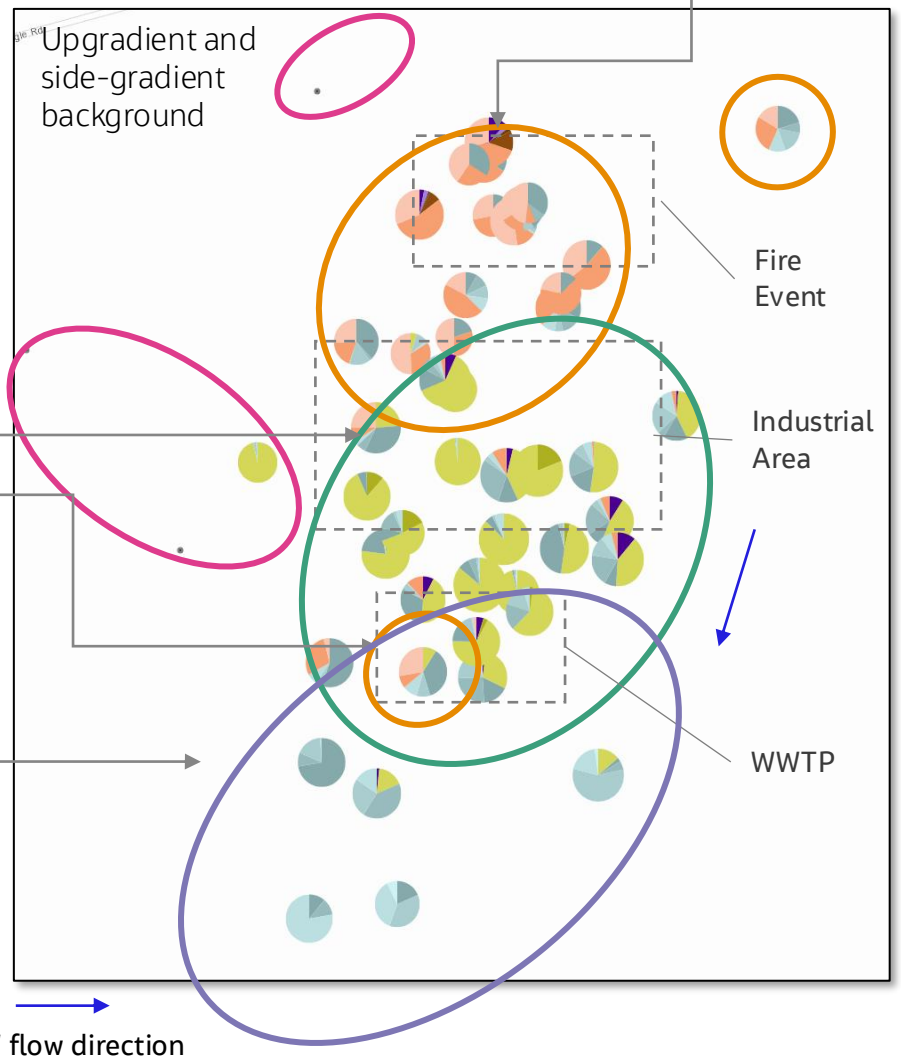
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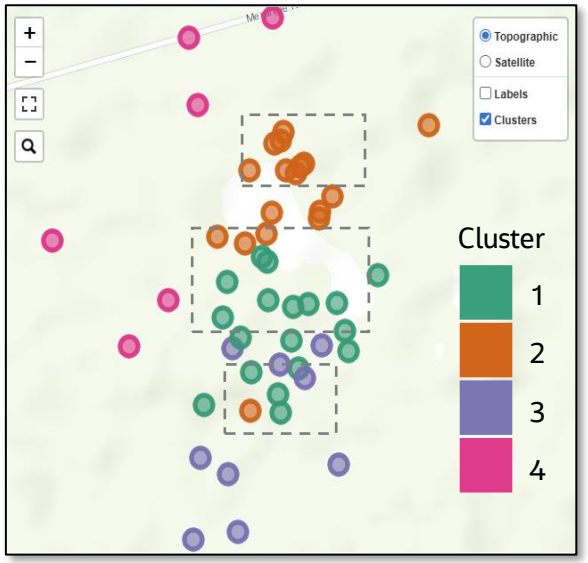
Overlapping of 2 clusters in the **Industrial Area**:
- AFFF signature
- FT dominant industrial area source

3 overlapping clusters at **WWTP**:
- Upgradient AFFF signature did not migrate further
- FT source from industrial area
- Precursor FTS transformation into terminal PFCA

Distinct signature **downgradient** from source areas, terminal PFCA dominant

Distinct AFFF signature at **Fire Event**:
- FASAAs, PFOS



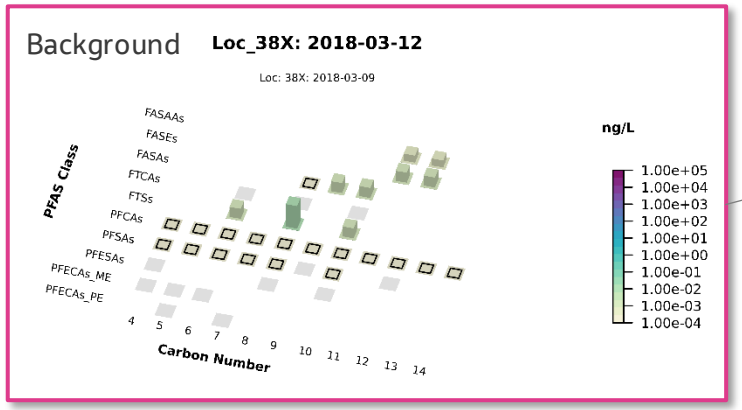


Chemical	Color
FASAAs	
NMeFOSAA	
NEtFOSAA	
FASAs	
FOSA	
NMeFOSA	
NEtFOSA	
FTSs	
62FTS	
82FTS	
PFCAs	
PFBA	
PFPeA	
PFHxA	
PFHpA	
PFOA	
PFSAs	
PFHxS	
PFOS	

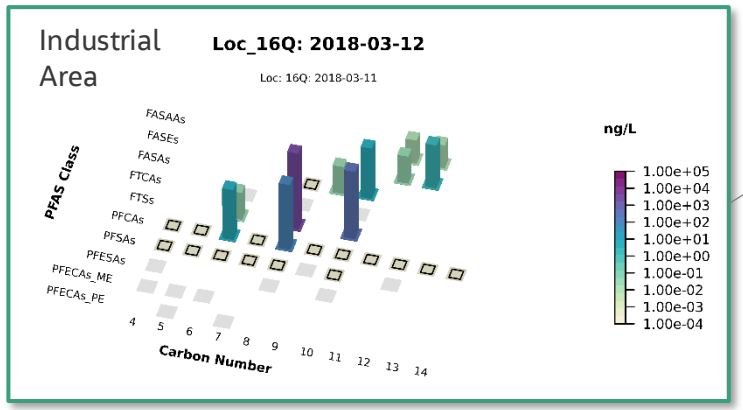
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Fingerprints & Clusters Explained

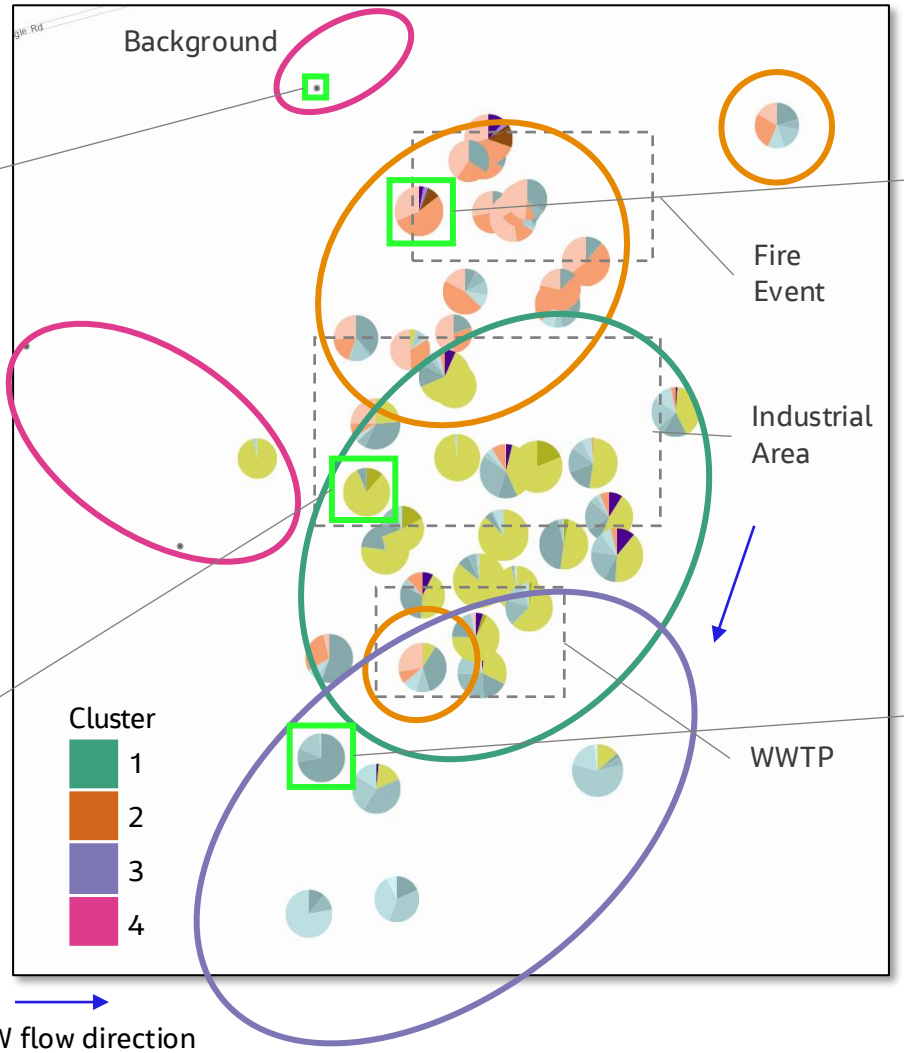
PFLUORENSICS

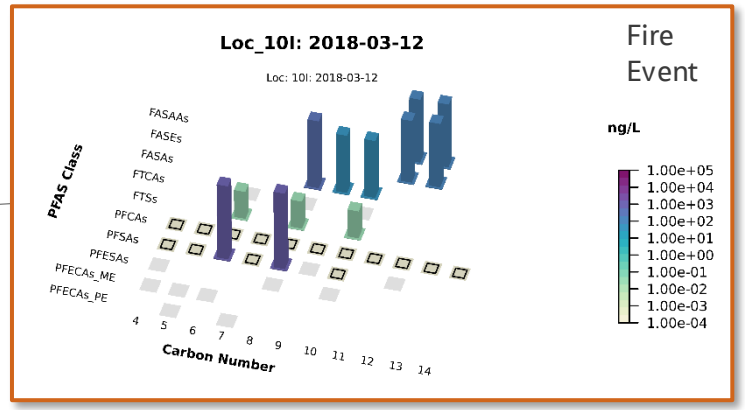


Minor FTSs; typical of atmospheric deposition

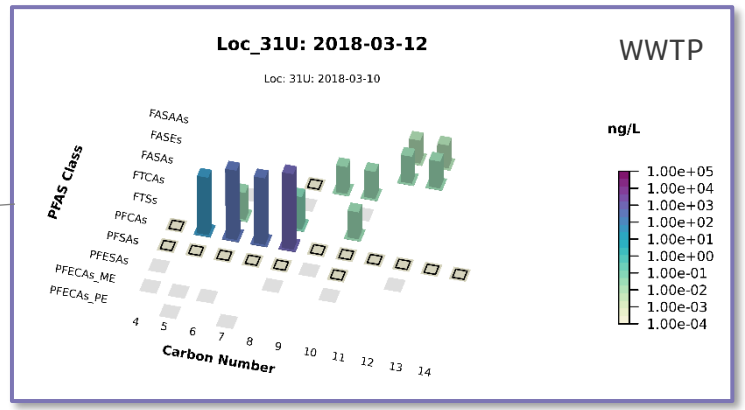


Long-chain PFCAs dominate with moderate FTSs; AFFF signature attenuated





Elevated FASAAs and PFOS (AFFF-type)



Conversion from precursors to terminal PFCAs

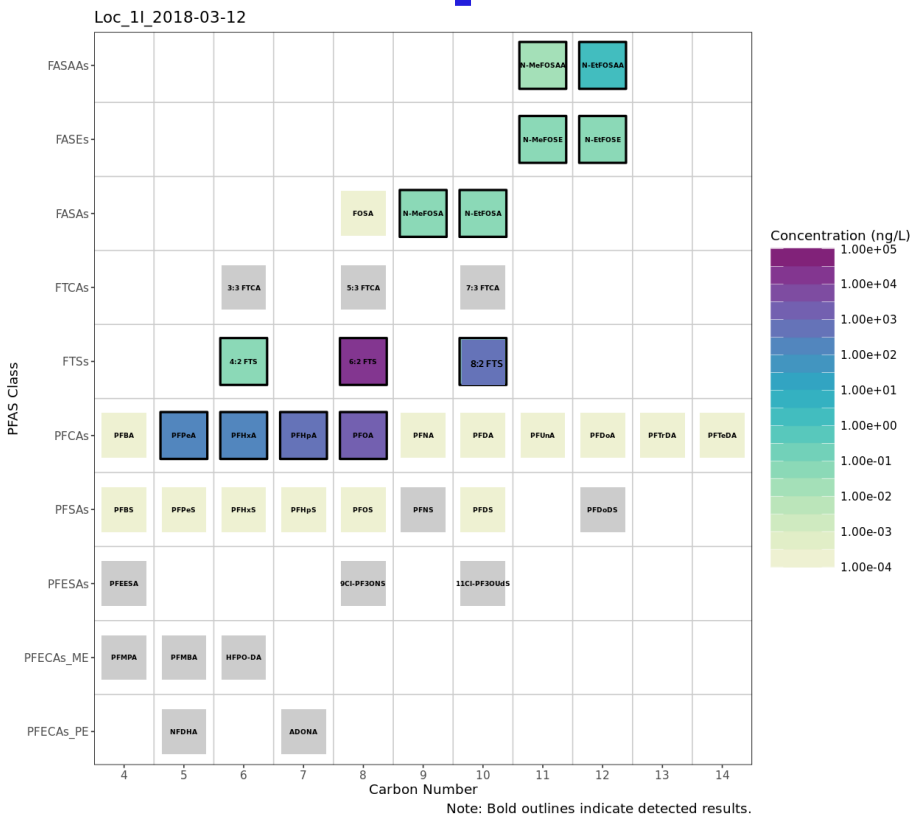
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Biotransformation

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Biotransformation can alter the PFAS profile.

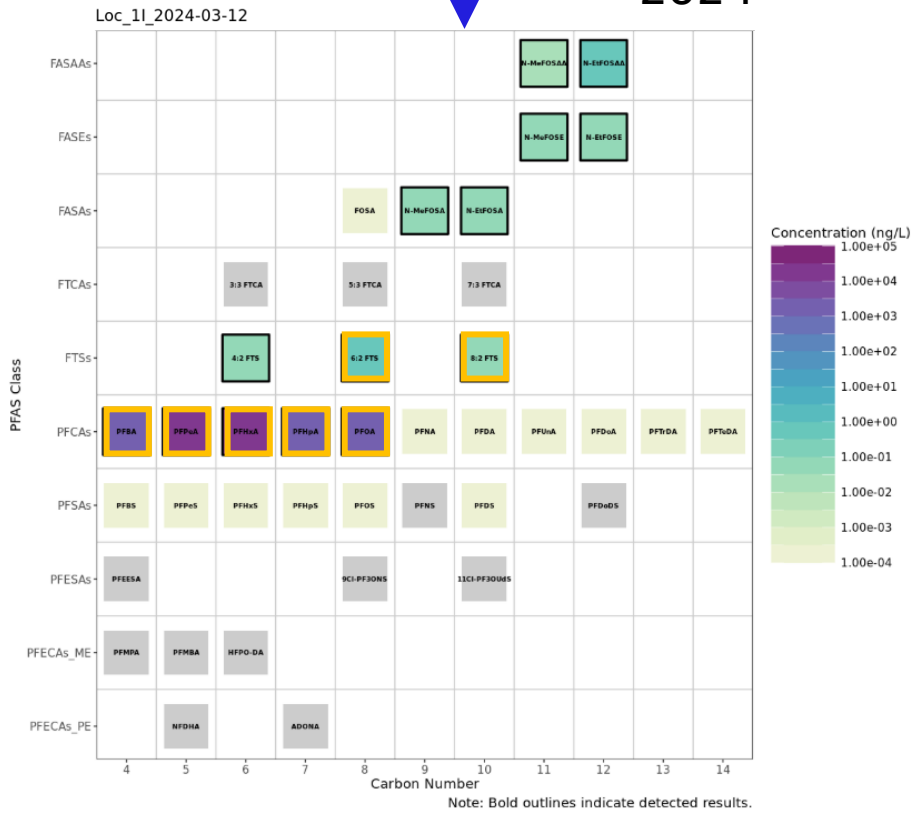
2018



Jacobs Biotransformation Database

Look for Biotransformation products of 6:2 FTS and 8:2 FTS

2024

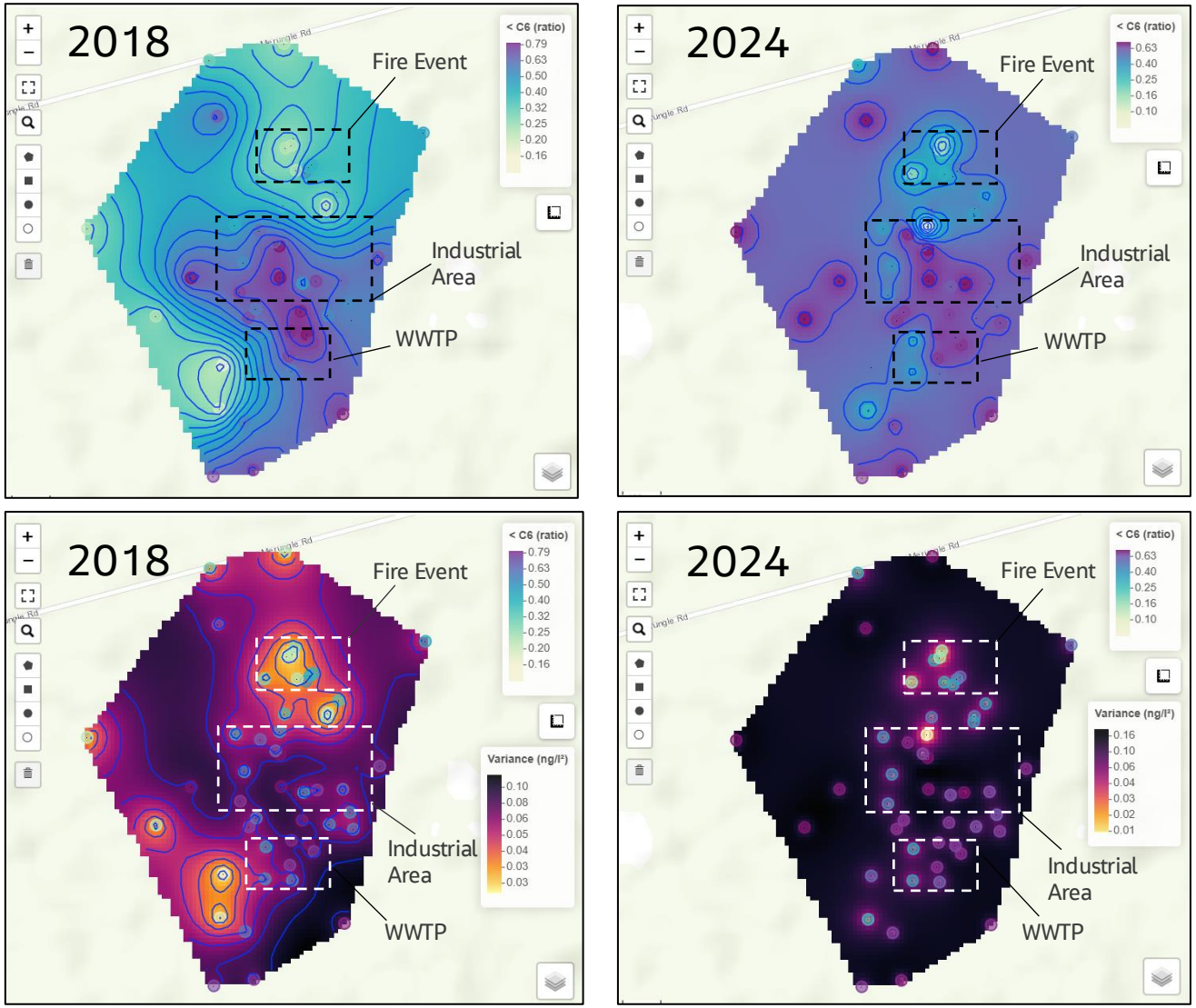


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Temporal changes in short-chain PFAS (≤C6)

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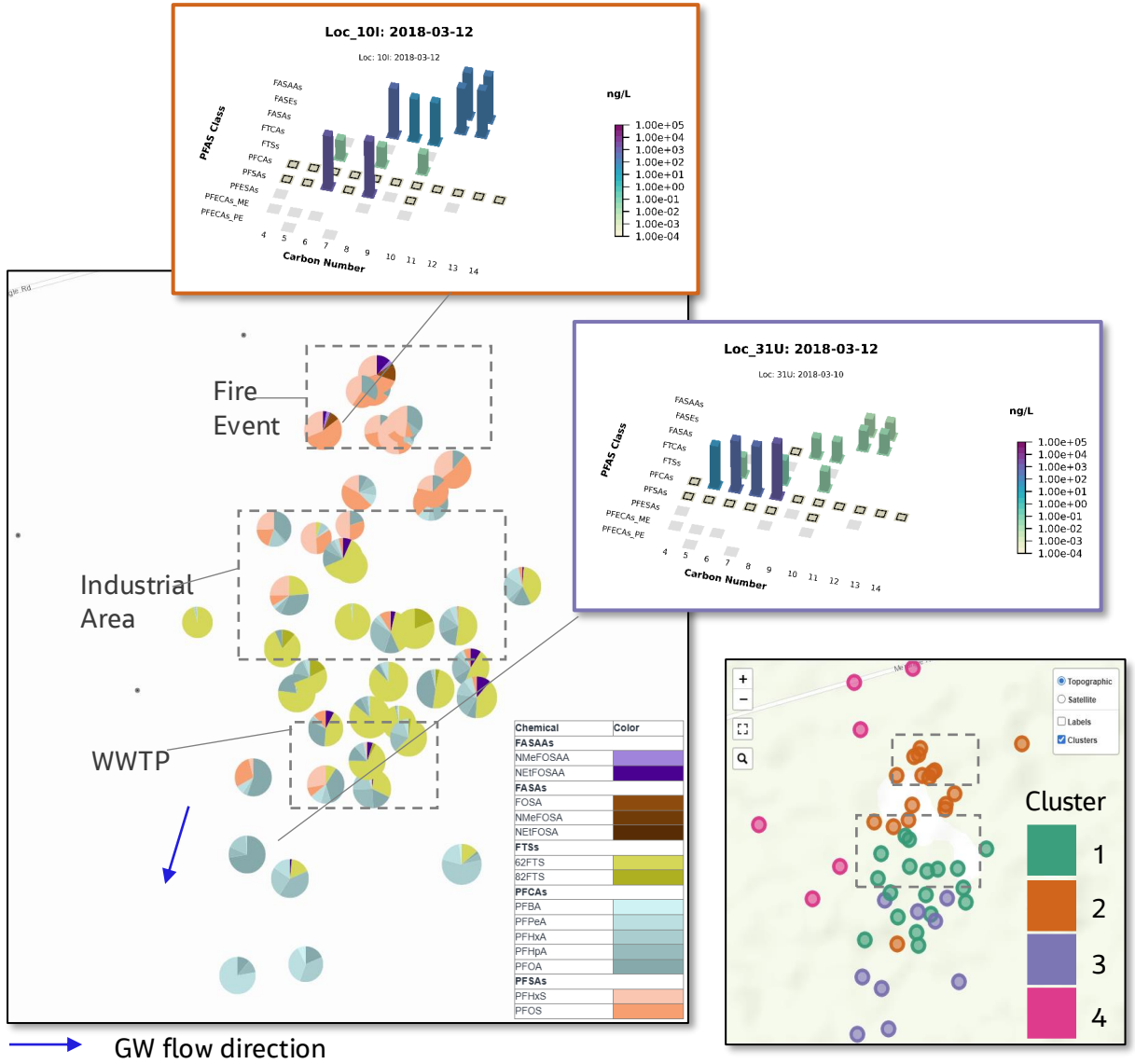
- ≤C6 Ratio
  - Proportion of total PFAS with six perfluorinated carbons or less
  - Precursors and replacements
- Composition
  - PFAS composition shifts from long-chain dominance to short-chain prevalence
- Spatial Patterns
  - Source contrast has diminished
    - Progressive migration, transformation, and dispersion
  - Variance higher and more uniform over time
    - More homogeneous PFAS distributions over time



Case Study Summary

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- **Multiple PFAS sources identified**, including AFFF use, industrial operations, and WWTP inputs with overlapping composition signatures.
- **Spatial heterogeneity has diminished** between 2018 and 2024, indicating progressive migration, transformation, and dispersion.
- **PFAS composition has shifted** from long-chain dominance to short-chain prevalence, reflecting transformation and replacement trends.
- Cluster analysis identifies **convergence of AFFF- and fluorotelomer-type sources** near the WWTP
- **Increasingly homogeneous PFAS distributions** and terminal PFCA dominance suggest plume aging and compositional evolution over time



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Translating Contamination to Solutions

Translating Contamination into Solutions

PFLUORENSICS

- Currently conducting similar evaluations in source water, collection systems, and through treatment plants
- Source mitigation is first priority!
  - More concentrated, lower volumes to treat
  - Prevent environmental impacts
  - Significantly reduce impacts on downstream users
  - Stakeholder engagement
- Concentration, fingerprint, and discharge patterns drive treatment selection
  - Low versus high PFAS levels
  - Long chain versus short chain PFAS
  - Carboxylates versus sulfonates
  - Consistent sources versus temporal patterns

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Questions?

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Reinventing tomorrow.