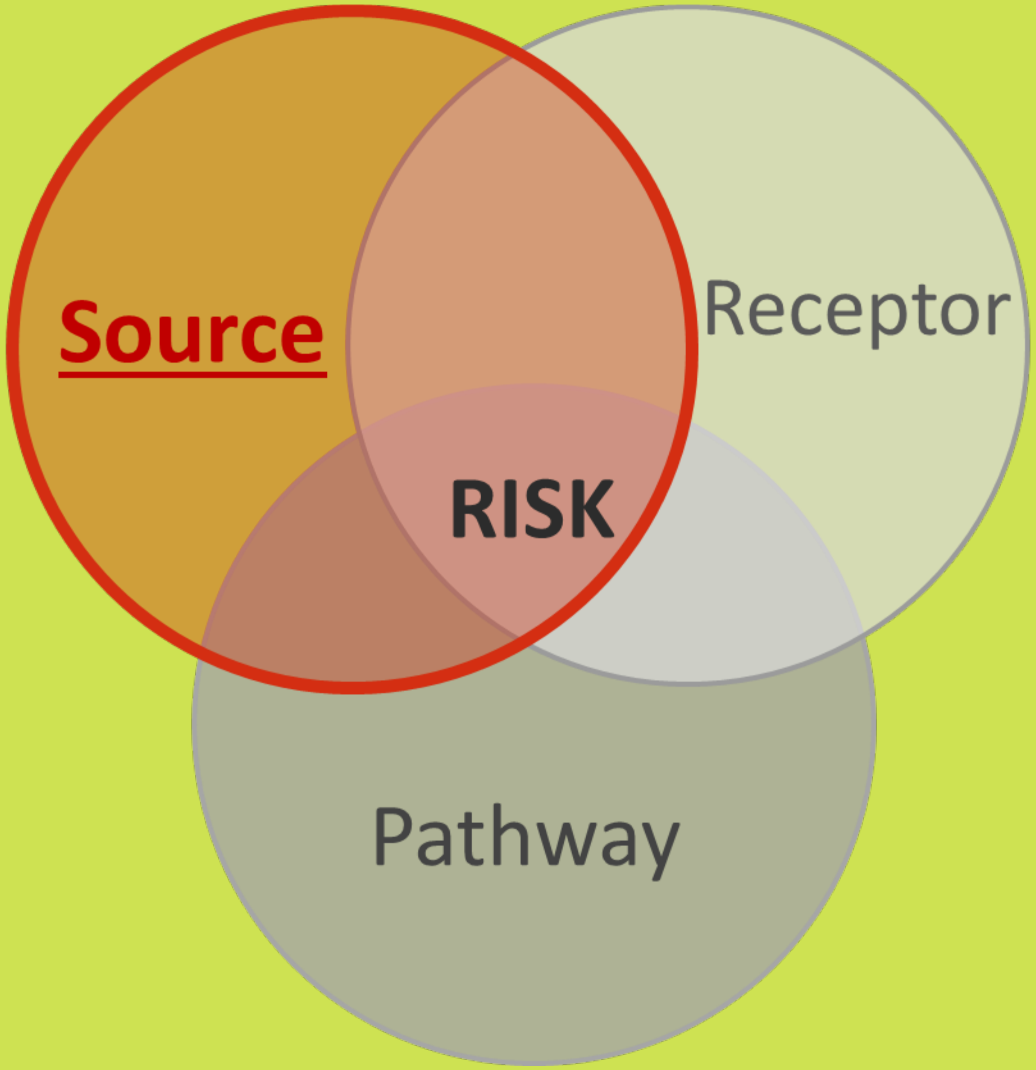
DEVELOPMENT OF A USER FRIENDLY FRAMEWORK FOR GEOSPATIAL IDENTIFICATION OF POTENTIAL PFAS SOURCE ZONES

Jennifer Guelfo, PhD

June 12, 2017



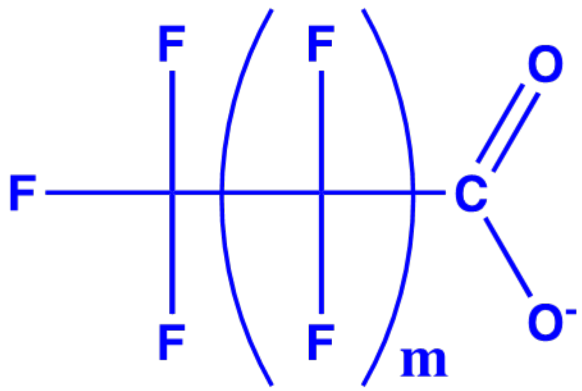
BROWN

PRESENTATION OVERVIEW

PFAS Overview	PFAS in U.S. Drinking H_2O	Source Zone Evaluation
• Terminology/chemistry • Uses/regulation	• UCMR3 data • Knowledge gaps	• Key PFAS sources • Geospatial eval. framework

PFAS OVERVIEW: TERMINOLOGY & STRUCTURE

Perfluoroalkyl carboxylates:



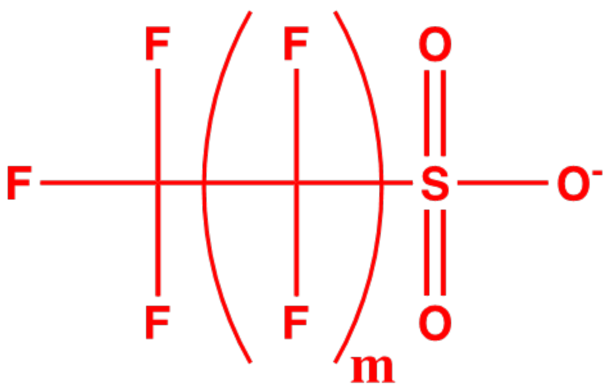
Examples:

m=2 PFBA

m=4 PFHxA

m=6 PFOA

Perfluoroalkane sulfonates:



Examples:

m=3 PFBS

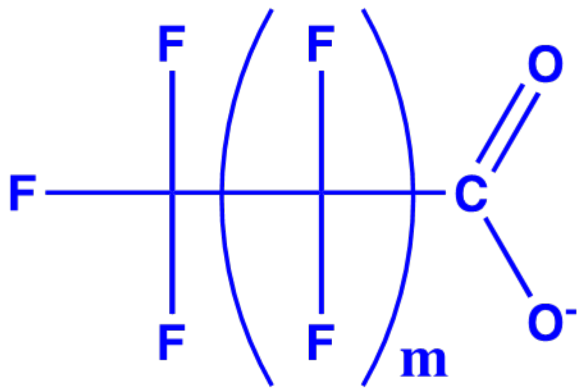
m=5 PFHxS

m=7 PFOS

Per = fully fluorinated alkyl tail.

PFAS OVERVIEW: TERMINOLOGY & STRUCTURE

Perfluoroalkyl carboxylates:



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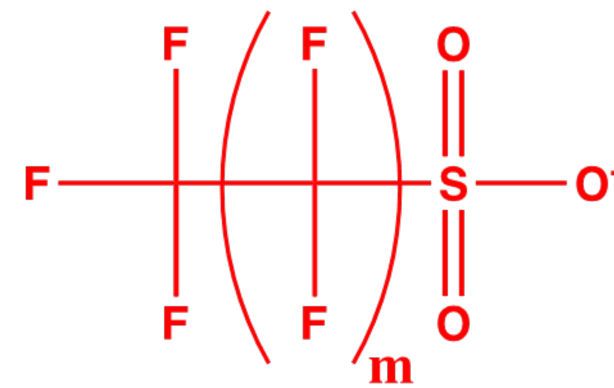
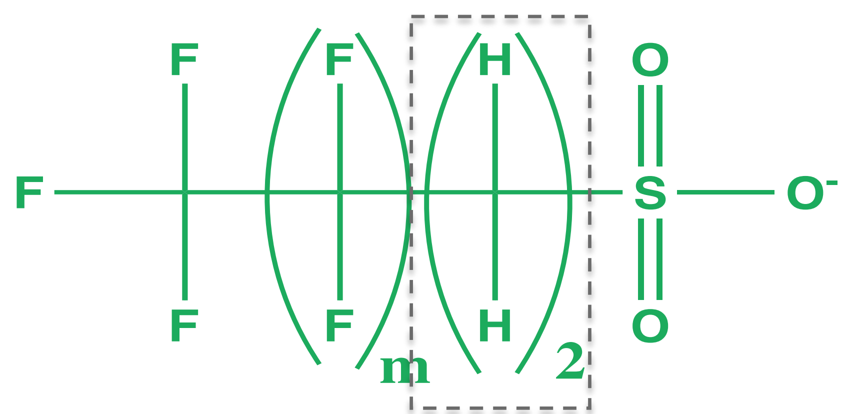


Examples:
m=3 PFBS
m=5 PFHxS
m=7 PFOS

Poly = partially fluorinated alkyl tail.

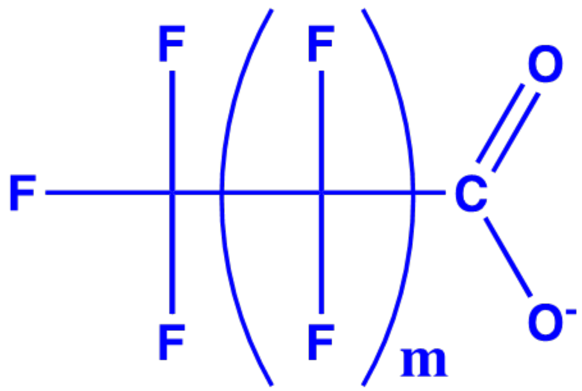
Polyfluoroalkyl substances:



m=5 6:2 FtS
m=7 8:2 FtS

PFAS OVERVIEW: TERMINOLOGY & STRUCTURE

Perfluoroalkyl carboxylates:



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m=2 PFBA
m=4 PFHxA
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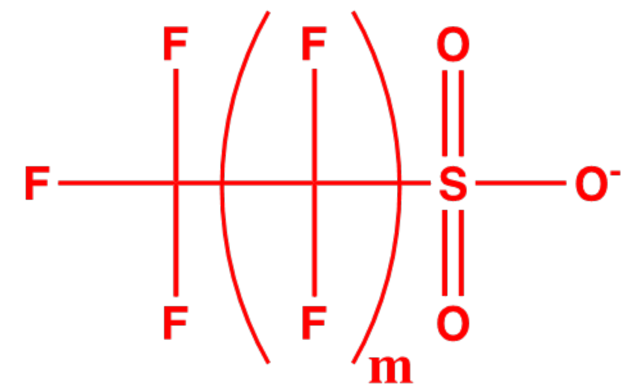
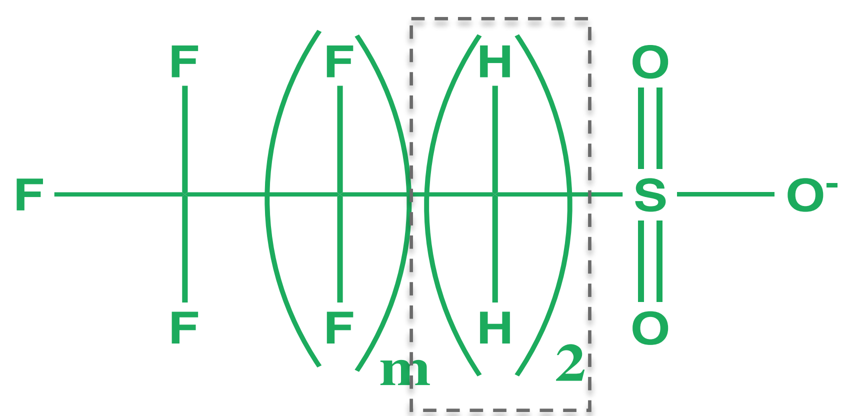


Examples:
m=3 PFBS
m=5 PFHxS
m=7 PFOS

Per + Poly =

<u>Per</u> & <u>poly</u>fluoro alkyl substances (PFAS)

Polyfluoroalkyl substances:



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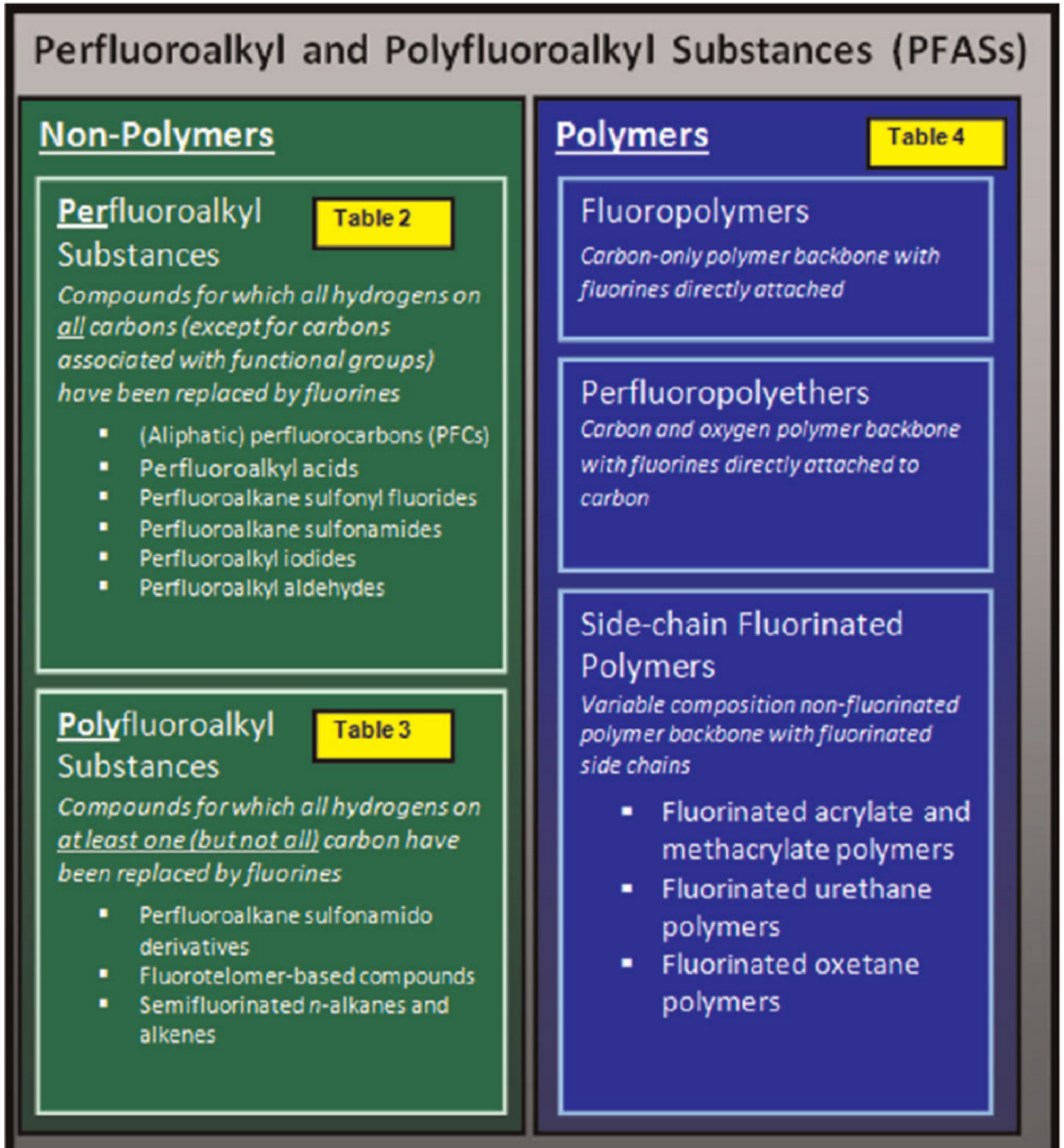

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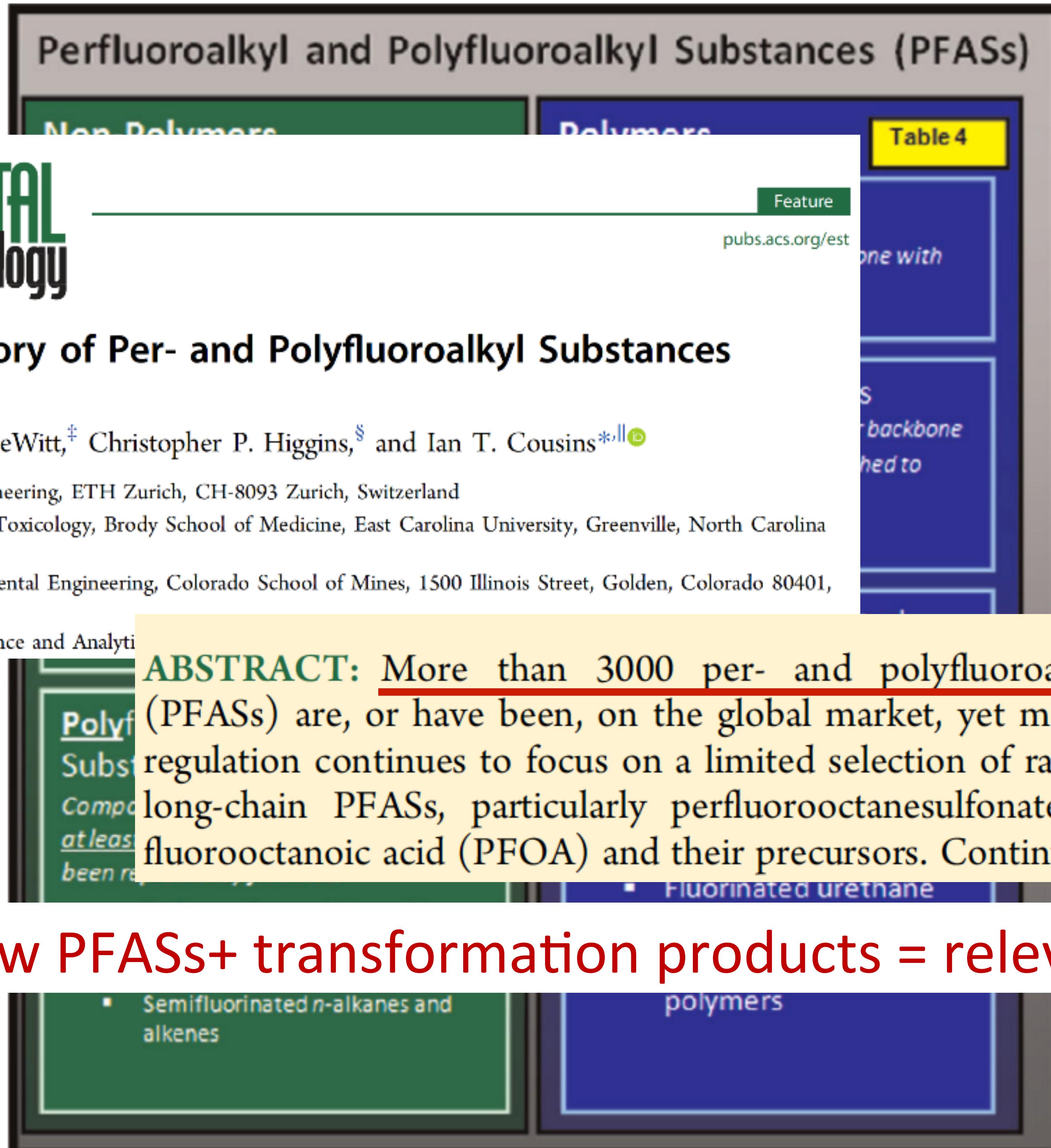

Environmental Science & Technology
Feature
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A Never-Ending Story of Per- and Polyfluoroalkyl Substances (PFASs)?

Zhanyun Wang,[†] Jamie C. DeWitt,[‡] Christopher P. Higgins,[§] and Ian T. Cousins*,[∥]

[†]Institute for Chemical and Bioengineering, ETH Zurich, CH-8093 Zurich, Switzerland
[‡]Department of Pharmacology and Toxicology, Brody School of Medicine, East Carolina University, Greenville, North Carolina 27834, United States
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[∥]Department of Environmental Science and Analyti

ABSTRACT: More than 3000 per- and polyfluoroalkyl substances (PFASs) are, or have been, on the global market, yet most research and regulation continues to focus on a limited selection of rather well-known long-chain PFASs, particularly perfluorooctanesulfonate (PFOS), perfluorooctanoic acid (PFOA) and their precursors. Continuing to overlook

3000 + new PFASs+ transformation products = relevant PFASs

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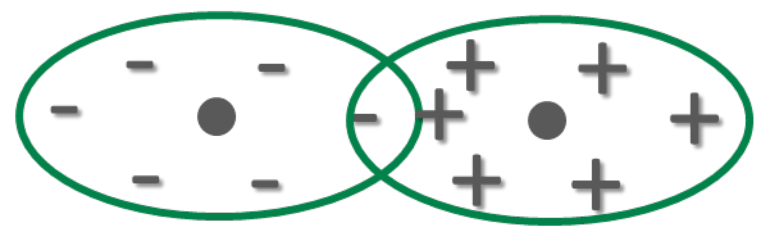
PFAS OVERVIEW: CHEMISTRY & USES

$$\overset{\delta^+}{C} - \overset{\delta^-}{F}$$

Electronegativity = strong, polar covalent bond

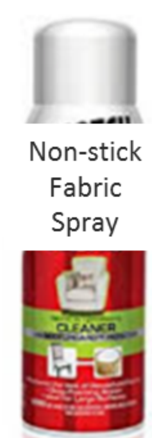


Not polarizable = weak intermolecular interactions

Small size of fluorine = F shields C

Resulting PFAS properties:

- Strong acidity (low pK_a)
- Thermal stability
- Chemical stability
- Hydrophobic & lipophobic
- Surfactant



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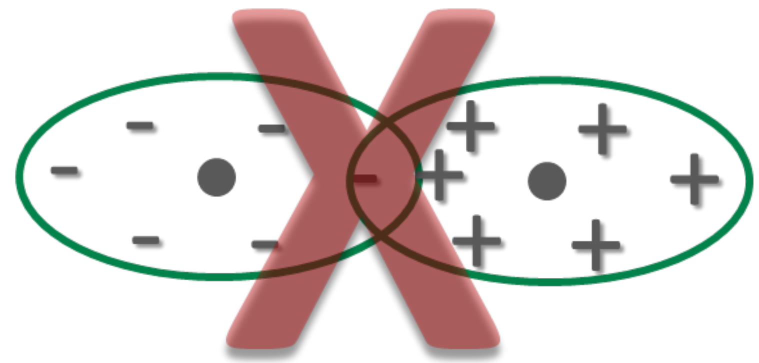
Banks, Ronald Eric, Bruce E. Smart, and J. C. Tatlow, eds. *Organofluorine chemistry: principles and commercial applications*. Springer Science & Business Media, 2013.

PFAS OVERVIEW: CHEMISTRY & USES

$$\underset{\delta^{+}}{C} - \underset{\delta^{-}}{F}$$

Electronegativity = strong, polar covalent bond



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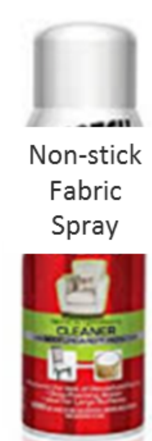

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PFAS OVERVIEW: REGULATION

Drinking Water Health Advisories for PFOA, PFOS

70 ng/L: individually or in combination

$$\frac{\text{RfD} * \text{Body Wt.}}{\text{DW ingestion}} * \text{Relative Source Contribution} = \text{Water Quality Standard}$$

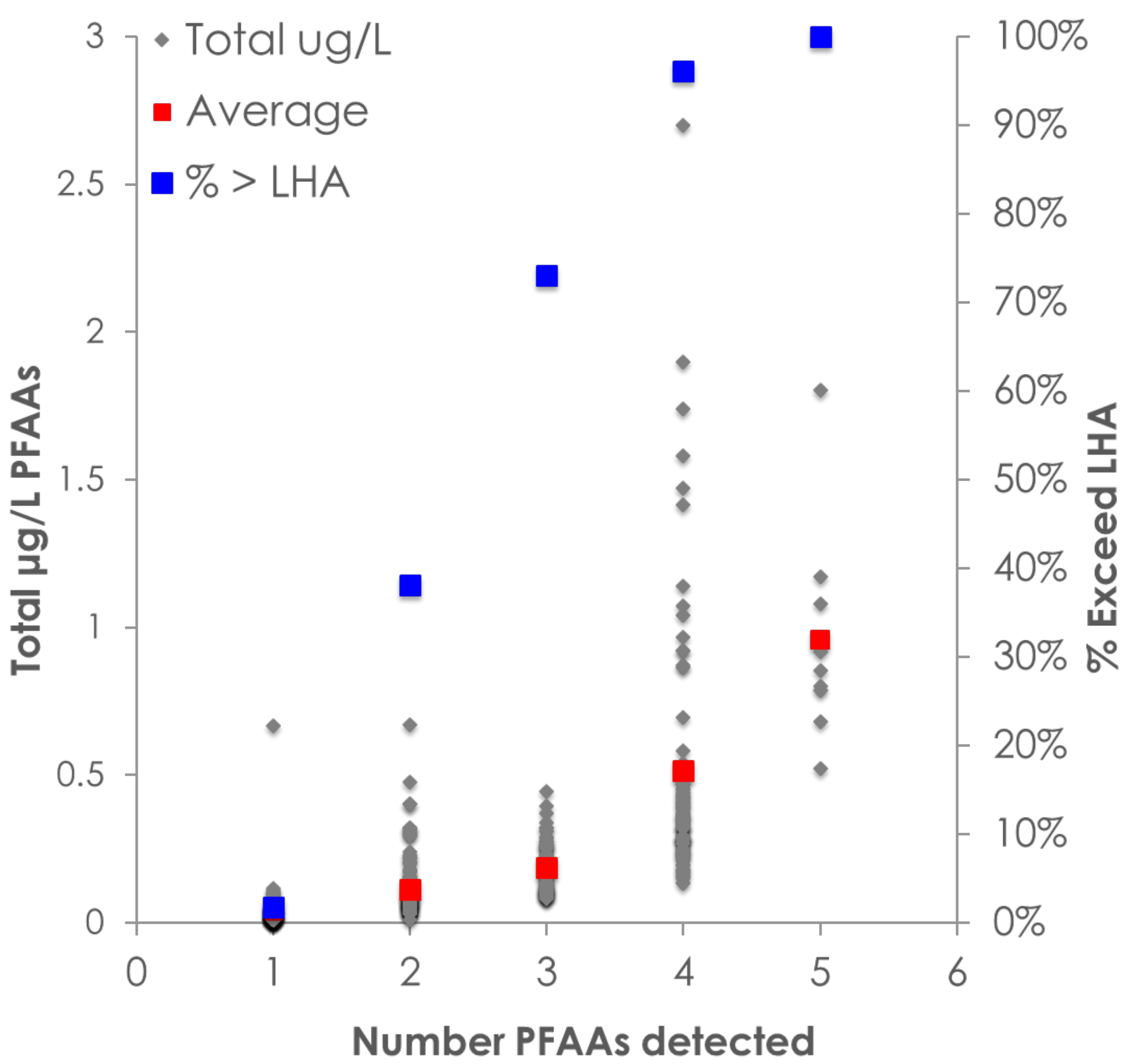
Advisory or standard	**Source**
70 ng/L ∑ PFOA, PFOS	USEPA LHA
20 ng/L ∑ PFOA, PFOS	Vermont
14 ng/L PFOA, 10 ng/L PFNA	New Jersey

Information courtesy of Dr. David Klein

Why the differences?

- VT: same RfD as EPA, different DW ingestion
- NJ: different RfD based different endpoint- liver weight vs. developmental delay.

PFAS IN THE U.S.: UCMR3 DATA



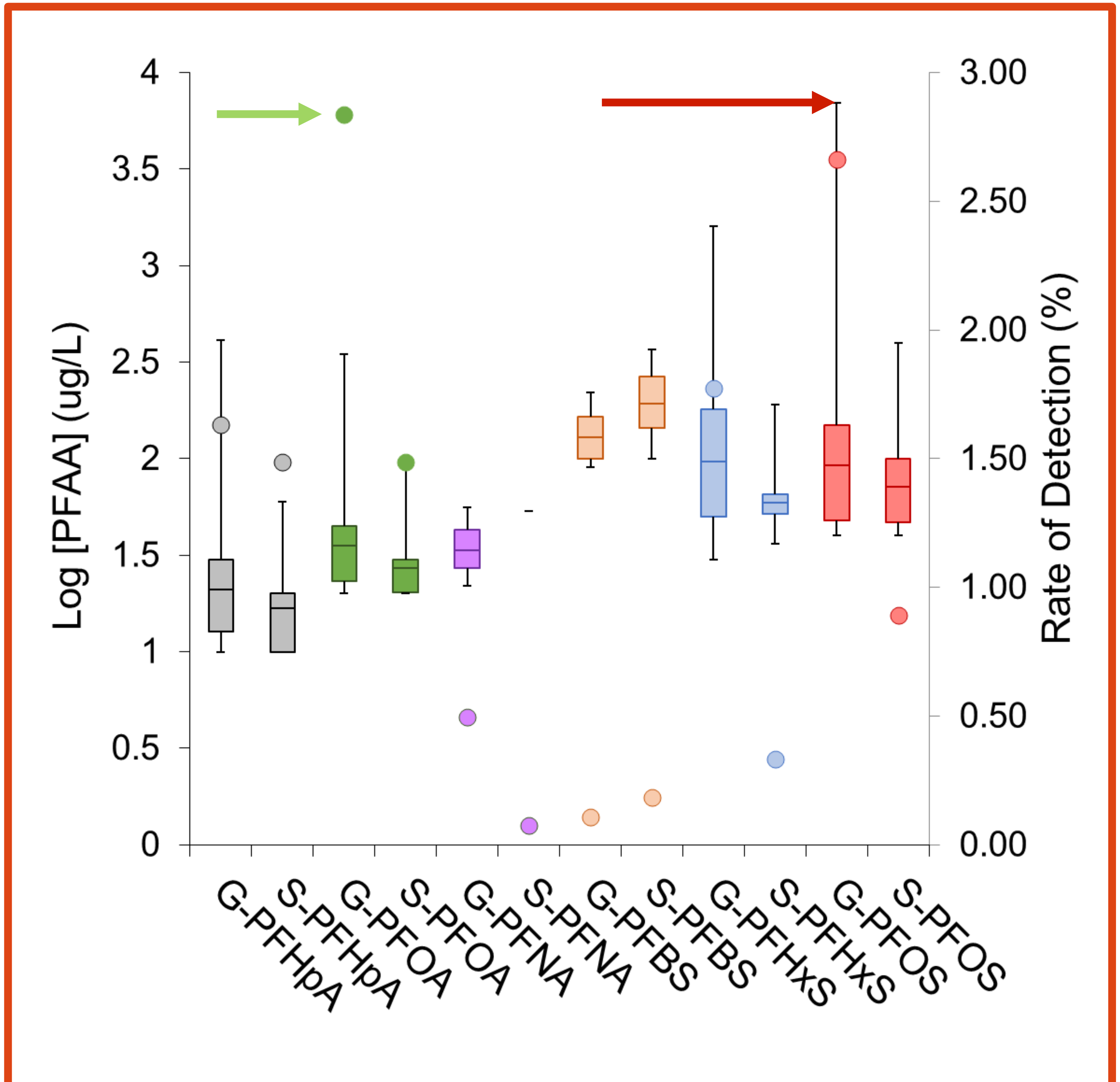
Data reflect only samples with PFAA detections

EPA UCMR Data 2013-2015:

- 4120 Systems > 10,000
- 800 systems ≤ 10,000
- No private systems
- Multiple PFAAs/sample
- 4% detection rate (~200); which are 'impacted'?
  - 64 systems > LHA
  - 122 systems > NJ (but MRL=20 ng/L)
  - 151 systems > VT

Hu, Xindi C., et al. "Detection of poly-and perfluoroalkyl substances (PFASs) in US drinking water linked to industrial sites, military fire training areas, and wastewater treatment plants." *Environmental science & technology letters* 3.10 (2016): 344-350.

PFAS IN THE U.S.: UCMR3 DATA



G = groundwater

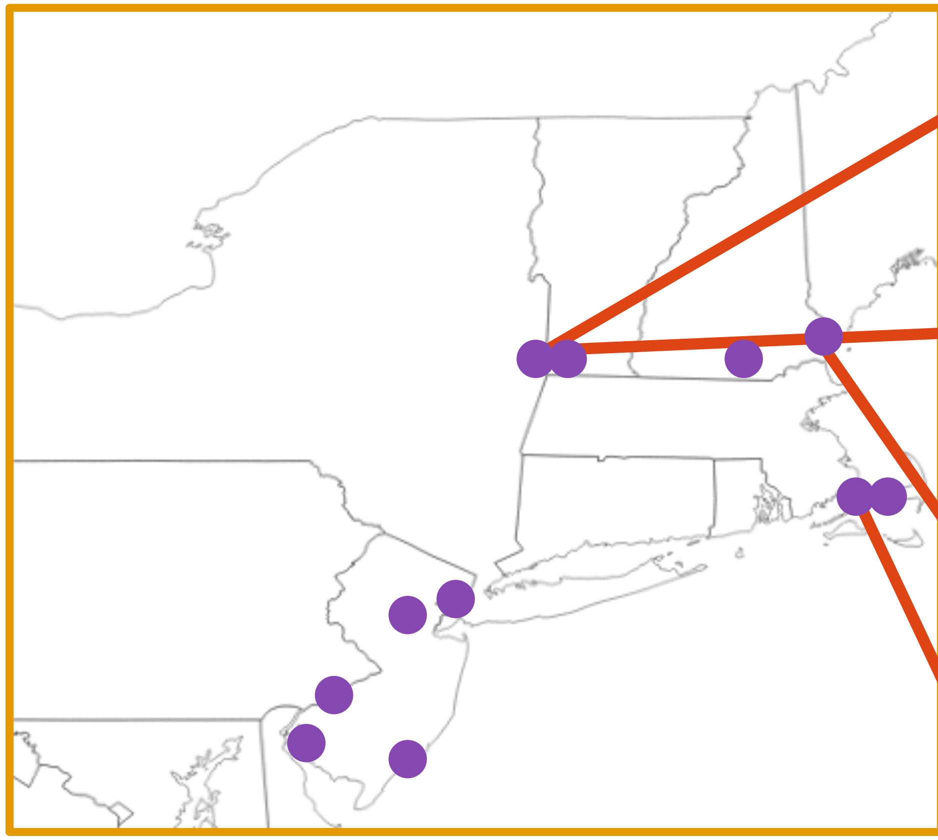
S = Surface water

O = Detection rate (right axis)

EPA UCMR Data 2013-2015:

- [PFAAs] 10-7000 ng/L
- [PFOS] = max overall
- PFOA most frequent detect
- Groundwater in ~80% of detects
- 2818 GW/GU systems, 2691 SW systems
- Average GW $[PFAA]_{tot}$ > SW $[PFAA]_{tot}$
- Overall: GW % detect > SW % detect

PFAS IN THE U.S.: UCMR3 DATA



Water Pollution in Hoosick Falls Prompts Action by New York State

By JESSE McKINLEY and VIVIAN YEE JAN. 27, 2016

Tainted-Water Worries Spread to Vermont Village

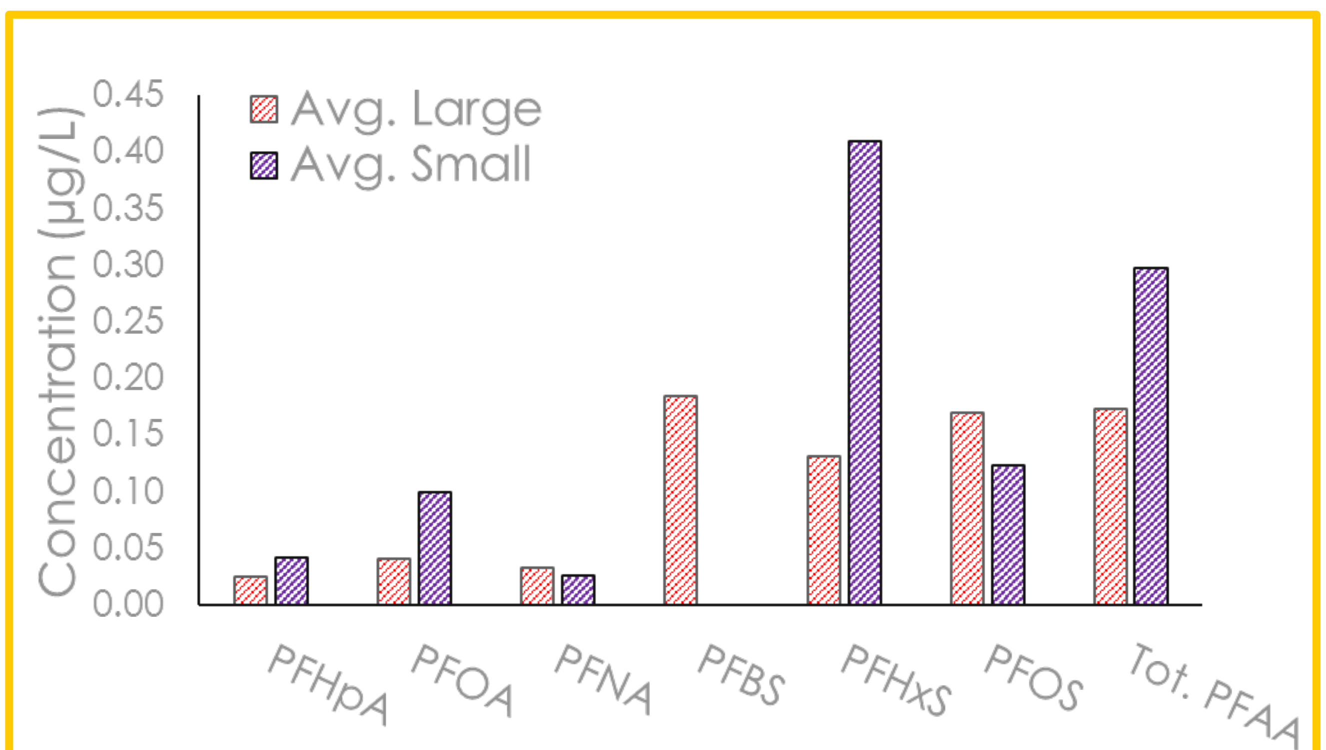
By VIVIAN YEE MARCH 14, 2016

Water Contamination in N.H. Addressing PFOA

By THE EXCHANGE • MAY 31, 2016

GLOBE MAGAZINE

Cape Cod's big drinking water problem



Is UCMR representative?

- No UCMR detects in VT, including Bennington, Pownal but impacts present
- Impacts present in areas not sampled (e.g. Hoosick Falls, NY)
- 0.5% of small systems in U.S. sampled (Hu, 2016)
- $[PFAA]_S > [PFAA]_L$ <u>but</u> S = small sample size

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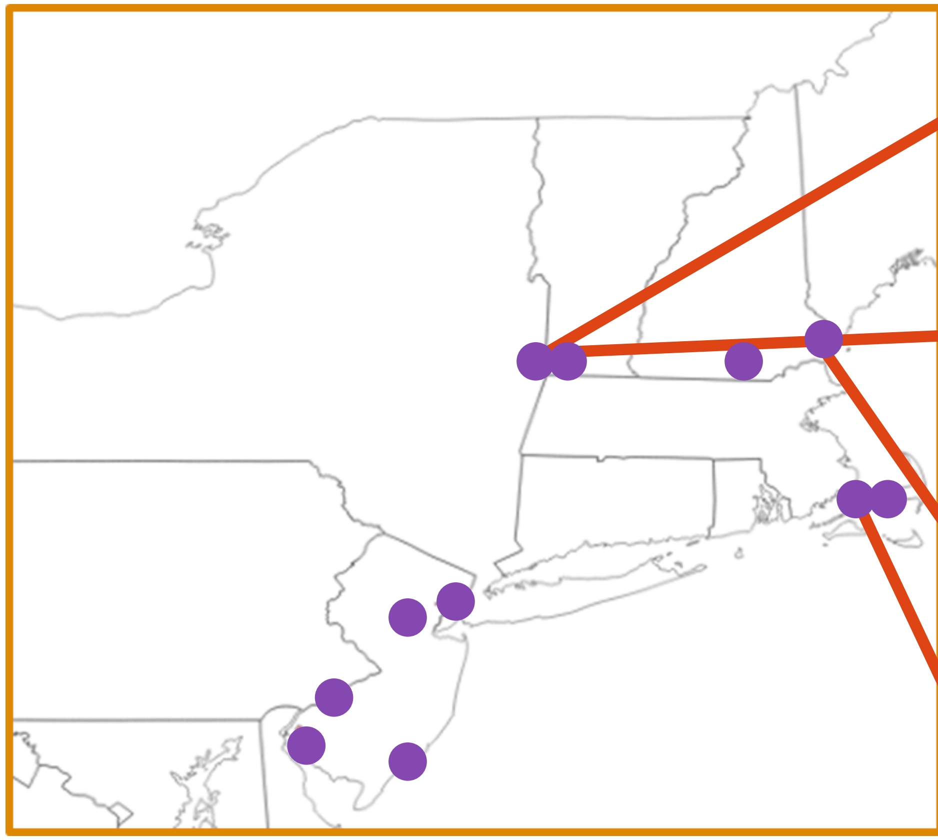

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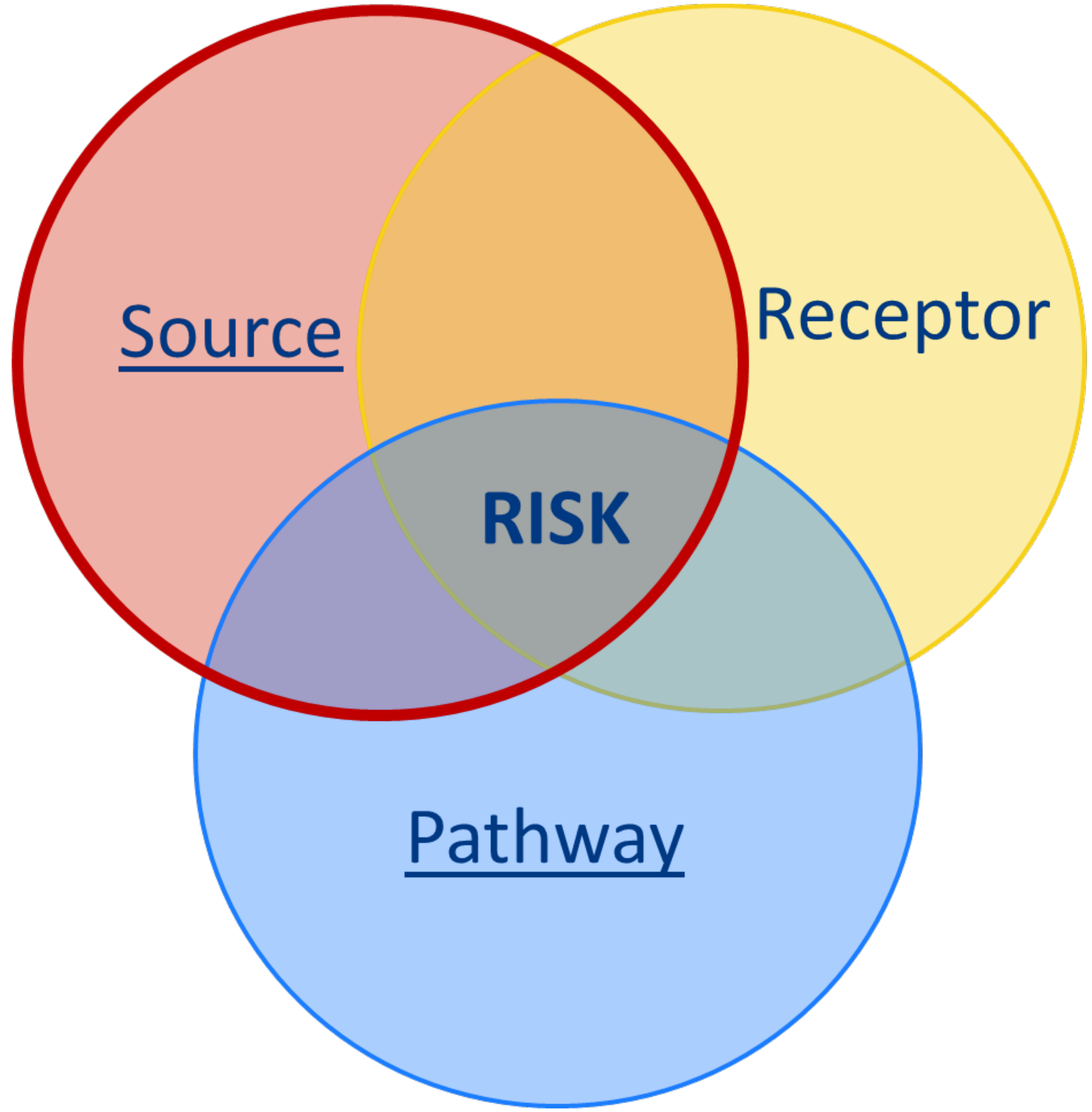
Data warrant targeted screening of community, private groundwater wells; need efficient, effective design of well screening programs.

PFAS IN THE U.S.: KEY CHALLENGES

Finding sources:

- Numerous uses/applications = numerous potential sources
- Low target concentrations = small releases, indirect sources relevant
- Unconsolidated or missing information on current, historical sources

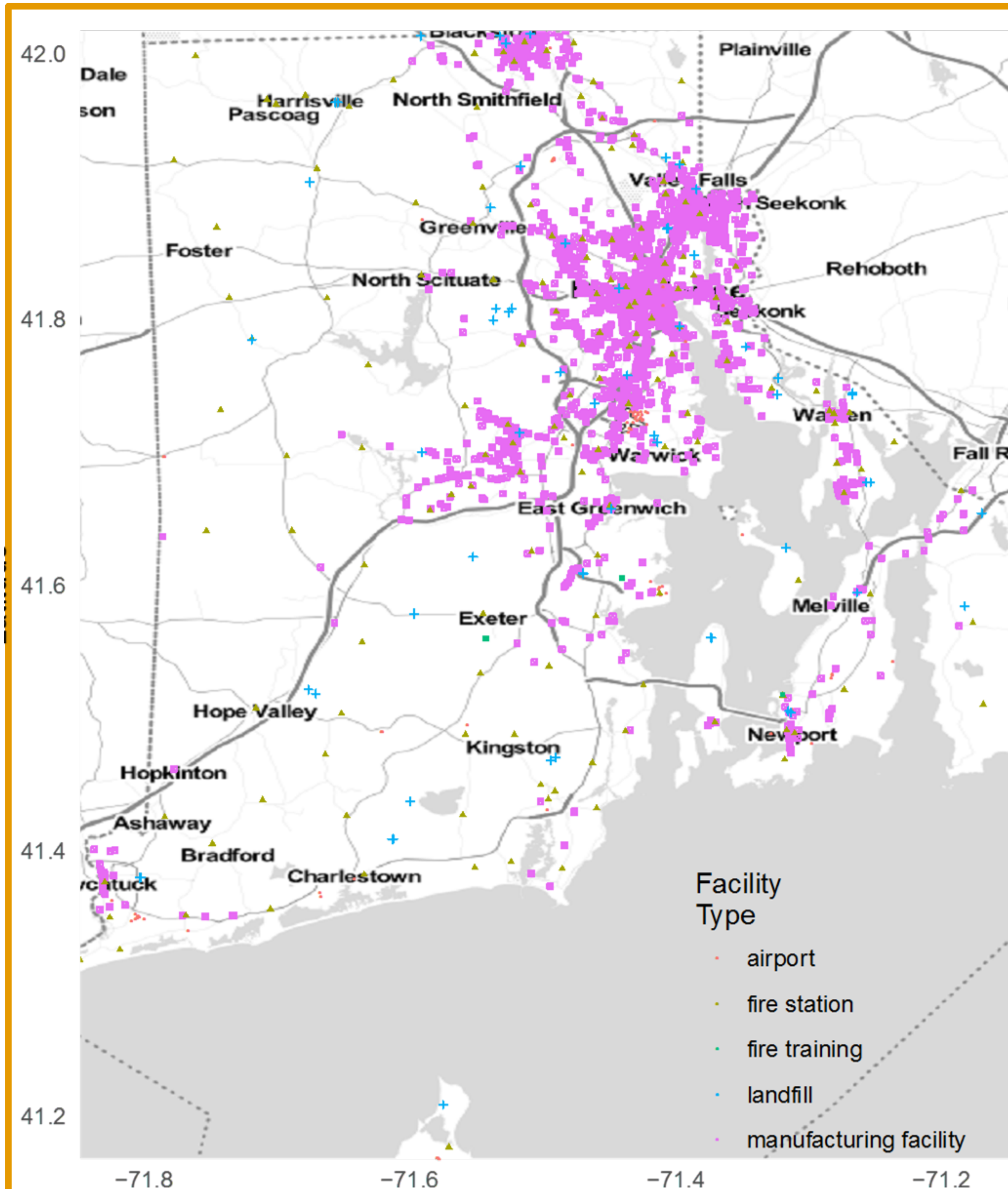


May cause: inefficient sampling plans, failure to ID all relevant sources, inability to determine source, increased time required to reduce risks to human health, environment

PFAS SOURCE ZONES: GEOSPATIAL FRAMEWORK

Data Sources:

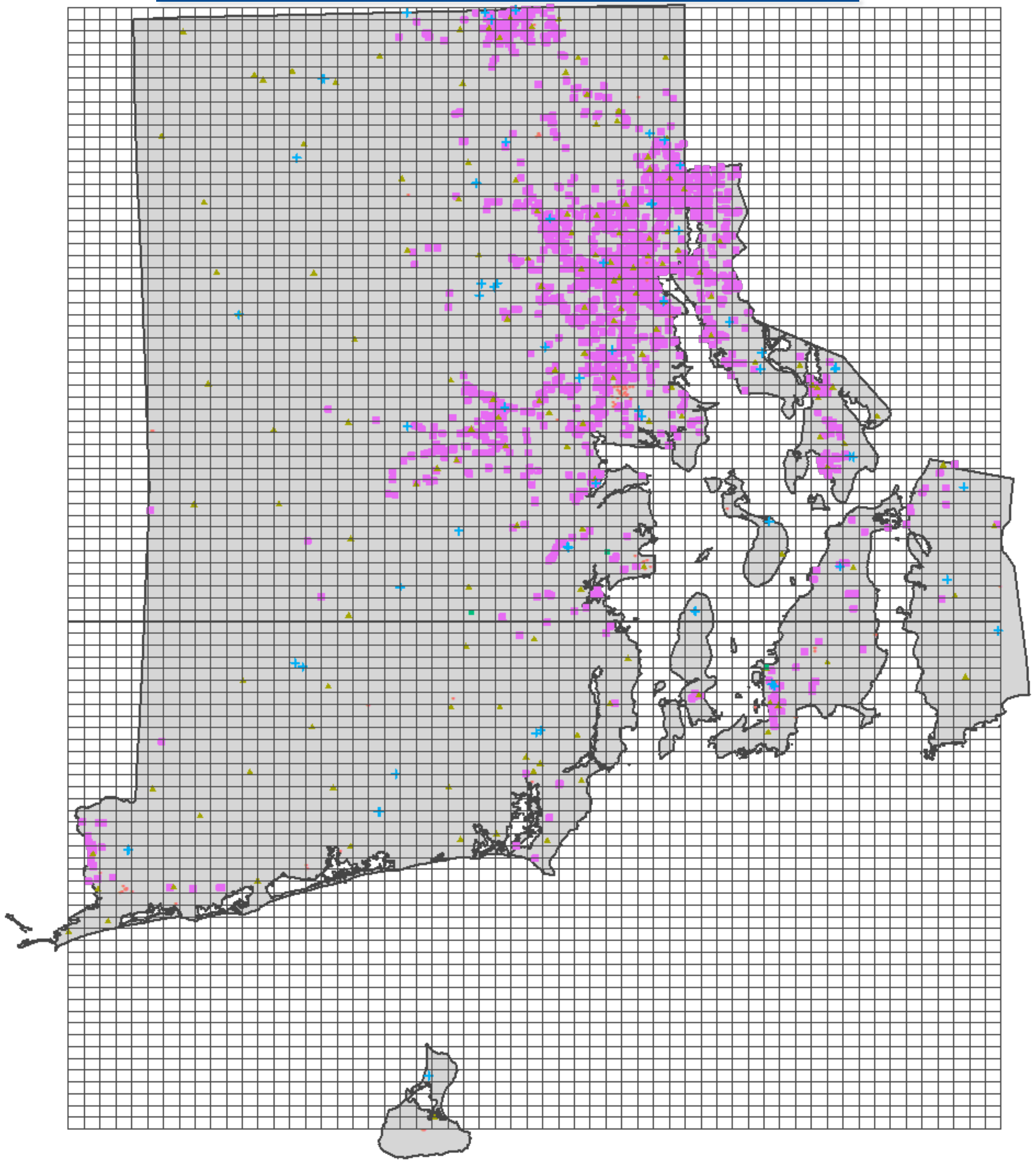
- Landfills
- Fire stations
- Fire Training Areas
- Airports
- Manufacturing facilities 1960-2012
    - Identified industrial codes known to use or produce PFAS



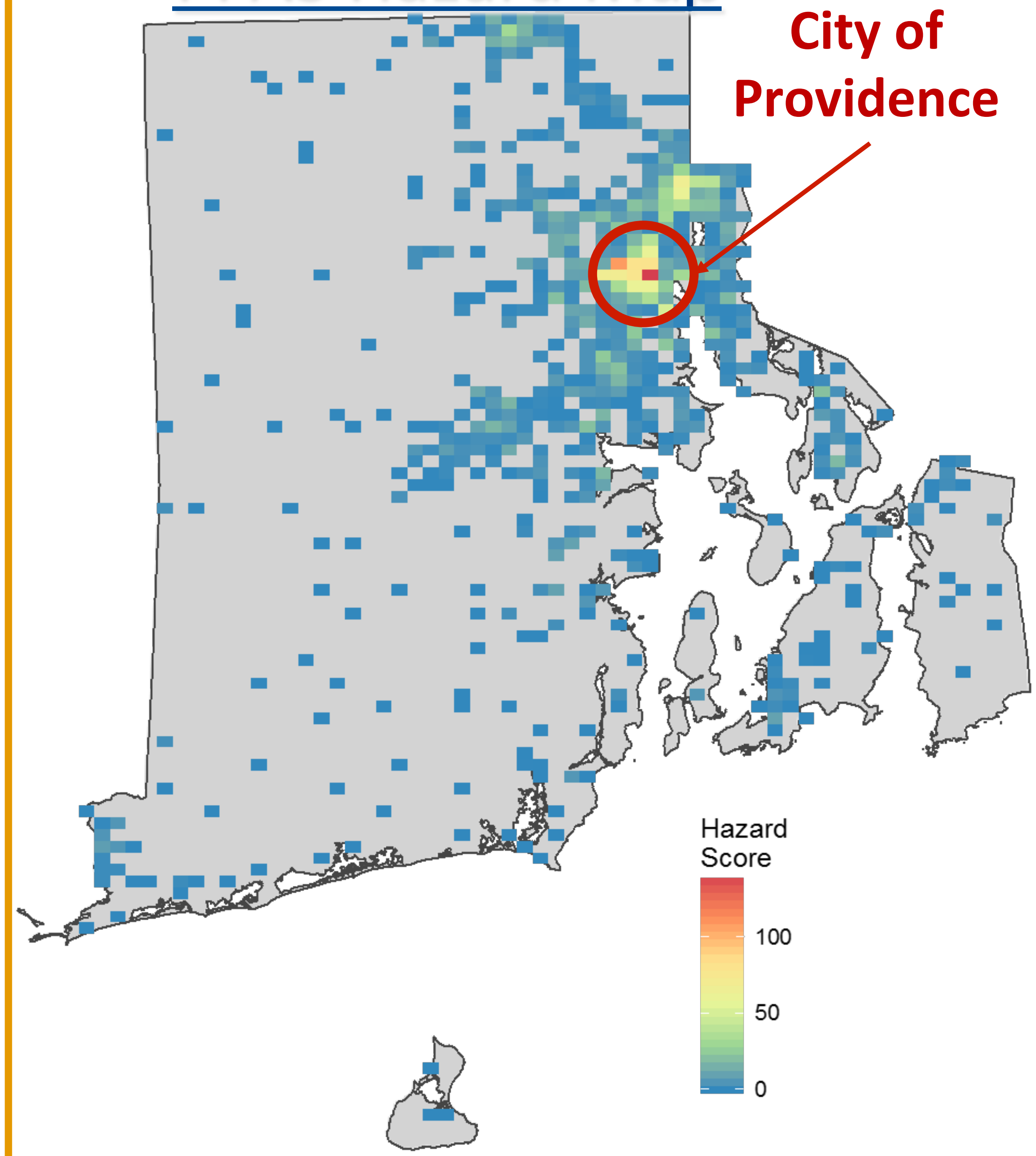
Hazard = (Release Prob.) * (Years of Operation)

PFAS SOURCE ZONES: GEOSPATIAL FRAMEWORK

Raster Grid and Points

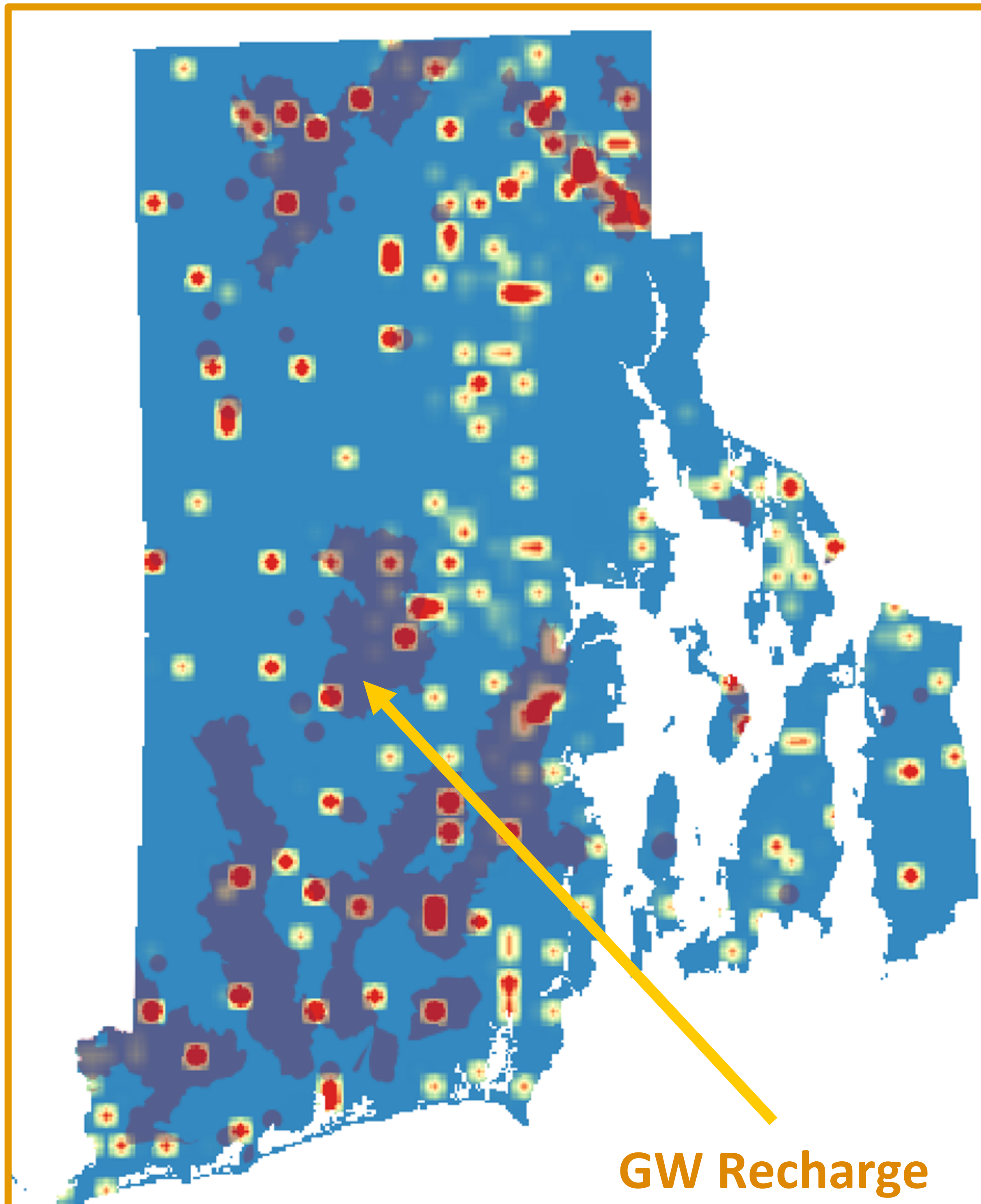


PFAS Hazard Map



How do hazards compare to groundwater vulnerability?

PFAS SOURCE ZONES: GEOSPATIAL FRAMEWORK



Vulnerability based on proximity to:

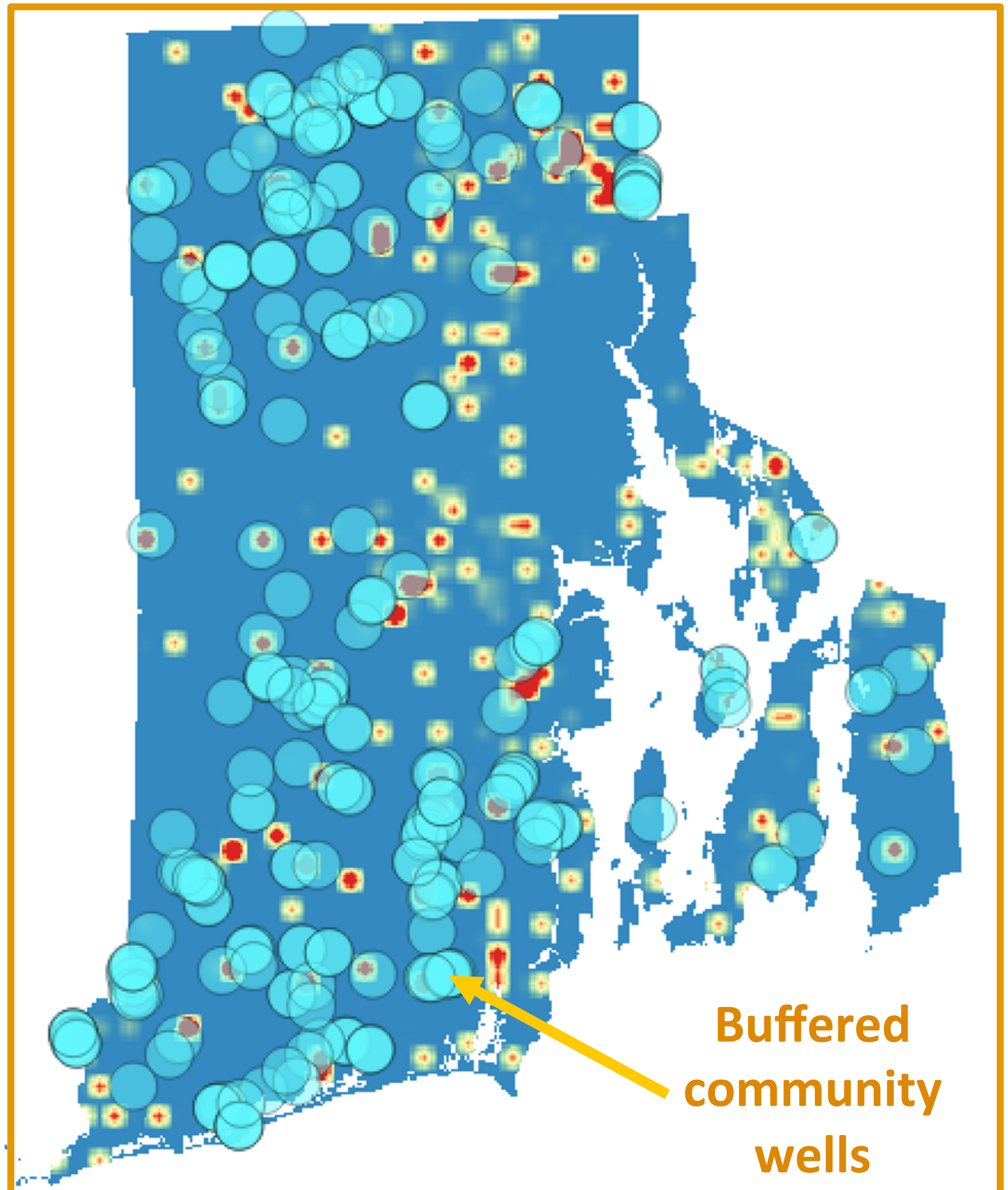
- Drinking water aquifers
- Wellhead protection areas

Hazard vs. Risk:

- ↑ Hazard in pop. centers but…
- GW not classified for drinking
- ↑ Risk in rural areas for small, community scale systems

Risk = Hazard * Vulnerability

PFAS SOURCE ZONES: GEOSPATIAL FRAMEWORK

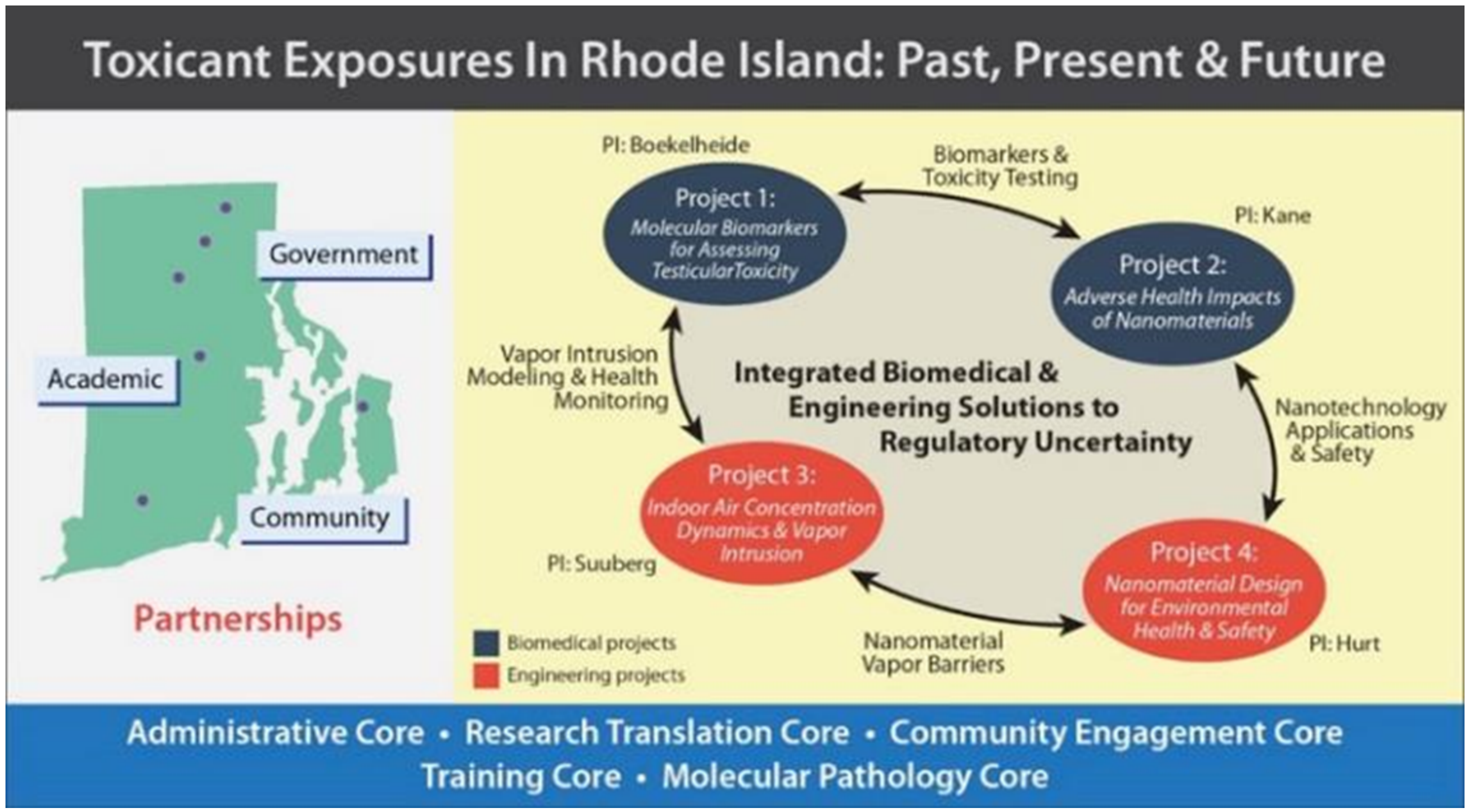


Geospatial future work:

- Assist in sample point selection, sampling, analysis
- Ground truth geospatial analysis
- Pending ***source data availability***, implement in regions w/GW data
- Key questions:
  - Can we evaluate based on potential for release vs. known use/release?
  - Relative importance of location info for each source type

Wells = exposure potential

Brown University Superfund Research Program



- Dr. Scott Frickel
- Thomas Marlow
- Amy Parmenter, RIDOH
- Dr. Eric Suuberg
- Suuberg lab group

NIH National Institute of Environmental Health Sciences
Superfund Research Program

NEWMOA

Rhode Island Department of Health

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Fluorine

Questions?