

2024 Battelle Chlorinated Conference

June 2-6, 2024 | Denver, Colorado

Interactive Dashboard Toolboxes with Coupled Data Based Mass Flux Models for High Resolution PFAS Conceptual Site Models

CDM Smith ¹

Dr. John Stults¹

Dr. Tamzen McBeth¹

June 5, 2024





Overview

1. Introduction

- PFAS Background

2. HR-CSMs for PFAS

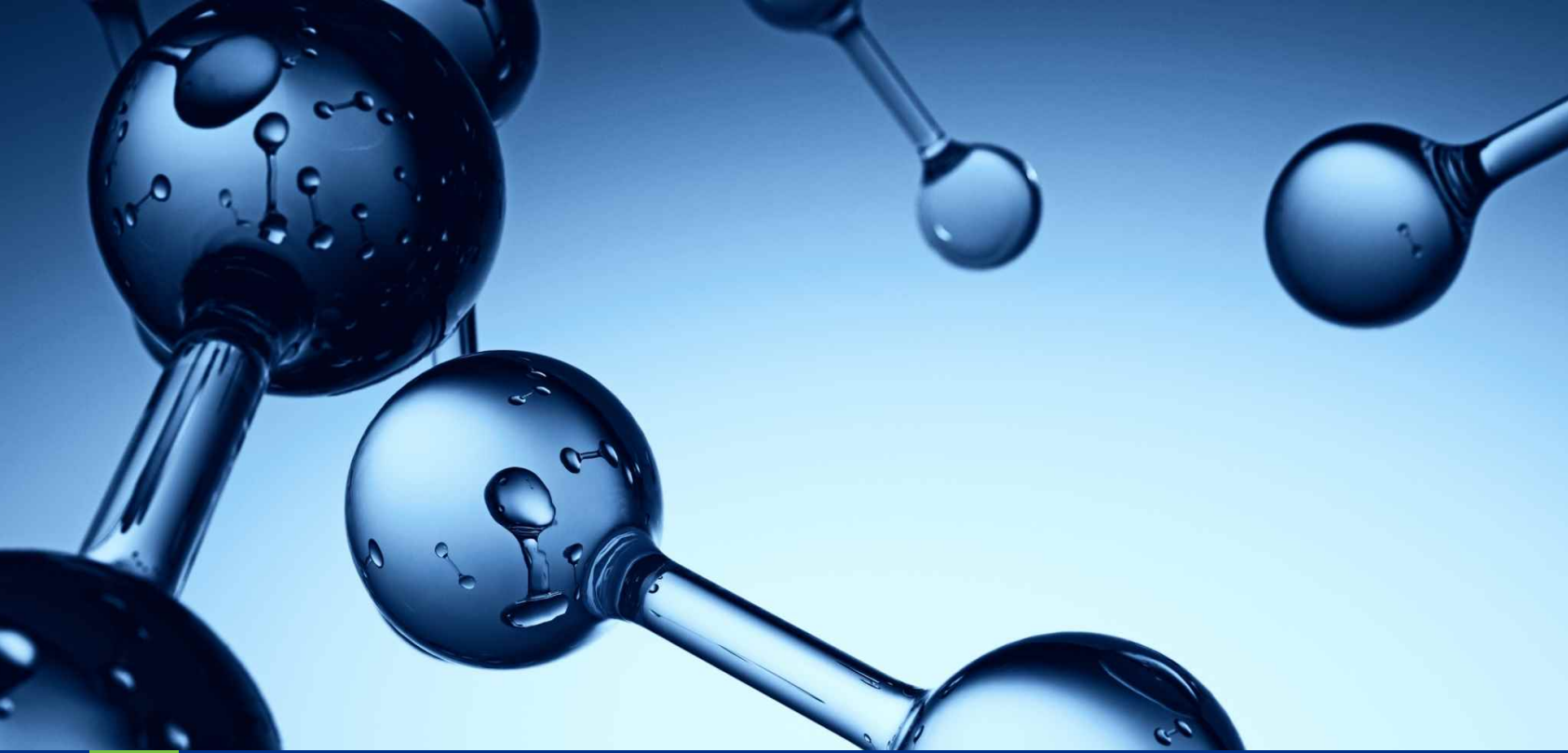
- Example of AFFF contaminated site

3. Analytics Tools for HR-CSM

- Dashboard Tools Overview and Reasoning

- Practical Analytics
- Vadose Zone Leaching Models
- Groundwater Plume Evaluation
- 3D Visualization

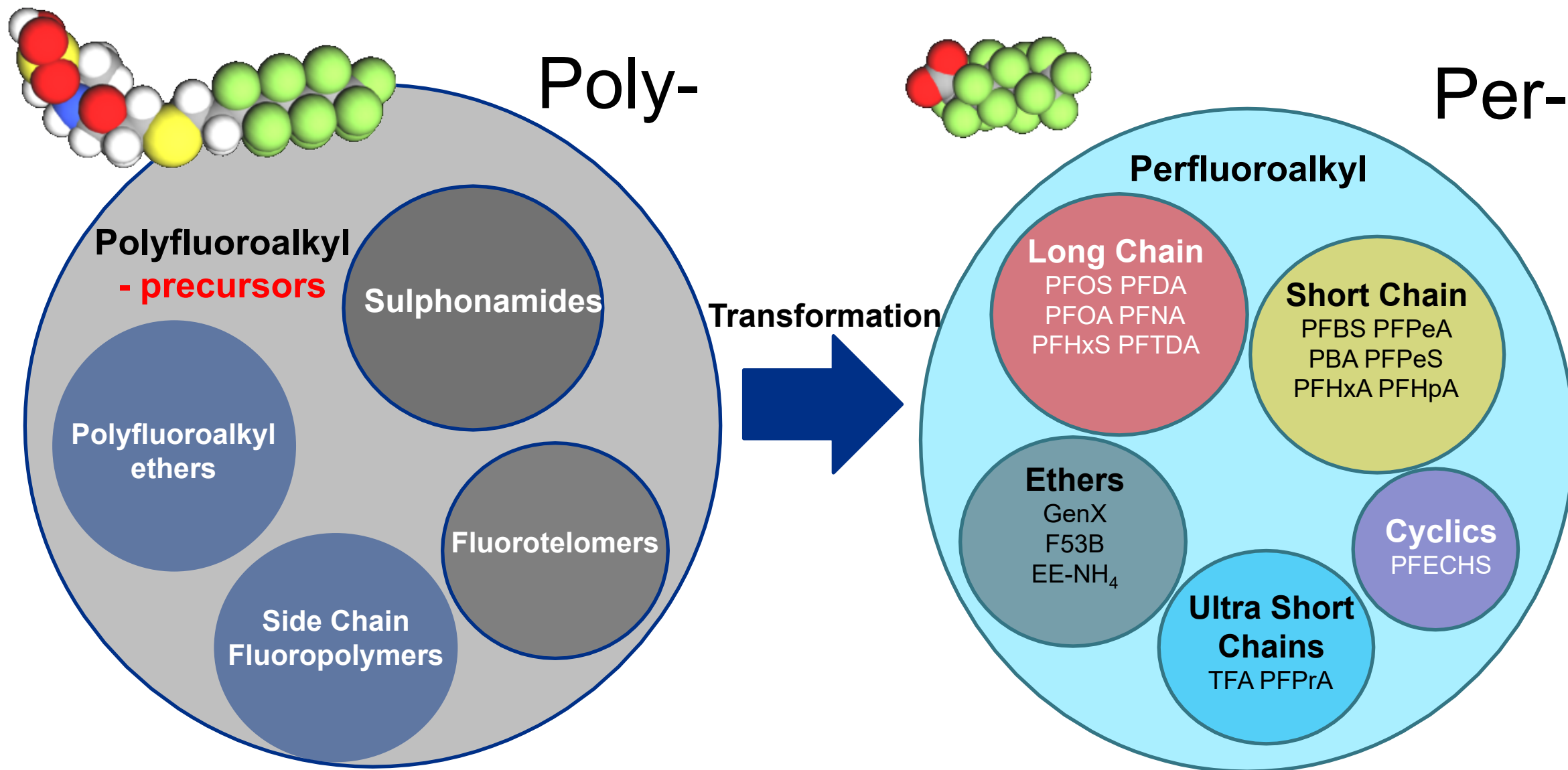
4. Demonstration



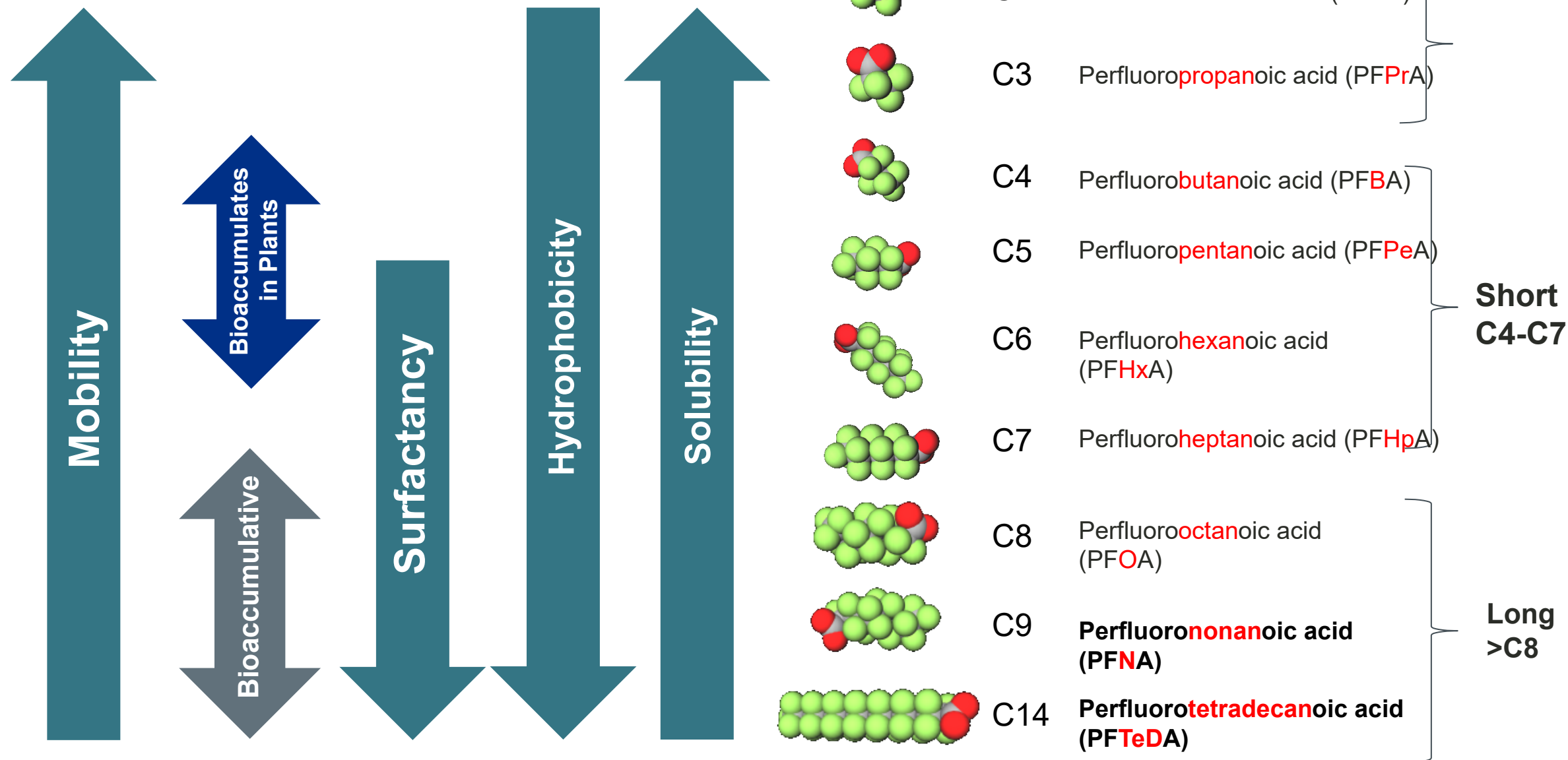
Introduction

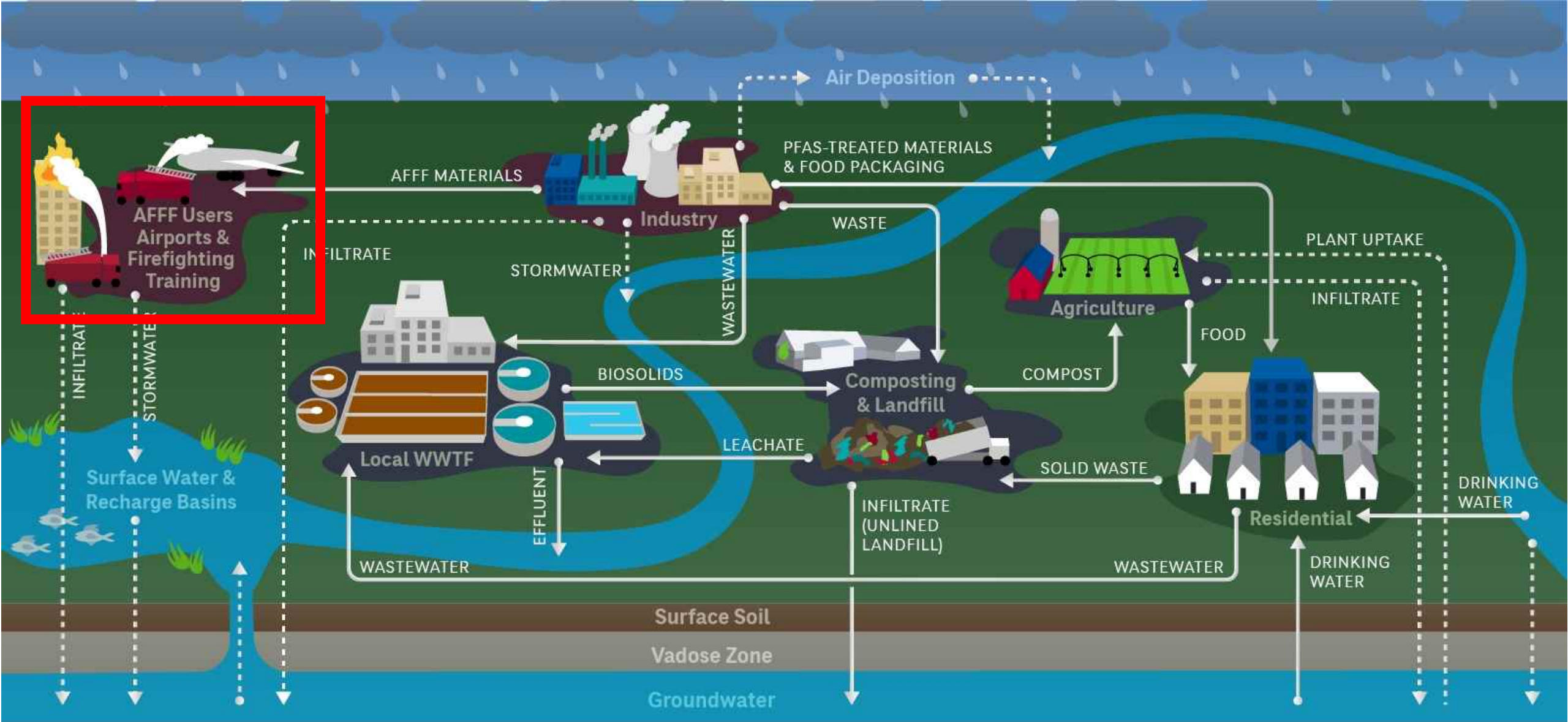


1.1. PFAS Background - Categories



1.1. PFAS Background - Mobility





PFAS Life Cycle

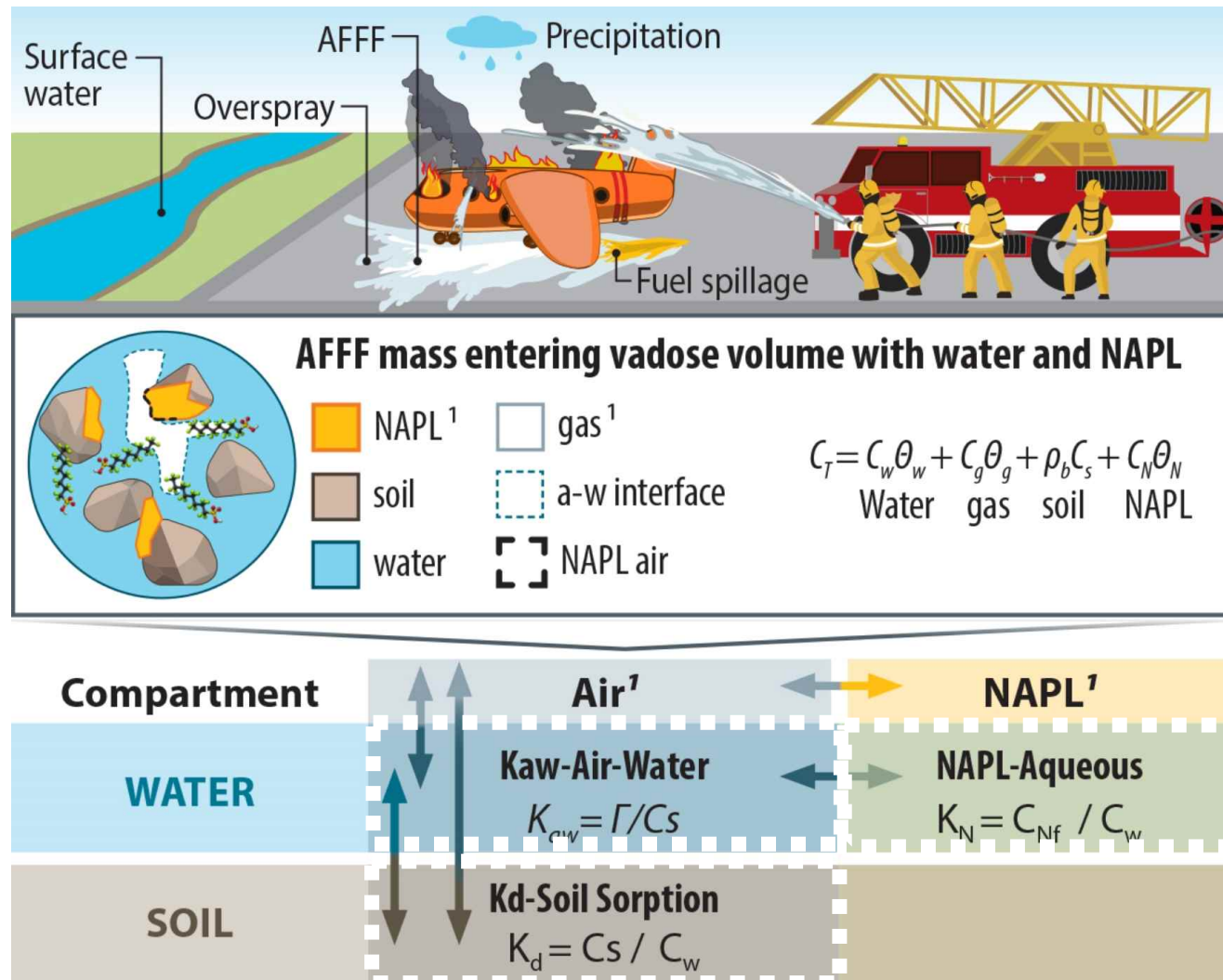
KEY

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

1.1. AFFF Source Zones

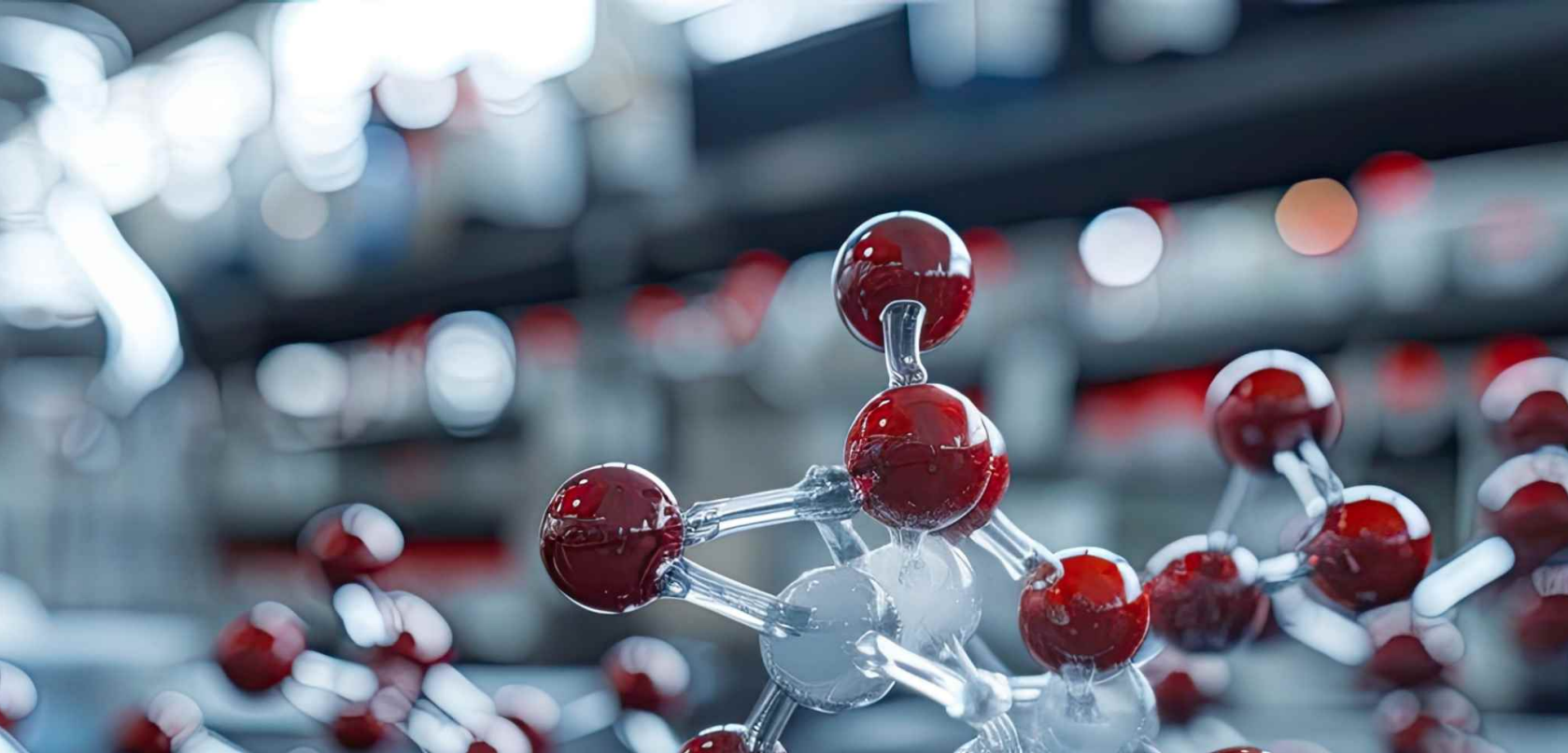


1.1. PFAS Partitioning and Transport



- Regulated PFAS are generally fluorosurfactants (amphiphiles)
- Surfactants accumulate on surfaces and at interfaces including:
 - Air: water / Solid: air / Solid: water / Aldair / NAPL: water
- PFAS can form highly stable assemblies/films on surfaces or at interfaces
- Amphiphilic PFAS have unique fate & transport properties

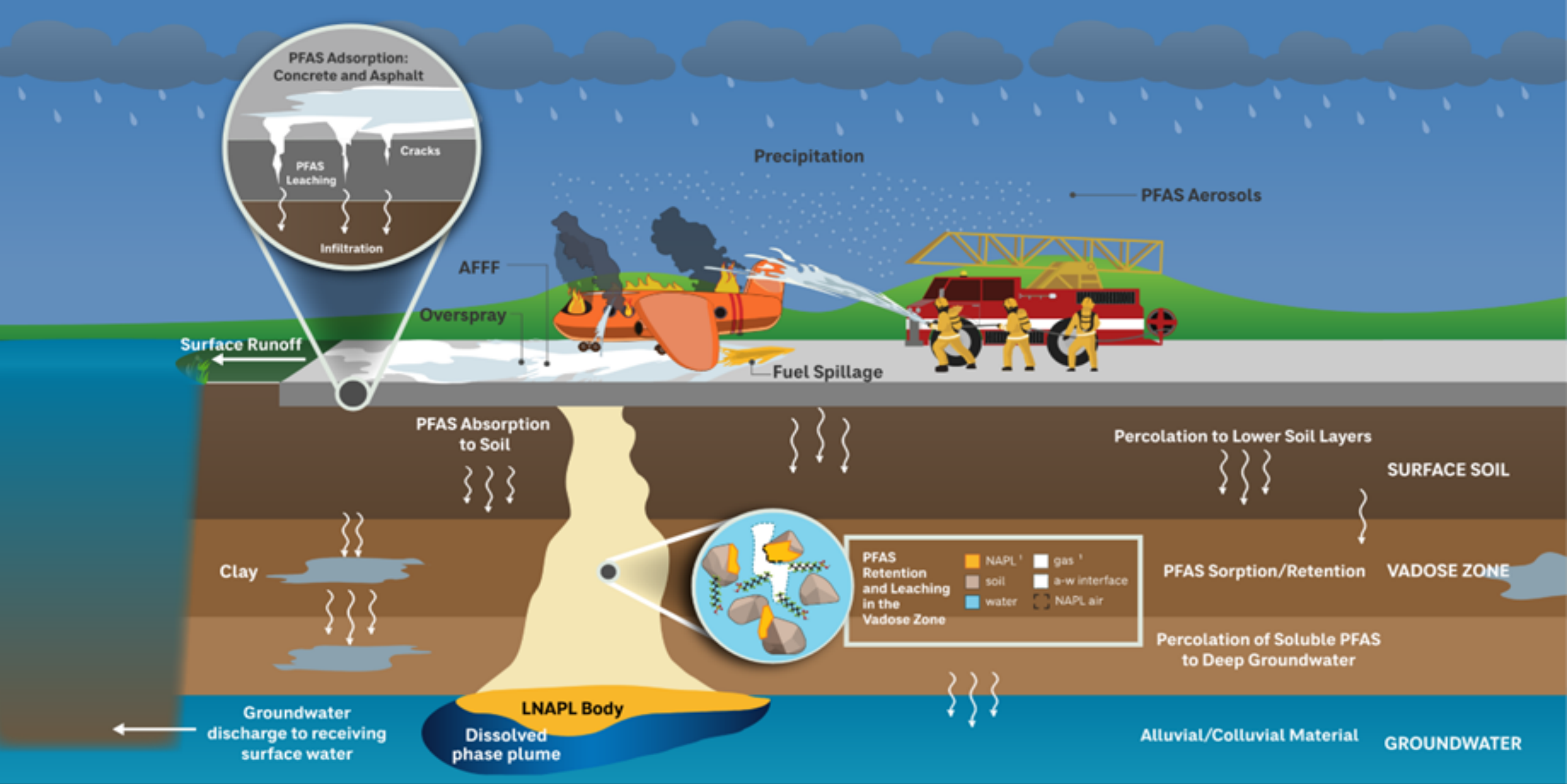
$$M_{\Sigma \text{ PFAS mass total}} = C_w (\theta_w + K_{dp} + K_{aw_c} + A_{aw} + K_N \theta_{NAPL})$$



HR-CSM for PFAS Source Zones

The Case for Dashboard Tools



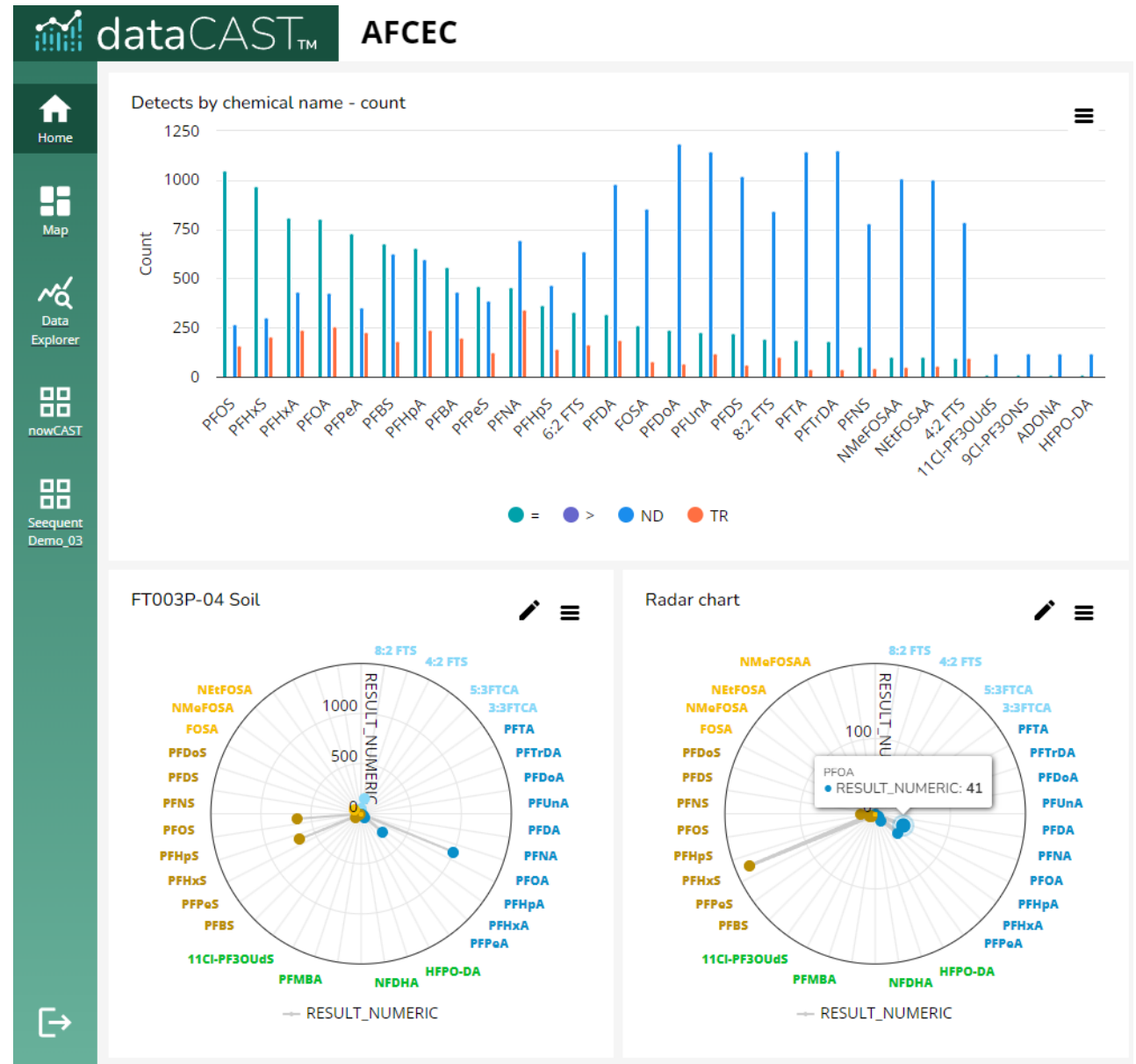


PFAS Conceptual Site Model

2.1. Evaluation Needs for AFFF HR-CSM

Why Dashboards? Convenient analysis of multiple data sources in one place

- Temporal trends in data
- PFAS distributions
- Concentration distributions
 - Kriging
 - Bar charts
 - Detect/non-detect analysis
- Media Heterogeneity
 - 3-D modeling
- Risk analysis
 - Flux models and analytical tools





Dashboarding Options and Implementation



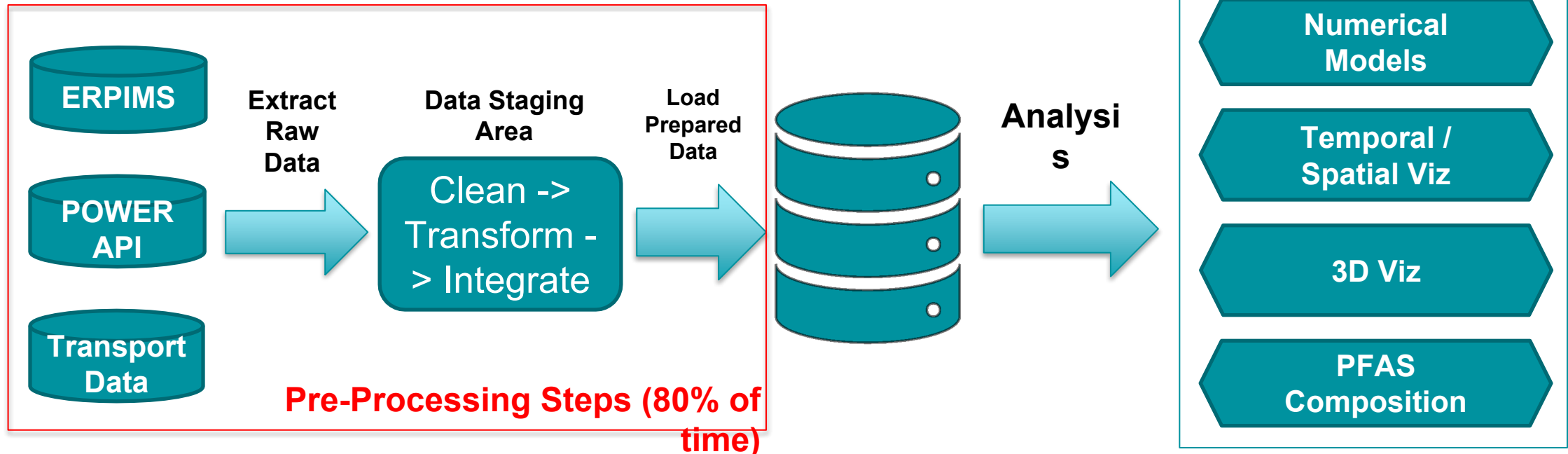
3.1. Dashboard Tools - Workflow

■ Significant effort developing data pipeline for advanced analytics

- 80:20 Rule – 80% of time spent on pre-processing; 20% on Analysis

■ Involves Ingesting & standardizing multiple data sources

- **ERPIMS** – PFAS/Site Specific Data
- **POWER API** – Agroclimatalogical Data
- **Transport Data** – Literature & other public sources



3.1. Dashboard Tools - Reasoning

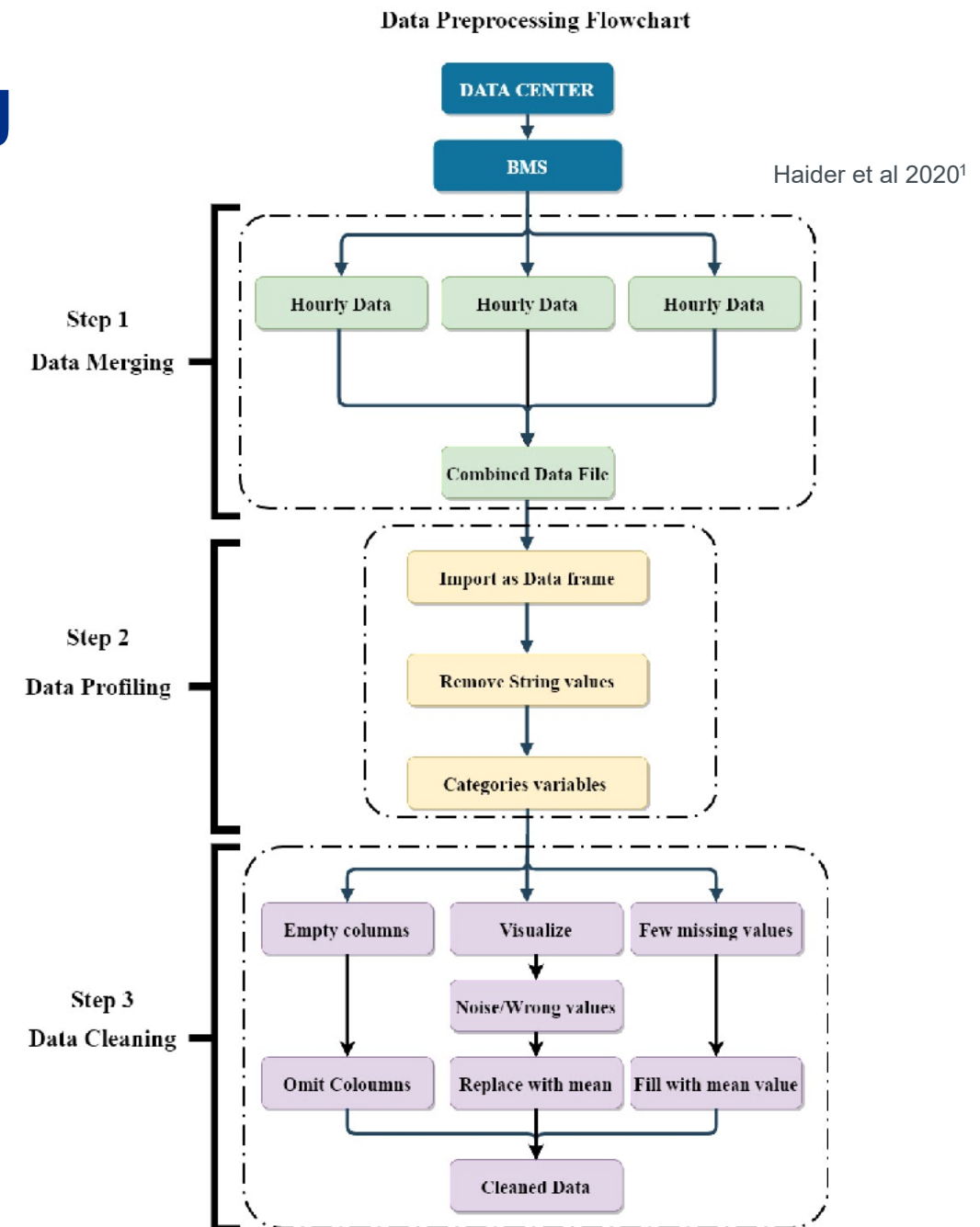
■ Implementation of dashboard tools requires automating preprocessing

- 80 % of the time in most applications

■ Allows for users to focus on analysis & decision making

■ 3 major steps

- Figure out the data scheme
- Create algorithms to import/export data to a central repository
- Test and validate



¹Haider, S. N.; Zhao, Q.; Meran, B. K. Automated Data Cleaning for Data Centers: A Case Study. In 2020 39th Chinese Control Conference (CCC); IEEE: Shenyang, China, 2020; pp 3227–3232. <https://doi.org/10.23919/CCC50068.2020.9189357>

3.1. Dashboard Tools – Data Cleaning

1. Import Raw Data Set



3. Merge w/ Central Data Set

[illegible]

Identify Consistent Cleaning Needs

[illegible]

Algorithmic Cleaning

Activity Identifier	Latitude	Longitude	PAH Chemical Name	Result	MR Result	MR Fish Species
NAUPCA-1005-017-0707190000-0631C	44.8007500000	-51.7827000000	Perfluorooctanoic acid	0	0	Blingli
NAUPCA-1005-017-0707190000-0631C	44.8007500000	-51.7827000000	Perfluorooctanesulfonamide	0	0	Blingli
NAUPCA-1005-017-0707190000-0631C	44.8007500000	-51.7827000000	Perfluorooctanoic acid	0	0	Blingli
NAUPCA-1005-017-0707190000-0631C	44.8007500000	-51.7827000000	Perfluoroundecanoate	0	0	Blingli
NAUPCA-1005-017-0707190000-0631C	44.8007500000	-51.7827000000	Perfluorooxleic acid	0	0	Blingli
NAUPCA-27-0040-00-100.0805180000-01757	44.9555500000	-51.1088000000	Perfluorooctanesulfonamide	2170	5,170000	Blingli
NAUPCA-27-0040-00-100.0805180000-01757	44.9555500000	-51.1088000000	Perfluorooctanoic acid	2220	5,210000	Blingli
CST_SHPD-TN6917-FT-2008-09-12-126879	35.8782800000	-89.5577180000	Perfluoroundecanoate	2400	2,400000	Blue cefish
NAUPCA-27-0031-00-100.0805180000-00257	44.9421100000	-51.1120000000	Perfluoroundecanoate	2420	2,410000	Blingli
NAUPCA-27-0040-00-100.0805180000-01757	44.9555500000	-51.1088000000	Perfluorooctanoic acid	2420	2,420000	Blingli
NAUPCA-27-0040-00-100.0805180000-01757	44.9555500000	-51.1088000000	Perfluorooctanesulfonamide	2480	2,480000	Blingli
NAUPCA-27-0042-00-100.0805290000-00355	43.0172000000	-51.1363000000	Perfluorooctanoic acid	2500	2,500000	Blingli
CST_SHPD-DE018-FT-2008-08-05-321119	36.8187100000	-55.6292000000	Perfluoroundecanoate	2500	2,500000	Largemouth bass
CST_SHPD-AG644-FT-2008-08-18-528949	32.1168800000	-90.3951000000	Perfluorooctanoic acid	2500	2,500000	White bass
CST_SHPD-NH417-FT-2008-07-10-521713	43.4301300000	-72.3904100000	Perfluoroundecanoate	2500	2,500000	Smallmouth bass
CST_SHPD-W0468-FT-2008-07-29-530443	44.8834800000	-87.4572000000	Perfluoroundecanoate	2500	2,500000	Smallmouth bass

Join Data

Clean
Dataset 1

Clean Dataset 2

Clean Dataset 3

Clean Dataset 1

Clean Dataset 2

Clean Dataset 3

3.1. Dashboard Tools - Options

Open Source

- **Pros:** Customizable and flexible
- **Cons:** Labor-intensive startup, programming, **internal deployment**



Proprietary

- **Pros:** No programming knowledge, out of the box
- **Cons:** Pay for service, inflexible, **internal deployment**



Power BI



+ a b | e a u

DataCast

- **Pros:** Customizable and flexible out of the box; deployment managed by 3rd party
- **Cons:** CDM Smith/Trinnex Proprietary

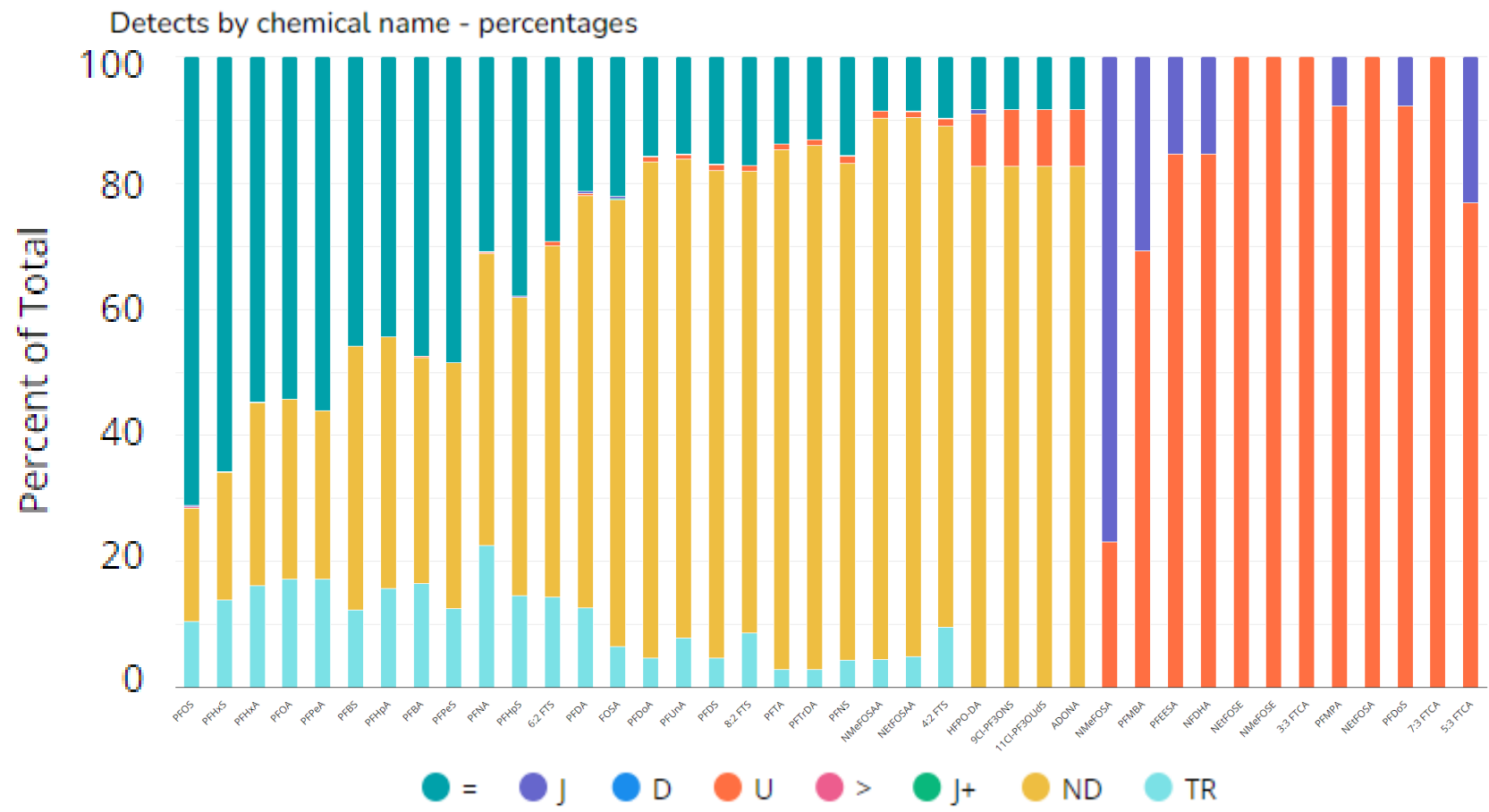


	Maturity	Simplicity	Adaptability	Focus	Language Support	Capital Cost	Labor Cost
Streamlit	C	A	C	Dashboard	Python	\$	\$\$
Dash	A	B-	A	Dashboard	Python, R	\$	\$\$\$
Shiny	A	B+	B	Dashboard	Python, R	\$	\$\$
PowerBI	A	A	C	Dashboard and Data Management	Python, R	\$\$\$	\$
DataCast	A	A	A	Dashboard and Data Management	Python	\$\$\$	\$

3.1. Analysis Tools - Detections

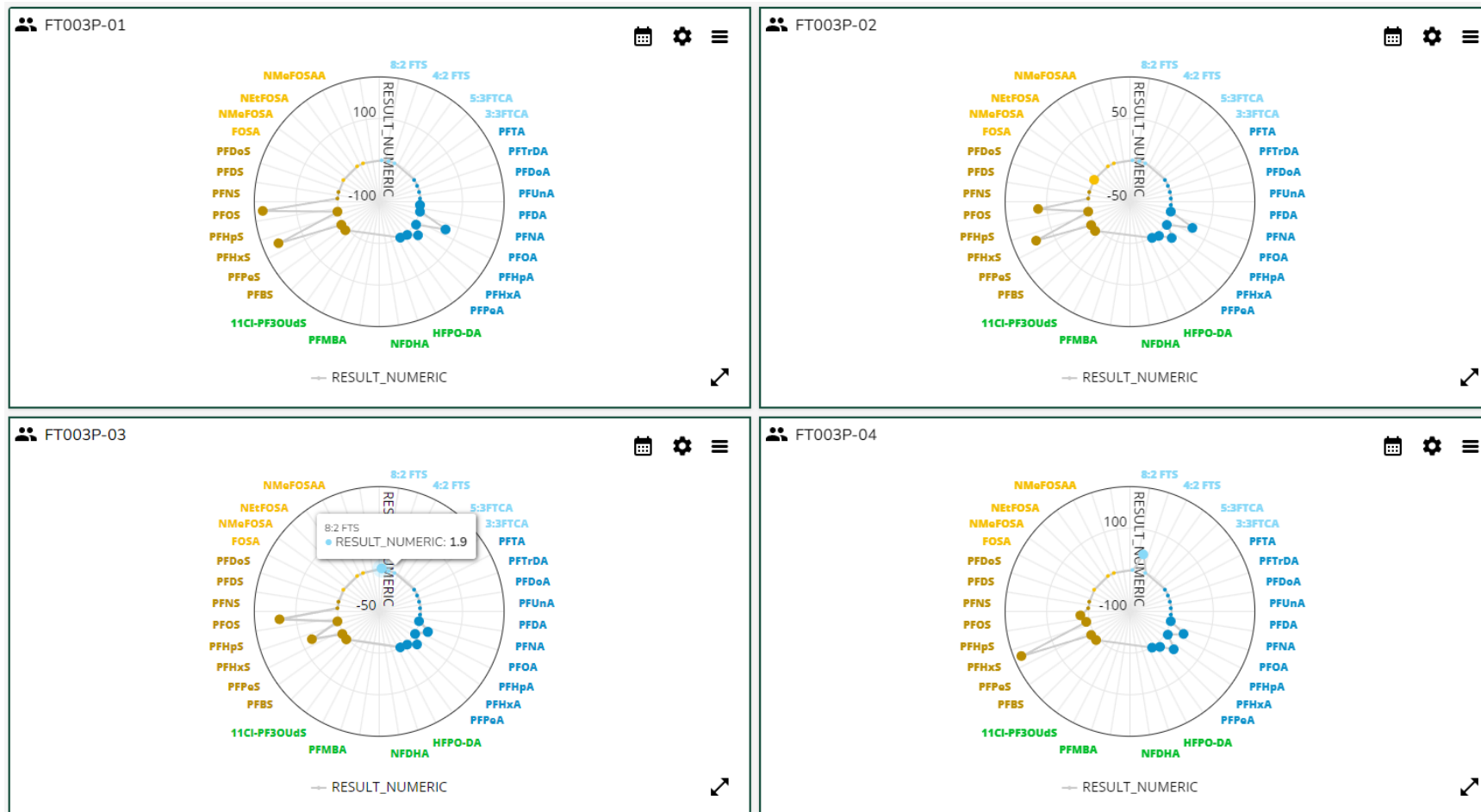
■ **Goal:** Determine what PFAS are likely to present

■ **Tool:** Detect Percentages



3.2. Analysis Tools – PFAS Distributions

- **Goal:** Determine types of PFAS present
- **Tool:** Distribution chart of 1633 components

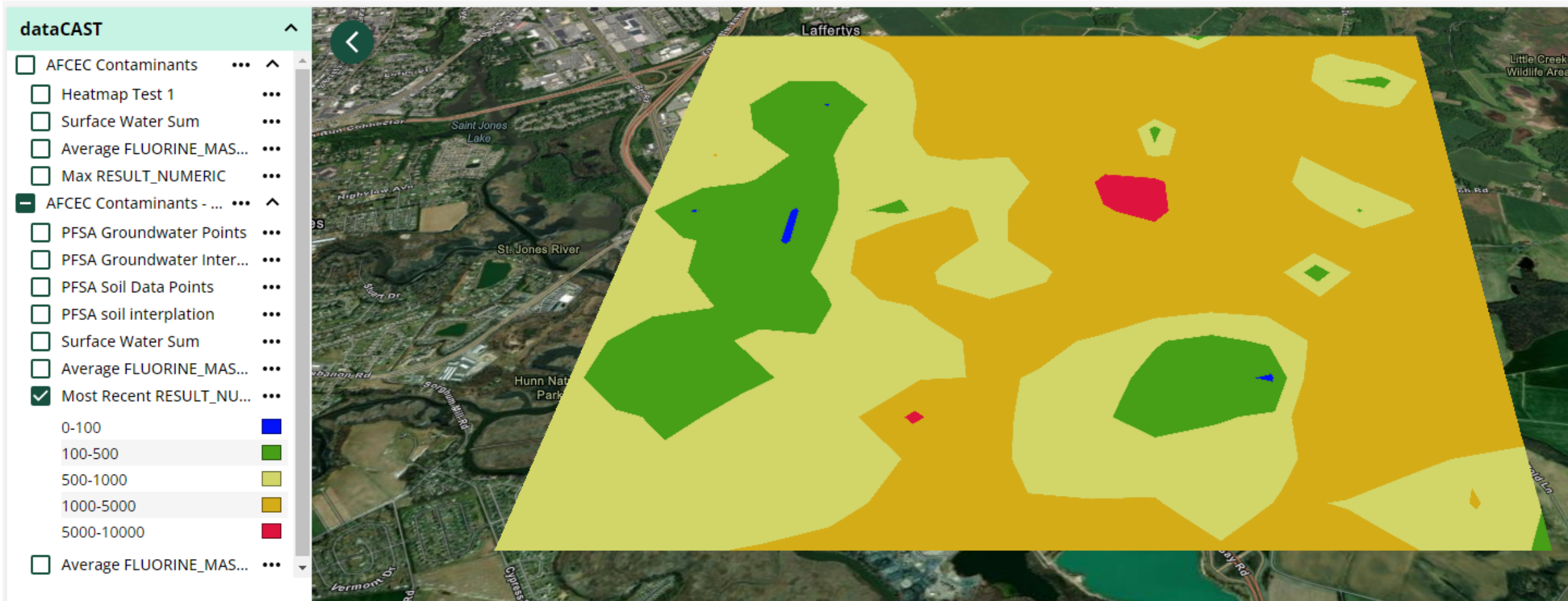


3.2. Analysis Tools – Mapping Values

- **Goal:** Determine general locations of high detects
- **Tool:** General mapped values with color bars

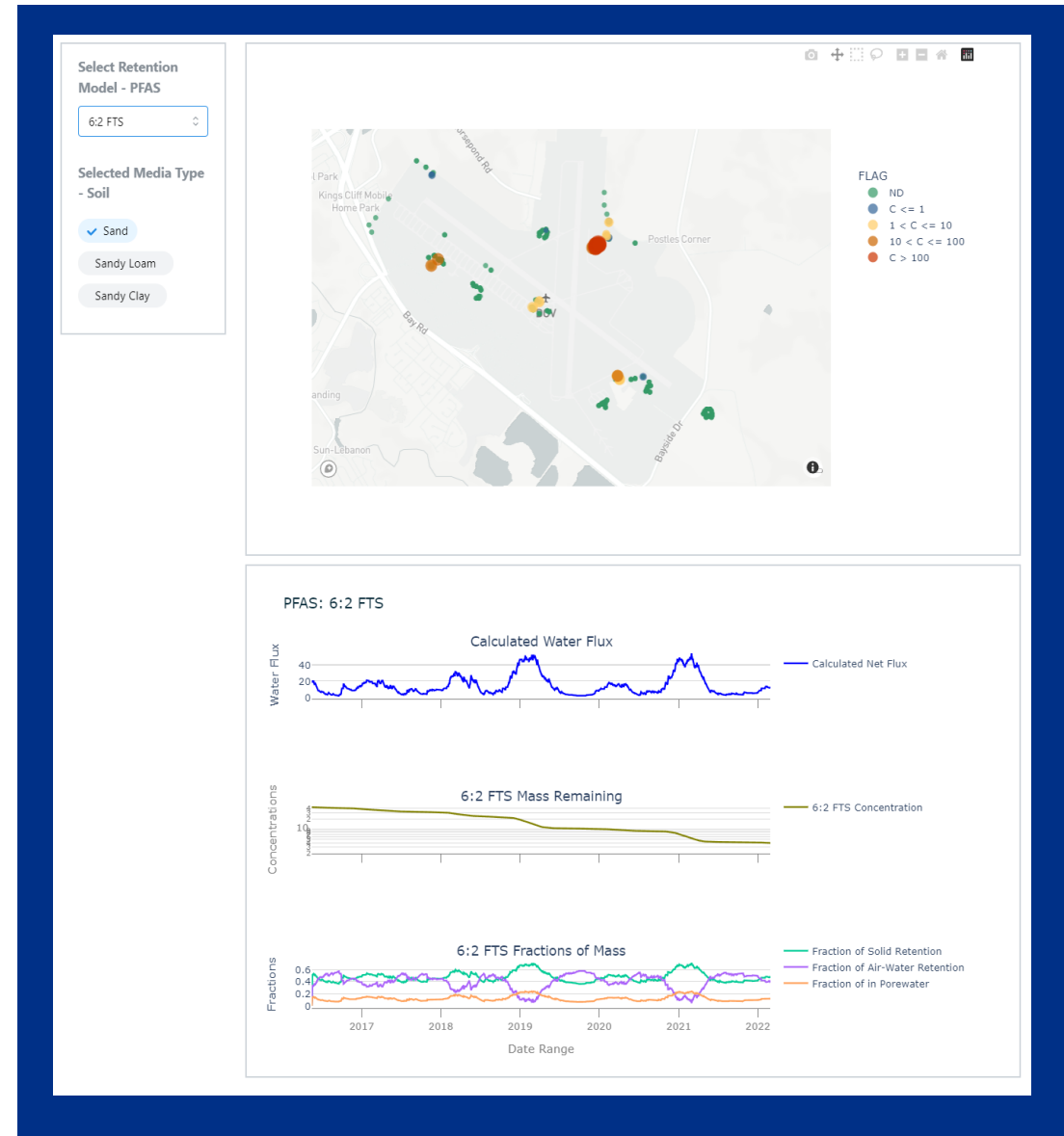


3.3. Analysis Tools – Mapping Plume extents

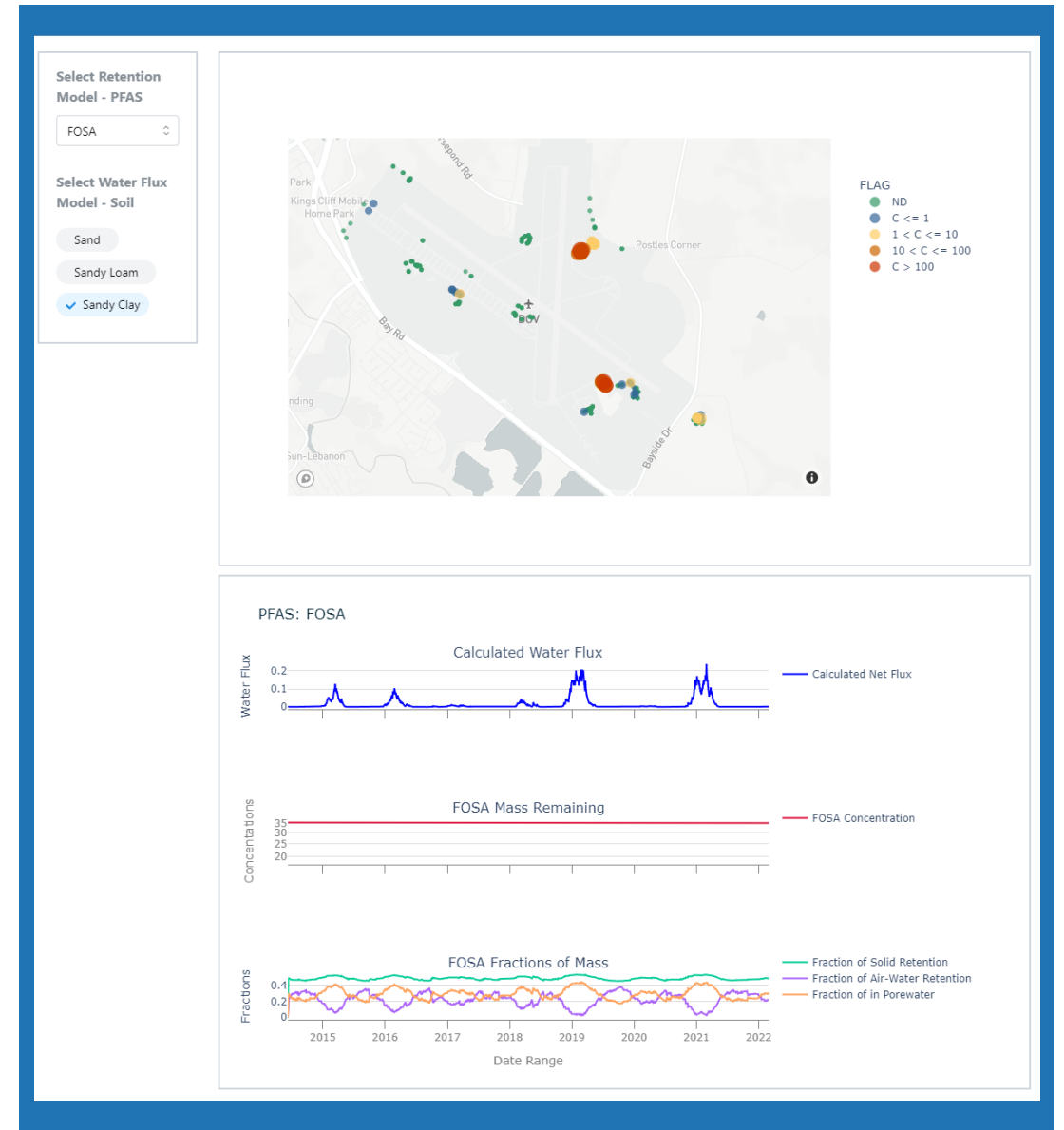
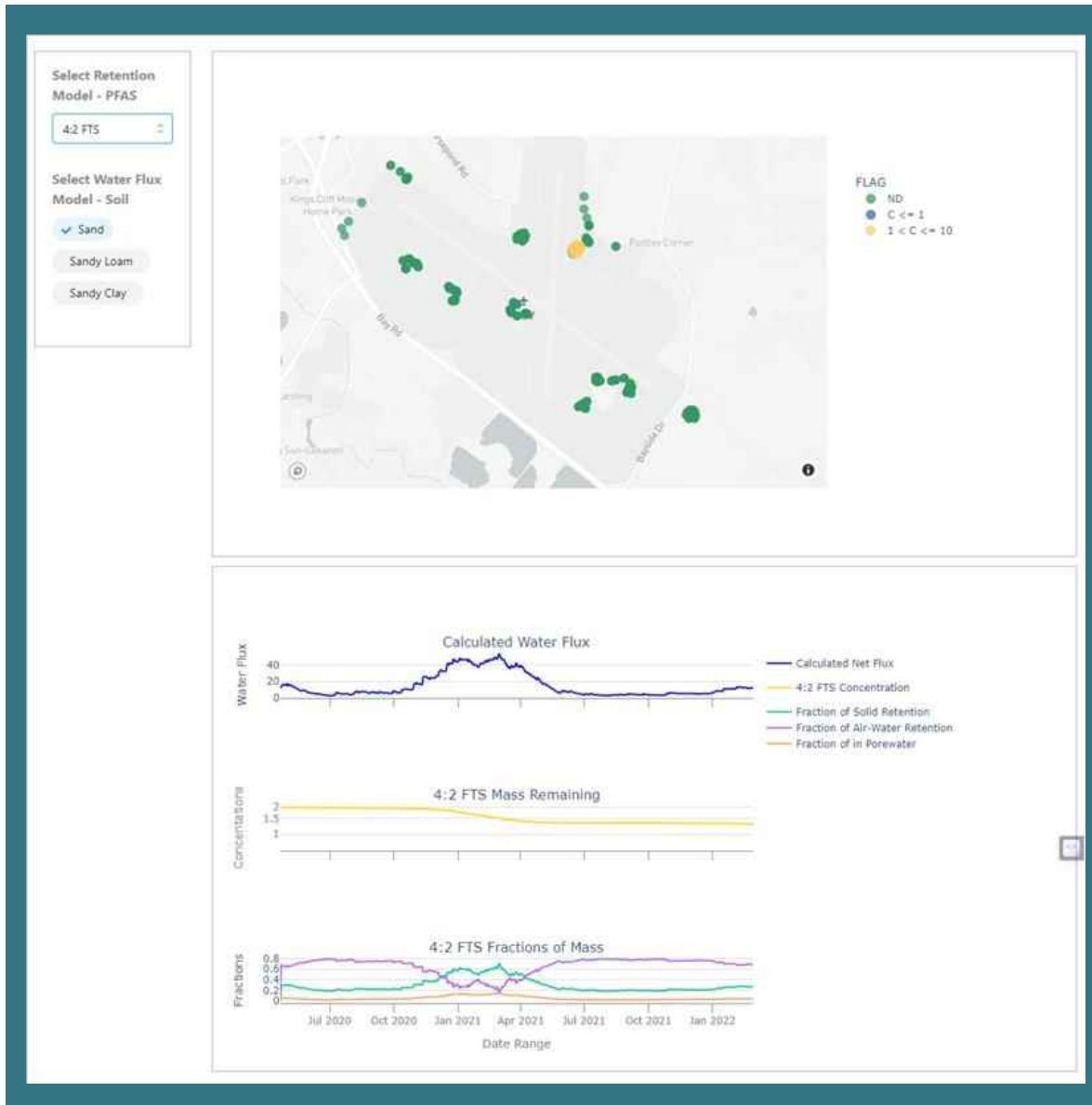


3.4. Risk Analysis – Leaching Model

- **Goal:** Determine leachability of PFAS from source zones to the underlying aquifer
- **Tool:** Simplified, data-based model running in real time



3.4. Risk Analysis – Leaching Model Other Displays



3.4. Risk Analysis – Leaching Model

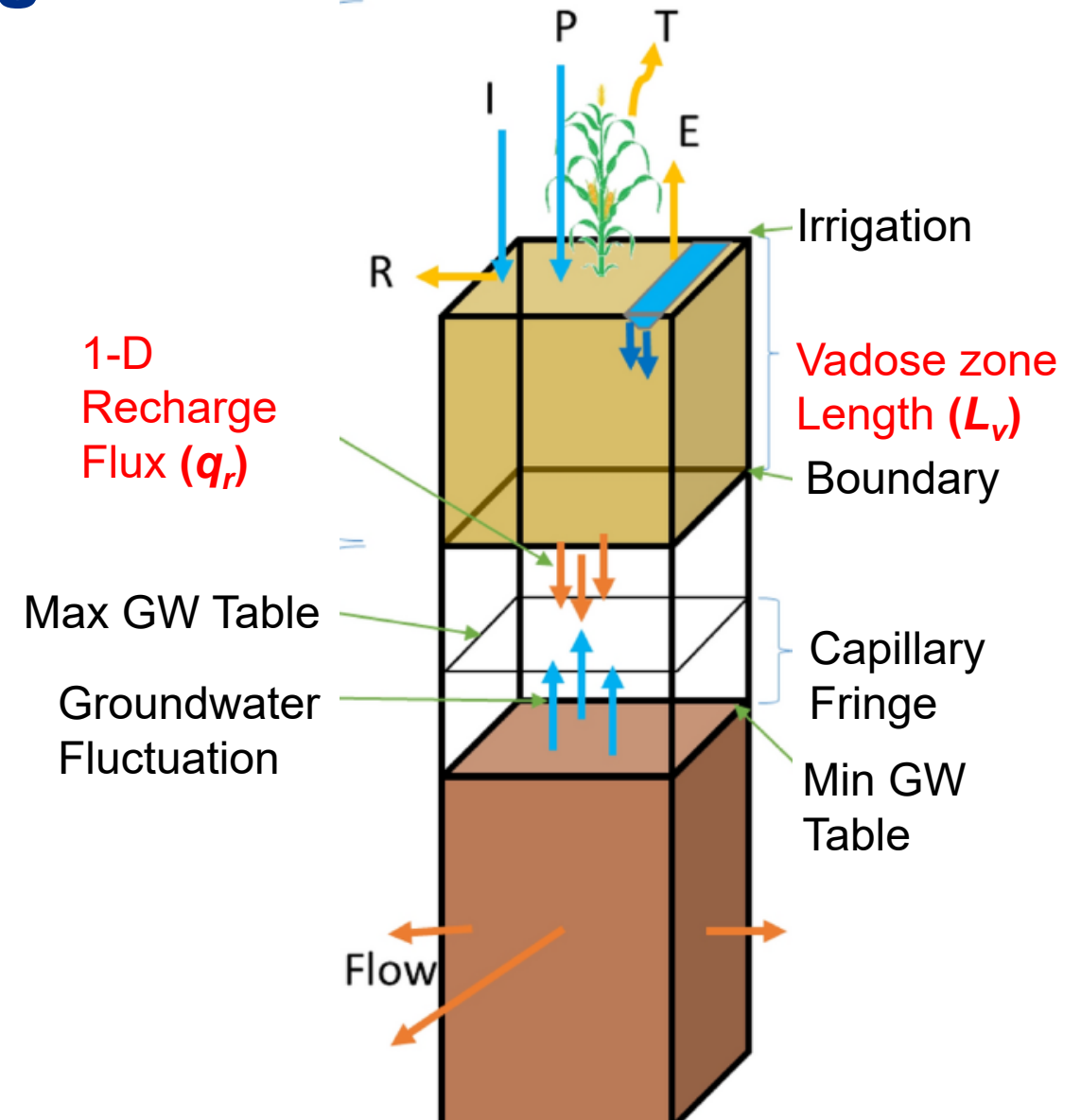
C_T = Total PFAS Conc.

C_p = Mobile porewater Conc

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

$$C_T = C_p \frac{\theta_w}{\rho_b} R$$

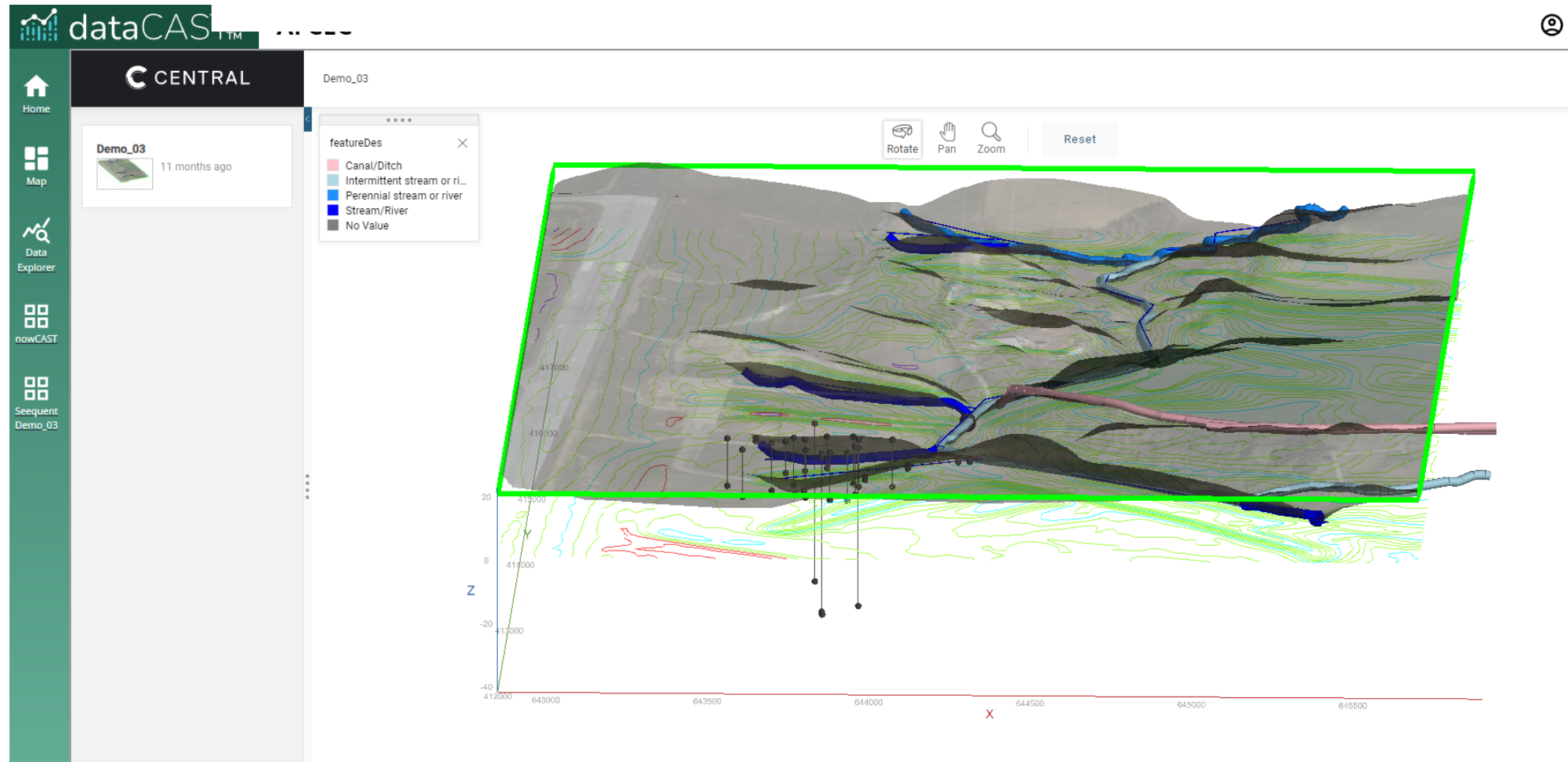
- Real time sensor and satellite data feeds into model
- Requires integration of multiple data libraries



3.5. 3-D Visualization

■ **Goal:** Determine effects of heterogeneity and contextualize the site

■ **Tool:** 3-D Viz with Leapfrog embedded in DataCast





Demonstration

<https://trinnex.cloud/datacast/map>



Thank you!



To learn more, contact:

John Stults

CDM Smith

StultsJF@cdmsmith.com