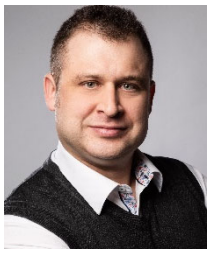
Advantages of Passive Sampling as a Decision-Making Tool and its Application to Contaminated Groundwater Upwelling



Brent Pautler
SiREM

Virtual SMART Remediation Seminar Series 2021
February 25, 2021

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Advantages of Passive Sampling as a Decision-Making Tool and its Application to Contaminated Groundwater Upwelling

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SMART Remediation

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(SiREM)
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(Geosyntec Consultants Inc.)
Steven Aufdenkampe
(Norfolk Southern Corporation)

siremlab.com

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Introduction to SiREM

Founded in 2002 in Guelph, ON
In 2020 expanded to Knoxville, TN

Provide products and testing services to support and improve site remediation

Further information: siremlab.com

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Passive Sediment Porewater Sampling Service

- Porewater sampler for dissolved organic and inorganic compounds
- Easy to use off the shelf sampler ready for deployment
- Includes Performance Reference Compounds



SP3 SPeeper

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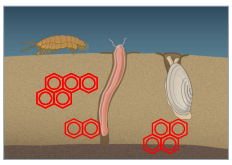
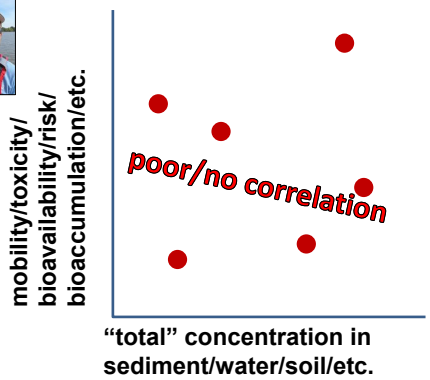
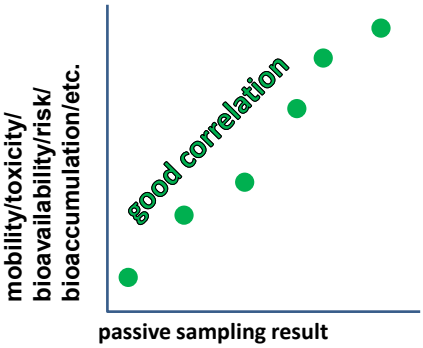
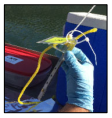
Why Porewater by Passive Sampling?



Availability







…dozens and dozens of papers over the past 20 years

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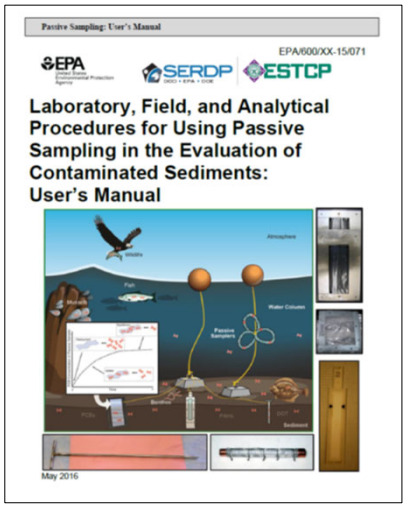
Regulatory Perspective



- USEPA and many state regulators are actively promoting the use of passive sampling to answer key decision-making questions
- Several examples of decision-making uses of C_{free} (bioavailable concentration) at State and Federal sediment sites

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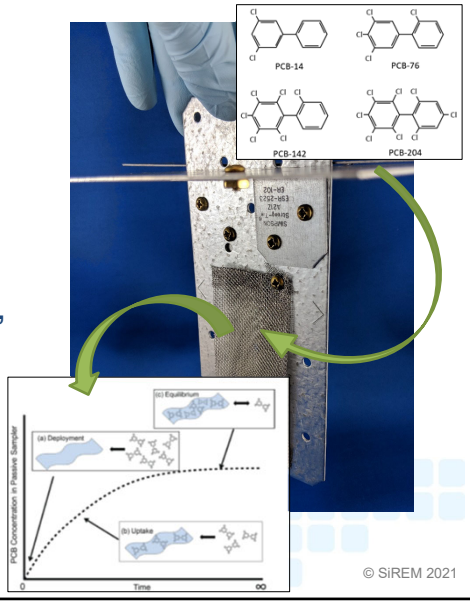
SP3™: Passive Sampler for Hydrophobic Organics

- Polyethylene-based passive samplers for PCBs, PAHs, Dioxins and Furans, total petroleum hydrocarbons (TPH) and organochlorine pesticides (OCPs)
- Equilibrium-based partitioning sampler
- End to End service for supply of samplers, assist with deployment/retrieval (optional), analytical chemistry and C_{free} calculation



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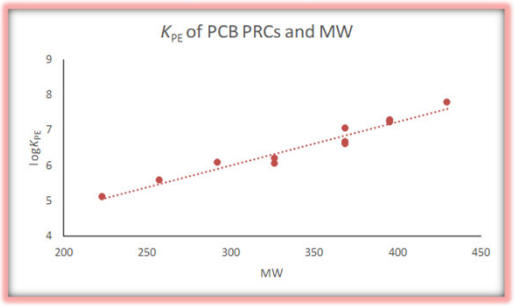
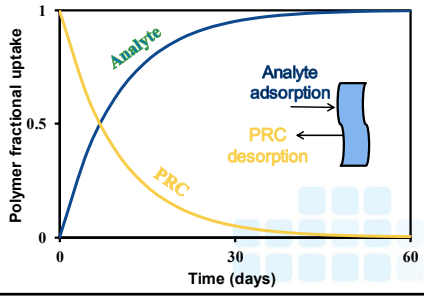
Performance Reference Compounds (PRCs)

- Standard PRCs for SP3™ are 10 rare PCB congeners
  - Specific congeners can be removed if they are incompatible with the analytical lab or present at the site
  - Used to correct for non-equilibrium
- Data analysis models are based on K_{PE} values





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Custom Configurations & Deployment

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Analysis and Data Processing

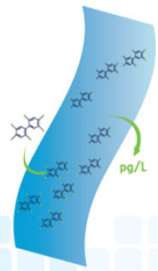
- Concentration in polyethylene converted to liquid concentration (e.g., pg/L)
  → "available concentration"
  → "porewater concentration"
  → "freely-dissolved concentration (C_{free})"

- Food-web/risk models
- Predict/understand bioaccumulation
- Risk-based threshold concentrations
- Fate/remediation models
- Etc.

$$C_{free} = \frac{C_{sampler}}{(1 - e^{-k_e t}) \times K_{sampler}}$$

$$k_e = \ln\left(\frac{C_{PRCi}}{C_{PRCf}}\right) \times \frac{1}{t}$$

$$COC_D = \frac{COC_{PS}}{K_{PS-D}} * 1000$$



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GROUNDWATER UPWELLING IN PUMP SLOUGH
FORMER WOOD PRESERVING SITE, LOUISIANA

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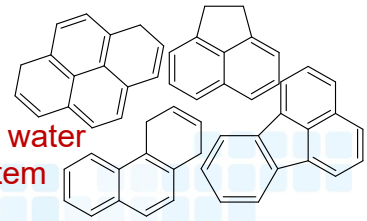
Former Wood Preserving Site, LA

- Parent and Alkylated PAHs detected in groundwater adjacent to and sediment in Pump Slough
- Horizontal and Vertical groundwater gradients suggested that the sands beneath the Pump Slough are in hydrogeologic communication with the Pump Slough
  - Groundwater primarily discharges to pump slough with brief period of recharge over the period of record
- Does contaminated GW discharge into sediment & surface water?
- Is the discharge significant or above acceptable levels?



Overall Goal – Ensure that there are **NO** surface water or sediment impacts on human health or ecosystem

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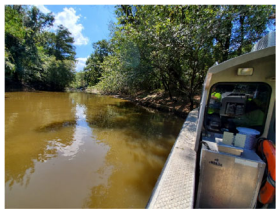
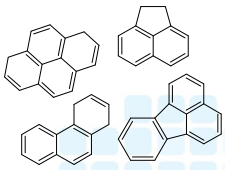
Approach

- Determine C_{free} of parent & alkylated PAHs
  - 24 SP3™ samplers (19 sediment, 2 surface water, 3 trip blanks)
  - Deployed 30 days
  - Analyzed by modified EPA 8270 method (ID-0016; PAHs by GC/MS Isotope Dilution)
- Use C_{free} values and USEPA final chronic values (FCVs) derived from the equilibrium partitioning (EqP) approach to determine toxic unit (TU)
- Use C_{free} values and multivariate statistics to cluster results and provide another line of evidence to EqP and TU approach





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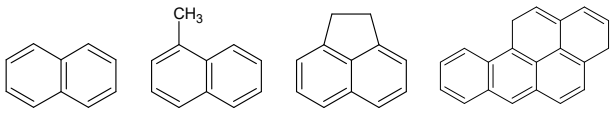
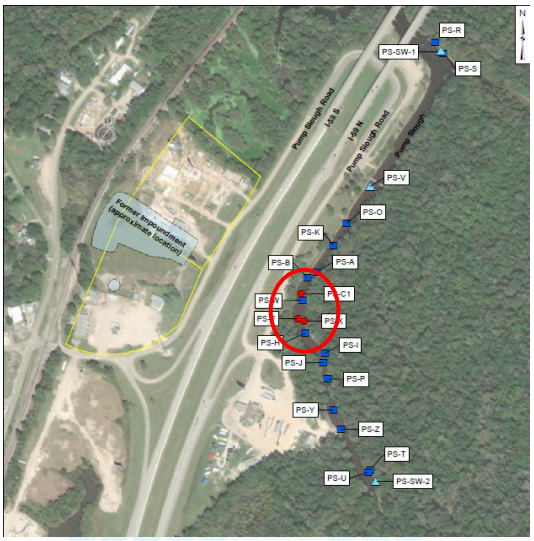
PAH Mixtures and Toxic Units

$$TU = \frac{[PAH_1]}{FCV_1} + \frac{[PAH_2]}{FCV_2} + \cdots + \frac{[PAH_n]}{FCV_n}$$

C_{free} data available from SP3™, TU data more representative estimate of potential toxicity than one-carbon EqP

PS-C1, PS-F, PS-X TU ranged from 1.84 – 3.88. (TU > 1 possible risk to benthos)





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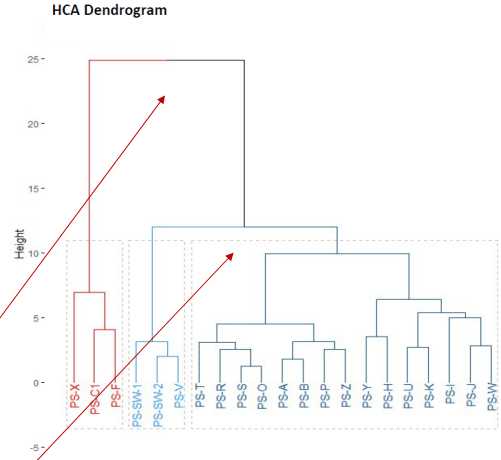
Analysis of Results – Multivariate Statistics

Hierarchical cluster analysis (HCA) that can identify common groups of samples (clusters) within a large data set based on PAH concentration compositions

1. Begin assuming each sample is own cluster
2. Identify the closest two clusters (based on similarity across PAH concentrations) and combine them into one cluster
3. Repeat the above step until all the data points are in a single cluster

Euclidean distance across PAH concentrations used for similarity/closeness quantification



Two Distinct Clusters of passive sampler locations

Cluster 2 divided into two sub-groups

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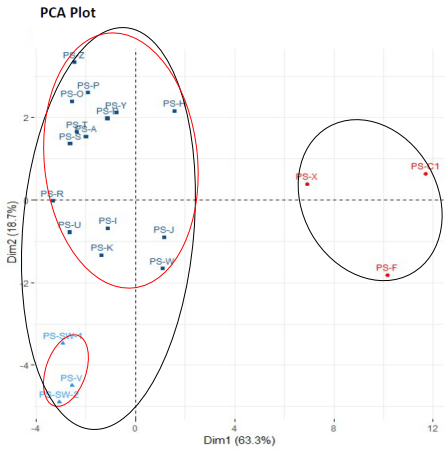
Analysis of Results – Multivariate Statistics

Principal Component Analysis (PCA) summarizes variation in the data set that consists of multiple correlated variables.

1. Reduces the number of variables by transforming them into smaller sets of uncorrelated variables without the loss of information
2. New variables correspond to a linear combination of the original variables called principal components (PC)
3. Samples that plot near each other in PC space have similar variable distributions, farther away have less similar distributions



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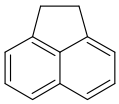
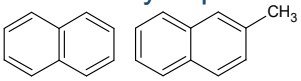
PAH Concentrations & Composition

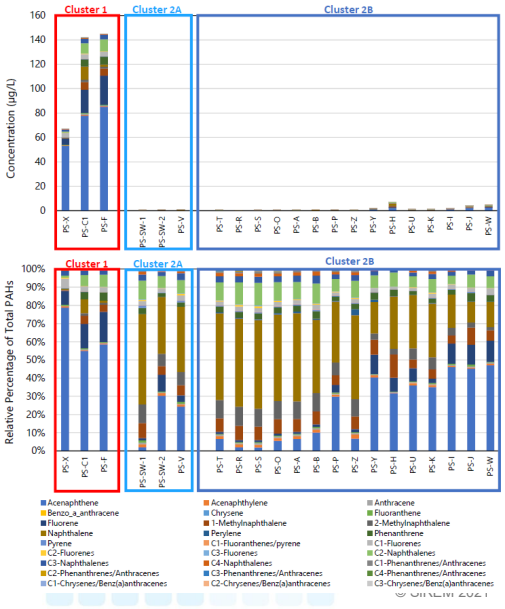
Cluster 1 – Highest concentrations and major contributor: acenaphthene



Cluster 2 – Total concentration are 1 to 2 orders of magnitude lower than cluster 1 and major contributors: naphthalene and 2-methylnaphthalene



Clustering consistent with TU > 1 (Cluster 1 samples), and are clearly distinguishable from remainder of samples



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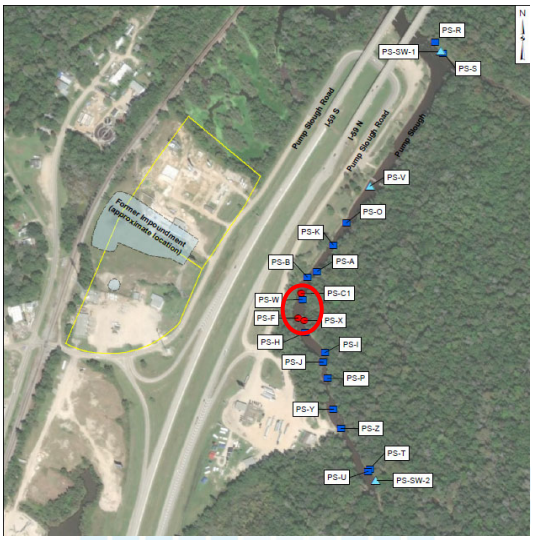
Recommendations

- Groundwater discharges into Pump Slough indicate that the discharge is contained along southern bend
- All other areas have very low C_{free}
  - Consistent with previous bulk chemistry sediment data in terms of totals
  - SP3™ able to distinguish from background where bulk chemistry could not



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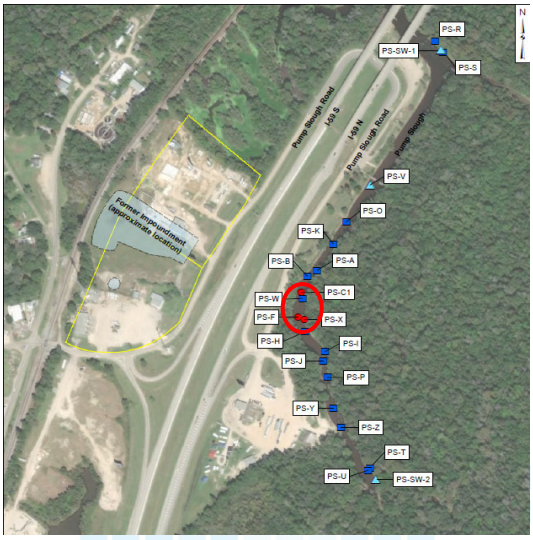
Summary

- SP3™ identified locations and concentrations of COC flux with multiple lines of evidence
- Previous work over-estimated the need for corrective action at this site
  - SP3™ able to reduce potential remediation costs and planning

If corrective action required, would be confined to a small area



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Further Information

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