U.S. DEPARTMENT OF ENERGY

Initial DOE PFAS Research Plan: Summary of National Laboratory Research and Development Areas

December 2022

Plan, Scope and Purpose

<u>Scope:</u>

This is an initial DOE Research & Development Plan, as called for in the DOE PFAS Roadmap (August 2022). The initial plan will be updated periodically with an expected finalization by the 1st quarter of FY 2025.

<u>Purpose:</u>

To inventory active PFAS R&D activities across the DOE enterprise and to identify gap areas.

<u>R&D Plan Maturity:</u>

In accordance with the DOE PFAS Roadmap objectives, the plan will mature over time to identify additional capabilities that DOE National Laboratories can bring to fill gap areas and to establish research priorities to ensure a coordinated effort across the National Laboratories and other federal research partners.

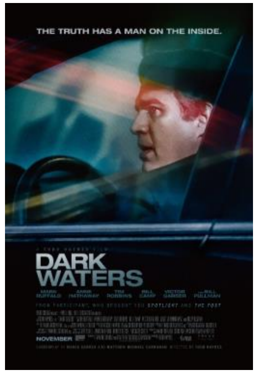
There is an increased urgency in dealing with the PFAS problem

U.S. HOUSE OF REPRESENTATIVES COMMITTEE ON
SCIENCE, SPACE, & TECHNOLOGY
Eddie Bernice Johnson, Chairwoman • Frank Lucas, Ranking Member

FOREVER CHEMICALS: RESEARCH AND DEVELOPMENT FOR ADDRESSING THE PFAS PROBLEM

SUBCOMMITTEE ON ENVIRONMENT & SUBCOMMITTEE ON RESEARCH AND TECHNOLOGY
DATE: TUESDAY, DECEMBER 7, 2021

Credit: HBO



Credit: Focus Features

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LEGISLATION

US legislation would limit PFAS in industrial wastewater

Measure would also expand EPA's definition of PFAS

by Cheryl Hogue
July 15, 2022

EPA United States Environmental Protection Agency

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EPA Announces New Drinking Water Health Advisories for PFAS Chemicals, $1 Billion in Bipartisan Infrastructure Law Funding to Strengthen Health Protections

Agency establishes new health advisories for GenX and PFBS and lowers health advisories for PFOA and PFOS

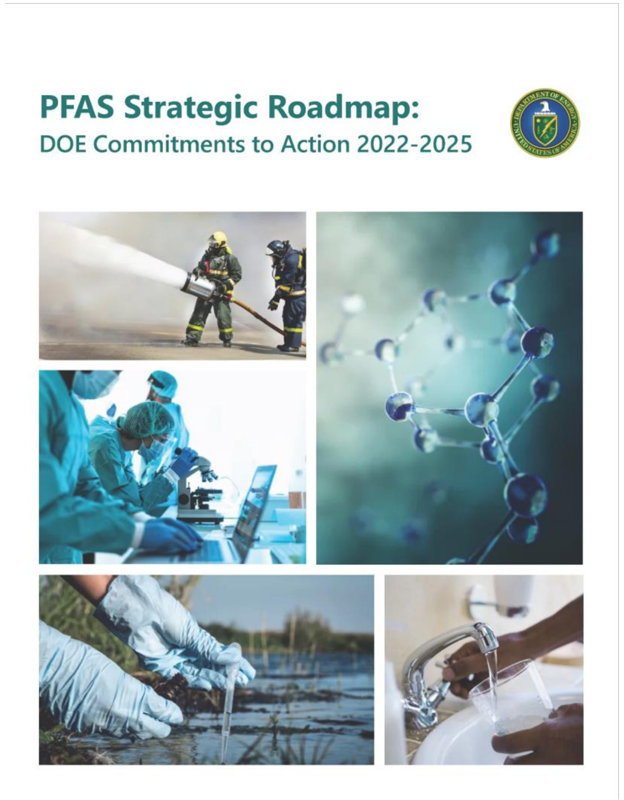
June 15, 2022

Current Federal PFAS Research Activity

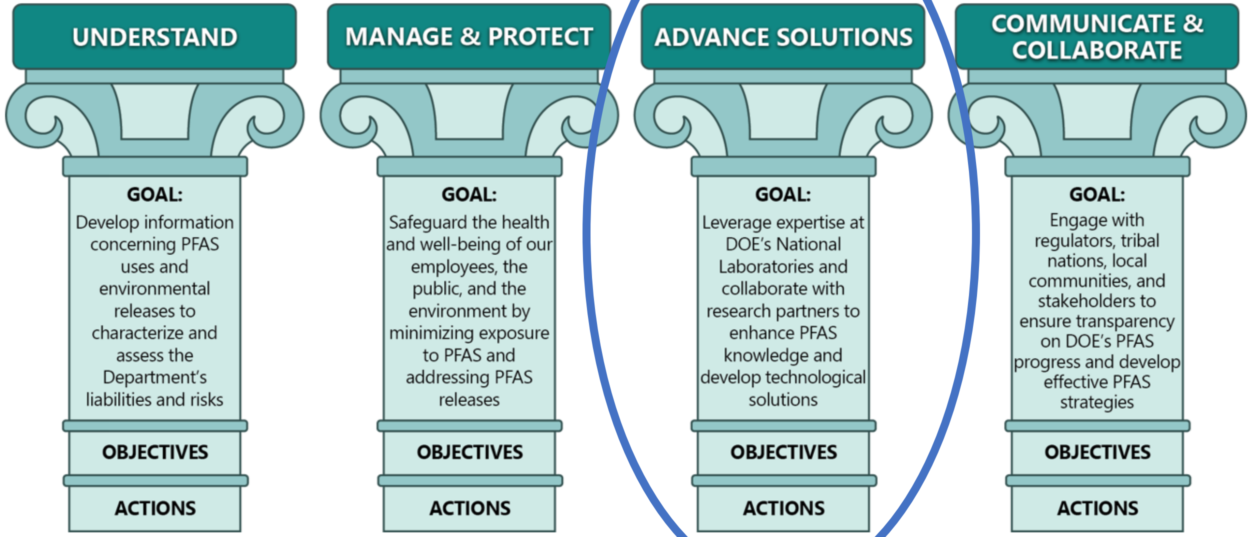
Numerous federal agencies support or are engaged in PFAS research:

- **Federal Aviation Administration (FAA)**
- **United States Department of Agriculture** (**USDA**)
- **Environmental Protection Agency** (**EPA**)
- **Department of Defense** (**DOD**)
  - Strategic Environmental Research and Development Program (**SERDP** - with DOE, EPA)
  - Environmental Security Technology Certification Program (**ESTCP**)
- **Health and Human Services** (**HHS**)
  - National Institutes of Health (**NIH**)
    - National Institutes of Environmental Health Sciences (**NIEHS**)
  - Agency for Toxic Substances and Disease Registry (**ATSDR**)
  - Centers for Disease Control (**CDC**)
  - Food and Drug Administration (**FDA**)
- **Department of the Interior** (**DOI**)
  - U.S. Geological Survey (**USGS**)
- **Department of Transportation** (**DOT**)
- **Department of Homeland Security** (**DHS**)
- **National Aeronautics and Space Administration (NASA)**
- **National Science Foundation (NSF)**
- **Department of Commerce (DOC)**
  - National Institute of Standards and Technology **(NIST)**

PFAS Strategic Roadmap: DOE Commitments to Action 2022-2025



4 Pillars and Goals



Leverage National Lab expertise and collaborate with research partners to enhance PFAS knowledge and develop technical solutions

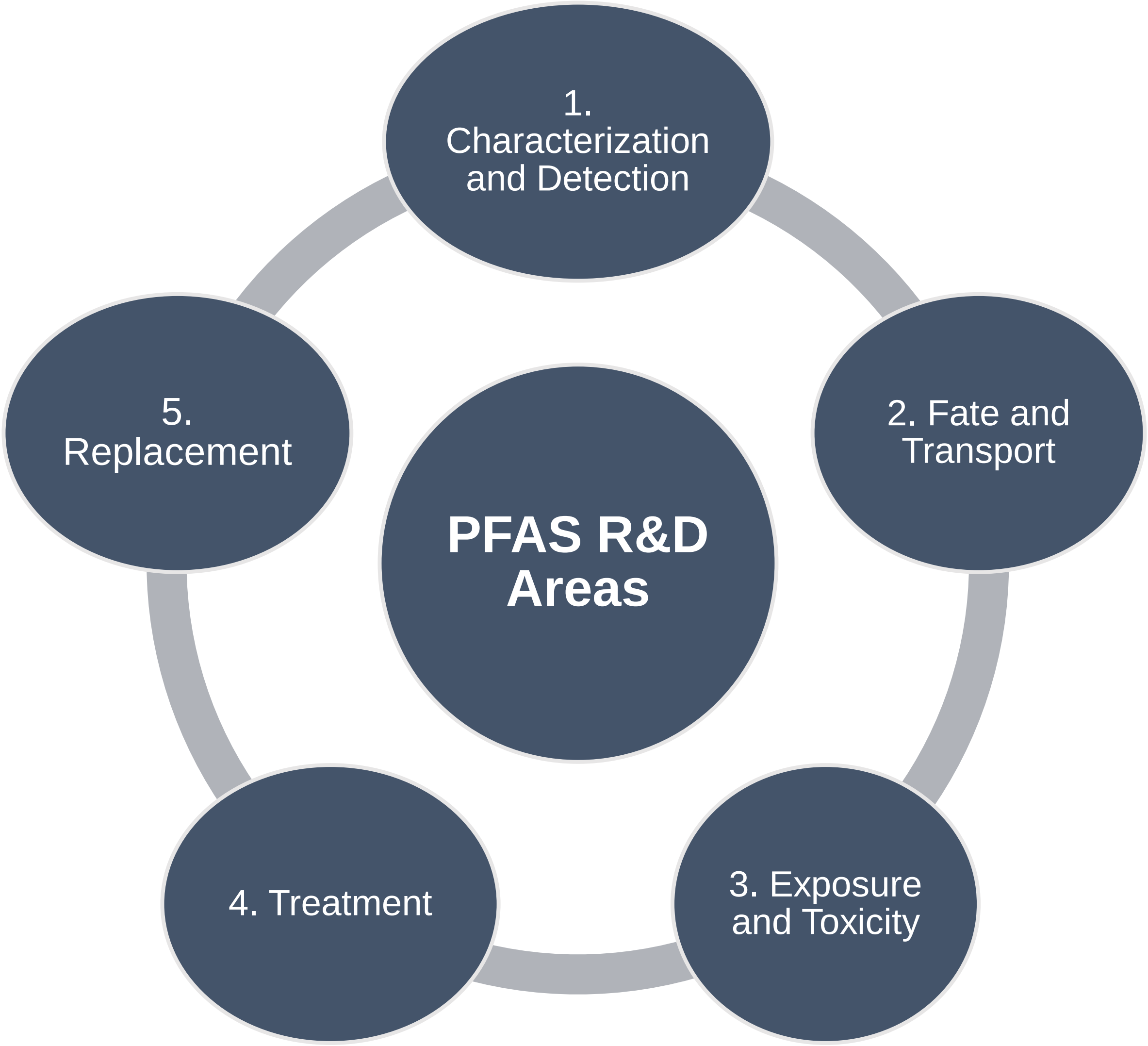
- Initial Plan due by end of Q1 FY23
- Update to Plan by end of FY25

SCAN ME

Link: DOE PFAS Strategic Roadmap: DOE Commitments to Action 2022-2025 (energy.gov)

Working list of R&D priorities for DOE planning and corresponding National Lab research efforts

Overview: PFAS Research and Development Areas



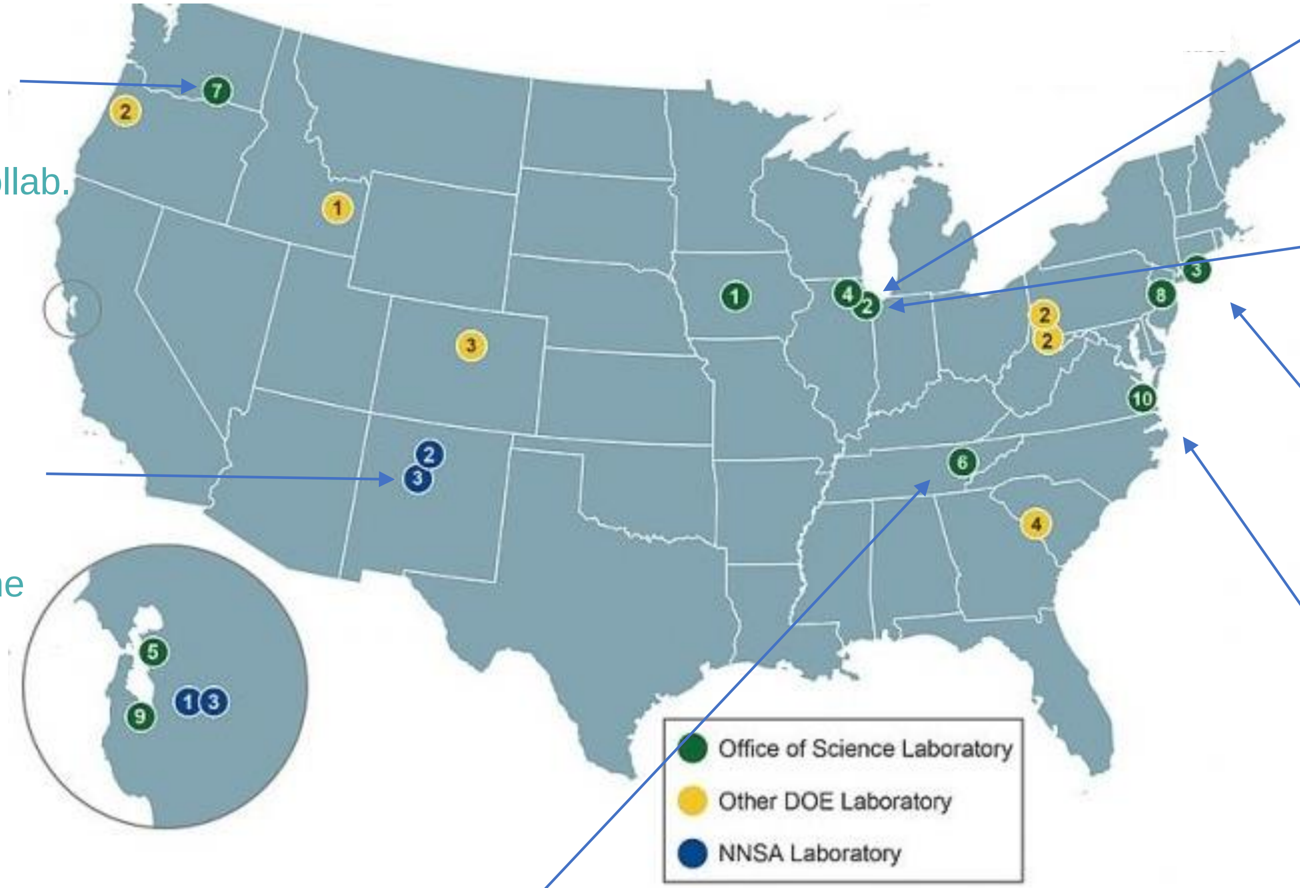
Most government agencies and other research institutions that are actively engaged in PFAS research have identified similar areas, each with a different emphasis.

DOE's PFAS research emphasis, outlined in the DOE PFAS Research Plan, will leverage the unique facilities and expertise of the National Labs and partnering institutions.

Overview: Summary of DOE National Lab PFAS activity

Pacific Northwest National Laboratory
PFAS capture probe
DOD ESTCP sensor collab.
PFAS destruction

Sandia National Laboratories
Advanced oxidation technologies for PFAS destruction, low cost PFAS sorbents, halt the migration of plumes in the subsurface



Fermi National Accelerator Laboratory
Electron beam destruction (with BNL)

Argonne National Laboratory
FET+AI/ML PFAS detection
Sensors and sorbents
Multiple treatment train
PFAS destruction
Ecological Screening Values for DOD
AI for PFAS toxicity predictions

Brookhaven National Laboratory
Plasma-based destruction, in collaboration with the State University of NY at Stony Brook (SBU).

Thomas Jefferson National Accelerator Facility
Electron beam destruction

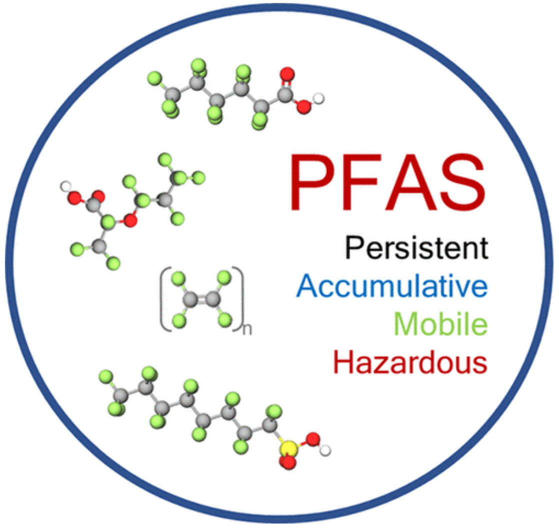
Consortium for Risk Evaluation with Stakeholder Participation (CRESP)
DOE-funded, Vanderbilt University, TN
PFAS leaching test and evaluation
Membrane separation to concentrate PFAS
Methods to mobilize PFAS
Efficacy studies of landfill liners

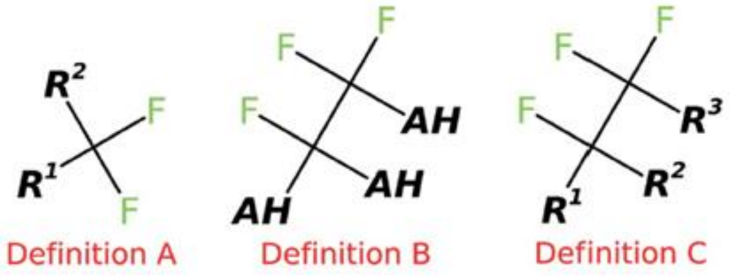
1. Characterization and Detection

Background The estimated number of PFAS compounds that may be in the environment are in the thousands yet only ~70 are currently uniquely detectable in certain media. Some parameters such as adsorbable organic fluorine (AOF), extractable organic fluorine (EOF), and total fluorine (TF) can help quantify hidden PFAS, but it is hard to identify the specific compounds. State-of-the-art liquid chromatography with tandem mass spectrometry (LC-MS/MS) works well when the target compound is known. Additionally, several unknown precursors and their transformation products exist in the environment that we lack understanding. For detectable PFAS, current detection limits may not be low enough for public health thresholds.

Possible Research Topics

- Improved methods to identify unknown PFAS, including an environmental forensics approach to identify non-AFFF sources
- In-situ detection for broad range of PFAS in various media (water, air, soil, dust, biota, food etc)
- Lower detection limits to keep pace with evolving thresholds





Examples and various definitions of PFAS

Image credit:
Barnabas et al. *Digital Discovery* **2022**
Kwiatkowski et al *Environmental Science & Technology Letters* **2020**, *7*, 532-543

1. Characterization and Detection: Current Lab R&D Activities

- **ANL** is currently developing a field-effect transistor platform for rapid electronic detection of PFAS in water, including the use of AI/machine learning for the design of molecular probes toward selective detection and separation of PFAS. These efforts are ongoing.
- **ANL** research continues on the development of additional PFAS selective sensors and sorbents.
- **PNNL** created a PFAS capture probe that is tailored for highly selective analyte recognition and detection which can also be used for quantification. PNNL's capture and sensor efforts were patented.
- **PNNL** is part of a recent DOD Environmental Security Technology Certification Program project award with ARCADIS and New Jersey Institute of Technology on "Field-Scale Demonstration of a Novel Real-Time Sensor for PFAS," where PNNL is working on detecting six different PFAS molecules using the PFAS sensor.
- DOE is supporting PFAS research activities through the Consortium for Risk Evaluation with Stakeholder Participation (**CRESP**), based at Vanderbilt University in Tennessee. CRESP is pursuing development and demonstration of EPA leaching test and evaluation methods.

2. Fate and Transport

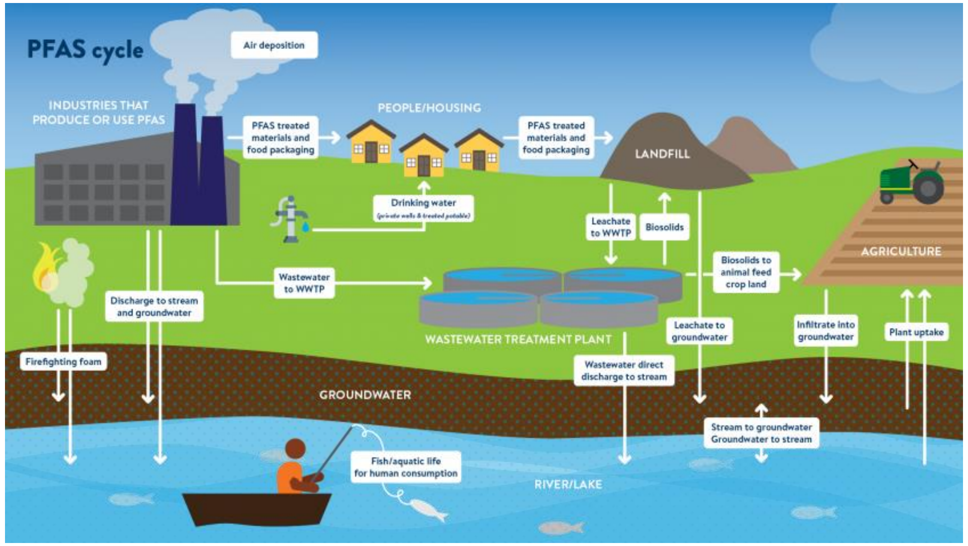
Background: PFAS releases into the environment can result in migration throughout the environment (e.g., AFFF releases to groundwater via migration through soil). PFAS precursors also create challenges with their transformation in the environment or by anthropogenic processes. For example, precursors like fluorotelomer alcohols can be converted to perfluorinated carboxylic acids (e.g., PFOA) in nature and by wastewater treatment. Basic fate and transport research is underway at other federal agencies and research institutions.

Possible Research Topics

- Understand basic subsurface transport characteristics of AFFF at DOE sites (specifically PFAS comingled with radionuclides)
- Identify precursors with the ability to transform to PFAS in the environment (in soil, water and atmosphere)
- Understand impacts PFAS have on soil wettability (i.e., hydrophobicity), impacting vadose zone transport at shallow contaminated sites

Lab R&D Capacity

- Various modeling tools for biogeochemical transformation and transport are available and can be adapted for PFAS



Cursory PFAS Conceptual Site Model Image credit: MPCA

Current Lab R&D Activities

-Discussions between Brookhaven National Laboratory and the U.S. EPA are underway to examine PFAS Fate and Transport using BNL as a case study.

-CRESP: Development, demonstration, and evaluation of EPA leaching test and evaluation methods.

3. Exposure and Toxicity

Background: PFAS has been associated with altered immune and thyroid function, liver disease, lipid and insulin dysregulation, kidney disease, adverse reproductive and developmental outcomes, and cancer. Perfluorinated acids are generally found in blood plasma and the liver, bound to proteins. The limited studies to date have been human studies focused on legacy PFAS. Little is known about emerging PFAS and interactions of PFAS mixtures on human health and the environment. DOE expects to play a supporting research role to lead health effects research agencies.

Possible Research Topics

- Better understanding of the toxicity and accumulation of emerging PFAS and mixtures in the body
- Transformation processes in the body
- Establish priorities for environmental monitoring/remediation based on toxicity and exposure routes

Lab R&D Activities

- ANL has developed the Ecological Screening Values (ESVs) for eight PFAS for surface water and soil for the Air Force and other DOD services. ESVs were developed for ecological receptors with the participation of EPA, Army, Navy, and Air Force ecological risk experts.
- ANL has developed an Artificial Intelligence (AI) workflow using deep learning methods, which has also been developed for PFAS toxicity predictions and tested for 8163 PFAS.

4. Treatment

Background: C-F bonds are highly stable, preventing degradation by microorganisms or conventional oxidation processes. Reduction (e.g. e-beam, plasma) and thermal treatment can lead to C-F bond cleavage with the loss of a fluoride (F^-) but the transformation products or byproducts of these treatments may be just as persistent and toxic. There is a lack of understanding of all the products or how to achieve complete destruction of all C-F bonds in an energy-efficient manner.

Standard water treatment methods such as Granular Activated Carbon (GAC) filters and ion exchange resins work well to remove PFAS, at least for longer-chain (legacy) PFAS. Current evidence suggests that standard methods are less effective against emerging short chain PFAS compounds. Furthermore, there is evidence that conventional biological wastewater treatment can make the PFAS problem worse, by transforming precursors into more harmful PFAS. In-situ treatment is even less understood. Treatment methods are also challenged by lower thresholds creating a “moving the goal post” scenario.

Possible Research Topics

- In-situ treatment methods for soil and groundwater
- Methods to treat water and soil for emerging PFAS and precursors and improved treatment of studied PFAS to achieve lower concentrations
- Address transformation of precursors, byproducts, and products incidental to combustion during treatment
- Methods to mobilize PFAS in the subsurface for accelerated removal
- Seek out energy-efficient and economical approaches for PFAS treatment
- Understand long term effectiveness of blocking PFAS migration with caps (local contamination) or barriers (landfill)

4. Treatment Current Lab R&D Activities

WATER / WASTEWATER

- **BNL** is developing a plasma-based technique to destroy PFAS and related components in water. The main advantage of the plasma-based technique is that the energy requirements are very favorable.
- **Fermilab and BNL**: Research is being conducted on the degradation of PFAS in water via a high power, energy-efficient electron beam accelerator. Results to date have established that an electron beam is effective at breaking down PFAS compounds and work continues on how to best incorporate this technology in water treatment.
- **TJNAF** is collaborating with Hampton Roads Sanitation District (regional wastewater utility company) on electron beam irradiation of PFAS-contaminated water samples. Preliminary results indicate the breakdown of long-chain PFAS compounds in wastewater effluent matrices following electron beam irradiation at a relatively low dose. Further studies are ongoing. Concepts for compact industrial irradiation facilities based on the latest accelerator technology are being developed.
- **ANL** uses an electrochemical oxidation process for destruction of PFAS in wastewater.
- **ANL** is pursuing a design of treatment train to combine multiple ANL technologies including selective adsorbent sponges for PFAS capture, membrane-wafer-assembly electrodeionization for waste-stream reduction by extracting PFAS into concentrated waste stream for destruction, and use of low-temperature atmospheric pressure plasma for > 95% decontamination and destruction of PFAS in an adsorbent medium and surfaces.
- **CRESP** is developing membrane separation approaches to concentrate PFAS from groundwater to make subsequent destruction technologies more efficient by providing a smaller volume and more concentrated feed, and is performing leaching test on cement-encapsulated PFAS.
- **SNL** is investigating advanced oxidation technologies for PFAS destruction
- **SNL** is developing novel low cost PFAS sorbents

4. Treatment Current Lab R&D Activities (continued)

IN-SITU

- **CRESP** researchers are investigating techniques to mobilize PFAS to facilitate more efficient recovery from the vadose zone and groundwater
- **PNNL** is developing and demonstrating Electrical Resistivity Tomography (ERT) methods to quantify the delivery of activated carbon particles to remediate PFAS in underground aquifers.
- **SNL** is testing in-situ permeable reactive barriers to halt the migration of PFAS plumes in the subsurface

SOIL / SOLIDS

- **PNNL** is evaluating soil additives and other tools that can improve the sustainability of thermal decomposition of PFAS compounds while using infrared spectroscopy to monitor, and potentially reduce, the formation of problematic volatile organic fluorine (VOF) gases.
- **ANL** uses low-temperature atmospheric pressure plasma for >95% decontamination and destruction of PFAS in adsorbent medium and surfaces

DISPOSAL

- **CRESP** is testing the efficacy of liners for retaining PFAS when used in landfill disposal containment/leachate systems
- **SNL** has developed high-performance, inexpensive engineered barrier materials for various organic and inorganic contaminants that may be applicable to PFAS disposal (capacity)

5. Replacement

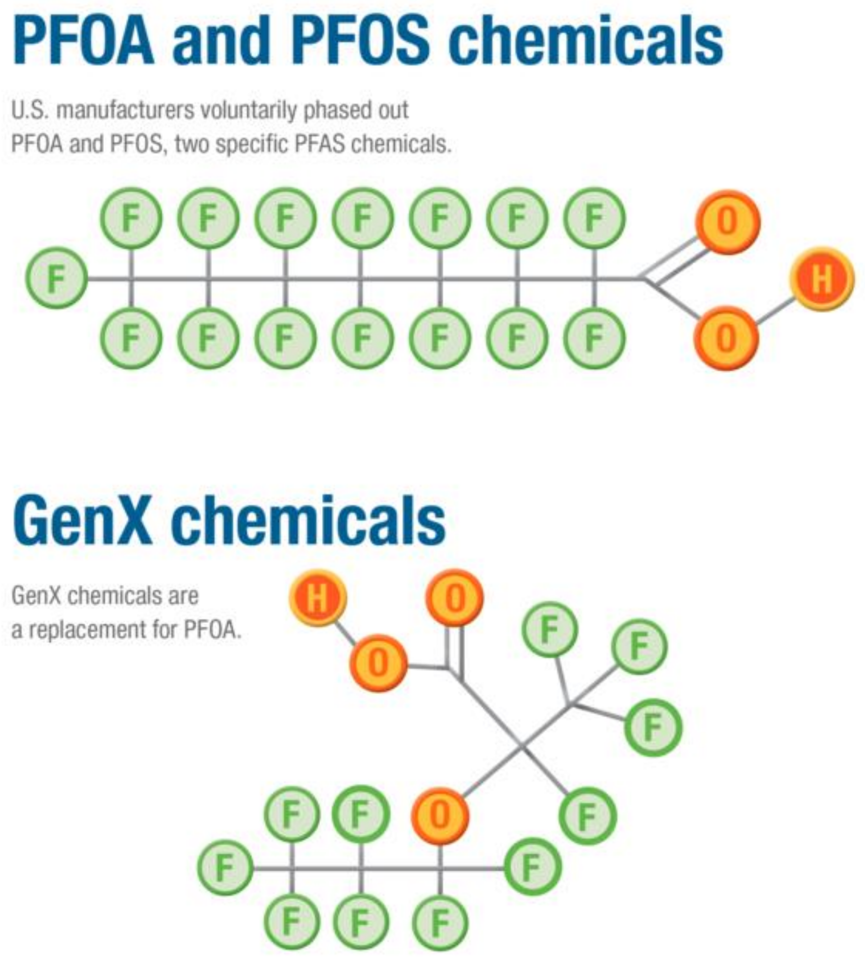
Background: The move to short chain PFAS (butyl, hexyl) has not resolved persistence in the environment and toxicity issues identified with long chain PFAS. Short chain "GenX" PFAS may also be harder to remove (e.g. with GAC) and easier to take-up into plants. These newer chemicals are found in many commercial products (e.g. food packaging and stain-resistant carpets and textiles). There is an imperative to 'turn off the tap' for all but essential uses. A third generation of materials that offer the same characteristics as PFAS and could be considered less toxic (e.g. resistant to protein-binding), more treatable, easier to detect, or naturally decaying is needed.

Possible Research Topics

- Revisit fundamental molecular-level design rules for ease of capture/destruction, lack of bio-accumulation/toxicity and transformation to support alternative chemicals
- Evaluate uses and releases of PFAS in DOE missions, including plastic bonded explosives (PBX) research and production, fuel cells research and production, and materials science research

Current Lab R&D Activities

- None



Examples of legacy (long-chain) and emerging (GenX) PFAS, the latter of which may be just has persistent, harmful and harder to capture

Image credit: https://yourscvwater.com/pfas/

Additional Lab R&D Capacity

The **Office of Science** (SC) provides foundational knowledge and state-of-the-art capabilities in support of DOE's mission with a focus on innovation. SC's Office of Basic Energy Sciences (BES) stewards capabilities that can be used to provide foundational knowledge for design of new approaches for PFAS capture and conversion, though BES does not support research specifically focused on PFAS. Capabilities in experimental and computational chemical sciences relevant to PFAS research include research programs in separation science, with a focus on understanding the molecular mechanisms of selective separation processes, and catalysis science, with a focus on mechanistic understanding of catalytic transformations that produce targeted products.

The **Office of Environmental Management** supports independent technical assessments and analysis involving environmental remediation through the Network of National Laboratories for Environmental Management and Stewardship.

Summary of R&D Possible Research Topics

R&D Area	R&D Need
Characterization and Detection	• Improved methods to identify unknown PFAS • In-situ detection for broad range of PFAS in various media (water, air, soil, dust, biota, food etc) • Lower detection limits to keep pace with evolving thresholds
Fate and Transport	• Understand basic subsurface transport characteristics of AFFF at DOE sites (specifically PFAS comingled with radionuclides) • Identify precursors with the ability to transform to PFAS in the environment (in soil, water and atmosphere) • Understand impacts PFAS have on soil wettability (i.e., hydrophobicity)
Exposure and Toxicity	• Better understanding of the toxicity and accumulation of emerging PFAS and mixtures in the body • Transformation processes in the body • Establish priorities for environmental monitoring/remediation based on toxicity and exposure routes
Treatment	• In situ treatment methods for soil and groundwater • Methods to treat water and soil for emerging PFAS and precursors and improved treatment of studied PFAS to achieve lower concentrations • Address transformation of precursors, byproducts, and products incidental to combustion during treatment • Methods to mobilize PFAS in the subsurface for accelerated removal • Seek out energy-efficient and economical approaches for PFAS treatment • Understand long term effectiveness of blocking PFAS migration with caps (local contamination) or barriers (landfill)
Replacement	• Revisit fundamental molecular-level design rules for ease of capture/destruction, lack of bio-accumulation/toxicity and transformation to support alternative chemicals • Evaluate uses and releases of PFAS in DOE missions, including plastic bonded explosives (PBX) research and production, fuel cells research and production, and materials science research

Summary and Next Steps

- **This is an initial Plan that**:
  1) Identifies five PFAS R&D areas
  2) Provides an inventory of the current ongoing PFAS R&D efforts across the DOE enterprise
  3) Identifies potential gap areas (research needs)
- **The initial plan was shared with the DOE PFAS Coordination Council members as well as the PFAS InterAgency working group to validate the R&D areas and the R&D gaps**.
- **The next iteration of this plan will be to**:
  1) Distribute a survey to DOE field offices and other federal research networks seeking information on research gap areas
  2) Conduct a workshop to assemble the DOE R&D community and members from EPA and DOD to develop the R&D priorities (As described on the next slide and the Notional framework for the workshop provided as attachment #1)
  2) Develop the prioritized R&D plan
  3) Create a DOE PFAS R&D community of practice
  4) Facilitate collaborative opportunities between DOE Labs and external organizations (Federal and non-Federal)
  5) Examine opportunities for DOE facilities to address their own current PFAS challenges through R&D capabilities/possibilities

Phase 1: Conduct a Survey of PFAS R&D Needs

The Purpose of the Survey will be to:

- Understand PFAS research needs at DOE field offices
- Identify non-DOE labs for collaboration efforts on existing and future research
- Use the information from the survey to inform the R&D Workshop (Phase-II)

The conceptual framework for the workshop is found in Attachment A to this plan

Phase 2: Conduct a DOE PFAS R&D Workshop

The Purpose of the workshop will be to:

- Bring the National Laboratory community together
- Invite select federal & non-Federal PFAS R&D organizations
- Identify potential areas where Laboratory capabilities can fill some of the identified gap areas
- Identify collaboration opportunities with other Federal Agencies and non-Federal entities also performing PFAS R&D
- Use the information from the workshop to establish DOE’s PFAS research priorities
- Use the information to help address some of the immediate PFAS challenges at DOE sites.
- Facilitate initiation of small R&D efforts where funding is currently available

The conceptual framework for the workshop is found in Attachment A to this plan

Some Useful Resources

Active Government-Funded PFAS Research Topics

NIH NIEHS

https://www.niehs.nih.gov/research/supported/exposure/pfas/researchers/index.cfm

EPA

https://www.epa.gov/chemical-research/research-and-polyfluoroalkyl-substances-pfas

SERDP DOD • EPA • DOE | ESTCP

https://www.serdp-estcp.org/Featured-Initiatives/Per-and-Polyfluoroalkyl-Substances-PFASs

General PFAS information

PFAS CENTRAL
A PROJECT OF GREEN SCIENCE POLICY

https://pfascentral.org/

PFAS-TOX DATABASE

https://pfastoxdatabase.org/

Attachment A

Conceptual Framework for the DOE PFAS R&D Workshop

Purpose of Proposed PFAS Workshop: Foundation for the PFAS Research Plan

Write a workshop report to set out DOE Priority Research Topics to guide future DOE R&D efforts across DOE National Laboratories and affiliates.

The Report should:

- Validate, modify and append (if appropriate) the identified PFAS “Possible Research Topics” identified in this initial plan
- Inform and close knowledge gaps by inclusion of experts from DOE, National Laboratories, Federal Agencies (i.e. EPA, DoD) and industry collaborators
- Develop a more complete understanding of DOE National Laboratory capabilities and current activities.
- Develop R&D priorities for DOE, informed by:
  - General knowledge gap priorities
  - DOE-specific risks and challenges for PFAS contamination or use
  - Topics where other Federal or State agencies have expertise/jurisdiction
  - Topics where DOE National Laboratories provide capabilities or can collaborate

Participants in Proposed PFAS Workshop

- DOE Stakeholders, Subject Matter Experts, PFAS Coordinating Committee (PCC)
- DOE National Laboratory representatives, especially for National Laboratories with current PFAS remediation or R&D activities
- Subject Matter Experts (e.g. as speakers) from EPA, DoD, other Federal agencies or partner institutions (e.g., universities)

Structure of Proposed hybrid PFAS Workshop

1.5 days (+ 1/2 day for chairs and report writers)

- Day 1 morning
  - General PFAS research needs and national priorities
  - Current PFAS activities across the federal government
  - PFAS challenges in the DOE complex (results from PFAS R&D survey)
- Day 1 afternoon
  - Current National Lab activities
  - National Lab capabilities relevant to PFAS research
  - Breakout session 1: Characterization/Detection, Fate/Transport, Exposure/Toxicity, Treatment, Replacement
  - Discussion: Seek overlap between PFAS research gaps, NL capabilities, DOE complex needs while reducing overlap with other federal agencies. Decide on DOE priority research areas
- Day 1 evening
  - Chairs gather to discuss DOE priority areas and assign groups for next breakout session
- Day 2 morning
  - Introduce the identified DOE priority areas
  - Breakout session 2: DOE priority areas (~4-6 identified)
  - Discussion: Decide on plan for each priority area
- Day 2 afternoon
  - Chairs, writers etc.. assign tasks for report