



RemPlex Seminar

August 11, 2026

PFAS in the Environment: Transport Processes and Identifying PFAS Research Needs



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Today's Seminar and Speakers



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PFAS in the Environment: Transport Processes and Identifying PFAS Research Needs

AUGUST 11, 2026



Trey Fortner
Noblis



Ramona Iery
SERDP/ESTCP



Matthew Spurlin
Noblis



2026 PFAS Innovation Workshop

- DOE is convening:
 - Researchers
 - Site program managers
 - Industry
 - Academia
 - Regulators
- Accelerating progress
- Sparking cross-site collaboration
- Turning ideas into action



 **PFAS 2026**

DOE PFAS INNOVATION WORKSHOP 2026

AUGUST 25–26, 2026
Pacific Northwest National Laboratory

Be part of the community driving PFAS
solutions across the DOE complex.

 **PNNL**  U.S. DEPARTMENT
of ENERGY | Office of Environmental
Management

GWMR Special Issue

- **Topic:** “Vertical Characterization and Monitoring of Contaminants in Groundwater”
- Paper submission by 31-October 2026
- Co-editor: frederick.day-lewis@pnnl.gov
- <https://www.ngwa.org/publications-and-news/journals/groundwater-monitoring-remediation>




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Call for Papers

Vertical Characterization and Monitoring of Contaminants in Groundwater

Submission Deadline: Saturday, 31 October 2026

The National Ground Water Association is announcing a call for papers for a special issue of *Groundwater Monitoring & Remediation* on “Vertical Characterization and Monitoring of Contaminants in Groundwater.” We know that plumes are highly variable in the vertical dimension, with contaminant concentrations often varying by several orders of magnitude over intervals of centimeters to meters. Legacy methods involving long-screened wells and two-dimensional snapshot maps of plumes are insufficient for understanding contaminant fate and transport and may even be misleading. Despite the availability of modern tools for aquifer investigations, characterization of subsurface contamination in three dimensions is not yet standard in the groundwater protection industry. Moreover, monitoring of the concentrations and flux of subsurface contamination over time (i.e., the “fourth dimension”) at a spatial scale that matches the distribution of the contaminants is even less common. The focus of this special issue is on “**High Definition and Vertical Characterization and Monitoring of Contaminants in Groundwater.**” The issue will highlight the characterizing and monitoring of the vertical extent of natural and anthropogenic contaminants in the subsurface, leading to a true four-dimensional understanding of the nature, extent, and flux of the contaminants in the subsurface.

Topics of interest for this call for papers include but are not restricted to:

- Examples of diagnostic temporal performance monitoring of in situ contaminated groundwater remedies;
- Case studies where groundwater sampling and monitoring has been done along transects oriented perpendicular to the plume axis;
- Vertical characterization and monitoring at groundwater/surface water boundaries;
- Assessments focused on mass flux and contaminant mass discharge (CMD);
- Case studies where CMD has been monitored over time at contaminated sites;
- Characterization and temporal monitoring of contaminant concentrations and fluxes in the vadose zone;
- The role of high-resolution groundwater sampling and monitoring for assessing the risk of vapor intrusion from groundwater sources;
- Vertical profiling and long-term monitoring of contaminants in drinking water aquifers and wells;
- Case studies where engineered multilevel monitoring systems (e.g., Westbay, Solinst Waterloo, CMT, Flute and others) systems have been used;
- Case studies involving innovative depth-discrete monitoring of contaminant flux using passive flux meters (PFMs) and direct velocity measurement tools;
- Strategies and technologies for characterization and monitoring the vertical nature, extent, and flux of dissolved contaminants over time outside of North America;
- Geophysical methods for characterizing and monitoring contaminants in the subsurface;
- Novel technologies for vertical subsurface characterization and monitoring (e.g., fiber optics);
- Advances in remote sensing technologies to characterize and monitor contaminants in groundwater;
- Innovative technologies for vertical characterization and monitoring used in the oil and gas and mining industries;
- Technologies and strategies for characterizing and monitoring nuclear sites being decommissioned and the next generation of nuclear power plant sites.

Guest Editors:

Murray Einarson
Haley & Aldrich,
United States

Fred Day-Lewis
Pacific Northwest National Laboratory,
United States

John Heneghan
Sellafield Ltd.,
United Kingdom

Keywords:
Aquifer; environmental science; groundwater.

Submission Guidelines/Instructions:

Please refer to the [Author Guidelines](#) to prepare your manuscript. When submitting your manuscript, please answer the question “Is this submission for a special issue?” by selecting the special issue title from the drop-down list.

[Submit now](#)

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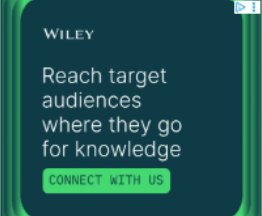
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Looking Forward with RemPlex

Upcoming Seminars in 2026-2027

- Data Readiness for AI/ML in Environmental Remediation (planning for Nov. 2026)
- Environmental Management Workforce Development
- Environmental Remediation in Deactivation and Decommissioning
- Drones for Site Characterization & Monitoring

Give us your thoughts on topics of interest!

For more information and to register for seminars, go to
<https://www.pnnl.gov/projects/remplex/seminars>

Save the Date: 2027 Global Summit on Environmental Remediation, Nov. 1-4, 2027 in Richland, Washington



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Watch for Call for Abstracts in 2027



Speakers and Talk Titles

- Ramona Iery, SERDP & ESTCP
 - “Development of Statement of Needs for SERDP & ESTCP”
- Trey Fortner, Noblis
 - “From Rocky Seas to Smooth Sailing: Which Path Will Your GSI Investigation Take?”
- Matthew Spurlin, Noblis
 - “Updated Best Practices for PFAS Soil-to-Groundwater Leaching Evaluations at USAF Installations”



Development of Statement of Needs for SERDP & ESTCP

Ramona Iery PhD P.E.
SERDP & ESTCP

for
RemPlex Seminar August 11, 2026

DoW's Environmental RDT&E Programs



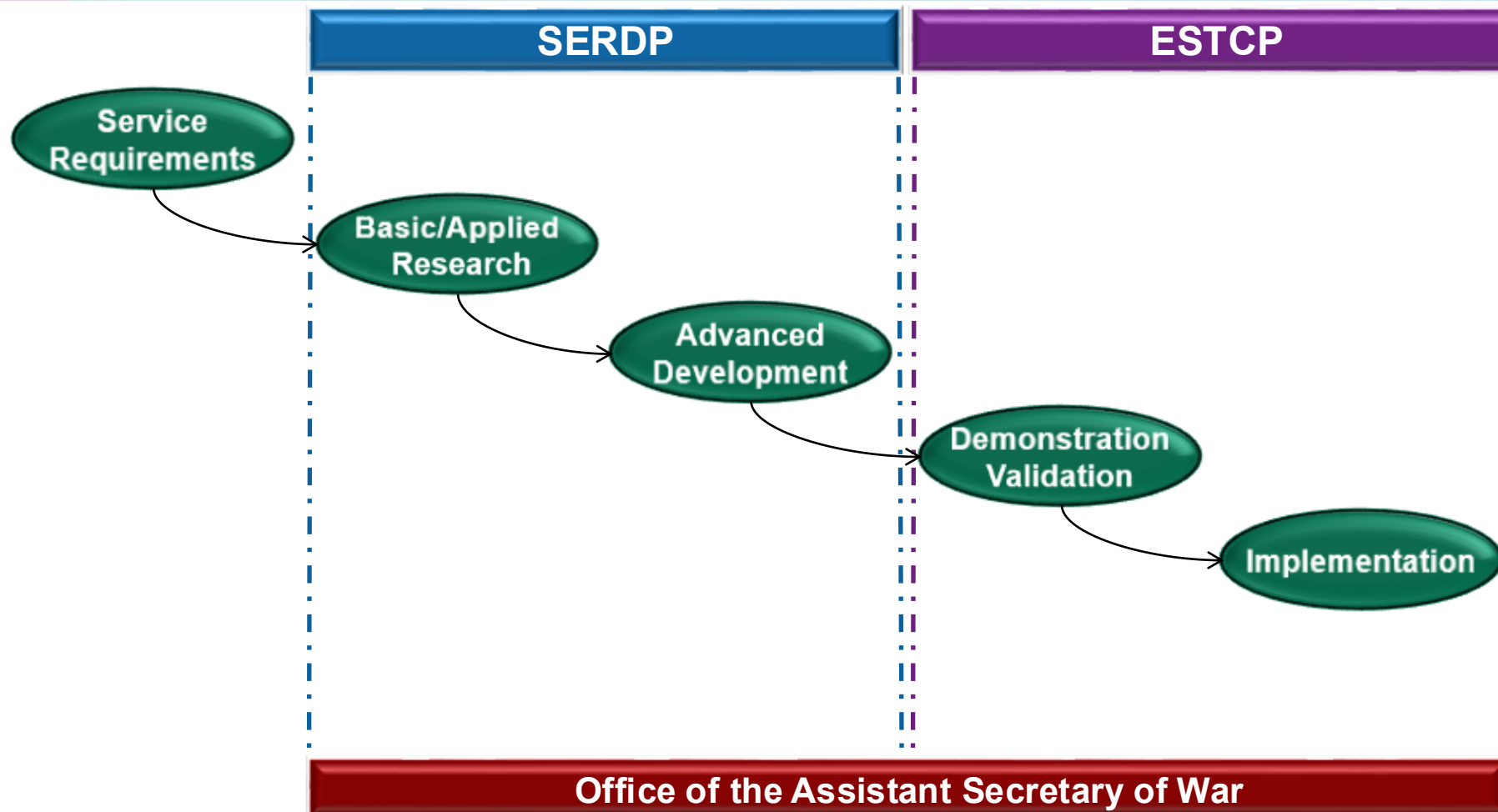
➤ Science and Technology

- Statutory research program established in 1991
- DoW, DOE, EPA partnership
 - Advanced technology development to address near-term needs
 - Fundamental research to impact real-world environmental management

➤ Demonstration and validation

- Demonstrate innovative and cost-effective technologies for improved environmental management
 - Transition technology out of the lab
 - Establish cost and performance
 - Partner with end-user and regulator
 - Technology transfer

Environmental Technology Development Process



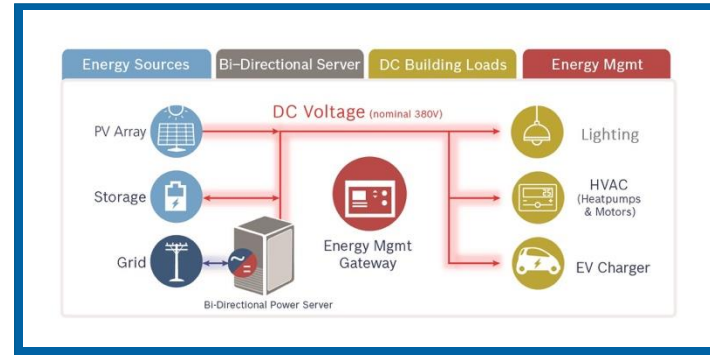
Program Areas

Weapons Systems & Platforms



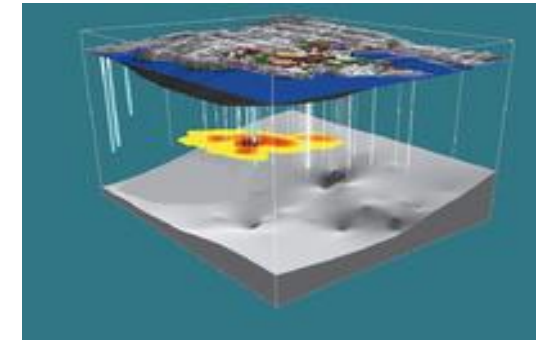
Resource Conservation & Resiliency

Installation Energy and Water



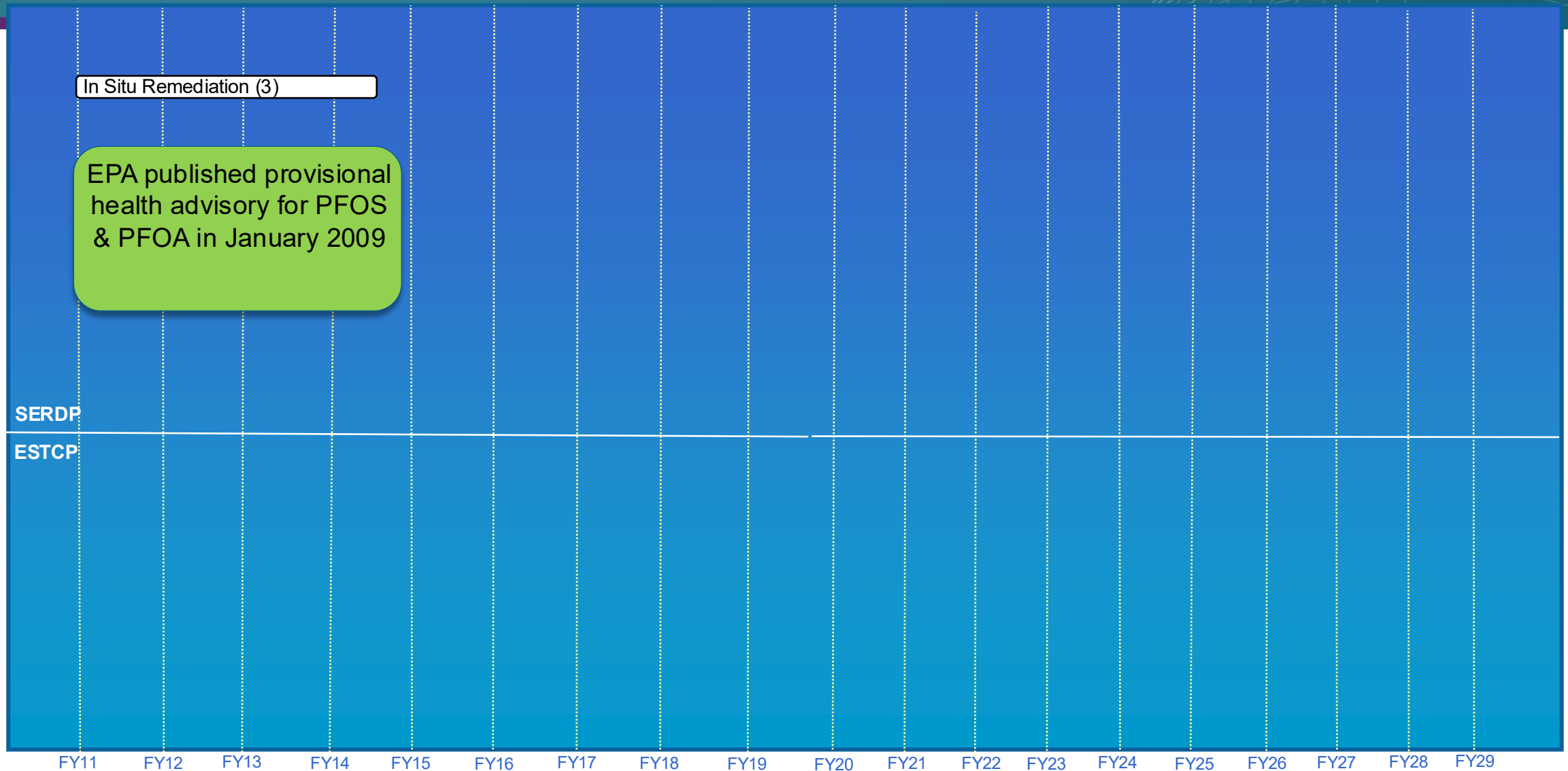
ESTCP Only

Environmental Restoration



Munitions Response

SERDP & ESTCP Efforts on PFAS



SERDP & ESTCP Efforts on PFAS

Long Term Mgmt
Workshop

PFAS Workshop

PFAS Ecotox
Workshop

Stormwater
Workshop

EPA published provisional
health advisory for PFOS
& PFOA in January 2009

Since 2011, over 300
projects funded, with over
\$300M invested

SERDP

ESTCP

In Situ Remediation (5)

Ecotoxicity (4)

Mixed Chemicals (5)

Next Gen AFFF (3)

Next Gen AFFF (6)

IDW Treatment (18)

Knowledge Gaps (6)

NIST AFFF Standards

Source Zones (5)

In Situ & Ex Situ Treatment (11)

Stormwater Impacts (3)

Sampling & Analysis (5)

Ecorisk Assessment (4)

DoD & EPA Multi-Lab Validation

Biodegradation (5)

Passive Samplers (8)

Leaching & Mobility (1)

Forensics (6)

Ecotox: PFAS-Free Firefighting
Agents (6)

Dev't: PFAS-Free Firefighting
Agents (9)

Training: Occurrence/Analytics

Nature & Extent of PFAS

Persulfate Oxidation and P&T

Ex Situ Destruction Life Cycle

Ion Exchange & Plasma

Real Time Analytical Methods

Concentration Technologies (2)

PFAS-Free AFFF Dem/Val (4)

In Situ Thermal Treatment

Ex Situ Destruction (2)

Concentration Technologies (3)

Monitoring & Characterization (2)

Firefighting System Cleaning (6)

PFAS-Free AFFF Dem/Val (5)

Thermal Destruction (11)

Amendment Effectiveness (8)

Mixture Ecotoxicity (4)

Avian Ecotoxicity (3)

Marine Ecotoxicity (6)

Treatment (27)

Enhanced PFAS-Free Agents (11)

Thermal Deg Polymeric PFAS in Munitions (1)

Transformation in Soil & Groundwater (13)

Stormwater Management (4)

AFFF-Impacted Concrete & Asphalt (8)

Performance: PFAS-Free Firefighting Agents (7)

Testing: PFAS-Free Firefighting Agents (2)

Sampling & Analysis (2)

Treatment: Concentration Technologies (1)

Treatment: Destructive Technologies (1)

Thermal Destruction Processes (3)

Fate & Transport (4)

Self-Assembly Behavior (2)

Enhanced PFAS-Free Agents (2)

Development: PFAS-Free Coatings (4)

In Situ Treatment (2)

Ex Situ Destruction (2)

Concentration Technologies (2)

Monitoring & Characterization (6)

App: Environmental Reg Criteria

Management of Impacted Soils and Waters (7)

Technology Transition (4)

In Situ Treatment (3)

Ex Situ Destruction (3)

Monitoring & Characterization (5)

In Situ Treatment (3)

Ex Situ Destruction (13)

Concentration Technologies (2)

Monitoring & Characterization (2)

PFAS-Free AFFF Dem/Val (2)

Technology Transition (3)

Monitoring & Characterization (4)

Ex Situ Destruction (6)

Concentration Technologies (3)

Microplastics Impacted with PFAS (4)

Physical-Chemical Properties of PFAS (4)

Treatment of Impacted Matrices (10)

Transformation in Soil & Groundwater (1)

Ecotoxicity (2)

Sensors for Detection and Quantitation (2)

FY11

FY12

FY13

FY14

FY15

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FY18

FY19

FY20

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FY26

FY27

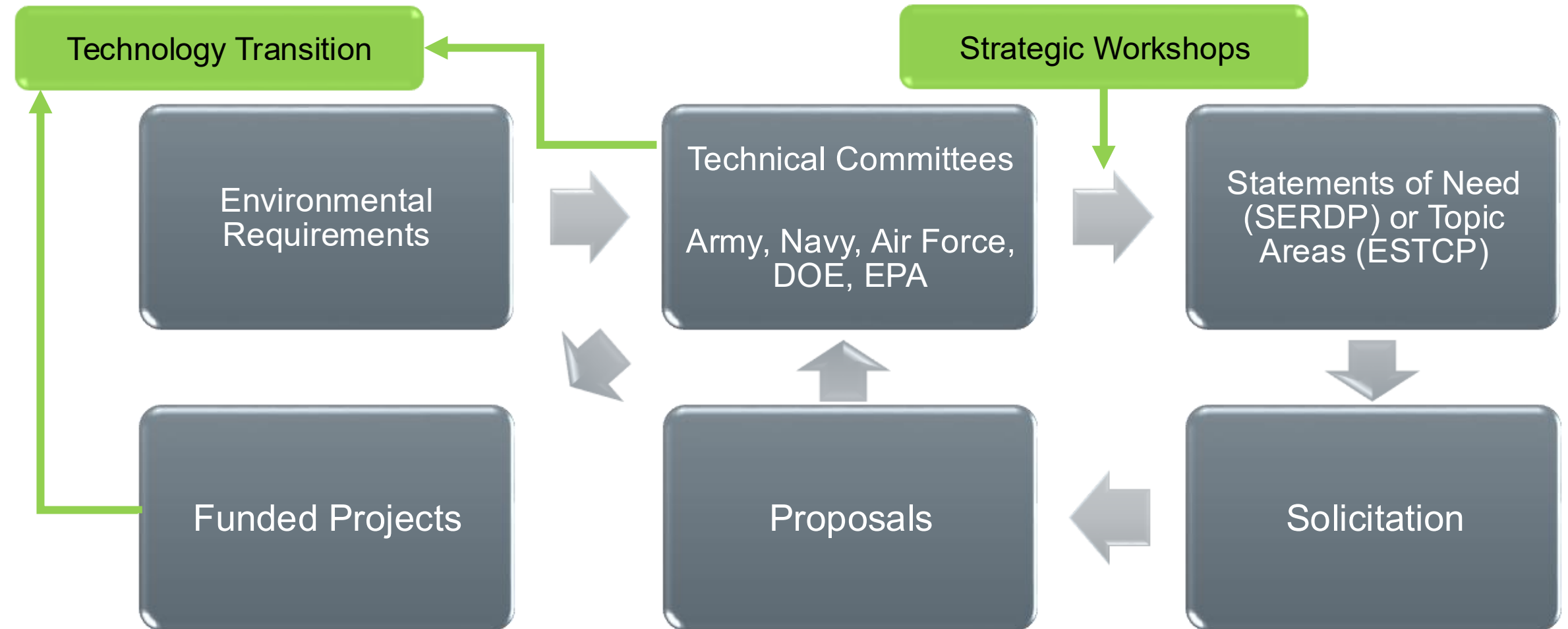
FY28

FY29

Primary Focus of PFAS Investments

- **PFAS Management in the Environment**
 - Treatment technology development & assessment
 - Sampling and analysis
 - Fate and transport
 - Ecotoxicity and ecological risk assessment
 - Stormwater management
- **AFFF Replacement: PFAS-Free Firefighting Formulations (F3)**
 - Development & demonstration of F3s
 - ARFF decontamination
 - Ecotoxicity of F3s

Strategic Process



Workshops

Key to identifying data gaps and research questions

Gather end users, policy makers
and technology implementers to
brainstorm for two days

Generate report summarizing
discussions and data needs

Feeds into SERDP & ESTCP
strategic plan



Stormwater Workshop 2026

- Two-day Meeting (invite only)
- 44 experts from DOW, EPA, Consulting and Academia

The overall objectives of this workshop:

- *Review the current state of the science and engineering in each of the topic areas for stormwater management.*
- *Evaluate whether currently available stormwater management practices meet users' needs and requirements.*
- *Identify and prioritize research, demonstration, and technology transition opportunities.*

Four Breakout Sessions

1. Predicting Stormwater Impacts
2. Stormwater Control and Treatment Practices
3. Chemicals of Concern
4. Innovations in Best Management Practices (BMP)/Stormwater Harvesting.

Charge questions related to Modeling, Implementation, Prioritization, Integration, Gaps.

Criteria for Prioritizing Research, Demonstration, and Technology Transition Needs

	Critical	High
Research	Research that potentially could have a significant impact on stormwater management within the next 1-3 years.	Research that is of high priority but may not be able to be initiated until critical research needs are addressed or may be more clearly defined after critical research needs are addressed.
Demonstration	Field demonstrations or assessments that can improve stormwater management within the next 1-3 years.	Field demonstrations or assessments that are of high priority but may not be able to be implemented until critical demonstrations or assessments are completed.
Technology Transition	Specific actions or documents that could be undertaken immediately to promote technology transition of key concepts or technologies.	Actions or documents that should be undertaken to promote technology transition of key concepts or technologies once specific research and/or demonstrations have been completed.

Workshop Report

- Strategic Workshop on Stormwater Management

Release date October 2026!

Congressionally Directed

Three congressional adds in past three years

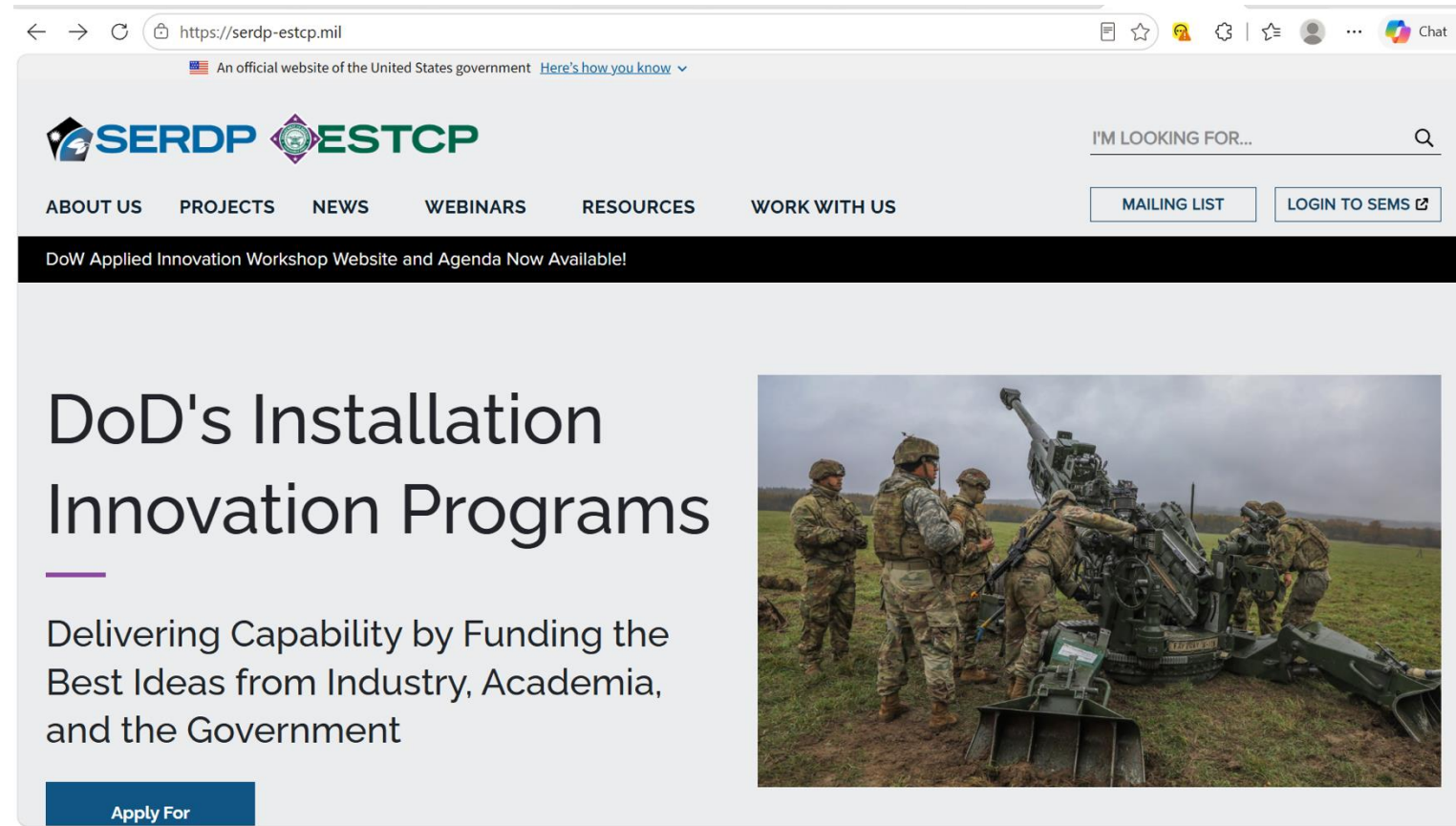
1. FY24 Treatment and Destruction of AFFF Concentrates (2022 NDAA)
2. FY25 Center for PFAS Remedial Technology Engineering
3. FY27 Improved Understanding of the Fate and Transport of Compounds Released from Tire Wear Particles to the Aquatic Environment

Summary

SONs developed by

- Regulatory Drivers
- NDAA – National Defense Authorization Act
- Learnings from Past Research Projects
- Expert Workshops
- Congressional Directives

<https://serdp-estcp.mil/>



Air Force Installation & Mission Support Center



From Rocky Seas to Smooth Sailing: Which Path Will Your GSI Investigation Take?

Everett Fortner III (Trey), PG (Noblis)
Amar Wadhawan, PhD (Noblis)
William Niemand (AFCEC/CZPR)

11 August 2026
RemPlex Seminar



GSI Pathway Investigations Outline



- **Why Do GSI Investigations Need a Tailored Strategy?**
- **Objectives**
- **Challenges and Approach**
- **Investigation Framework**
- **Key Takeaways**





Why Do GSI Inv. Need a Tailored Strategy?



- **Transport CSM** $\Rightarrow$ Migration through variable and interconnected pathways (e.g., groundwater to surface water, surface water to groundwater, storm sewer to surface water) with potential for bidirectional exchange and transport beyond the original source area
- **Contaminant Fate** $\Rightarrow$ Physical and geochemical conditions at the interaction zone drive contaminant transformation, sorption, and degradation, affecting mass and composition along transport pathways
- **Investigation Complexity** $\Rightarrow$ Interaction occurs across varying geologic settings and spatial/temporal scales, requiring phased, multi-method investigations for effective characterization

**GSI investigations require a skilled multidisciplinary team
and phased approach**

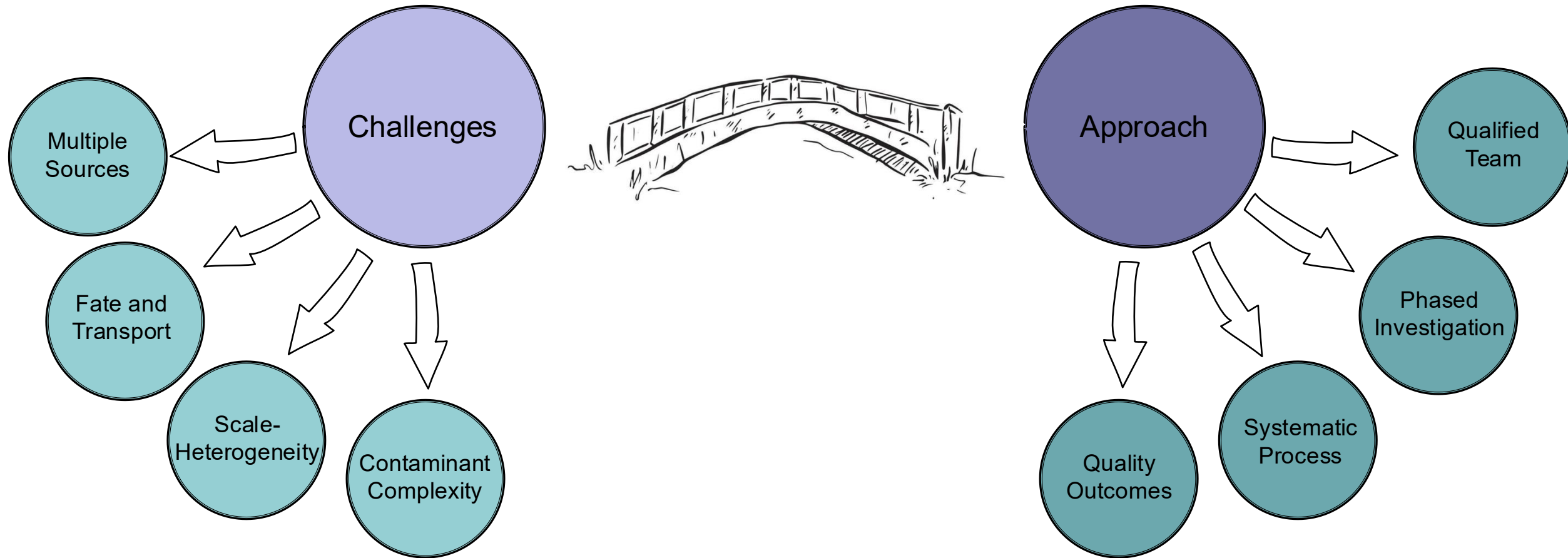


Objectives



- 1. Present a systematic framework for addressing common GSI investigation challenges through phased investigation approach and robust CSM development.**
- 2. Demonstrate method selection strategies that align investigation tools with site-specific conditions to achieve defensible results, efficient outcomes, and decision-ready data.**

Understanding the Challenges: Why Structured GSI Investigations Matter

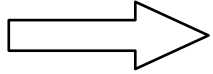




Challenges

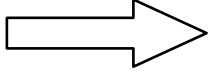


Multiple Sources



Distribution & Migration - widespread distribution, co-mingled plumes, offsite migration
Source Complexity - historical release timeframes, multiple source areas, active source release

Fate and Transport



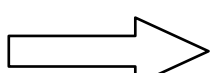
Transport Pathways - groundwater, storm sewer, seeps, wind, bidirectional exchange
Contaminant Fate - transformation, mixing zones (hyporheic), geochemistry, degradation

Scale-Heterogeneity



Spatial Variability - heterogeneity, variability along flow paths
Temporal Variability - seasonal fluctuations, storm events, climate

Cont. Complexity



Chemical Prop. - Ex. PFAS: ionic forms, partitioning, precursor trans., total oxidized precursor
Regulatory Framework - screening levels, exceedances with small magnitude discharge

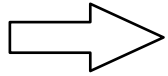
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Approach



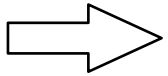
Qualified
Team



Expertise - hydrogeologist, hydrologists, SMEs, project/data managers

Team Dynamics - skilled evaluation, quality, defensible outcomes, efficient investigations

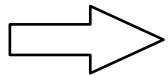
Phased
Investigation



Phased Framework - start small, manageable actions, break down complexity, data gaps

Method Strategy - spatial/temporal alignment, multiple lines of evidence, aligned with site setting

Systematic
Process



Integration - aligned SOW, stakeholder collab., regulator coord., logistics, data management

DQO Process - clear objectives in work plan, methods, quality control

Quality
Outcomes



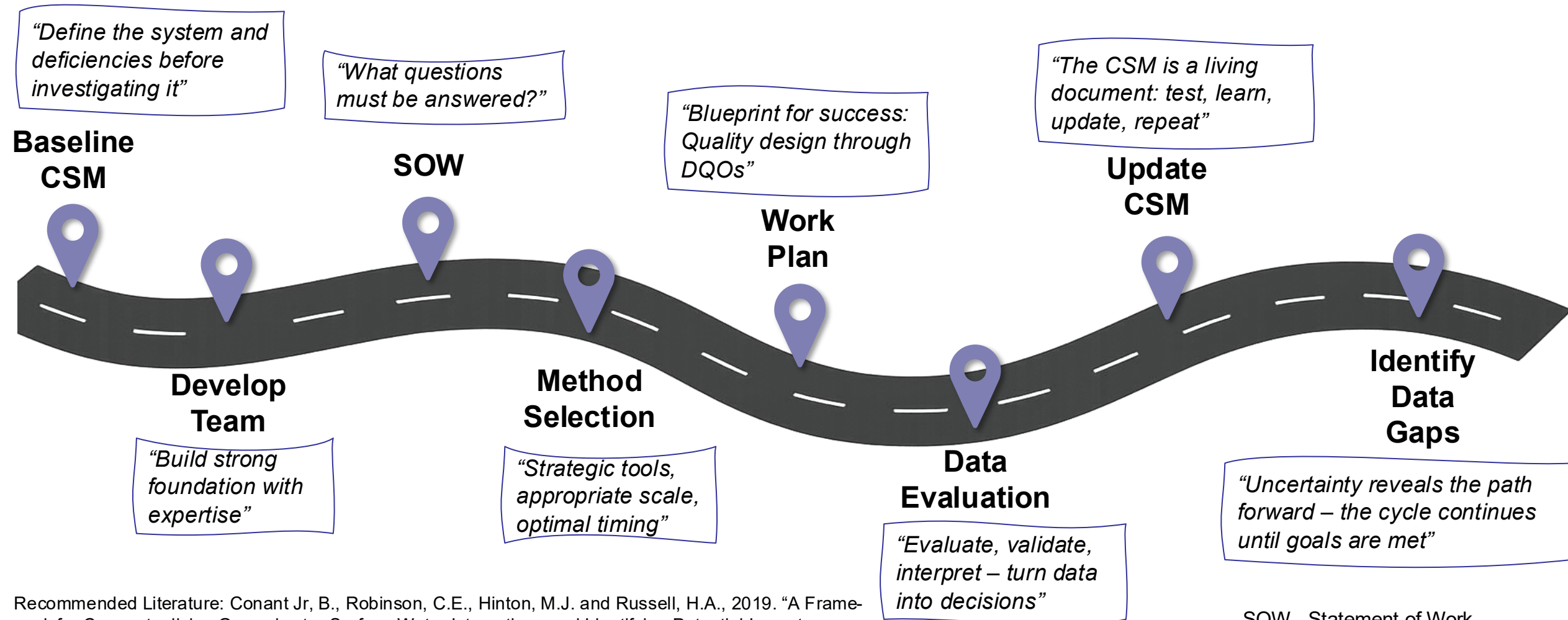
Results - def. findings, efficiency, reg. acceptance, actionable data (informed decisions)

Deliverables - robust CSM updates, support for modeling and feasibility studies

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Investigation Framework



SOW - Statement of Work
DQO - Data Quality Objective

Recommended Literature: Conant Jr, B., Robinson, C.E., Hinton, M.J. and Russell, H.A., 2019. "A Framework for Conceptualizing Groundwater-Surface Water Interactions and Identifying Potential Impacts on Water Quality, Water Quantity, and Ecosystems." *J. Hydrol.* <https://doi.org/10.1016/j.jhydrol.2019.04.050>



Investigation Framework - CSM Essentials



Baseline CSM

Typical Baseline CSM (Often Inadequate)

- ✓ Climate
- ✓ Source Area
- ✓ Plume Extent
- ✓ Geology/Hydrogeology
- ✓ Hydrology
- ✓ Groundwater Flow

Limited in supporting GSI evaluations

Data Collection and Evaluation



Data Gap

GSI-Specific CSM

- ✓ Detailed Surface Water Hydrology
- ✓ Preferential Pathways
- ✓ Hydraulic Connection
- ✓ Background Contribution
- ✓ Mass Flux/Discharge
- ✓ Temporal Variability
- ✓ Anthropogenic Influences/Elements
- ✓ Plume Transport - GSI
- ✓ Contaminant Specific Characterization (PFAS)

Updated CSM

Comprehensive Understanding

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Investigation Framework - SOW to Methods



SOW Foundation

- ✓ Review CSM
- ✓ Research Questions
- ✓ Data Gaps
- ✓ Investigation Goals
- ✓ Preliminary Method Screening

Work Plan Development 7 Step DQO Process

Method Selection Strategy

- ✓ Align Objectives and Setting
- ✓ Navigate Complexity
- ✓ Maintain Strategic Focus

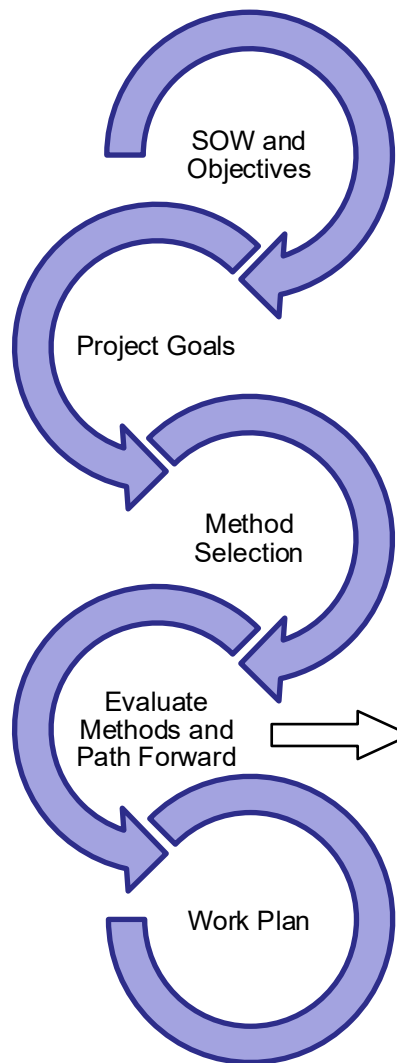
Problem Goal Inputs Boundaries Analytics Acceptance Plan

USEPA UFP-QAPP

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Inv. Framework - Method Selection Strategy



Updates to the tool
are Coming Soon!

Simplify Complex
Sites into Phases

Align with stakeholders
to build consensus

Hammett, S., Day-Lewis, F.D., and Trottier, B.R., 2021, U.S. Geological Survey Software Release for the GW/SW-MST: A Groundwater/Surface-Water Method Selection Tool, v1.0: U.S. Geological Survey Software Release, 27 January 2022.

2022 USGS GW/SW Method Selection Tool

EXAMPLE METHOD SELECTION LOGIC

STEP 1		STEP 2	
Method	Goal Question: Map geologic structure and other geologic attributes? Yes	Project Site Question: What is average depth of surface water in the area of data collection (m)? >3m	Project Site Question: Is the ground/bed armored or difficult to disturb? Yes
	Method Contributes to Goal? =IF(Bgoal="Yes",1,-1) Since answer is Yes, then cell value = 1 Since cell value =1, then conditional formatting symbol is	Method Made Infeasible by Site Parameter? =IF(DepthSW="<=1m",-1,1) Since answer is >3m, then cell value = 1 Since cell value = 1, then no conditional formatting symbol is displayed since the method is suitable for use at the project site	=IF(Armor="Yes",-1,1) Since answer is Yes, then cell value = -1 Since cell value =-1, then conditional formatting symbol is
	CSP – Continuous Seismic Profiling		
	Method Appropriate for Goals? ● Likely Appropriate/Effective ○ Not Likely Appropriate/Effective =IF(MAX(I25:V25)>=1,1,-1) ● Likely Appropriate/Effective	Method Effective at Site? ● Likely Appropriate/Effective ○ Not Likely Appropriate/Effective =MIN(W25:AQ25) ○ Not Likely Appropriate/Effective	Method Suitable? ✓ Potentially Suitable ✗ Not Likely Suitable =MIN(G9:H9) ✗ Not Likely Suitable
STEP 1b		STEP 2b	STEP 3



Key Takeaways



1. **Qualified Teams → Expertise drives quality**
2. **Phased Approach → Manages complexity systematically**
3. **Strategic Methods → Align tools to setting and objectives**
4. **Quality Process → DQOs ensure quality and defensible results**
5. **End Goals → Enable progress with optimal resources**

Success = Expert Collaboration + Systematic Planning

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Thank You



Questions?



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Air Force Installation & Mission Support Center



Updated Best Practices for PFAS Soil-to-Groundwater Leaching Evaluations at USAF Installations

PRESENTED BY
Matthew Spurlin, MS, CPG (Noblis)
11 August 2026



Acknowledgements



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Agenda



- Objectives
- Roadmap of Updated Approach
- Site-Specific Screening, Recharge & Mass Discharge Evaluations
- Guidelines for Lysimeter Investigations
- Guidelines for Data Modeling
- Data Collection Summary
- Soil Screening Level (SSL) Determination
- Data Gaps and Continued Research
- Next Steps



Objectives



- Updated guidance is needed to incorporate best practices that minimize uncertainties in data collection and interpretation.
- Should consider range of site conditions based on soil types and climate, and a more standardized set of best practices and tools.
- Provide a new tiered approach that provides an updated framework for determining SSLs that will address an immediate need for technical direction in scoping and conducting the next phase of PFAS RIs.

PFAS = per- and polyfluoroalkyl substances
RI = Remedial Investigation



Roadmap of the Updated Approach



- **Step 1 – Site-Specific Screening, Recharge, & Mass Discharge Evaluations**
 - 1a – If amenable to lysimeters and porewater available, estimate recharge, conduct mass discharge evaluation
 - 1b – If amenable to lysimeters and porewater not available, install minimum # of lysimeters, estimate recharge, conduct mass discharge evaluation
- **Step 2 – Pre-Installation Monitoring, Lysimeter Installation, & Sampling**
- **Step 3 – Site-Specific DF Estimation**
- **Step 4 – SSL Determination**
 - Method 1 – Linear Regression Using Paired Soil and Lysimeter Porewater Sampling Results
 - Method 2 – PFAS-LEACH Modeling Tool

■ Site setting and climate

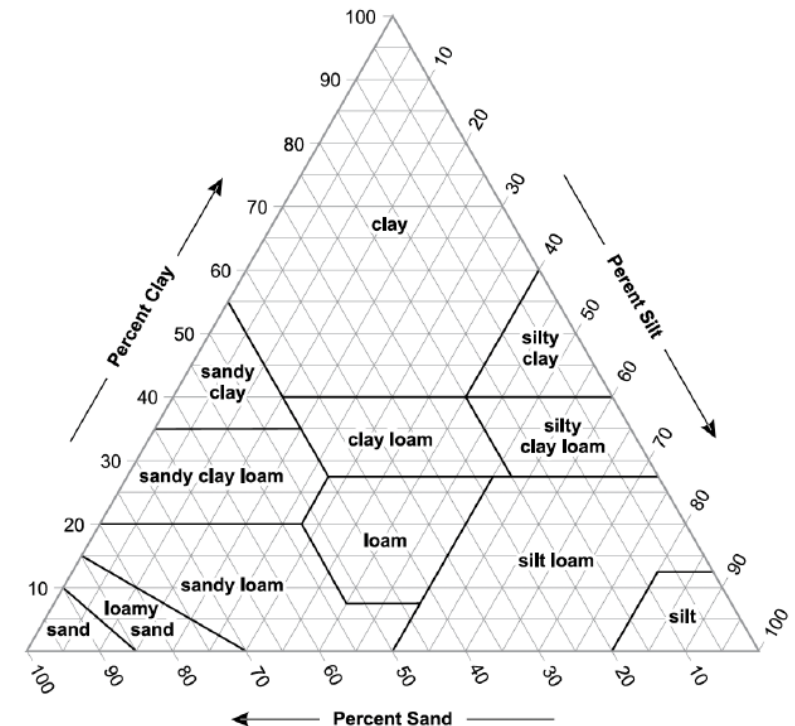
- Evaluate viability for lysimeter investigations based on climate category and depth to groundwater
- Support recharge and mass discharge evaluations

■ Geology and soil type

- Focus on dominant soil type
- Supports estimates of K_{sat} and van Genuchten parameters (pedotransfer functions, Web Soil Survey)
- Supports lysimeter data evaluation and modeling phases

■ Groundwater table

- Significant influence on viability of lysimeter investigations



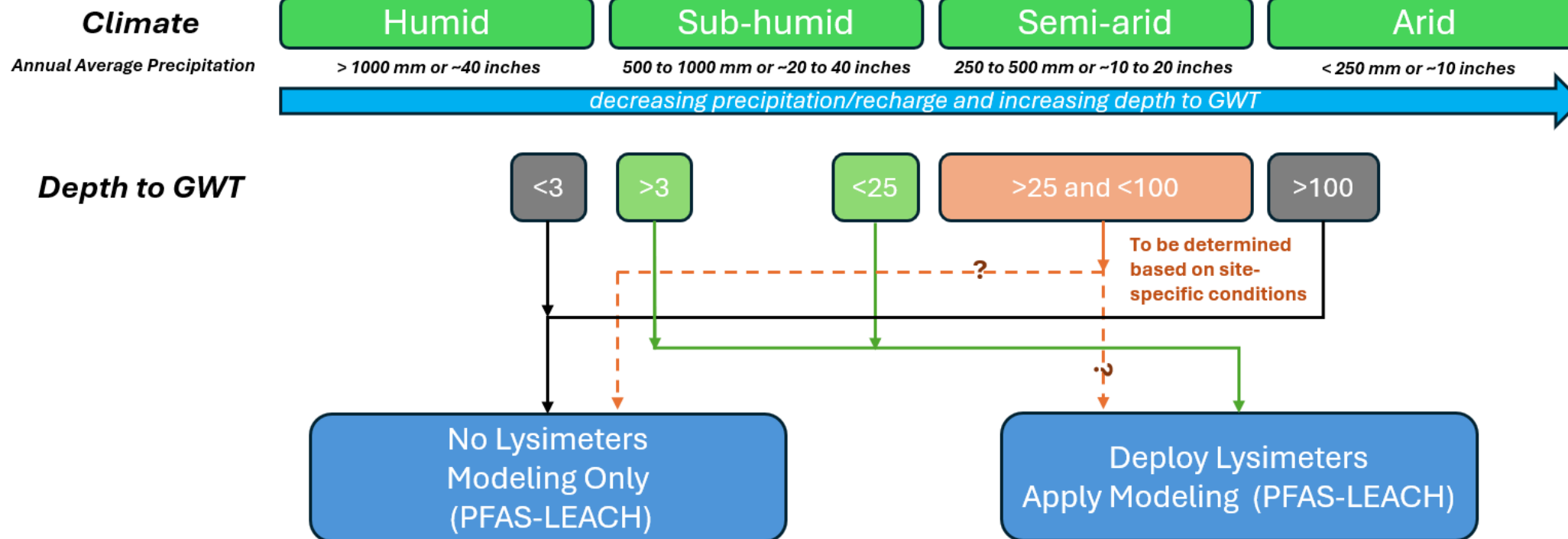
12 Basic Soil Classes (USDA)



Site-Specific Screening (cont'd)



Tiered Approach for Leaching Evaluations Based on Site Conditions





Recharge Evaluations



- Recharge is a significant component of downward PFAS mass flux from the vadose zone to groundwater
- 40 methods summarized, 15 methods recommended in Newell et al. (2023)
 - Tier 1 (4 types) – Low complexity, low cost
 - Tier 2 (6 types) – Advanced tools, moderate cost
 - Tier 3 (5 types) – Complex assessments, high cost
- Focused vs. diffuse recharge

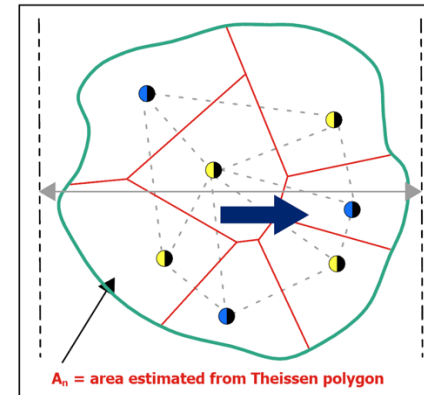
Determining groundwater recharge for quantifying PFAS mass discharge from unsaturated source zones

Charles J. Newell¹ | Emily B. Stockwell¹ | Jessica Alanis¹ | David T. Adamson¹ |
Kenneth L. Walker¹ | R. Hunter Anderson²

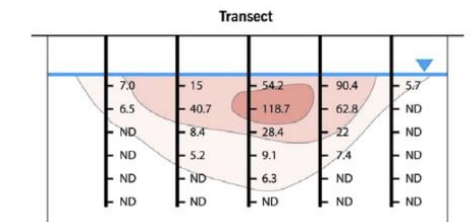
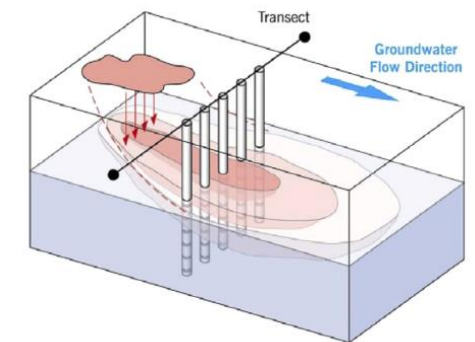
Mass Discharge Evaluations

- Why do we need mass discharge evaluation (M_d)?
 - Described in the 7-Step DQO process for UFP-QAPP Worksheet #11
- Vadose zone mass discharge
 - Annual precipitation, infiltration, porewater concentrations from source area, soil delineation boundary
 - Theissen polygon or PFAS-LEACH data modeling approaches
- Groundwater mass discharge
 - Groundwater concentrations, hydraulic conductivity (K), horizontal hydraulic gradient (i), impacted cross-sectional area (A)

Vadose Zone Mass Discharge



Groundwater Mass Discharge



Source: Newell et al. (2023)

DQO = data quality objective
UFP-QAPP = Uniform Federal Policy for Quality Assurance Project Plan

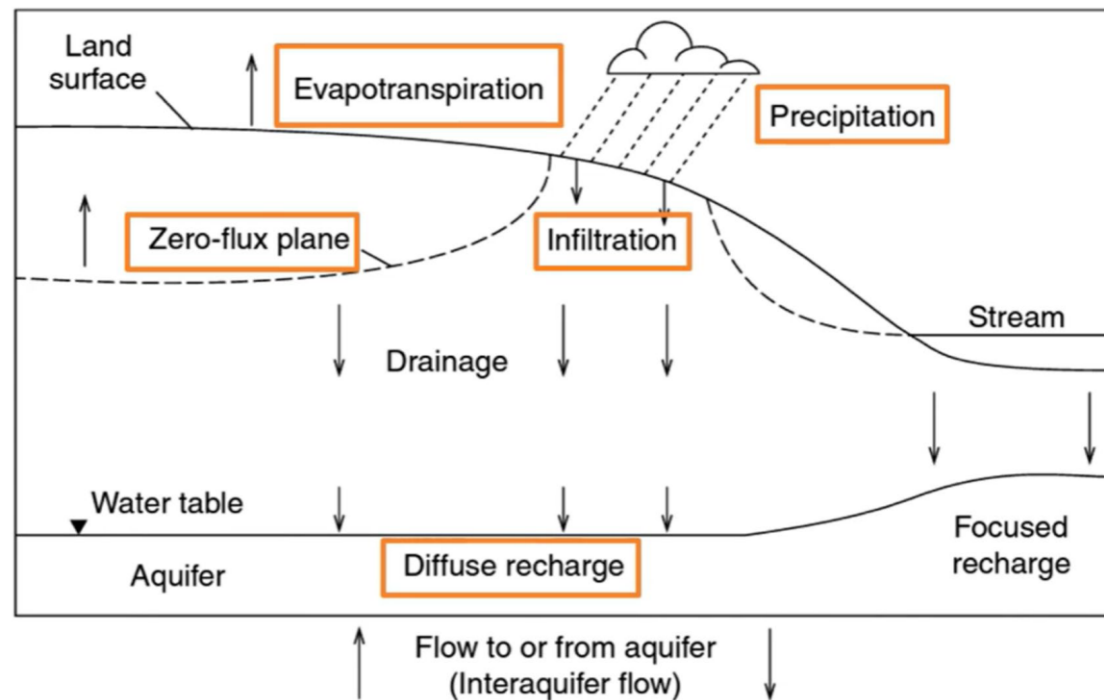


Guidelines for Lysimeter Investigations



- Planning and design
- Capillary fringe estimation
- Pre-installation monitoring
 - Soil sampling and analysis
 - Groundwater table monitoring
 - Paired tensiometers
 - Soil moisture probe
- Lysimeter installation and sampling
 - Paired soil and porewater samples
 - Minimum of 10 lysimeters per installation
- Additional lysimeter siting

Key Recharge Processes (Healy, 2010)





Guidelines for Lysimeter Investigations (cont'd)



■ Focused additional data evaluation based on lessons learned

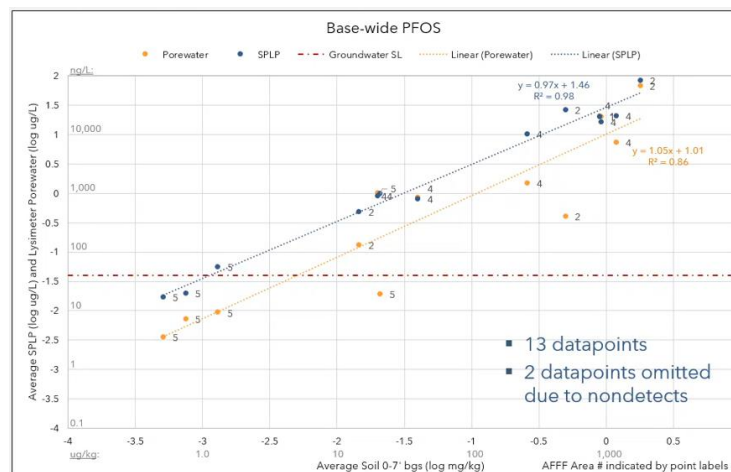
Correction of porewater sampling results using bromide tracer

$$CF = \frac{Br_{batch\ conc}}{Br_{batch\ conc} - Br_{PW\ conc}}$$

$$C_{PFAScorrected} = C_{PFASmeasured} \times CF$$

Statistical modeling with linear regression

- Exploratory data analysis (EDA)
- Evaluation of linear regression models and assumptions
- Sample size and high-leverage points



$$[\log C] = \frac{[\log C_w] - b}{m}$$

$$C_w = MCL \text{ (or TSL or RSL)} * DAF$$

Guidelines for Data Modeling

PFAS-LEACH – A Comprehensive Decision Support Platform for Predicting PFAS Leaching in Source Zones

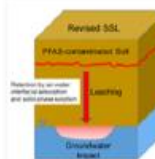
Bo Guo & Mark Brusseau, University of Arizona

- Four models spanning a wide range of complexity
- Comprehensive parameter selection module
- Documentation and user manual

Applications:

- Simulate retention & transport in multiphase systems
- Quantify mass discharge to groundwater
- Support risk assessments for soil-groundwater route
- Determine soil screening levels
- Determine remedial action targets
- Evaluate remedial action performance

Computational Cost & Input Parameters

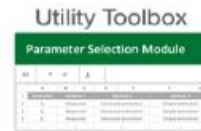
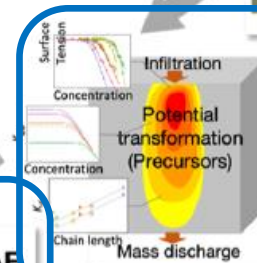


Tier 4 – PFAS-LEACH-DAP

Features: Revised EPA dilution-attenuation model

- Simplified mass-balance calculations

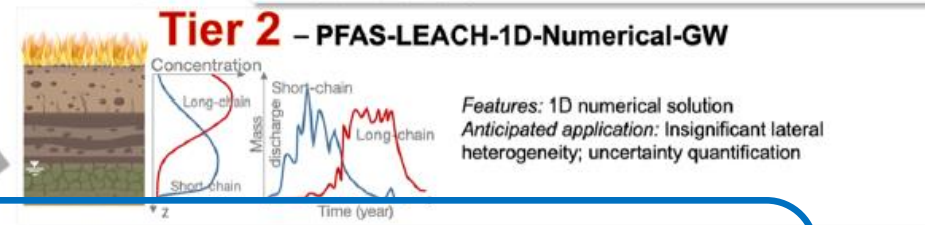
Anticipated application: Initial screening of sites



Tier 1 – PFAS-LEACH-COMP-GW

Features: Full-process model in 3D

- Anticipated application: Sites with sufficient data; complex spatial heterogeneity and/or source conditions

Tier 3 – PFAS-LEACH-Analytical-GW

Features: 1D analytical solutions Implemented in Excel

Anticipated application: Limited data; early stage of site management; order-of-magnitude estimate.



Model Complexity

“RI Data Only”
Approach

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Guidelines for Data Modeling (cont'd)

① Soil Properties and Site Conditions

Parameter	Value	Unit
Depth to groundwater*	300	cm
Contaminated site area (or unit area)	2500	m ²
Temperature	20.00	°C
Net infiltration*	25.92	cm/yr
Soil bulk density*	1.53	g/cm ³
Saturated hydraulic conductivity	44.87	cm/day
Residual water content	0.064	cm ³ /cm ³
Saturated water content*	0.370	cm ³ /cm ³
Median grain size	0.005	cm
Organic carbon fraction	0.41	%
van Genuchten parameter	0.018	cm ⁻¹
van Genuchten parameter	1.51	(-)
Longitudinal dispersivity*	13.42	cm
Water content*	0.219	cm ³ /cm ³
Air-water interfacial area scaling factor	4.7	(-)
Air-water interfacial area*	753.9	cm ² /cm ³

Soil Type: ☑ User defined

④ Initial PFAS Soil Conc. & Lysimeter Porewater Conc.

Interpolation Method: ☑ Piecewise Linear Interpolation Re-apply interpolation whenever datapoints are updated.

Soil concentration (ug/kg) vs Depth (cm) plot showing data points and a fitted curve.

② PFAS Properties

Parameter	Value	Unit
Surface tension parameter	62.1	mg/L
Surface tension parameter	0.19	(-)
Surface tension parameter	71.0	dyn/cm
Molar mass*	414.07	g/mol
Molecular diffusion coefficient*	4.90E-06	cm ² /s
Molar volume	237.20	cm ³ /mol
Organic carbon-water partition coefficient	136.2	cm ³ /g
Solid-phase adsorption coefficient*	0.56	cm ³ /g
Air-water interfacial adsorption coefficient*	3.69E-03	cm ³ /cm ²

PFAS Type: ☑ PFNA

NOTE: F_s and α_s are only needed for using the advanced solver.

③ Groundwater Dilution

Parameter	Value	Unit
Groundwater darcy flux	365.00	m/yr
Lateral site width	3.00	m
Saturated zone thickness	0.35	m
Vertical dispersivity	0.02	m
Mixing zone thickness	0.32	m
Dilution Factor*	151.0	(-)

⑤ Simulation Information

Parameter	Value	Unit
Simulation time (time series)*	100	yr
Output time interval (time series)*	1	yr
Output time points (profiles)*	5, 10, 30, 50	yr
Initial groundwater concentration*	0.004	ug/L

Lysimeter Data

(for estimating A_{gw} scaling factor in Box ①)

Depth (cm bgs)	Porewater conc. (ug/L)	Water content (cm ³ /cm ³)	A_{gw} scaling factor (-)
20	50	0.2	1.83
60	20		1.55
100	5	0.25	5.70

Diagram illustrating the lysimeter setup and groundwater flow parameters. Key parameters include: $I_f = 25.92$ cm/yr, $Z_{nw} = 300$ cm, $L = 3.00$ m, $U_{gw} = 365$ m/yr, $b_{sat} = 0.35$ m, and $\delta_{gw} = 0.32$ m.



Guidelines for Data Modeling (cont'd)



■ Model inputs

- Site soil properties, site conditions, PFAS properties, groundwater dilution, and PFAS soil concentrations
 - Module0 – base model for quantifying PFAS leaching and deriving SSLs
 - Module1 – adds the capability of parameter sensitivity analysis with left/right bound deviation from a median value
 - Module2 – adds the additional capacity for conducting Monte-Carlo-type uncertainty analysis on input parameters

■ Model outputs:

Algebraic solution

Analytical solution

Abbreviation	SSL Equation	Source
SSL _{EPA Standard}	$SSL_{EPA\ Standard} = C_{gw,a} \times DF \times \left[K_d + (\theta_w) \frac{1}{\rho_b} \right]$	USEPA, 1996a; USEPA, 1996b
SSL _{PFAS-LEACH Tier 4}	$SSL_{PFAS-LEACH\ Tier\ 3} = C_{gw,a} \times DF \times \left[K_d + (K_{aw}A_{aw} + \theta_w) \frac{1}{\rho_b} \right]$	Brusseau and Guo 2023
SSL _{PFAS-LEACH Tier 3}	$SSL_{PFAS-LEACH\ Tier\ 4} = C_{gw,a} \times AF_{vz} \times DF \times \left[K_d + (K_{aw}A_{aw} + \theta_w) \frac{1}{\rho_b} \right]$	Brusseau and Guo 2023



Data Collection Summary



Data Parameter	Method	Analysis	Requirement
Soil			
Soil Texture	NA	Vadose zone observed texture.	LI, DM
Grain Size Analysis	Laboratory	Sieve and hydrometer ASTM D6913/D7928/D422 AASHTO T88	DM
Bulk Density/Total Porosity	Laboratory	ASTM D7263	DM
Saturated Hydraulic Conductivity (K_{sat})	Laboratory	ASTM D5084/D5856/D2434	DM
TOC/Foc	Laboratory	Walkley-Black method as modified in Want et al. (2012)	DM
PFAS Concentration	Laboratory	USEPA Method 1633	LI
Matric Potential	Tensiometer	Time-series evaluation for assessment of recharge wave reaching the lysimeter depth location at applicable installations.	LI
Soil Moisture	Probe	Time-series evaluation with soil moisture conditions estimated to coincide with porewater lysimeter sample events.	DM
Water Retention Parameters	NA	Estimated from dominant vadose zone soil type.	DM
Porewater			
PFAS Concentration	Lysimeter	USEPA Method 1633	LI
PFAS Concentration	SPLP	USEPA SW846, Test Method 1312 and Leachate by USEPA Method 1633	LI
Groundwater			
PFAS Concentration	Laboratory	USEPA Method 1633	LI, DM
Groundwater Levels	Water level meter and pressure transducer	Synoptic and time-series evaluation for assessment of groundwater table flow/fluctuation and hydraulic gradient analysis.	LI, DM
Hydraulic Conductivity (K)	Pressure transducer	Hydraulic conductivity estimates calculated from testing results using method(s) that align with test type and response data evaluation.	DM
Climate			
Precipitation and Barometric Pressure	Weather Station or Equivalent	Time-series evaluation for seasonality and applicable data compensation or corrections for pressure transducers.	LI

TOC = total organic carbon
Foc = fraction of organic carbon

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LI = lysimeter investigation
DM = data modeling



Soil Screening Level (SSL) Determination



- **SSL determination:**
 - **Method 1 – Linear Regression Using Paired Soil and Lysimeter Porewater Sampling Results**
 - **Method 2 – PFAS-LEACH Modeling Tool**
- **PFAS anthropogenic background soil concentration for each PFAS compound with an MCL, TSL, or RSL should be estimated based on available information**
 - **If background > site-specific SSL, then background concentration will define response action for soil.**

MCL = Maximum Contaminant Level
TSL = Tap water Screening Level
RSL = Regional Screening Level



Data Gaps and Continued Research



- **Poorly understood complexities related to multi-phase retention of PFAS**
 - **Rate-limiting desorption-adsorption kinetics (non-equilibrium processes)**
 - **Precursor transformation effects on desorption-adsorption kinetics**
 - **Standardized batch desorption laboratory procedures**
 - **Metal oxide and oxyhydroxide retention**
 - **Efficacy of PFAS leaching evaluations in shallow fractured bedrock**
 - **PFAS sorptive losses to silica flour and/or ceramic suction lysimeter cups**
 - **Impact of a fluctuating groundwater table**
 - **Specific effects of heterogeneities on accelerated downward PFAS migration**
 - **Appropriate sample volume for evaluation of bromide tracer dilution**
 - **Use of multi-level lysimeters, microlysimeters and multichannel tubing (CMT) for porewater collection**



Next Steps



- Additional refinements are expected based on feedback from targeted external reviewers
- For additional information, please contact:
 - Matthew Spurlin, MS, CPG (Noblis, matthew.Spurlin@noblis.org)
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 - Kurt Lee, MS (AFCEC/CZPR, kurt.lee.3@us.af.mil)



Questions?



Questions?



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