Radial Diagram Visualization and Semi-Quantitative Forensic Methods for PFAS Site Characterization

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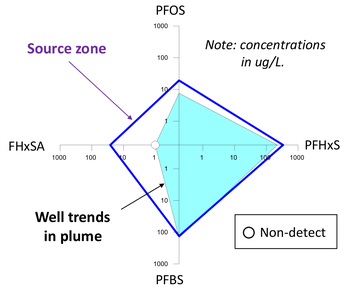
Abstract: Determining background concentrations and off-site origin(s) of PFAS plumes in groundwater is an important consideration at some sites. Radial diagrams are an effective approach for evaluating multispecies PFAS trends, including changes over time and space. For example, the ratios of short- and long-chain perfluorinated carboxylates (PFCAs) and sulfonates (PFSAs) may have distinct visual fingerprints for AFFF-impacted sources, relative to other types of sources such as wastewater treatment plants or landfills. Radial diagrams may also be applied to delineate redox zones where PFAS precursor biodegradation is favorable, and for visualizing the results of TOP assays that characterize the potential for precursor biodegradation in these redox zones.

The radial diagram visualization approach is demonstrated for several case studies based on data available in the literature, including:

1. Ellsworth Air Force Base PFAS trends based on data published by Houtz et al. (2013) and McGuire et al. (2014), including radial diagrams presented in the ITRC PFAS Guidance Manual.
2. Redox zone delineation at Wurtsmith Air Force Base based on data presented in Chappelle et al. (1996) and a new semi-quantitative approach for characterizing redox zones based on polygon area.
3. PFCA, PFSA, and precursor distribution in regional groundwater downgradient from former fire training areas in Uppsala, Sweden.
4. Quantification and visualization of PFCA and PFSA ratios to PFOS to compare source patterns in wastewater treatment plants based on data presented by Houtz et al. (2016).
5. Visualization of changes in PFCA and PFSA ratios to PFOS, and the correlation between polygon areas and the overall ratio of sulfonates to total PFAAs at 20 AFFF-impacted sites based on maximum groundwater concentrations reported in the SSEHRI PFAS database.

Radial diagrams are shown to be an effective tool when it comes to visualizing PFAS trends. This approach is useful not only for helping practitioners to analyze complex datasets, but also for illustrating key findings and concepts to non-technical audiences in support of regulatory and litigation projects. Ongoing research into this visualization approach includes further assessment of distinct graphical and semi-quantitative fingerprints associated with various types of sources. Visual Bio is a free radial diagram software tool available at our web site, and a new software tool specific for PFAS forensic analysis (Visual CHEM) is currently under development.

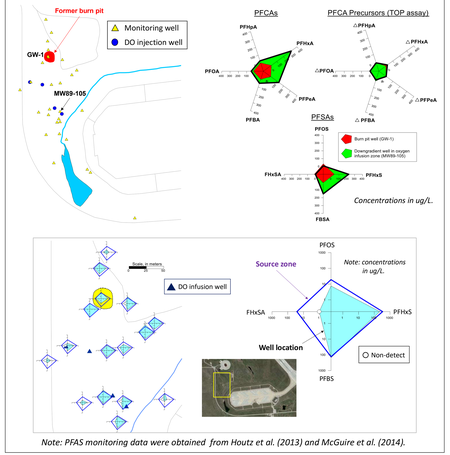
Example Elements of a Radial Diagram



Radial diagrams help to illustrate:

- Relative chemical concentrations or ratios at a single well
- Spatial trends using radial diagrams overlaid on maps
- Comparison of well trends to a Reference series that characterizes source zone or background conditions
- Temporal changes using multiple data series for different monitoring events
- Symbols to show where chemicals exceed cleanup criteria, or are non-detect

Example Radial Diagrams at an AFFF-impacted Site



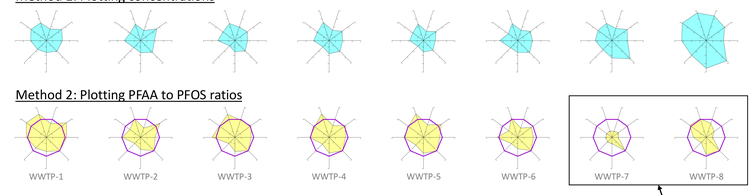
Note: PFAS monitoring data were obtained from Houtz et al. (2013) and McGuire et al. (2014).

Graphical Presentation of Wastewater Treatment Plant PFAS Data

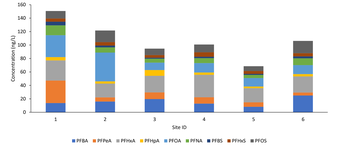
- Houtz et al.(2016) presented 2014 PFAS monitoring results for PFAS at eight sites (WWTP-1 to 8).
- WWTP-7 and 8 were apparently impacted by AFFF discharge from one or more upgradient sites.
- Radial diagrams were employed here to visualize trends for PFCAs and PFSAs at each WWTP.

Method 1: Plotting concentrations

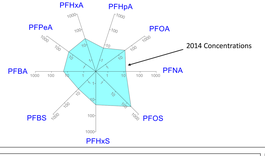
Method 2: Plotting PFAA to PFOS ratios



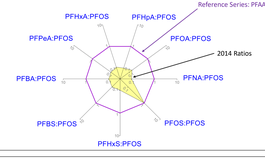
Note: Stacked bar charts are useful for illustrating total concentration differences, but less so for evaluating relative PFAS constituent concentrations.



Concentration Radial Diagram



PFAA:PFOS Ratio Radial Diagram

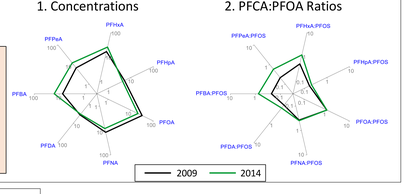


PFAA:PFOS ratios show that:

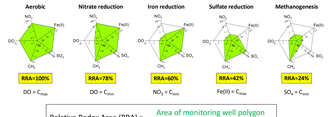
- Site 7 is impacted by ECF-based AFFF with little precursor biodegradation
- Site 8 is impacted by a mixture of ECF and telomer-based AFFF

2009 vs. 2014 Temporal Trend Analysis

Radial diagrams illustrate Houtz et al. (2016) finding that shorter-chain PFAAS are becoming more prevalent due to product composition changes.

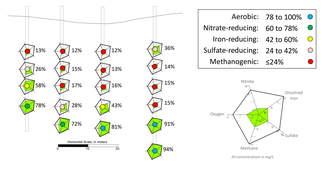


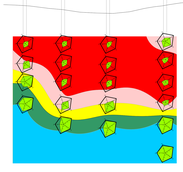
Semi-Quantitative Approach for Delineating Redox Zones



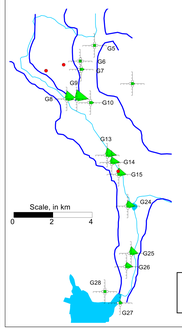
$$\text{Relative Redox Area (RRA)} = \frac{\text{Area of monitoring well polygon}}{\text{Area of reference polygon (Aerobic)}}$$

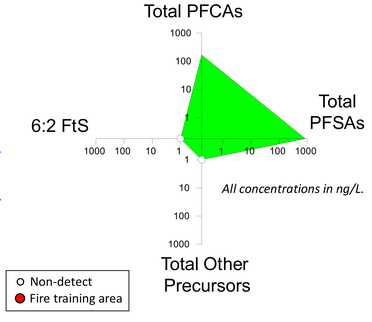
Ranges of polygon areas that represent each redox zone were distinguished based on Wurtsmith AFB data presented in Chapelle et al. (1996). These polygon areas were then used to delineate the extent of each redox zone in a transect of monitoring wells at the site.





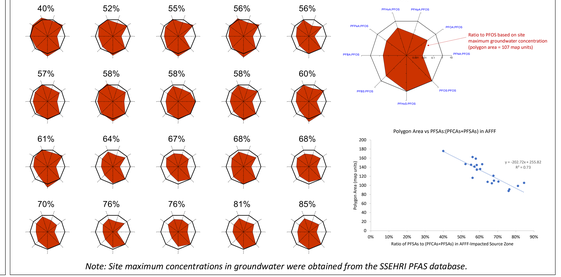
Regional PFAS Trends in Uppsala, Sweden





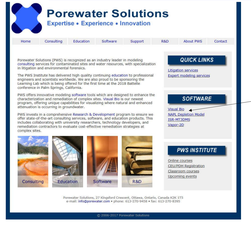
PFAA:PFOS Ratio Trends at 20 AFFF-Impacted Sites

Radial diagrams below represent AFFF-impacted sites ranked in order of the ratio of total PFSAs to total PFAAs



Note: Site maximum concentrations in groundwater were obtained from the SSEHRI PFAS database.

Free Download of Visual Bio Software



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