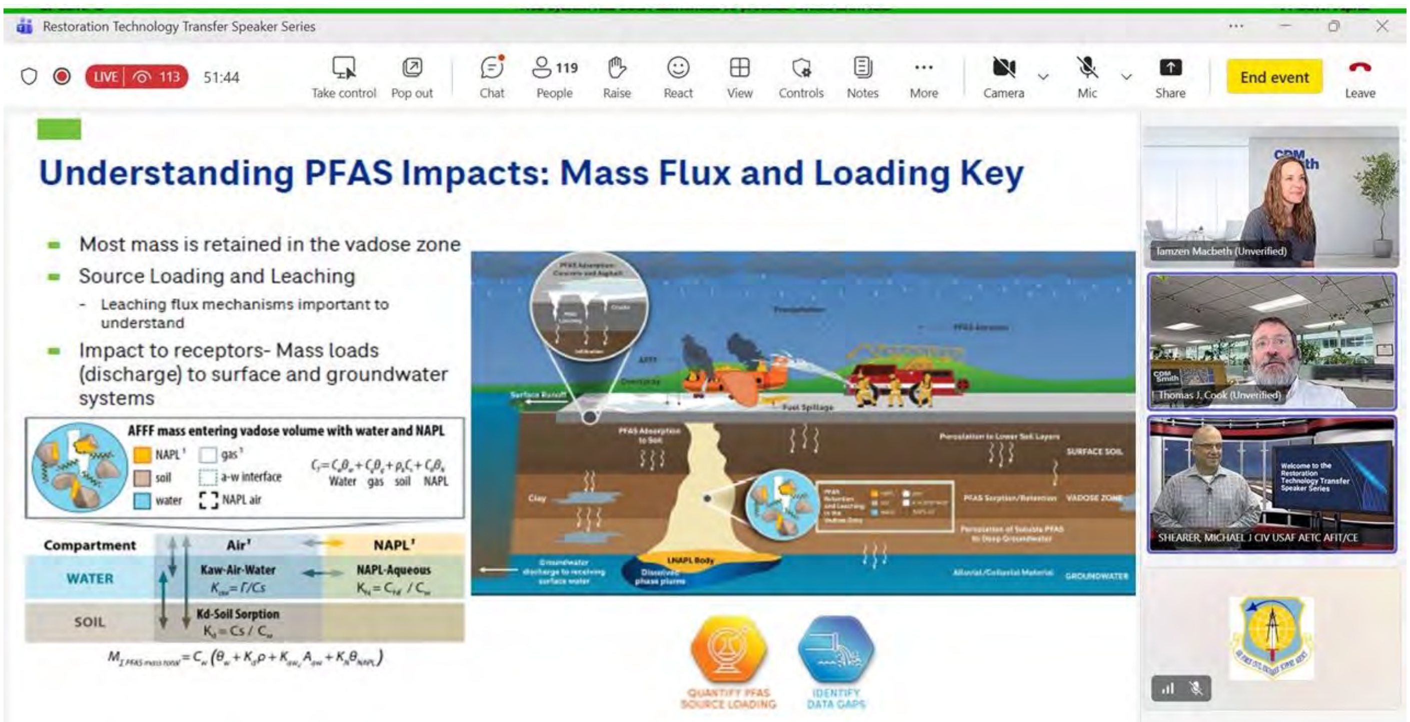
Restoration Technology Transfer Speakers Series
May 2026

Advanced Data Analytics and Forensics Framework (ADAFF): Driving Forward Environmental Solutions with Data Analytics

Presenters: Dr. Tamzen Macbeth & Tom Cook (CDM Smith)

This webinar highlighted results from an AFCEC BAA 2112 demonstration of an ADAFF that brings clarity to PFAS decision making by integrating historical data using advanced analytics, mass balance concepts, and modeling to quantify sources, transport, and source to receptor impacts. Using the former fire training area FT003 at Dover Air Force Base as a case study, the presentation illustrated how advanced analytics and visualization can improve confidence in PFAS conceptual site models, reduce uncertainty, and directly support remedy evaluation and performance assessment. AFCEC remedial project managers gained practical insights on how to move beyond data overload toward more transparent, and defensible decision support tools.



Dr. Macbeth and Mr. Cook discuss the conceptual site model of a source leaching to groundwater.

This event and future events are updated and posted on the AFIT website at: https://www.afit.edu/CE/index.cfm.

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Webinar Structure

	Restoration Technology Transfer Webinar Series – eDASH Archive
5 min	Welcome and Administrative Business
45 min	Main Presentation – CDM Smith *Advanced Data Analytics and Forensics Framework (BAA 2112)*
10 min	Questions and Answers
5 min	Final Thoughts

Advanced Data Analytics and Forensics Framework BAA 2112

Tamzen Macbeth, Ph.D., PE, BCEE
& Tom Cook
CDM Smith

May 2026

BAA-2112 Advanced Data Analytics and Forensics Framework

Driving Forward Environmental Solutions with Data Analytics

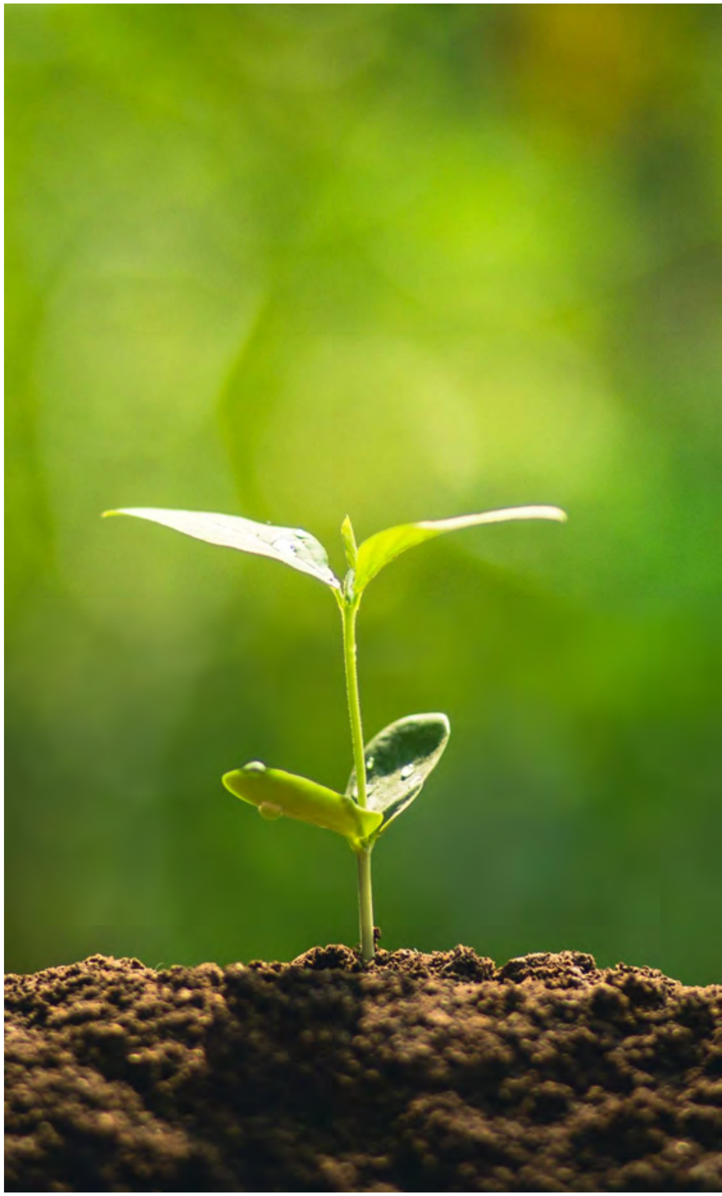
May 13, 2026

Tamzen Macbeth PhD, PE, BCEE

Tom Cook

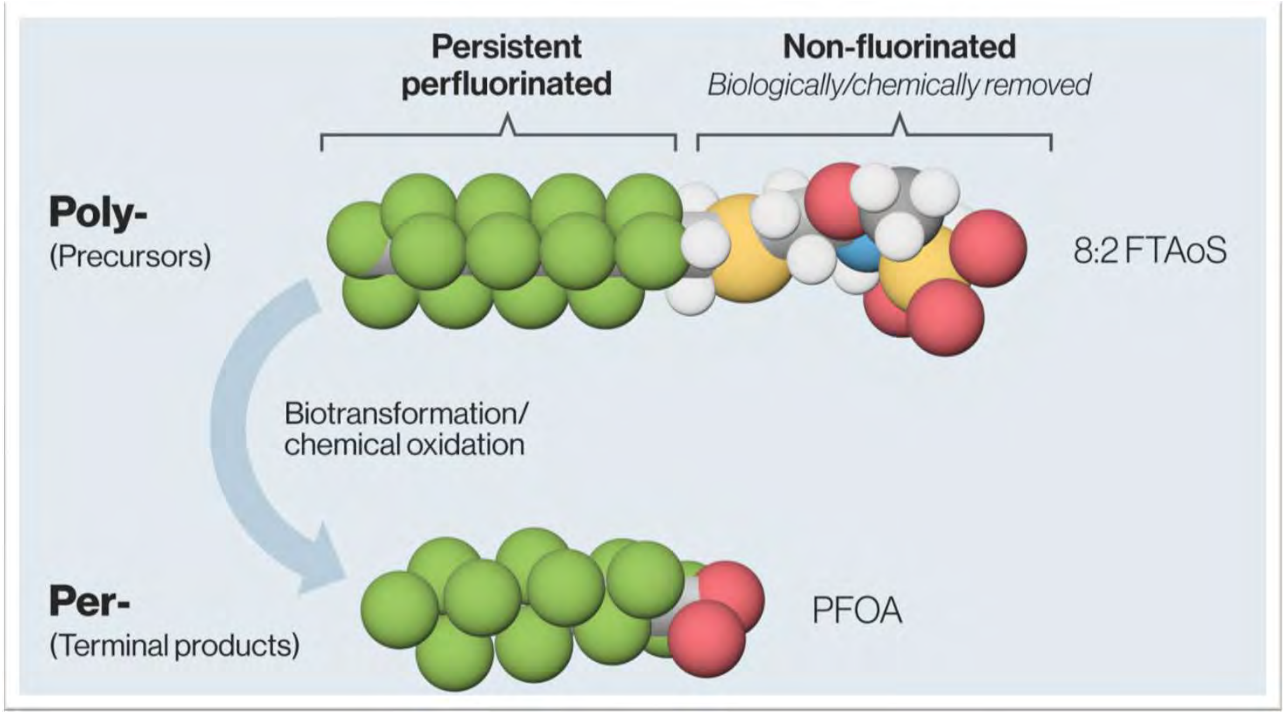
Agenda

- **Building PFAS Conceptual Site Models**
- **Data Analytics:**
  - How data analytics can aid in creating more accurate and comprehensive site models.
  - Insights into choosing the right tools for data visualization and managing the data pipeline effectively.
- **Decision Making and Modeling:** Exploring how data analytics can support decision-making processes.
- **Case Study:** AFCEC BAA project

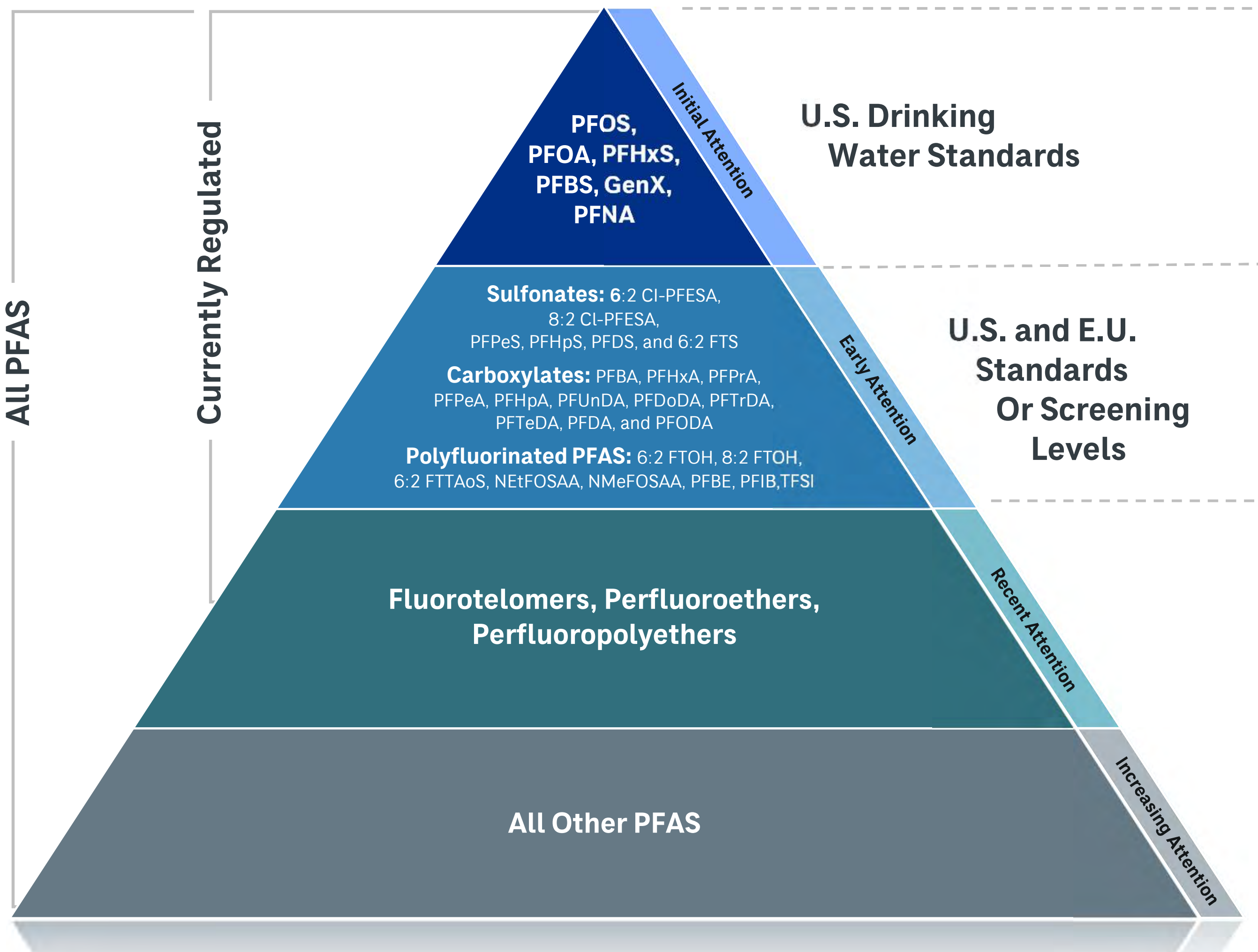


Introduction: Per- and Polyfluoroalkyl Substances (PFAS)

- **Extreme Persistence**
  Some PFAS half-lives in decades or centuries
- **Mobility**
  Soluble PFAS are mobile in the environment
- **Bioaccumulation**
  Some PFAS bioaccumulate and biomagnify up the food chain – long-chain PFAS concentrate in humans
- **Toxicity**
  There are very low (<4 ng/L) and diminishing regulatory acceptance criteria as more is known about the toxicity of specific PFAS.
- **Surfactants**
  Amphiphilic PFAS stick on surfaces and interfaces

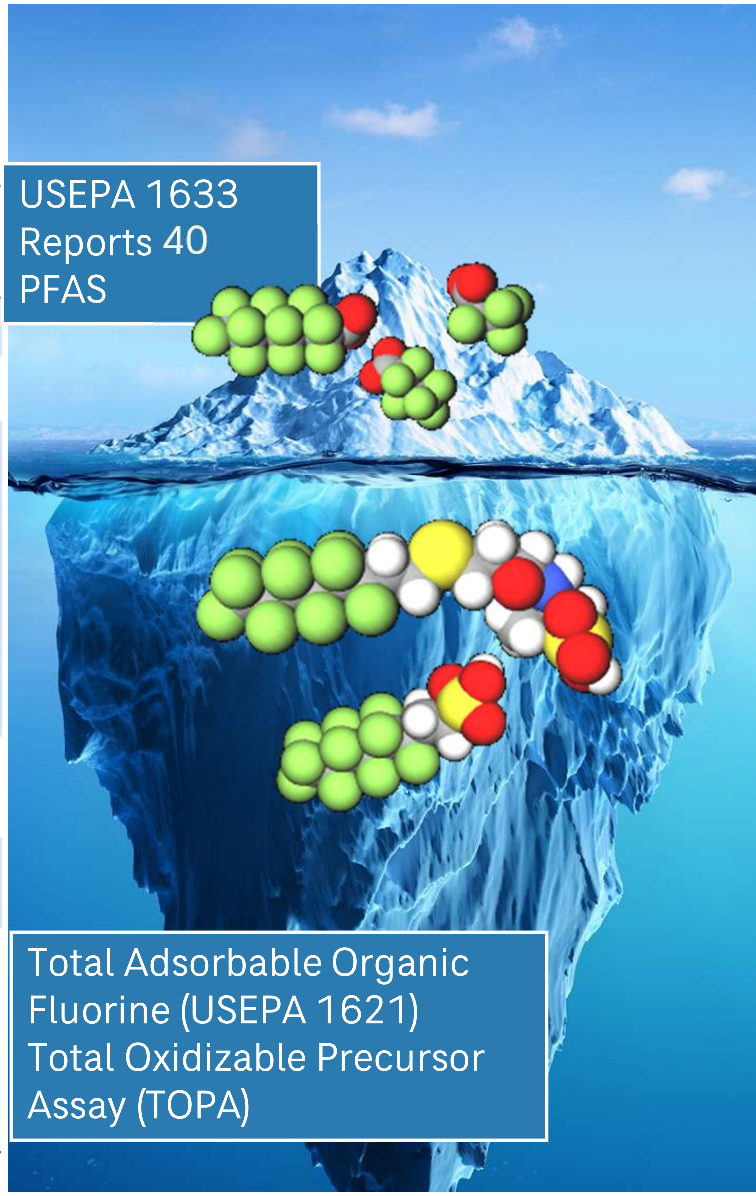


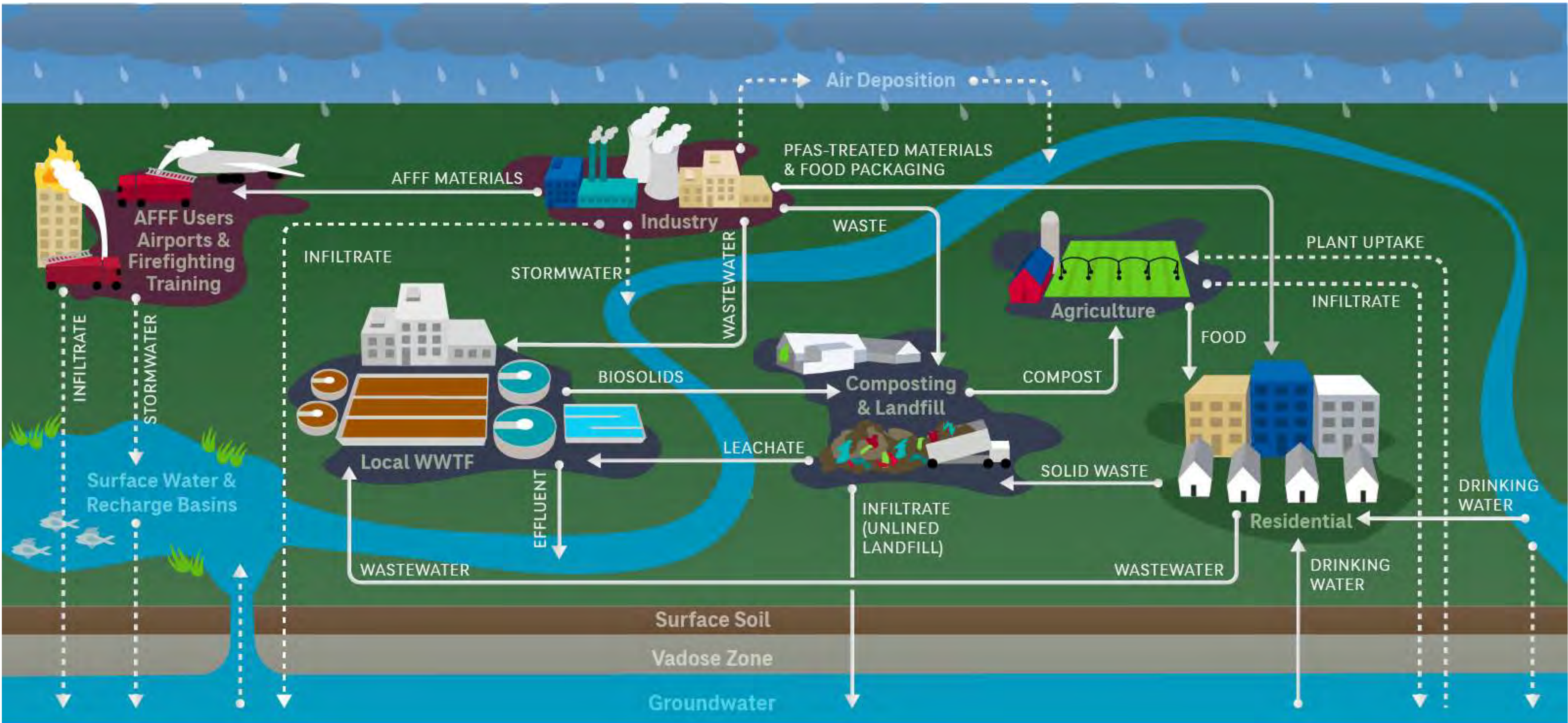
14,700 PFAS Chemicals....



PFAS Validated Analytical Methods

Method Name	USEPA 1633	USEPA 1621	TOPA
Released	January 2024	January 2024	In process
Data Type	Definitive	Screening	Screening
Matrix Analyzed	Surface water, groundwater, wastewater, soils, biosolids, sediment, landfill leachate, fish tissue	Surface water, groundwater, wastewater	Surface water, groundwater, wastewater, soils, biosolids, sediment, landfill leachate, fish tissue
Number of PFAS Quantified	40	NA- Nontarget Analysis	NA- Nontarget Analysis
Technology	LC-MS/MS	CIC	LC-MS/MS With Oxidation
Application to PFAS Monitoring Programs	Used in all DOD, CWA, e.g., NPDES permits	Used to assess presence of total organic fluorine as a surrogate for total PFAS	Used to assess presence of oxidizable precursors

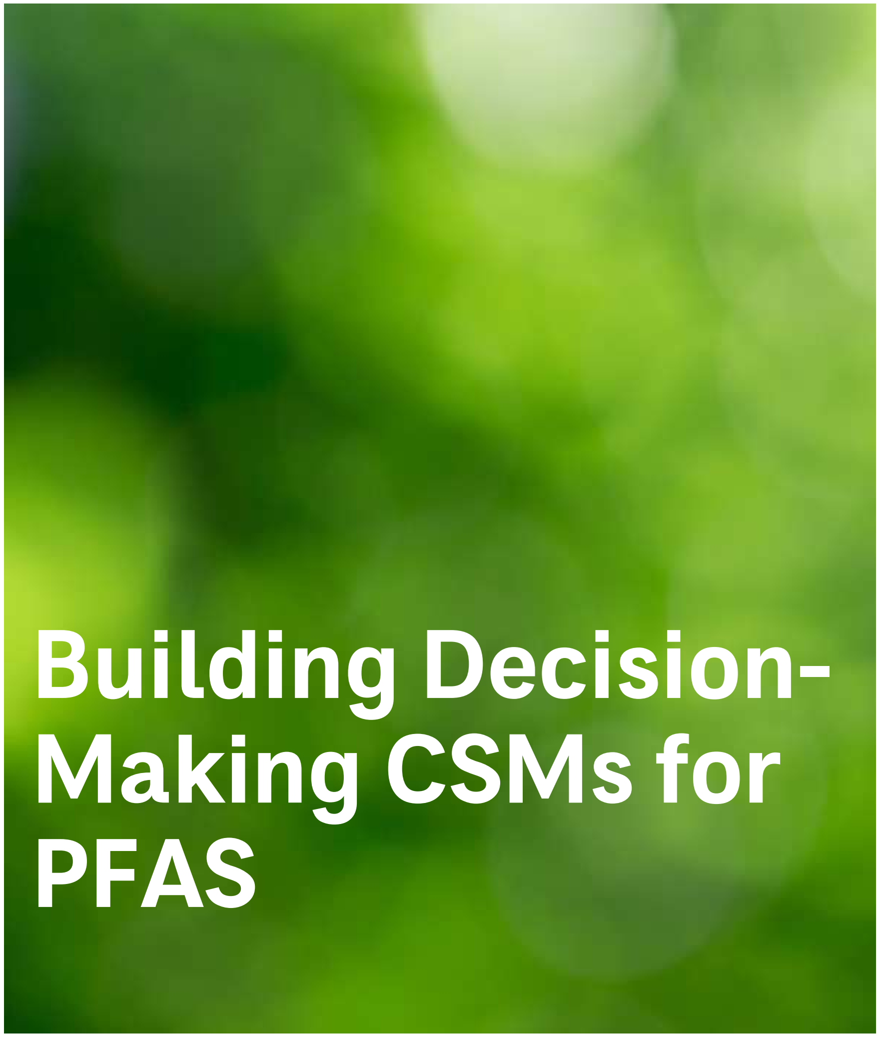




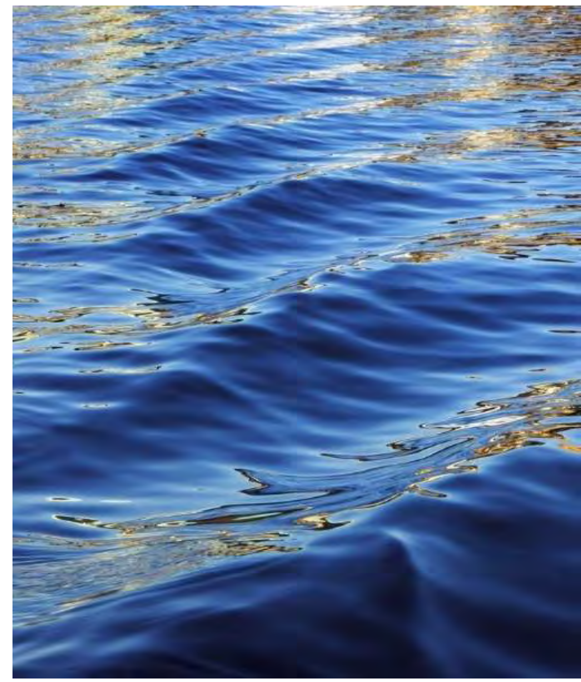
PFAS Life Cycle

KEY

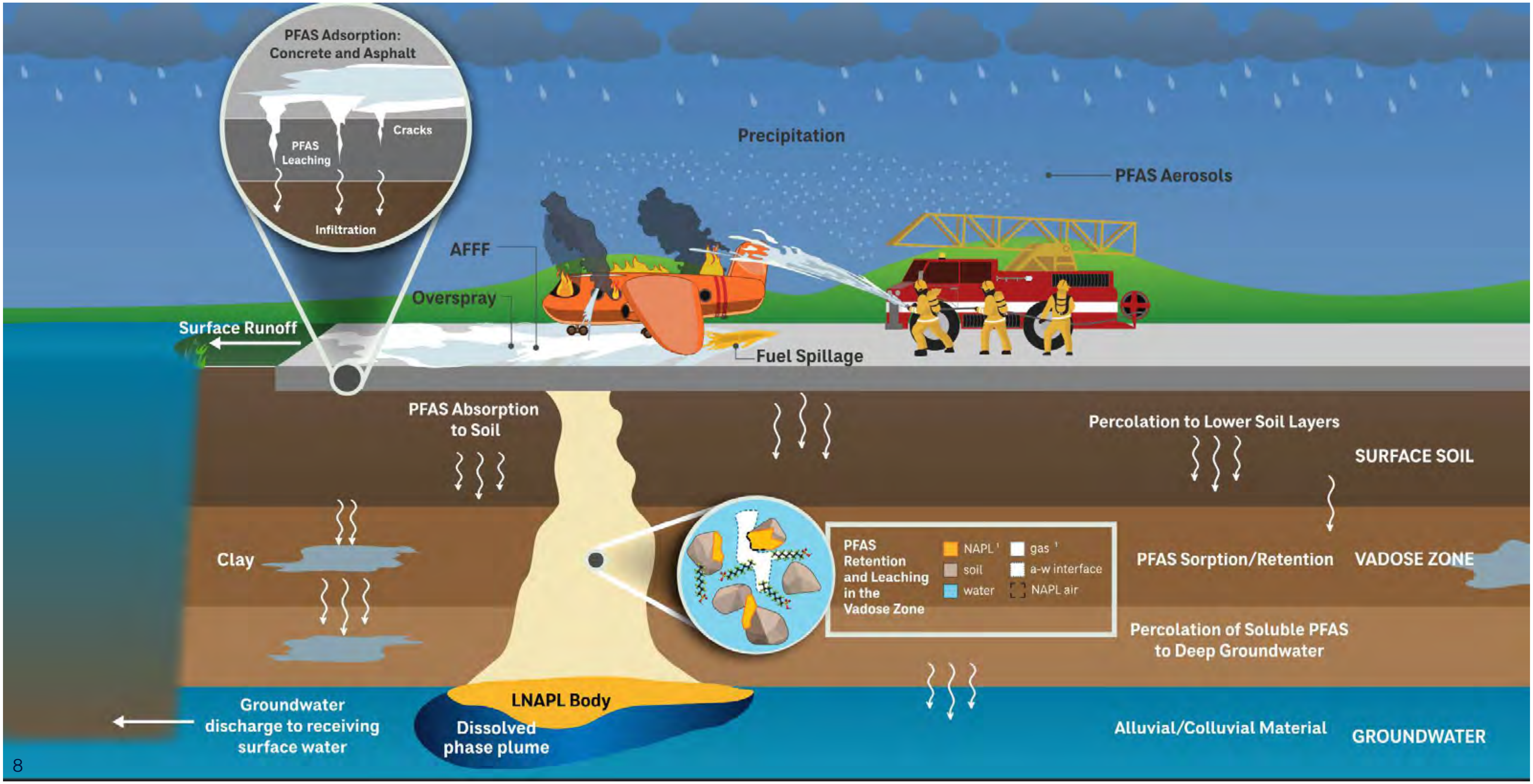
- Human Transport
- Environmental Migration
- Primary sources
- Secondary sources



Building Decision-Making CSMs for PFAS

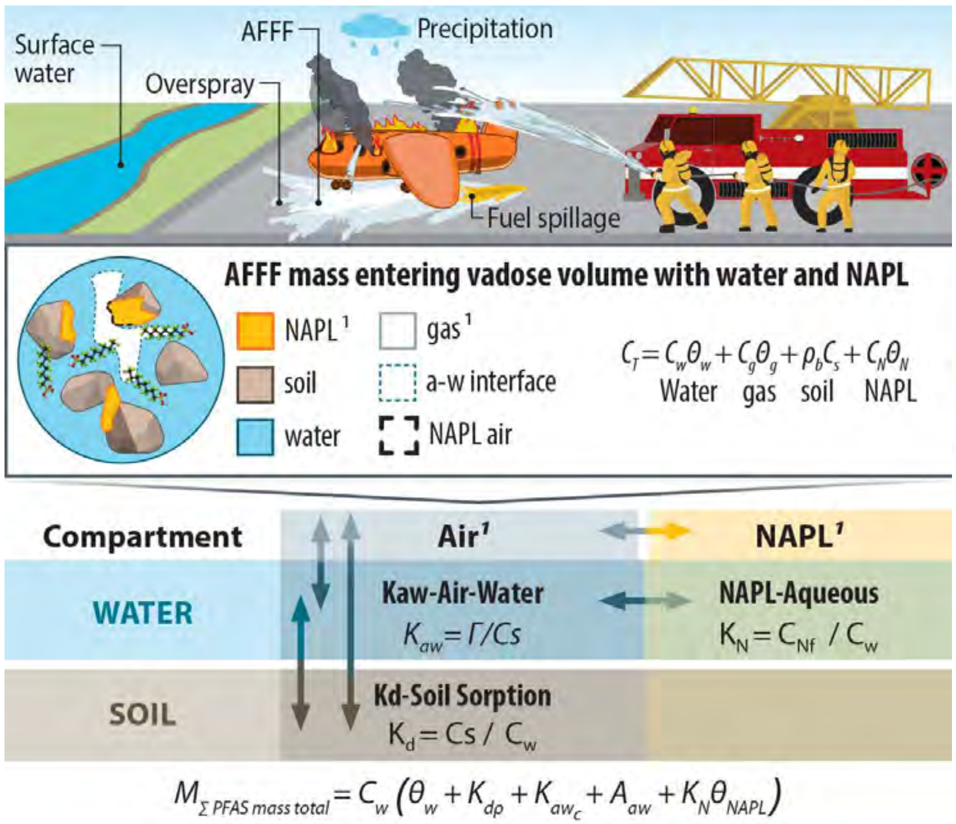


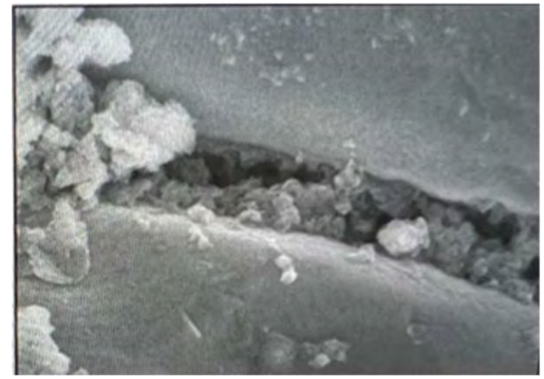
Building an AFFF Conceptual Site Model



Fate and Transport Considerations: Sources

- Surfactants accumulate on surfaces and at interfaces, including:
  - Air : Water
  - Solid : Air
  - Solid : Water
  - NAPL : Air
  - NAPL : Water





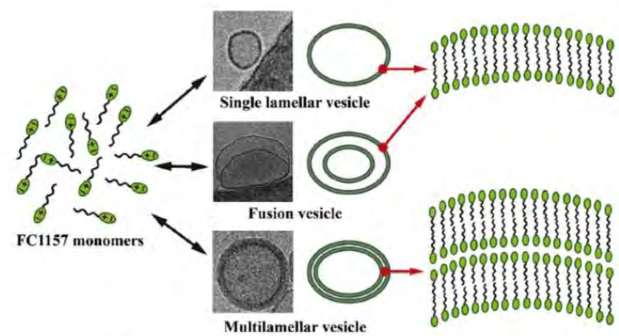
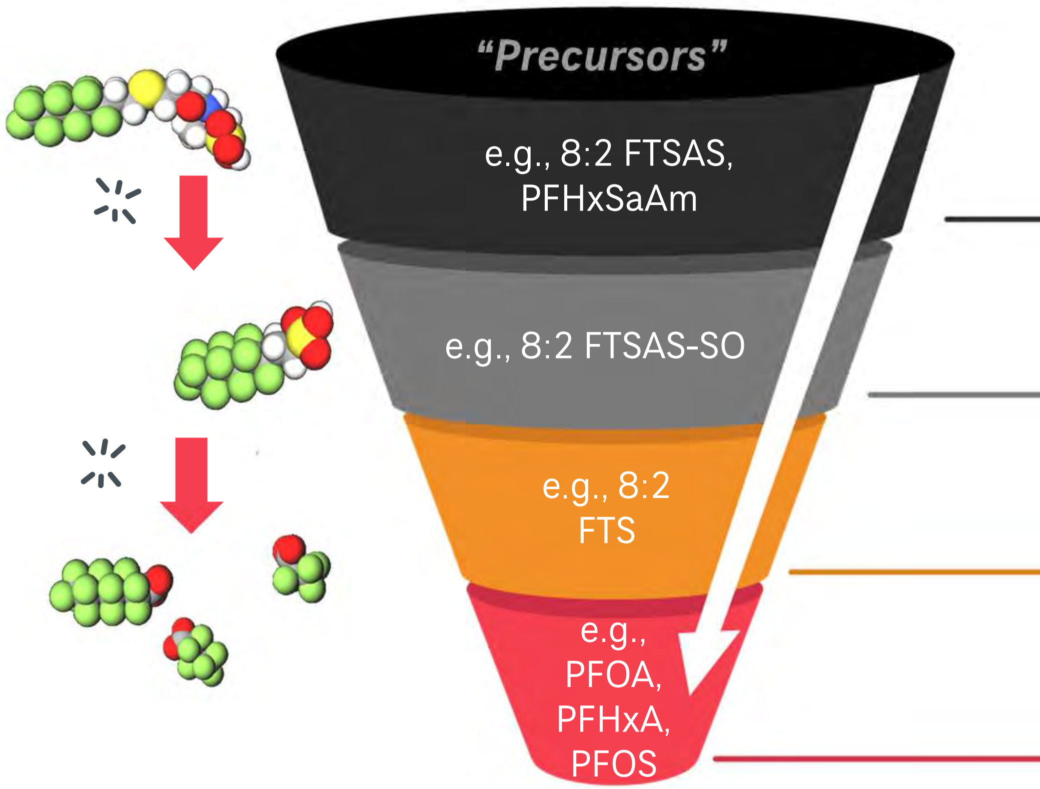


Fig. 14. A schematic illustration on the possible self-assembly structures of FC1157.

Yu et al., 2020

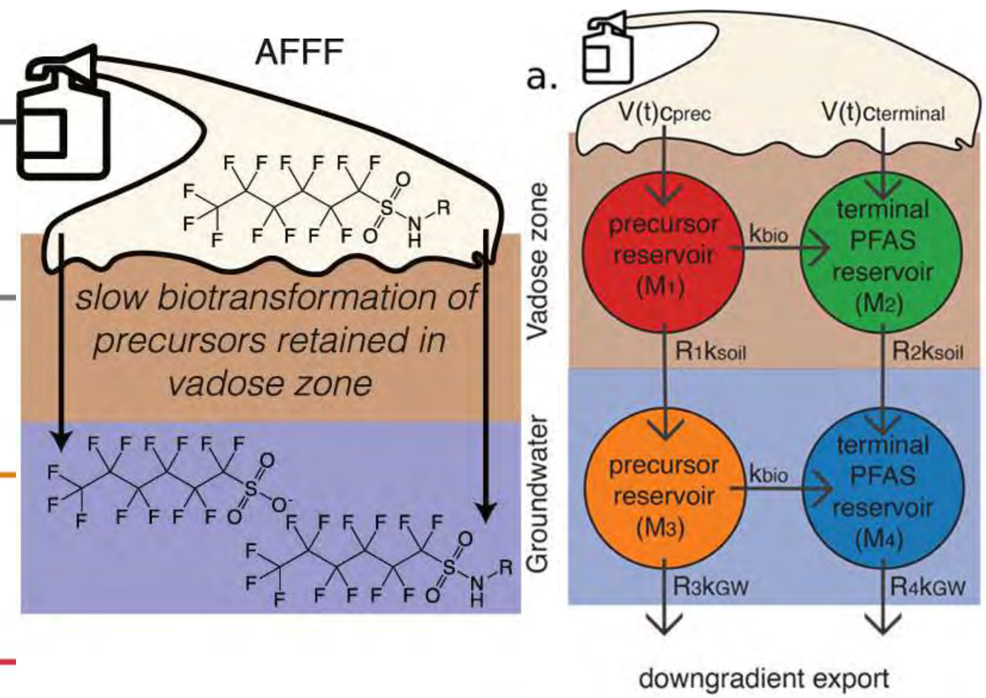
Some PFAS can form highly stable assemblies/ films on surfaces

Precursors Transformation: Sources



Centurial Persistence of Forever Chemicals at Military Fire Training Sites

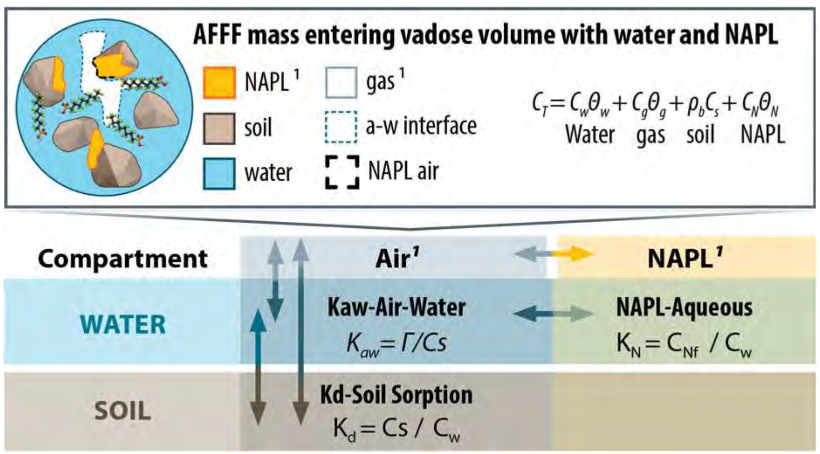
Bridger J. Ruyle*, Colin P. Thackray, Craig M. Butt, Denis R. LeBlanc, Andrea K. Tokranov, Chad D. Vecitis, and Elsie M. Sunderland



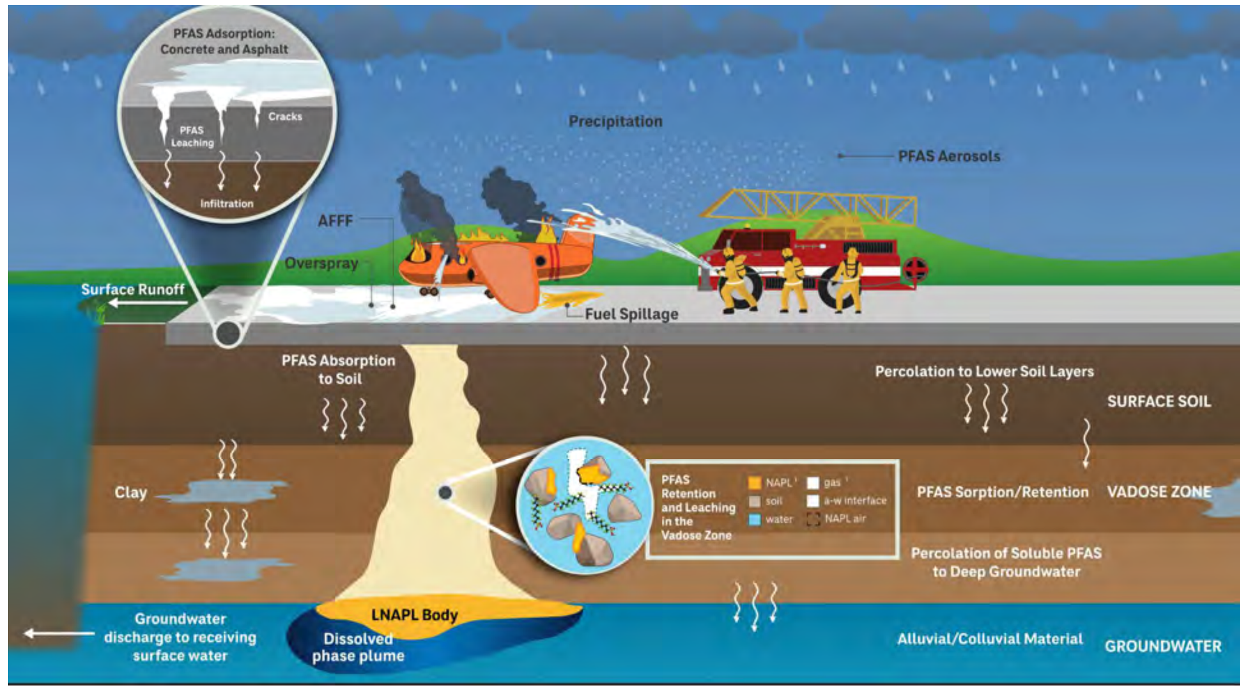
PFAS: Analytics Tools for CSMs and Evaluating PFAS Loads

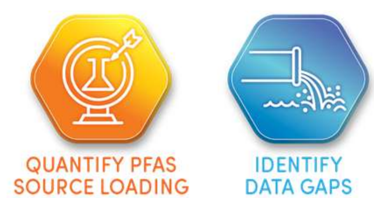
Understanding PFAS Impacts: Mass Flux and Loading Key

- Most mass is retained in the vadose zone
- Source Loading and Leaching
  - Leaching flux mechanisms important to understand
- Impact to receptors- Mass loads (discharge) to surface and groundwater systems



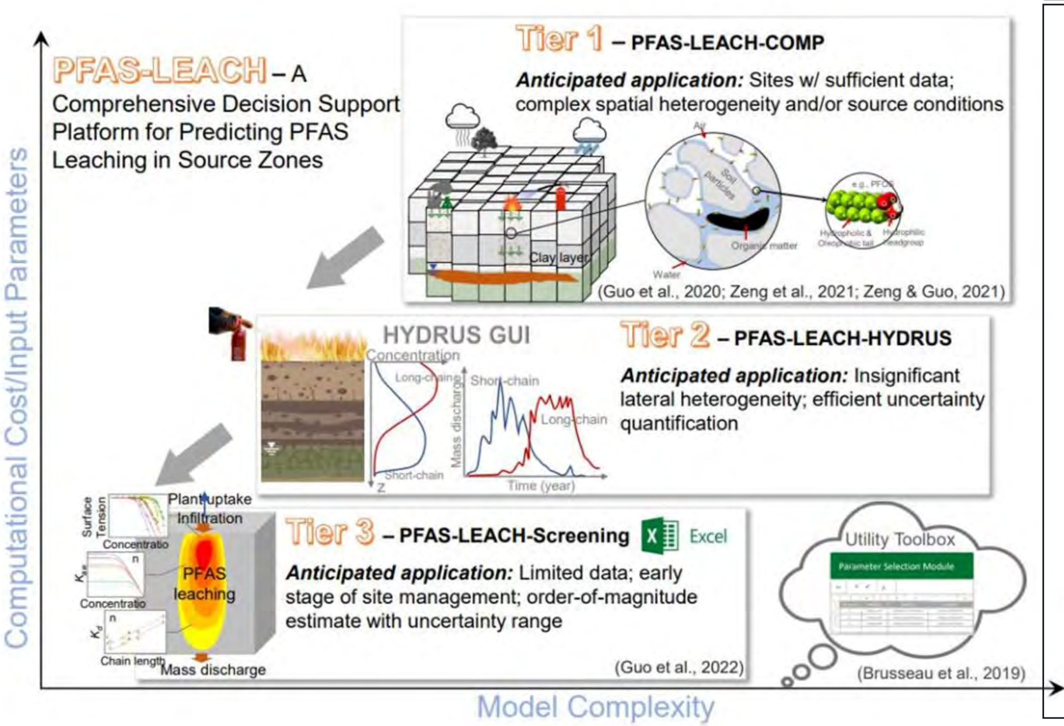
$$M_{\Sigma\,PFAS\,mass\,total} = C_w\left(\theta_w + K_d\rho + K_{aw_c}A_{aw} + K_N\theta_{NAPL}\right)$$





PFAS Leaching Modeling

Air-Water Interfacial Sorption



EPA

United States Environmental Protection Agency | Office of Solid Waste and Emergency Response Washington, DC 20460 | EPA/540/R95/128 May 1996

Superfund

Soil Screening Guidance: Technical Background Document

$$C_T = C_p\left(K_d + \frac{\theta_w}{\rho}\right)$$

Traditional approach

Measured in a soil sample — *Present in porewater*

$$C_T = C_p\left(K_d + \frac{\theta_w}{\rho} + \frac{k_{aw}a_i}{\rho}\right)$$

for PFAS (ER18-1204; ER20-5088)

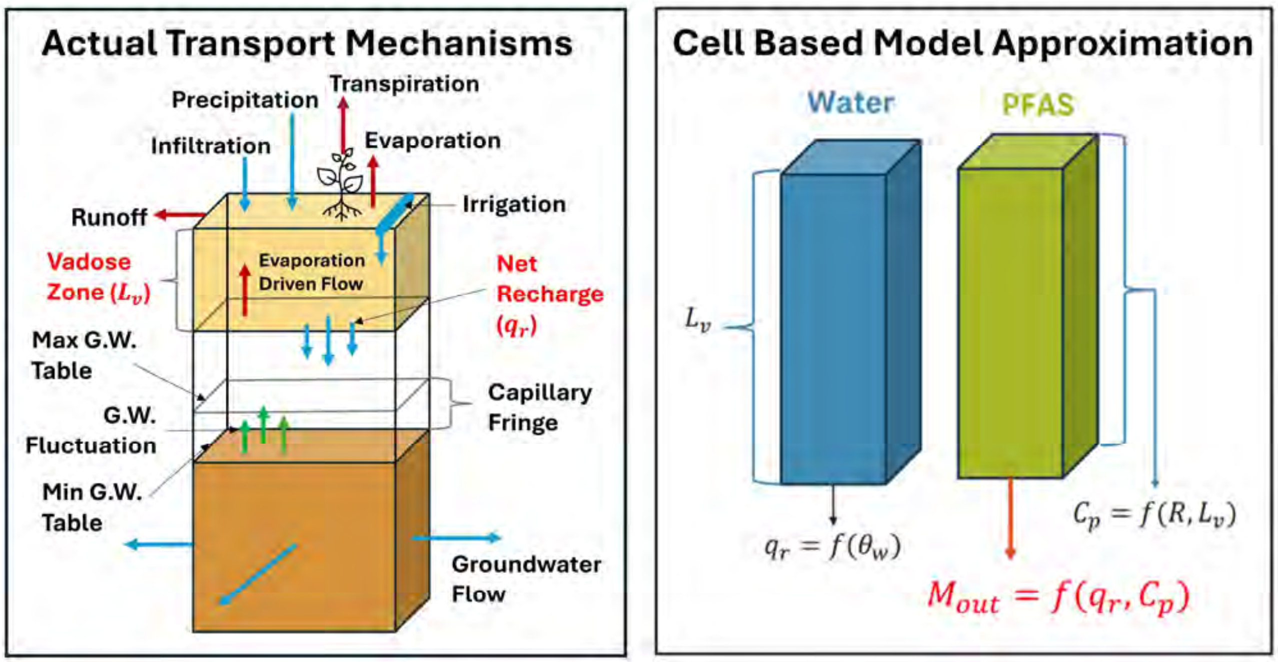
$$C_T = C_p\left(K_d + \frac{\theta_w}{\rho} + \frac{k_{aw}a_i}{\rho} + \underbrace{\frac{K_N\theta_N}{\rho} + \frac{k_{nw}a_{i-n}\theta_N}{\rho}}_{\text{May be in the form of emulsion/gel phase}}\right)$$

for PFAS with residual NAPL

Model Development – VZ Conceptual Model

- Two Potential Screening Models for PFAS
  1. PFAS LEACH Excel
     - Smith et al. 2024
  2. Cell Based Numerical
     - Stults et al. 2025
- Cell based numerical selected
  - Excel based screening tool requires manual calculation
  - Excel based tool is steady state, not based on real-time data

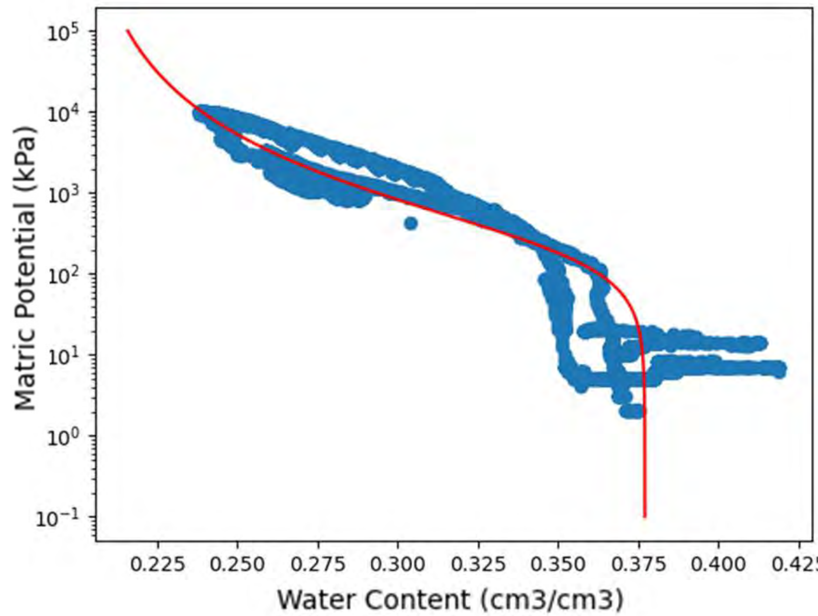
Stults et al. 2025



Vadose Zone Water Retention Calibration

- Multiple Field Sensors Deployed
- Paired water content and tensiometers to develop water retention function

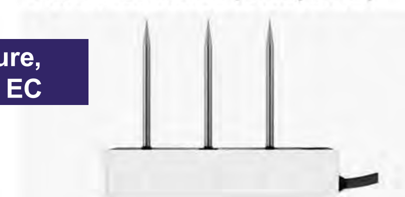
Tensiometer (matric potential)



Field Data Logger w/Sensor (Left)

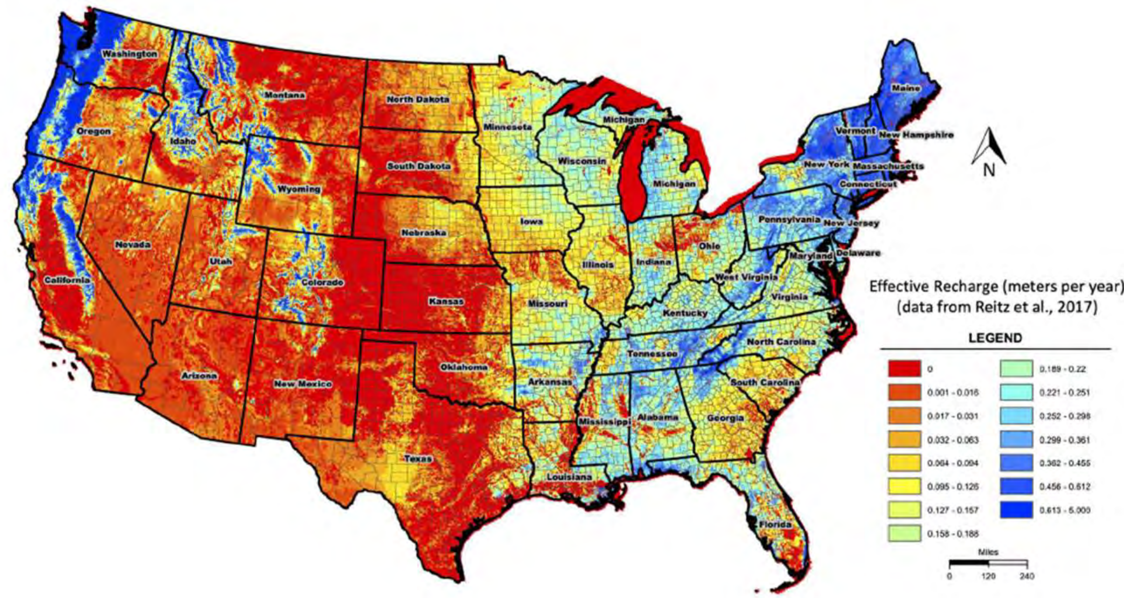
High Res. Field Logger and Sensors (Right)

Soil Moisture, Temp, and EC



Vadose Zone Hydraulic Flux Validation

Reitz et al. 2017 / Newell et al. 2023

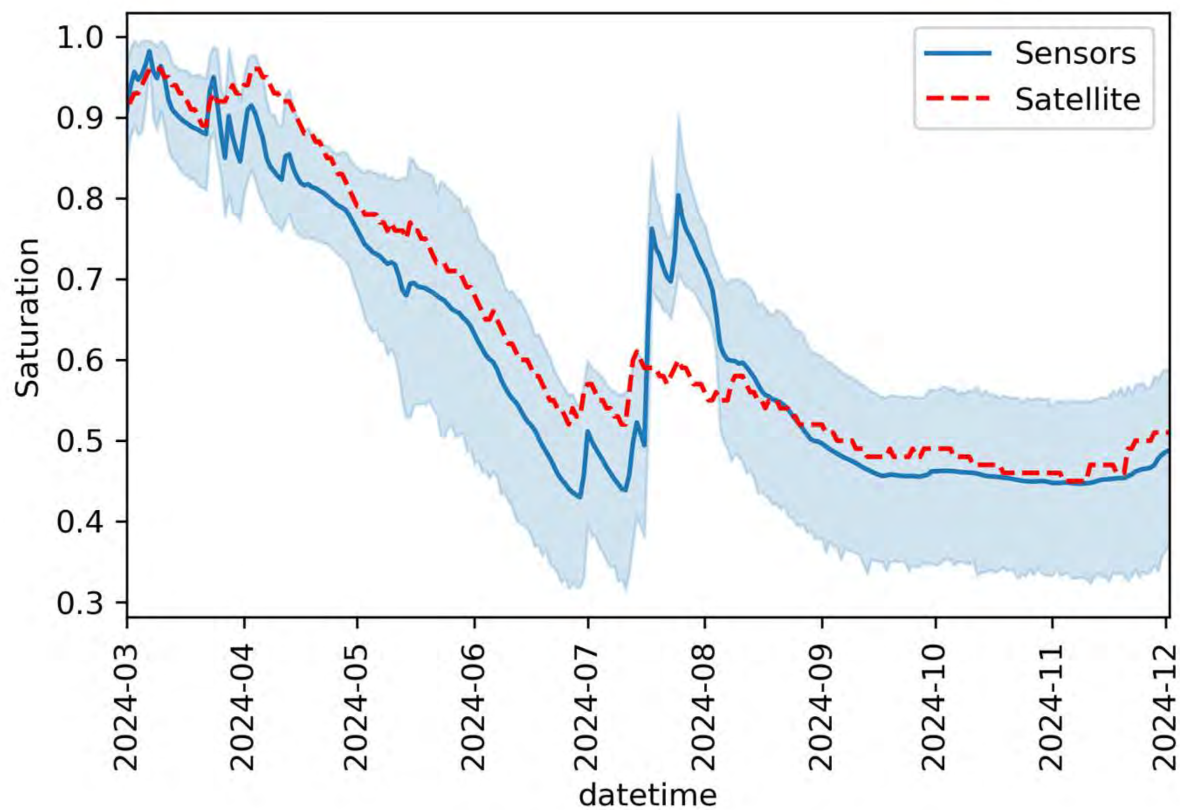


- 10-year period from 2015-2025
- Three Net Recharges compared
  1) Rietz et al. 2017
     - 200-400 mm/yr between 2003-2015
  2) Calibrated Flux Model
     - 225 mm/yr over 10 year
  3) Precipitation – Evapotranspiration
     - 761 mm/yr over 10 years
- Runoff/Lateral Flow Important

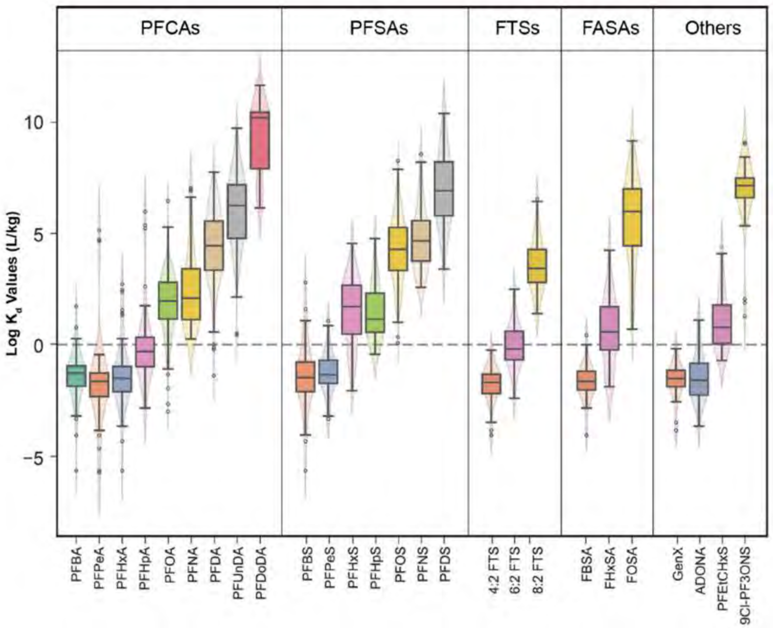
  ~2/3 of all net surface water
- Multiple Lines of Evidence Approach to Evaluate Recharge

Vadose Zone Satellite vs. Sensor Validation

- Sensor and Satellite Measured Saturated Well Correlated
- Good confidence in accuracy of historical data used for model
- Blue shaded is 95% CI of saturation.



Equilibrium PFAS Partitioning Database



Xie et al. 2024 – Solid Partitioning (Kd)

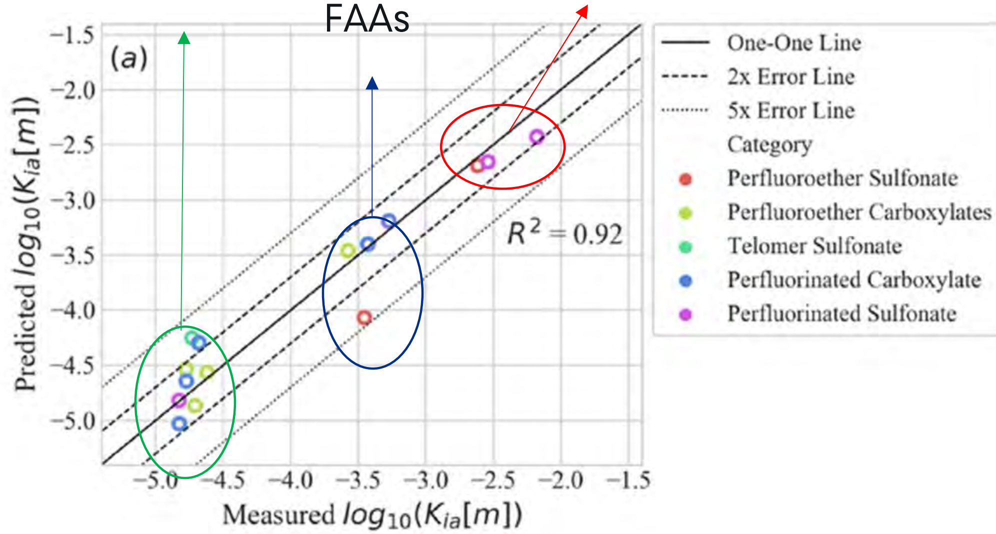
1. $R = 1 + \frac{K_d \rho_b}{\theta_w} + \frac{K_{ia} A_{aw}}{\theta_w}$

2. $v_{PFAS} = \frac{q}{\theta_w} \frac{1}{R}$

< C5 Ethers, telomers, PFAAs

C5-C6 Ethers, PFAAs

>C6 Ethers, PFAAs

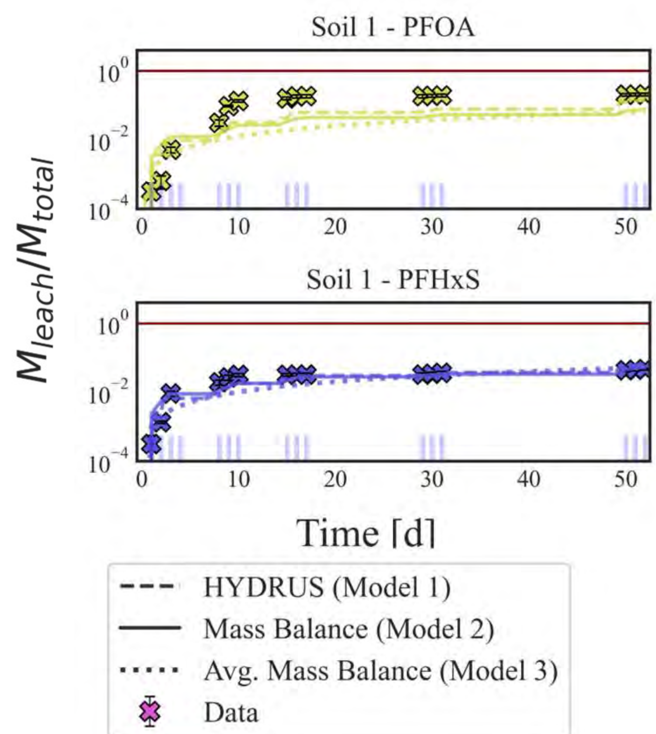


Stults et al. 2023 – Air-water interfacial Partitioning (Kia)

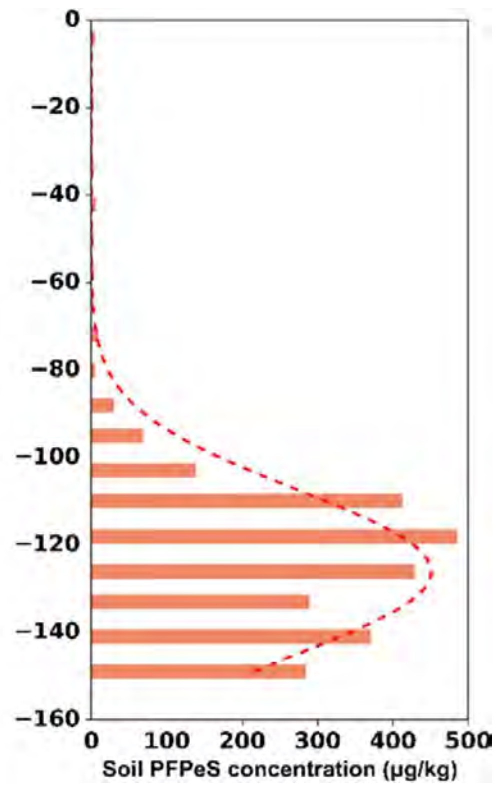
Xie et al. 2024 – Solid Partitioning (Kd)

Model Development – VZ Screening Validation

- Screening Model Validated for prediction of Mass Flux over extended periods of time.
- Similar performance to HYDRUS in lab and field settings
- Can couple with uncertainty analysis for capture of non-ideal processes



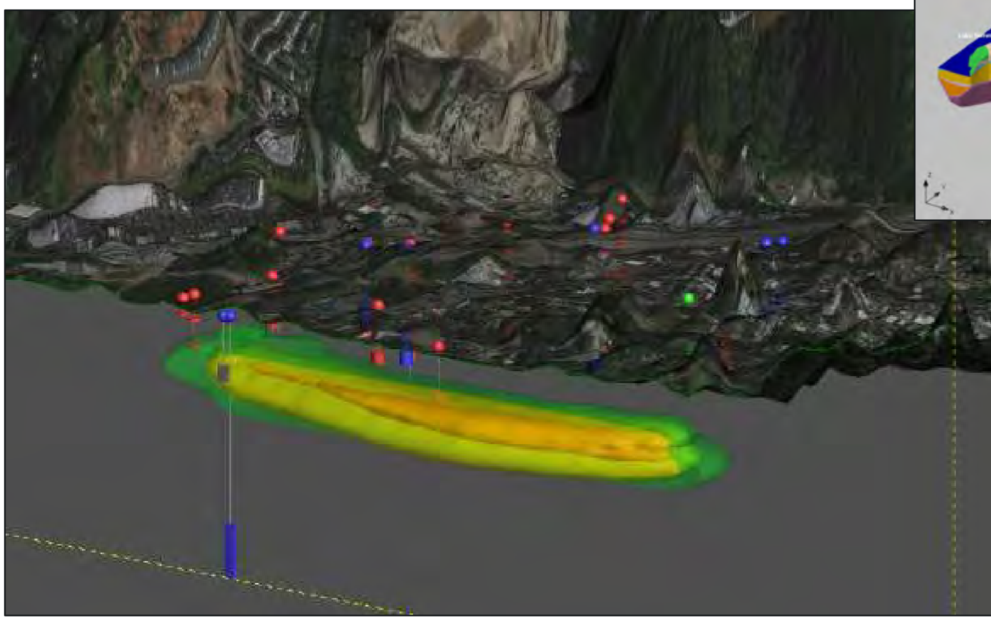
Stults et al. 2025 –
Laboratory Validation Against HYDRUS

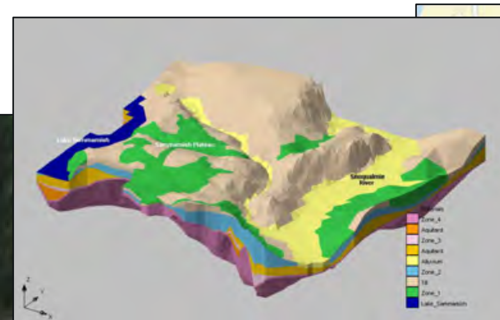


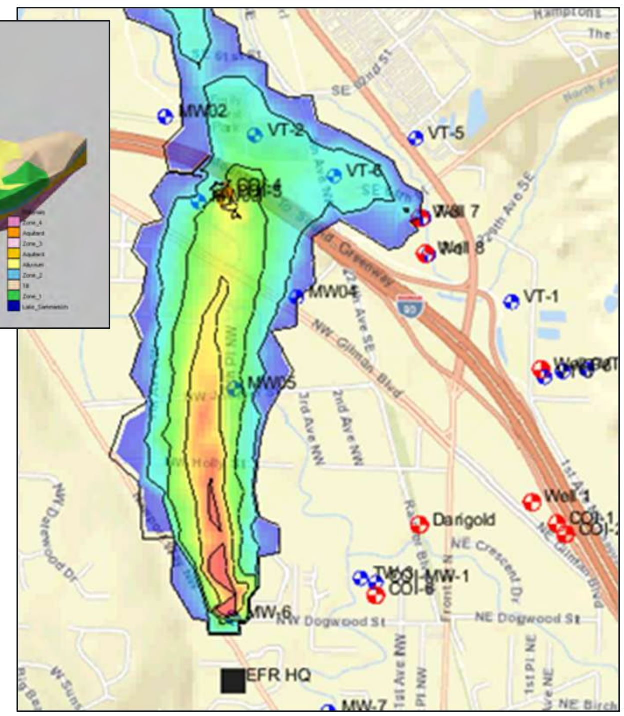
Bigler et al. 2024 –
Field Validation

Vadose Zone Model: PFAS Loads to Groundwater and Surface Water Models

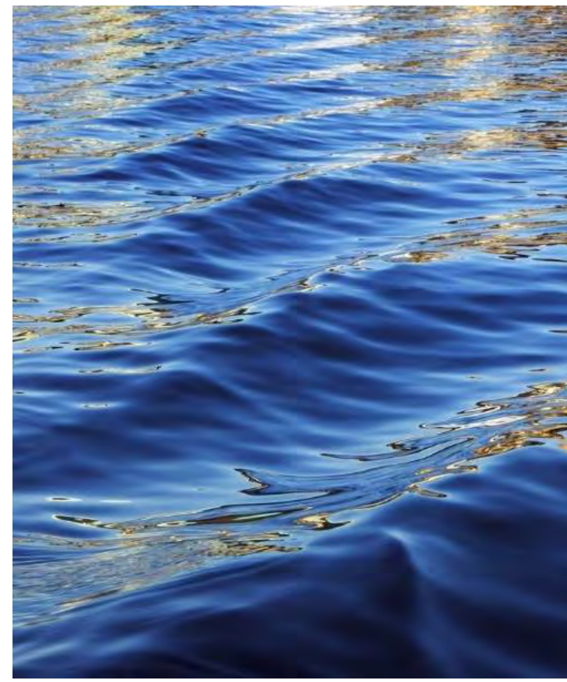
- **Link leaching loads to surface water** transport, e.g., HSPF
- **Link leaching loads to groundwater** PFAS loads to groundwater, which are then evaluated using transport module, e.g., MODFLOW,MT3D, RT3D
- **Load exchange between surface water and groundwater**







BAA-2112: Advanced-Data Analytics & Forensics Framework & FT003 Field Demonstration



The Challenge of Creating Large Data Sets

- PFAS data sets are growing in size and complexity.
- Collecting and managing environmental data presents many challenges.
- Ensuring data quality and completeness remains a key concern.
- Organizing data continues to be difficult.
- Technological advances are aiding in overcoming these issues.

Adaptive Tools for Decision-Making:
BAA-2112: Advanced-Data Analytics & Forensics Framework

DEFINE GOALS AND SELECT DATA ANALYTICS

ANALYTICS
- ESS
- Statistics
- 3D Model
- Geochemical Model
- Hydraulic Model
- Fate and Transport Model
- Dashboards
- Reports
- Chemical forensics

MINE EXISTING DATA AND BUILD DATA LIBRARY

Source Data

\+

Data Library

\+

Data Linkages

ANALYZE AND VISUALIZE

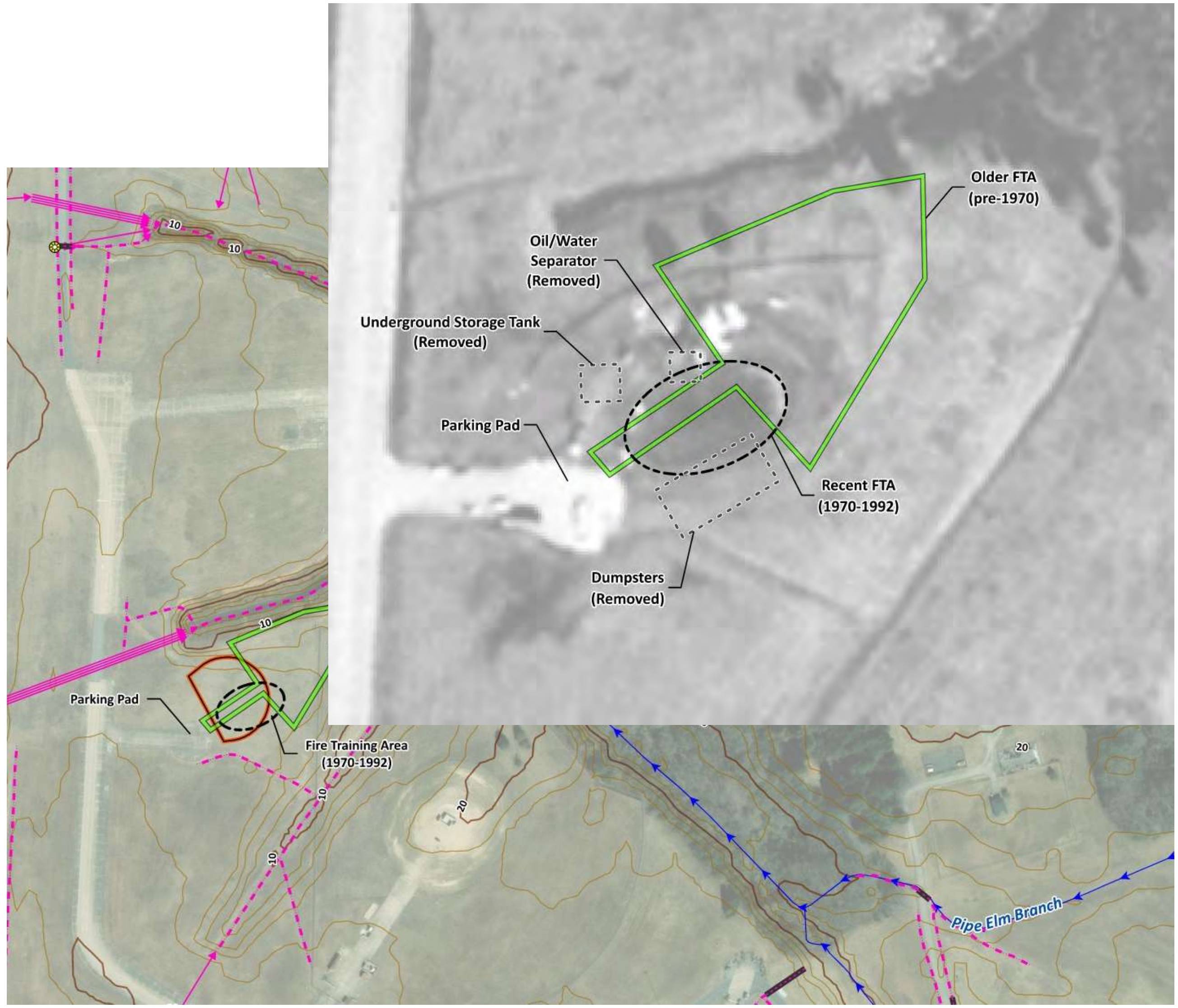
- **Chemical Fingerprinting**
- **Statistics and Predictive Modeling**
- **Background, e.g., PFAS**
- **Environmental Sequence Stratigraphy**
- **Attenuation Mechanisms**

REMEDIAL DECISION-MAKING

- **Select Remedial Technologies**
- **Evaluate treatment performance**
- **Optimize existing treatment systems**
- **Predict treatment timeframe**

FT003 History

- Former Fire-Training Area (FTA)
- Pre-1970- waste oil/fuel burned in an open pit
- 1970-1992- FTA moved southwest
  - Ignited 2X/week
  - Extinguished with AFFF, estimated 200 gallons

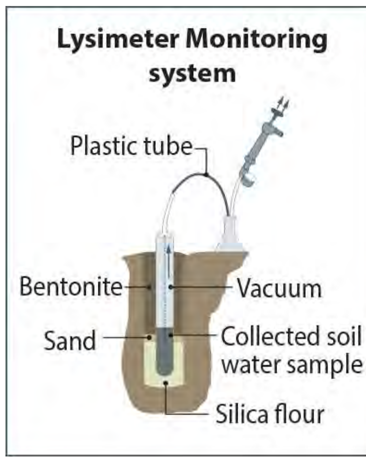


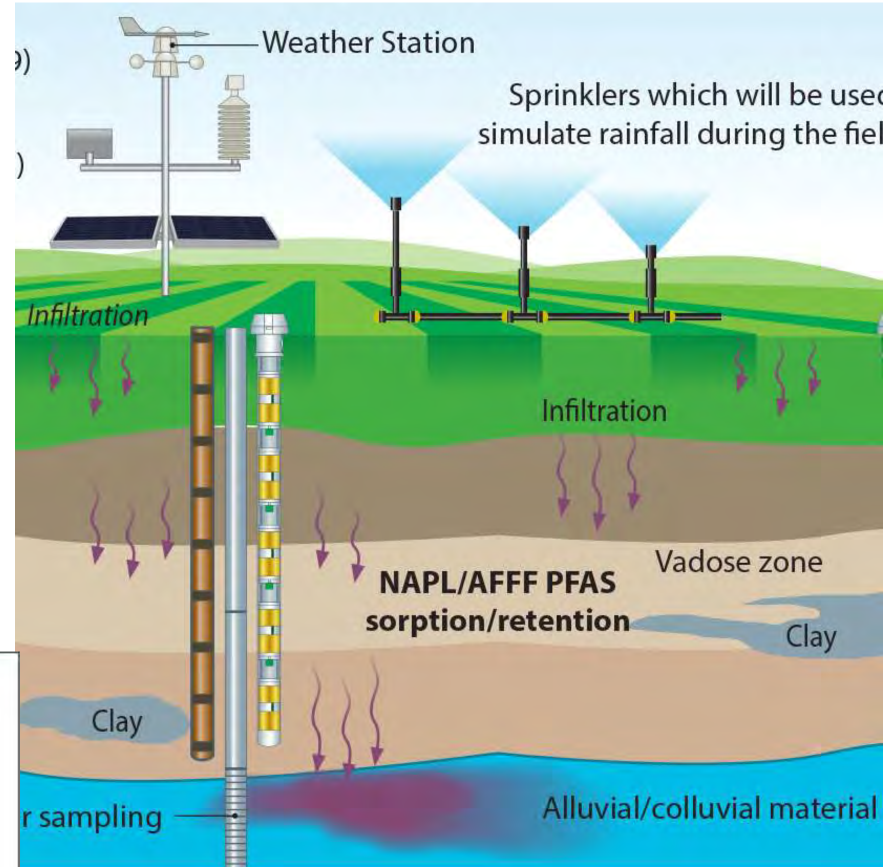
Elements of the PFAS Investigation

Generate a PFAS dataset incorporating all historical hydrogeologic, geochemical, contaminants and climate data to support new analytics.

Build a CSM: Evaluate Loads from Sources to receptors (Groundwater, surface water, stormwater, wetlands).

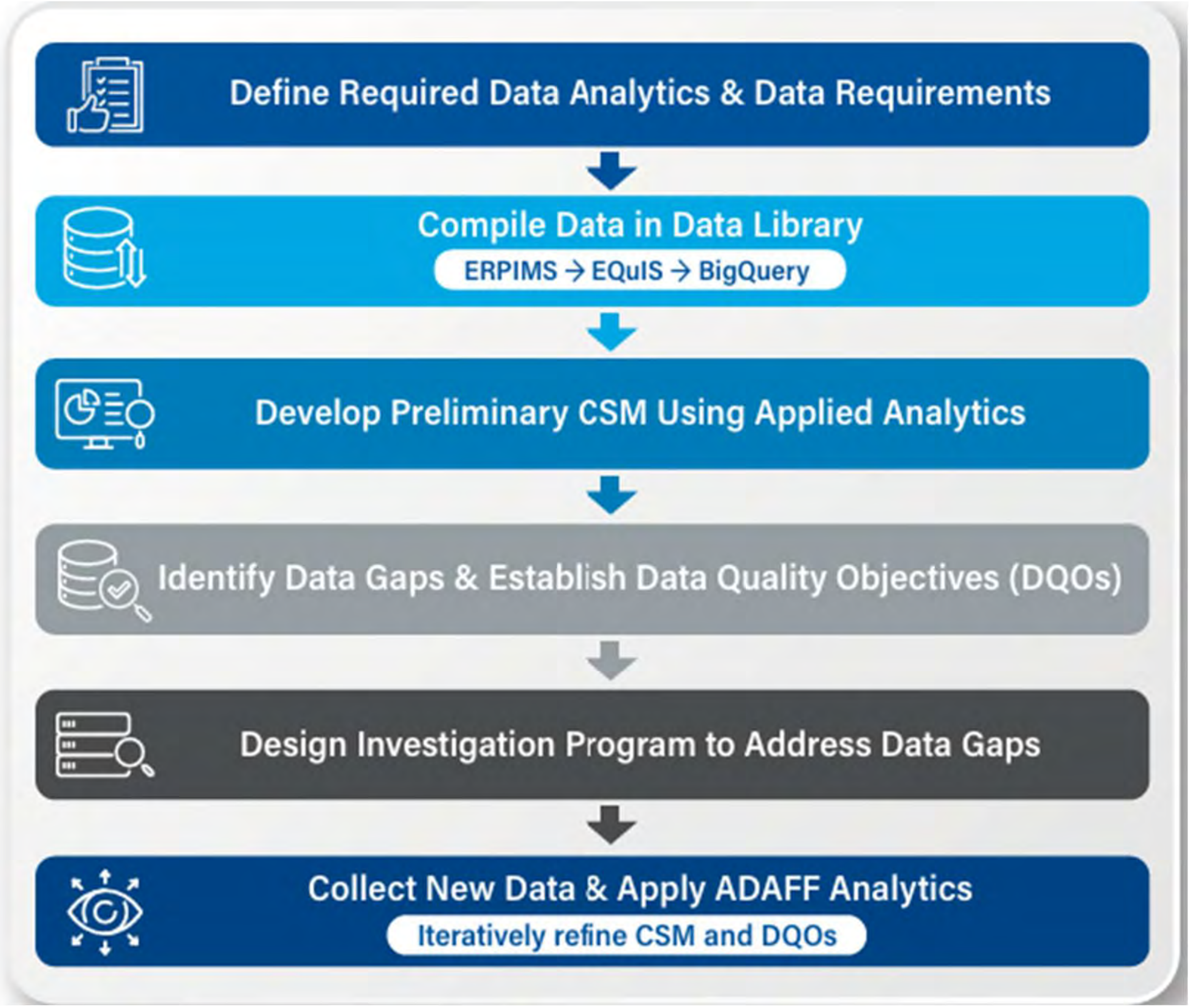
Identify data gaps to reduce uncertainties in PFAS CSM to support a future remedial investigations and risk assessment.



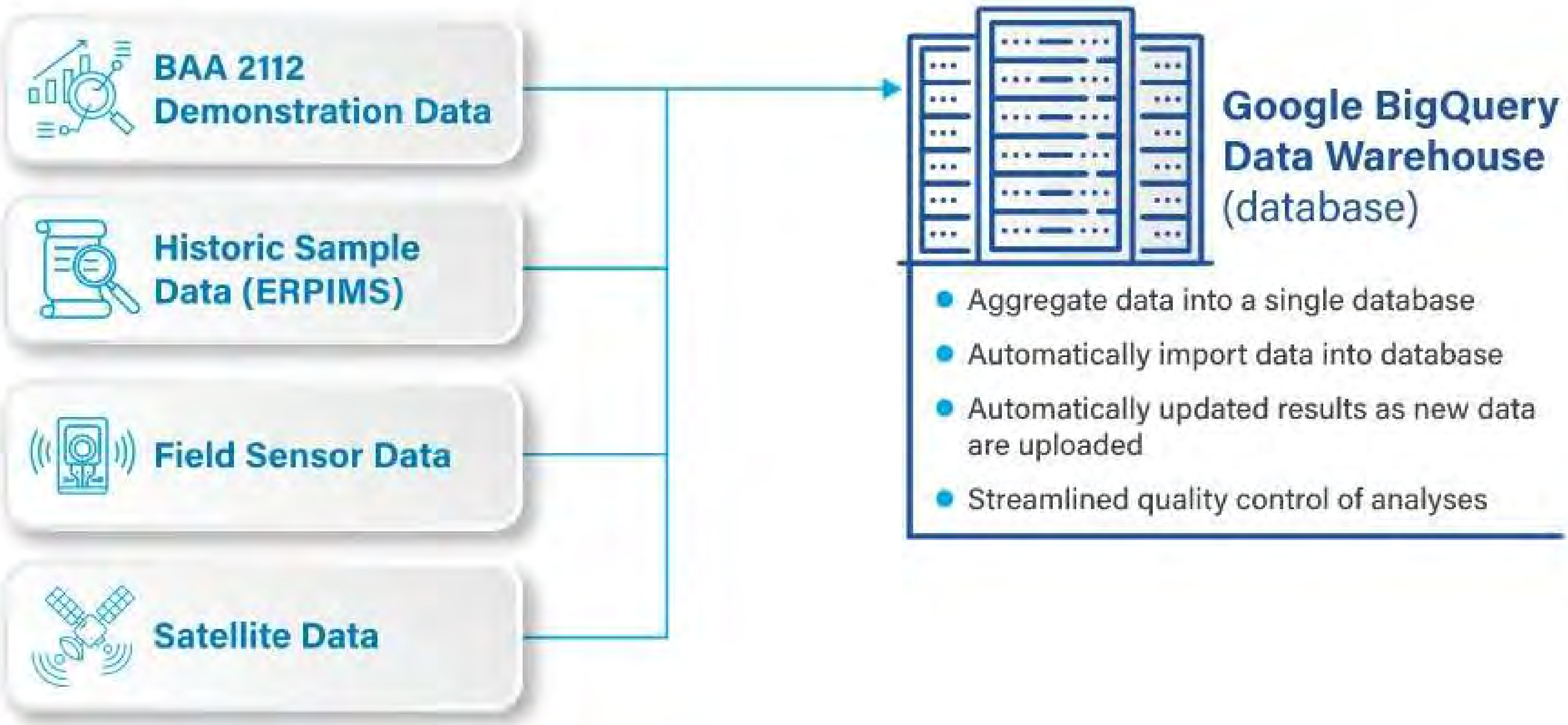


ESTCP: ER20-B2-5088, AFCEC: BAA-2108
Lysimeters can obtain a porewater sample for direct measurement of leaching and impacts to groundwater.

Planning Workflow for Data Compilation



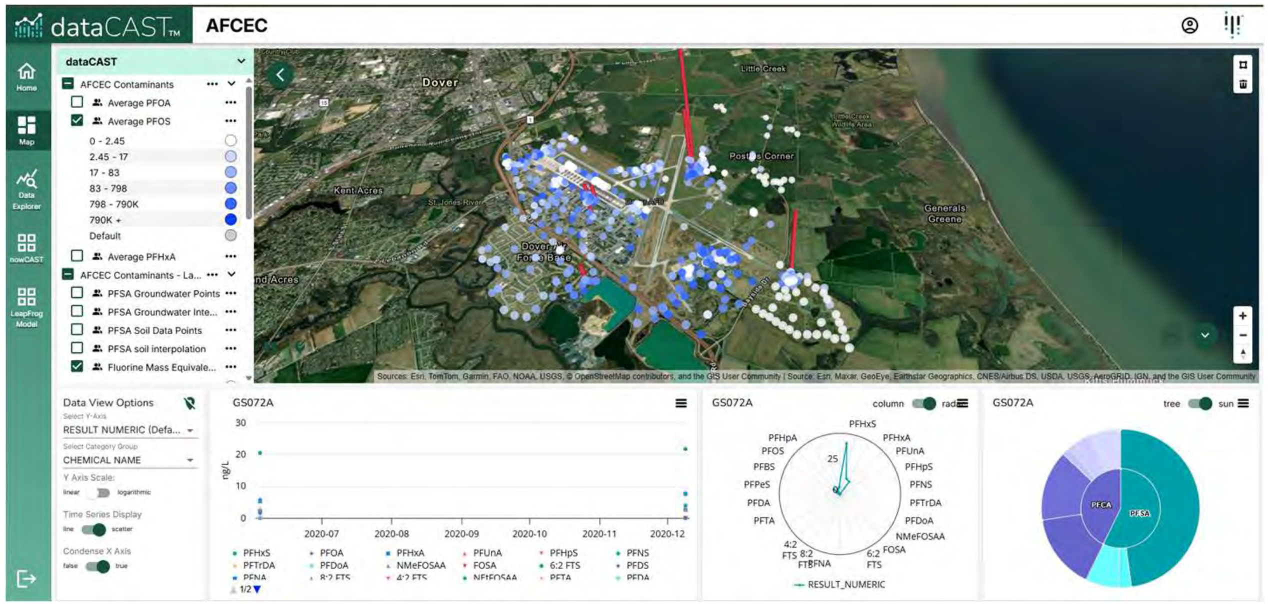
Centralized Database



Data Management Platform Needs

- Data management
- Analytics
- Custom visualizations
- Cloud-based, accessed via a web browser
- Secure with controlled user access
- Flexible for any kind of input data, e.g., spreadsheets, EDD, sensor, model output

dataCAST™



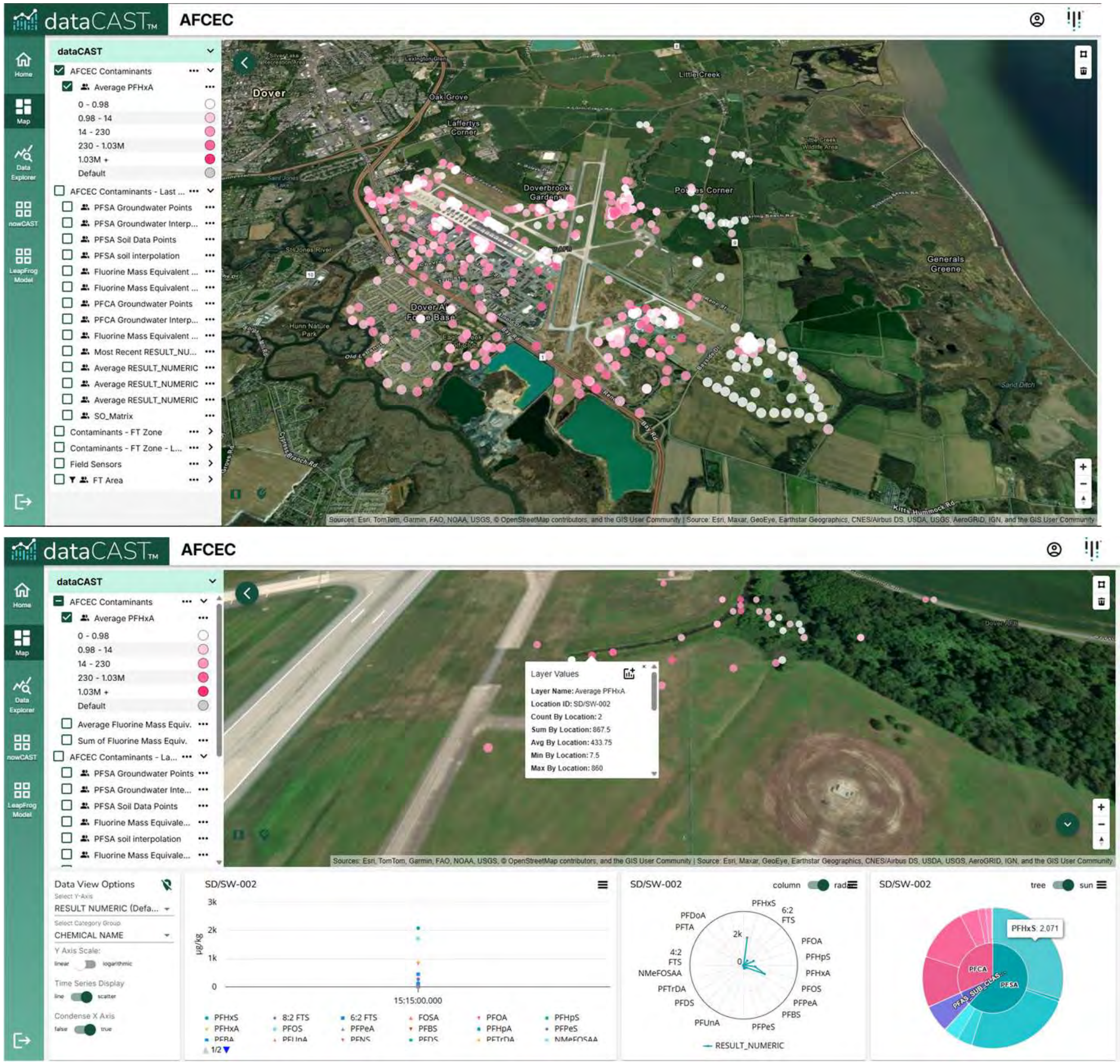
Key Benefits of Our Approach:

- Aggregated data into a single database
- Automatically updated results as new data are uploaded
- Shareable user-generated graphs
- Streamlined QC of analysis

DATACASTE DEMO:

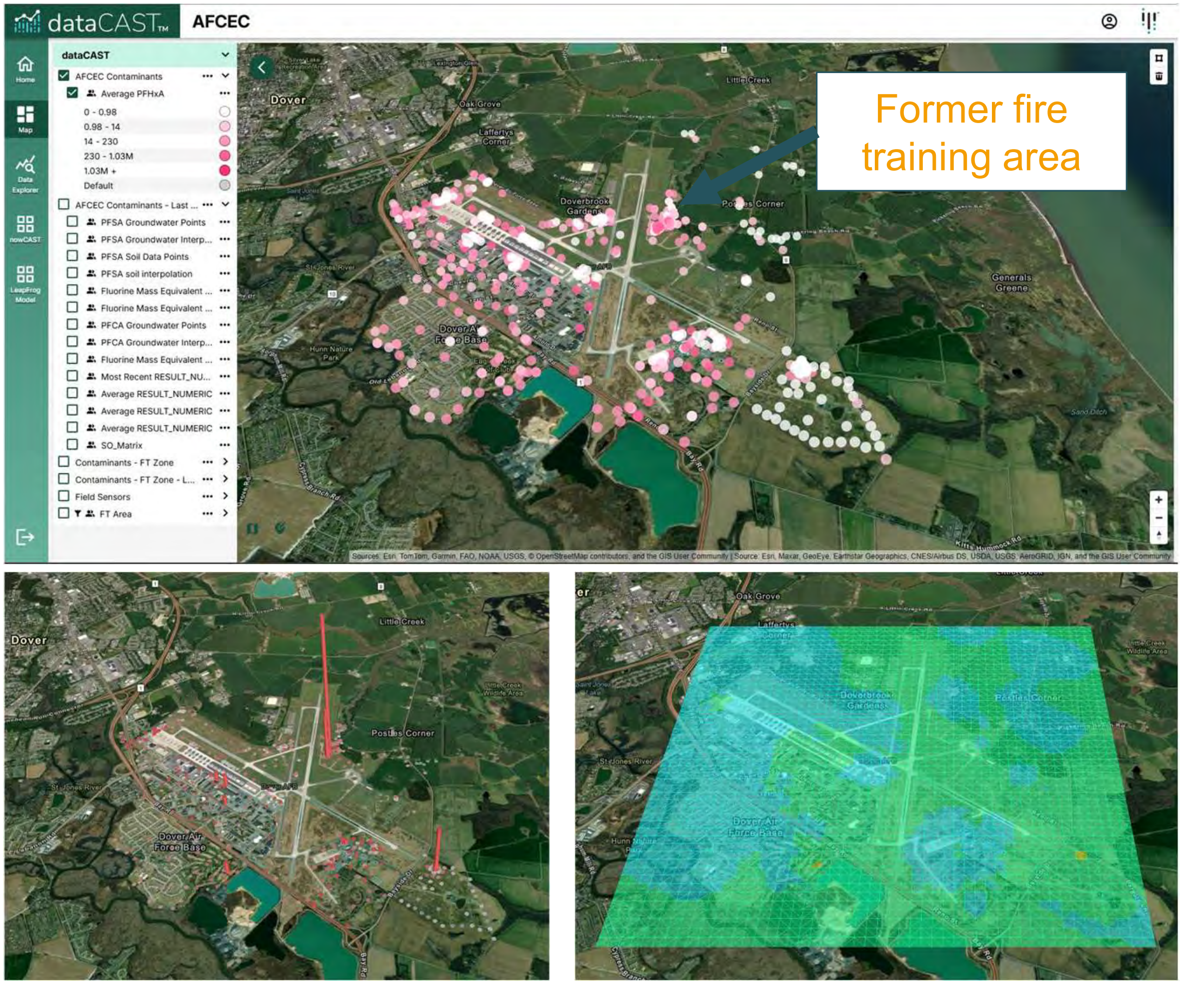
Interactive Sample Analysis

- Analyze specific sample locations and inspect PFAS **composition**
- Visualize proximity to receptors, e.g., surface water streams, drinking water wells
- Useful for spot-checking and answering **specific questions**



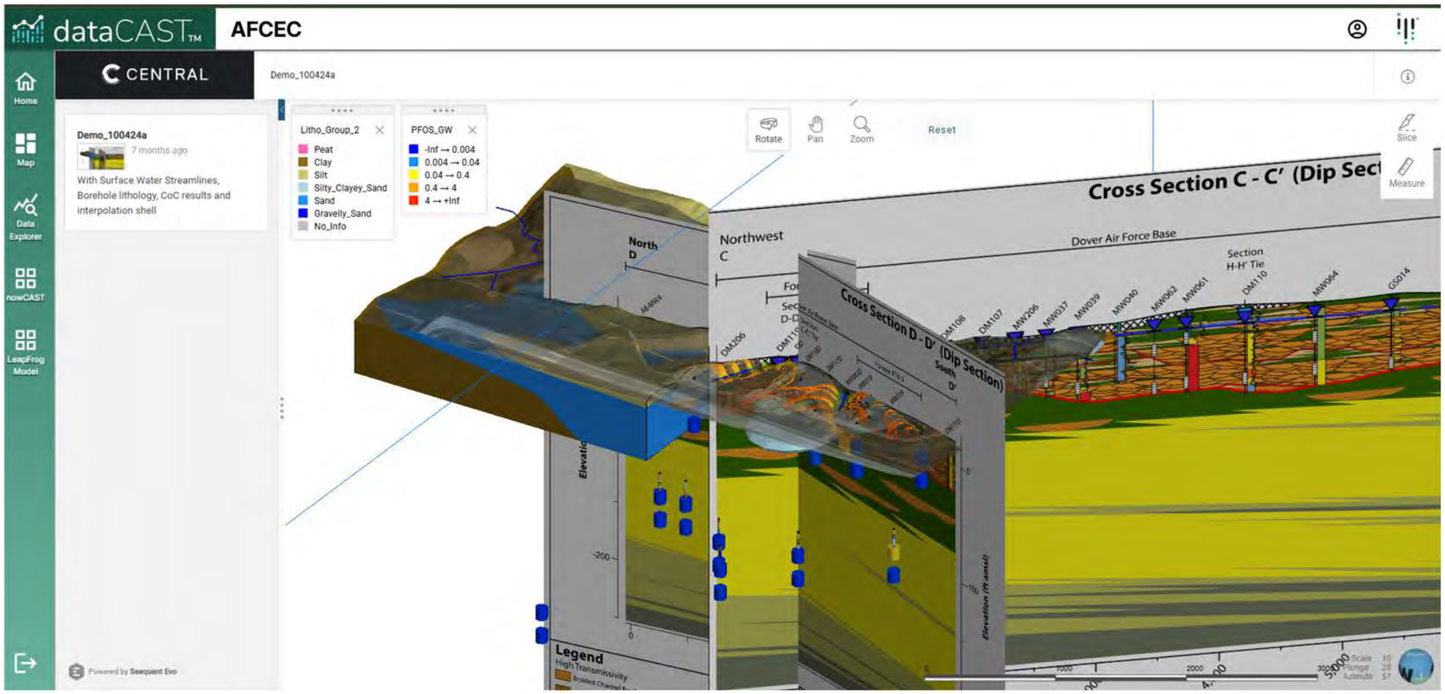
Spatial Analysis

- Create and share GIS **map layers** (e.g., average concentration of chemical X in 2024)
- Generate holistic views of site-wide PFAS contamination
- Layers **automatically update** when new data are uploaded



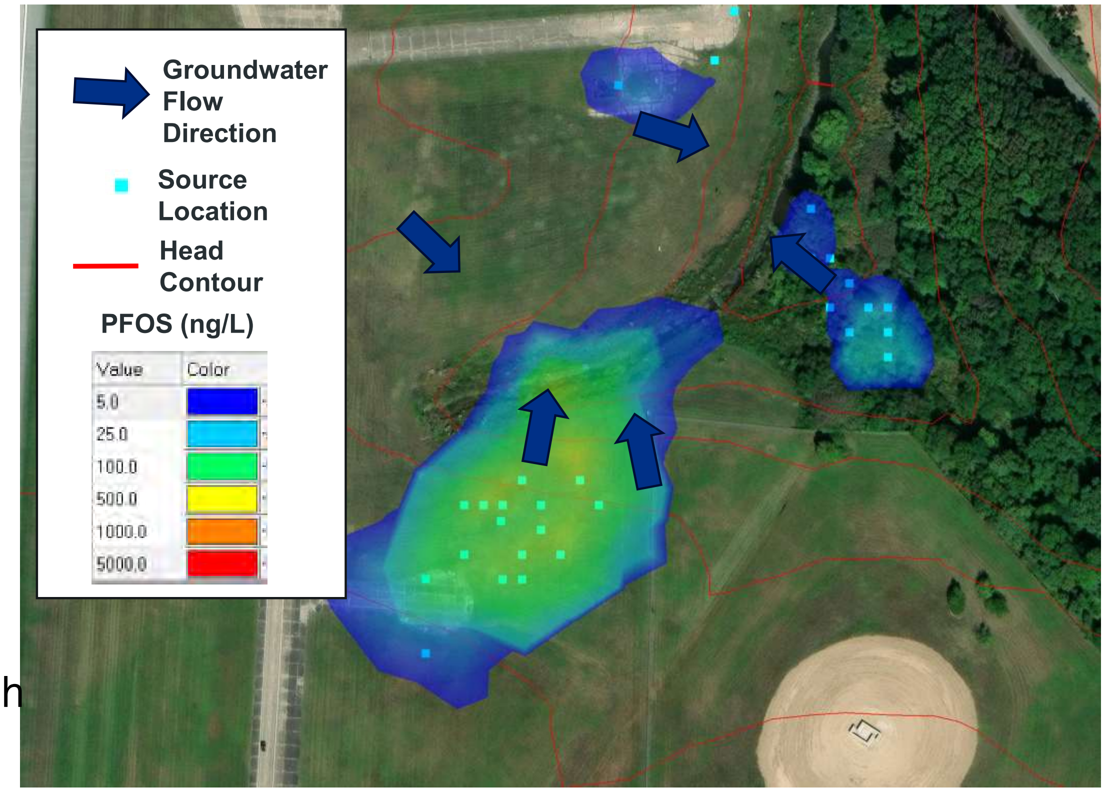
Custom Embedded Leapfrog

- 3D visualization
- Leverage Leapfrog to interpret cross sections
- Supports conceptual site model development



Groundwater Model Setup

- Constructed a simple groundwater model based on existing data
  - Ground surface
  - Material properties
  - Recharge
  - Boundary heads
  - Average conditions
- Steady state groundwater flow
- Groundwater flow near source areas is governed by surface water bodies
- Run transport for 8 PFAS from 2021 through 2025 using input from vadose zone model



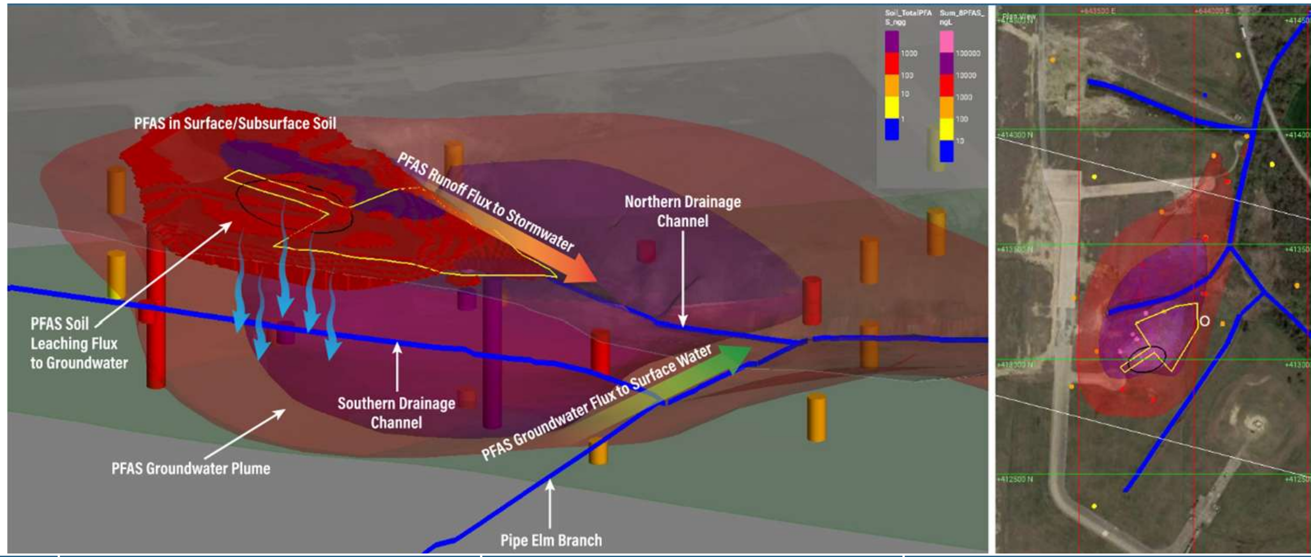
Results and Analysis from Coupled Models

2022-Year 0

PFOA	PFOS	PFHxA	PFHxS

CDM Smith

Source Longevity



Chemical	Mass Discharged by March 1, 2025 (lb)	Mass Discharged by March 1, 2055 (lb)	Mass in Vadose Zone Soil (lb)[1]	Time to Deplete Source Mass from Leaching (yr)
PFOS	0.017	0.165	20.88	401.3
PFOA	0.093	0.168	7.05	138.8
PFNA	0.001	0.003	0.22	242.0
PFHxS	0.164	0.427	12.69	97.8
PFBS	0.018	0.036	0.75	69.2
PFBA	0.006	0.009	0.26	93.4
PFHxA	0.068	0.159	3.47	71.7
6:2 FTS	0.024	0.038	1.35	117.2

Benefits of Data Analytics Approach

Quickly integrate multiple lines of evidence to fill data quality objectives

- Conventional tools (soil, groundwater, surface water sampling)
- In situ logging (HPT)
- Downhole geophysics (gamma)

Advanced and integrated 3D visualization, mapping and modeling presentations

Assess distribution of PFAS, fingerprint/composition, presence of PFAS precursors, and mass flux and discharge (leaching, groundwater and surface water transport)

Understanding loads and impacts to receptors for remedy decision-making

Acknowledgements

CDM Smith

- Travis Tomaselli
- John Stults
- Christine Pilachowski
- Riley Cotter
- Maxwell Hire
- Ernest Ashley
- Tom Cook
- Matt Gamache
- Teresa Nelis
- Shavonne Gordon

trinnex
Trust in what's next.

- Eoin Howlett
- Patrick Lewis
- Josh Soper

AIR FORCE CIVIL ENGINEER CENTER

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- Jeffrey Davis
- Kent Glover
- Miguel Gallegos

AFCEC Dover

- Leroy Demarest
- Robroy Young
- Gary Charyak

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Your Success is Our Mission!