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Evaluating the Challenges of Using Disparate Data Sets in Forensic Methods

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Why Combine Disparate Data Sets for Forensic Investigations?

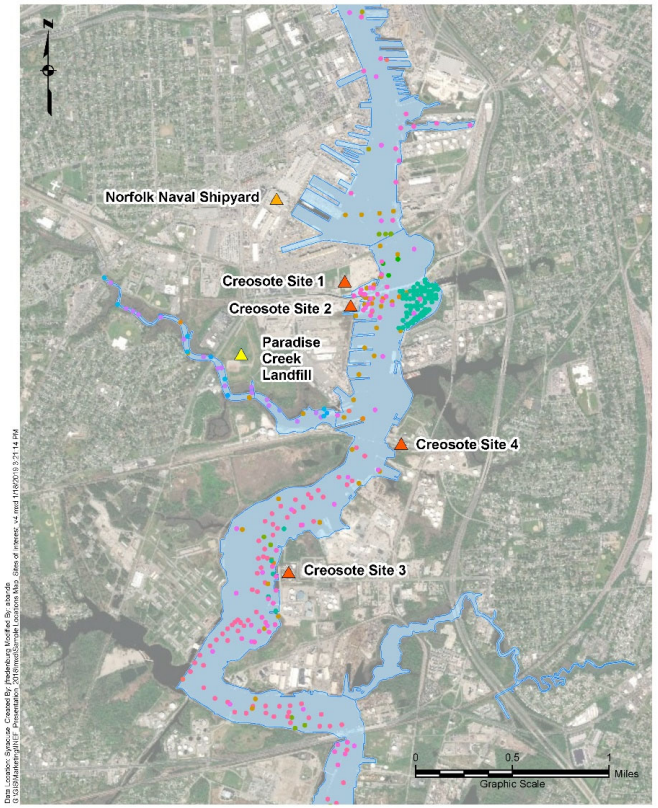
- Forensic methods are useful for identifying contaminant sources and assigning shares of costs in the allocation process
- The reasons for using and combining existing data sets include the following:
  - Providing a data set that is larger and has more coverage than any individual data set
  - Capturing data from historical sources that may have been removed or are no longer accessible
  - Avoiding the potentially prohibitive cost of additional studies/analyses
  - Informing future forensic sampling plans or investigations

Issues with Combining Data Sets for Forensic Investigations

- Available data are rarely collected with the aim of forensic analysis
- Some of the most common problems are:
  - **Varying contaminants analyzed**
  - **Censoring of data sets**
  - **Varying detection limits**
  - Variable units
  - Multiple contaminant names
  - Multiple analytical methods
  - Outliers
  - Distribution of sample locations due to study design
  - Lack of unique sample IDs within and between data sets
  - Inconsistent depth segmentation
  - Changes in surface elevation between studies
- **Combining data requires careful consideration of usability and harmonization**

Combining Data from Multiple Studies Provides Larger Data Set with Wide Coverage

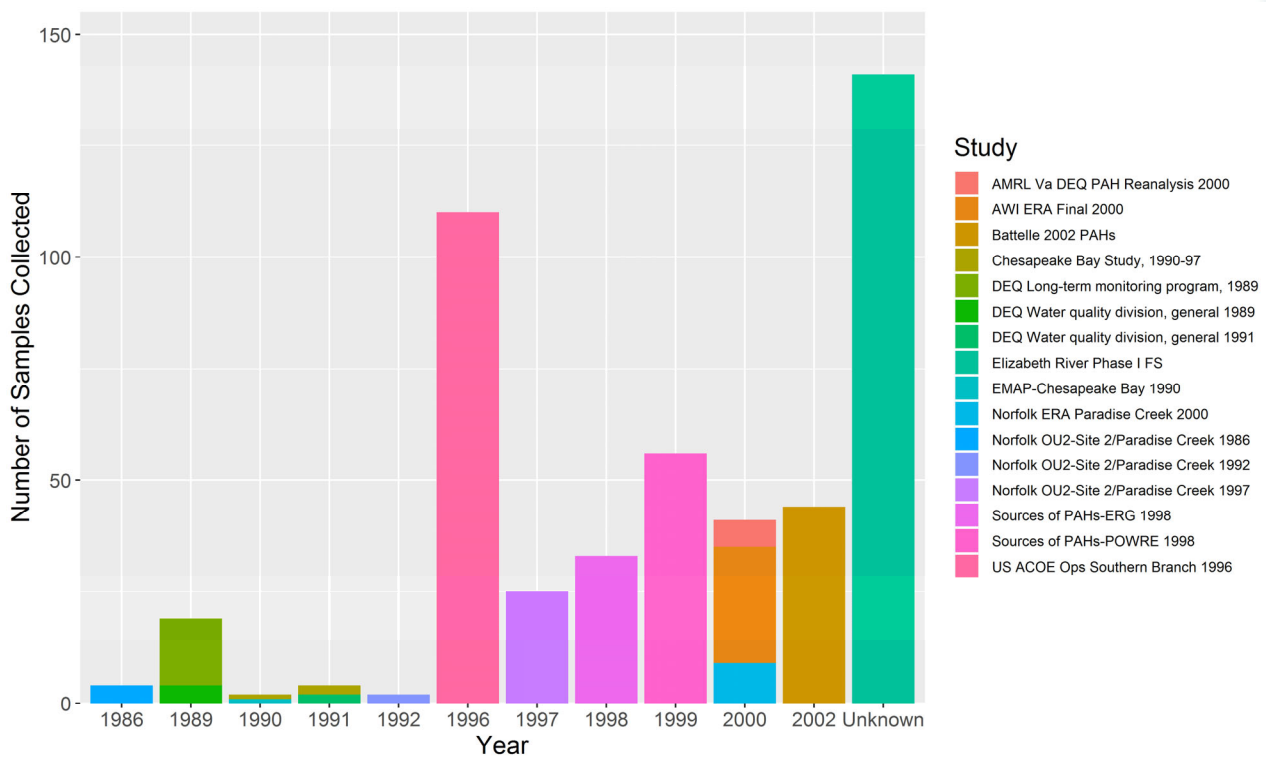
- Example data set from Southern Branch of Elizabeth River, VA
- All data came from National Oceanic and Atmospheric Administration's (NOAA's) Query Manager
  - NOAA's Query Manager addresses unit and analyte name consistency
- Multiple potential polycyclic aromatic hydrocarbon (PAH) sources identified in this area, so this example analysis was limited to PAHs



Multiple Studies Provide Extensive Historical Sampling

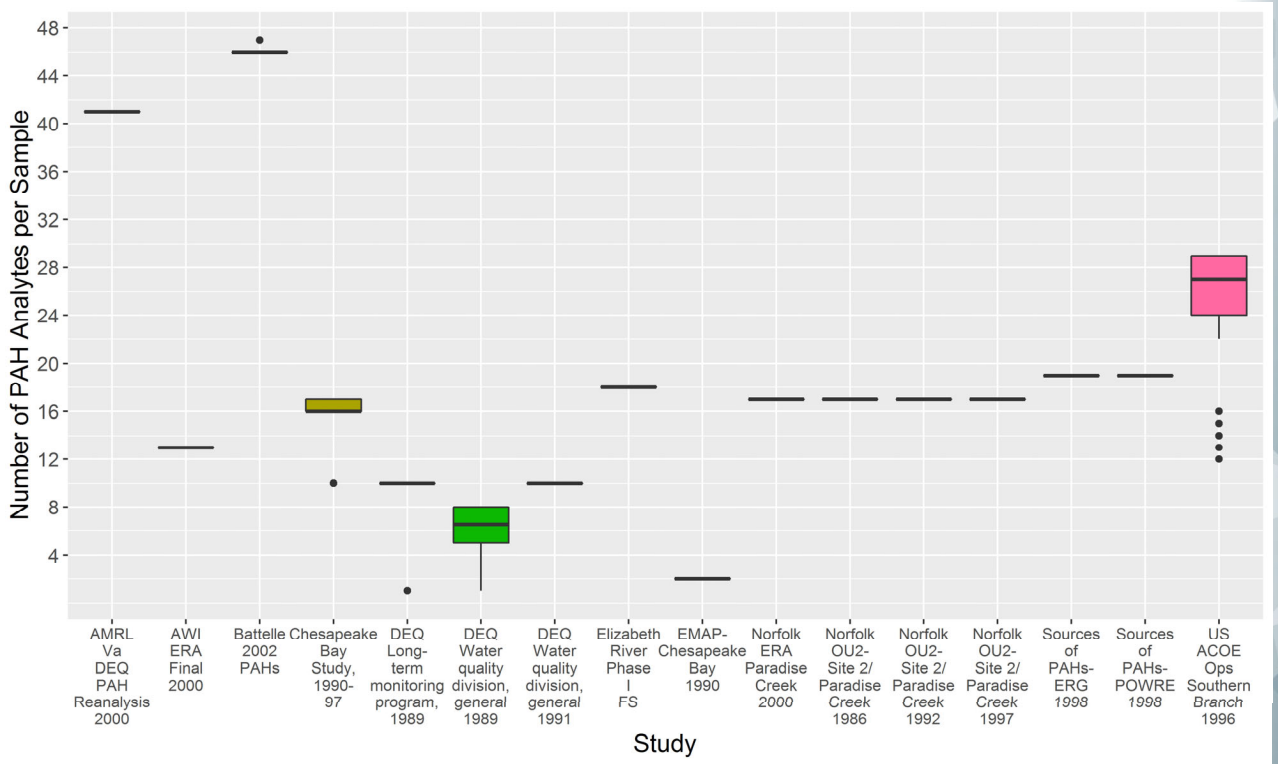
Elizabeth River PAH data

- Sampling events conducted over 16 years
- 16 studies
- 481 total samples
- 348 unique sample locations
- 10,246 results



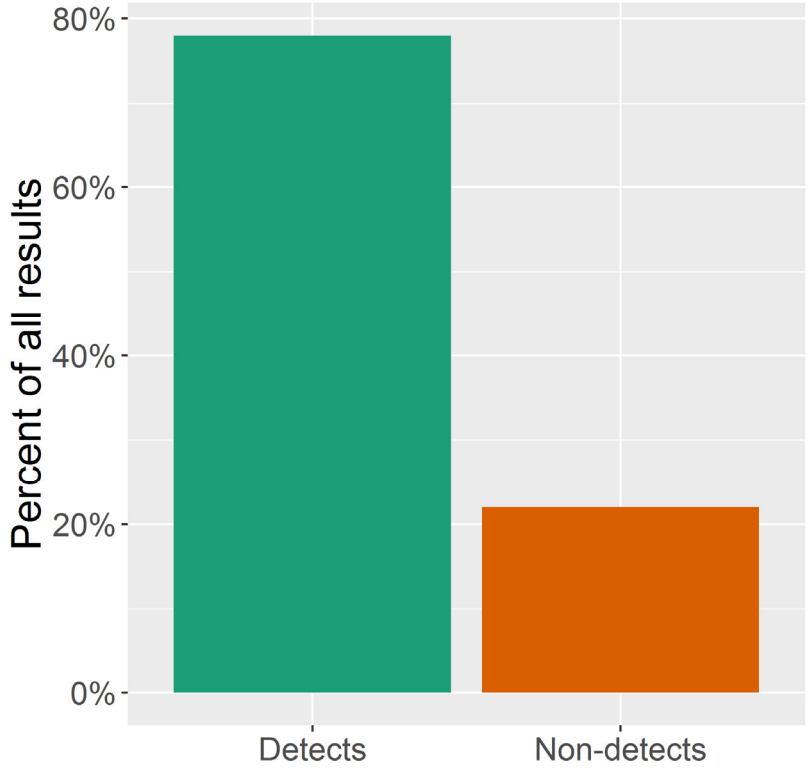
Different Studies Evaluate Different PAHs

- Number of PAHs analyzed per study ranges from 1 PAH (benzo[k]fluoranthene) to >40 PAHs (including methylated PAHs)
- Studies did not always analyze the same suite of PAHs



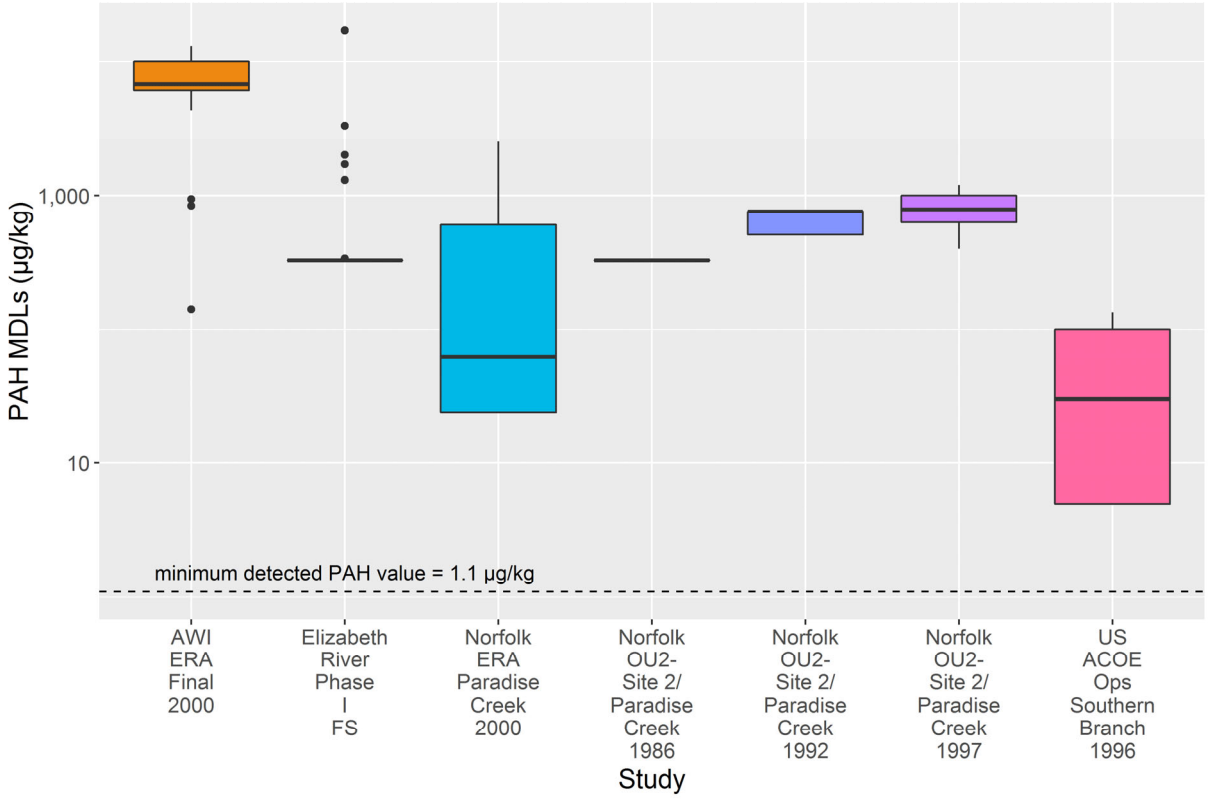
Combined Data Set Contains Censored Values

- More than one-fifth of all values are censored (below method detection limits [MDLs])
- Specific analytes may have:
  - High MDLs
  - No presence in sediments
- Specific studies may have:
  - High MDLs
  - Sampled non-contaminated locations



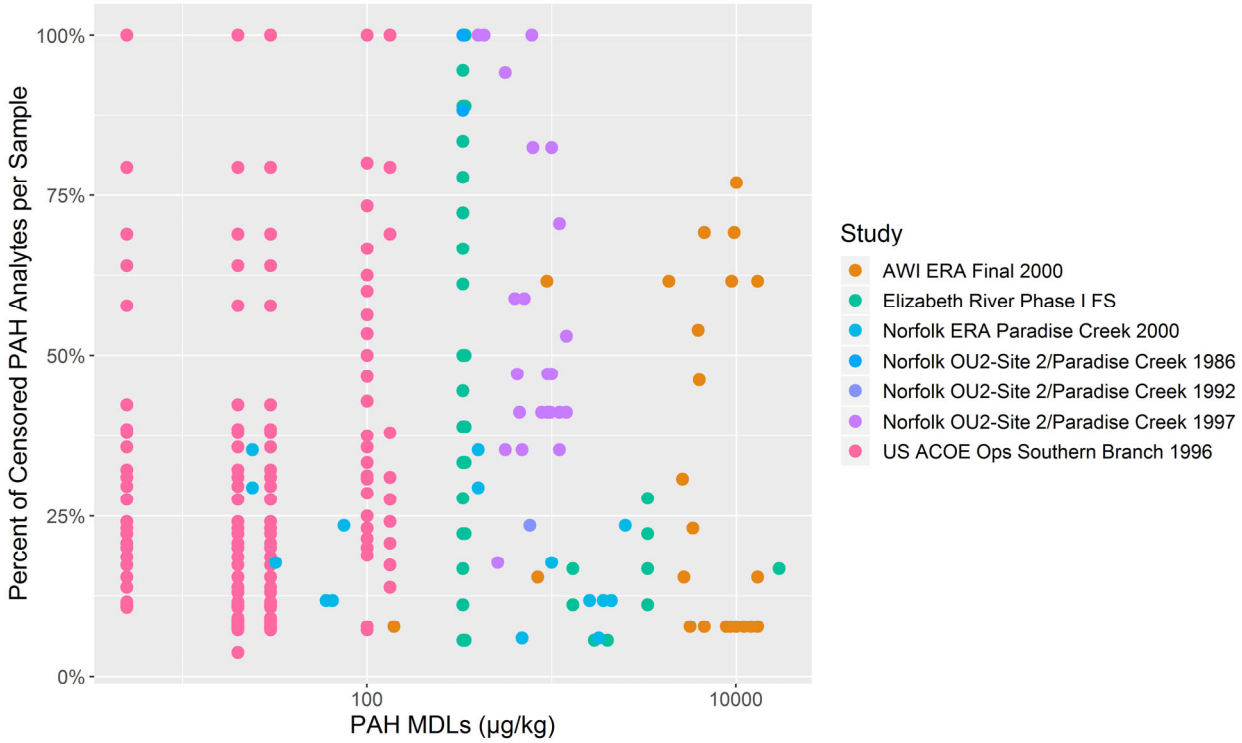
Studies Include Wide Range of MDLs

- MDLs only for non-detect results (7 studies)
- Wide range of MDLs potentially due to:
  - High concentrations
  - Lab quality/capabilities
  - Analytical method
- Does this affect censoring?



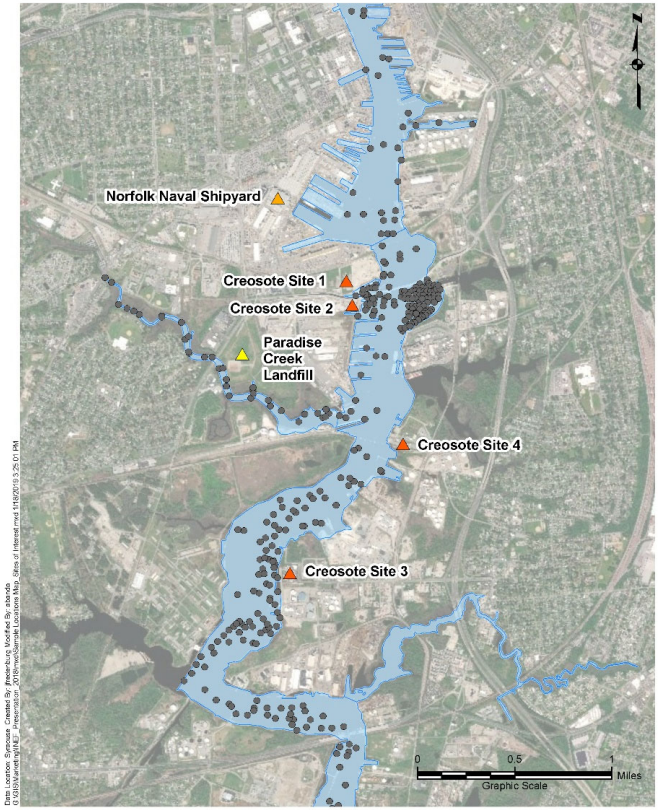
High MDLs Do Not Affect Censoring

- MDLs do not correlate with censoring
- Variability in censoring also potentially due to:
  - Matrix interference
  - Targeted study design



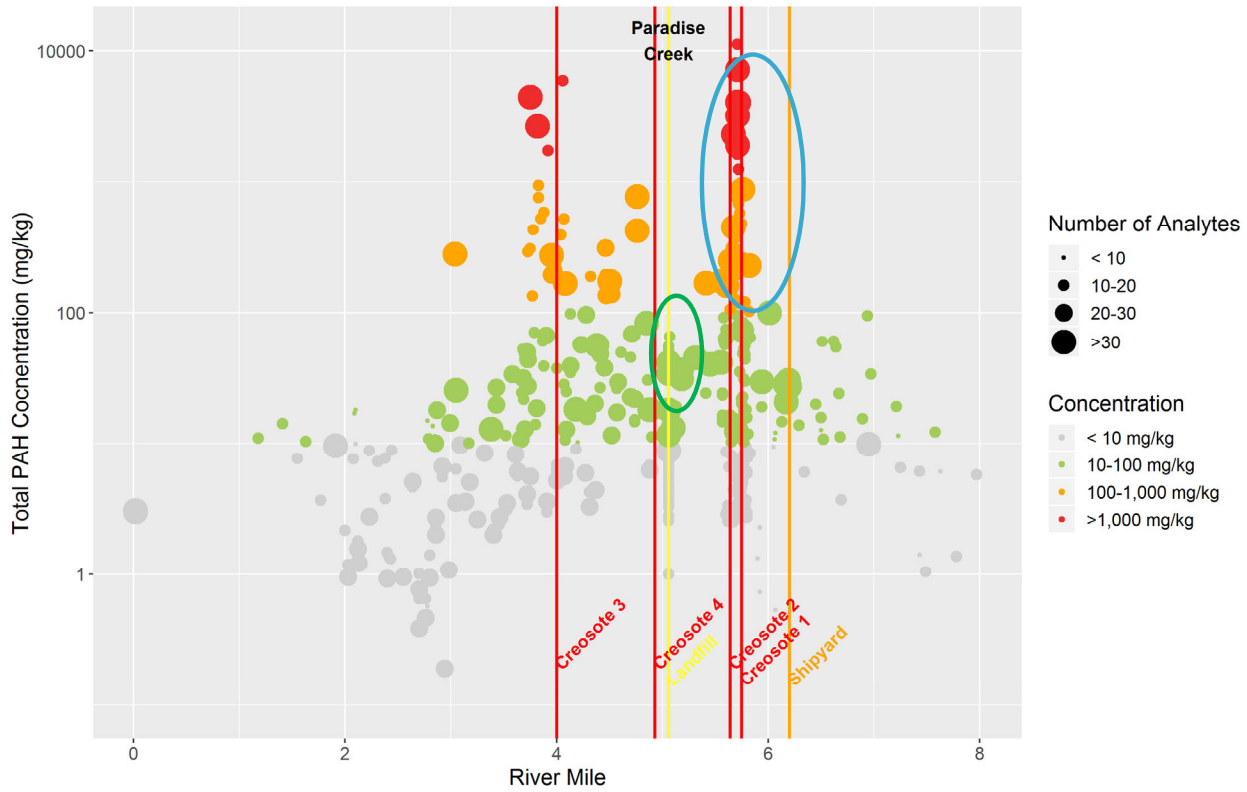
How Do Analyte and Censoring Issues Affect Forensic Analysis?

- There are multiple potential PAH contaminant sources in the Elizabeth River
- Analyte and censoring issues can result in drawing inappropriate connections between sources and analytical results



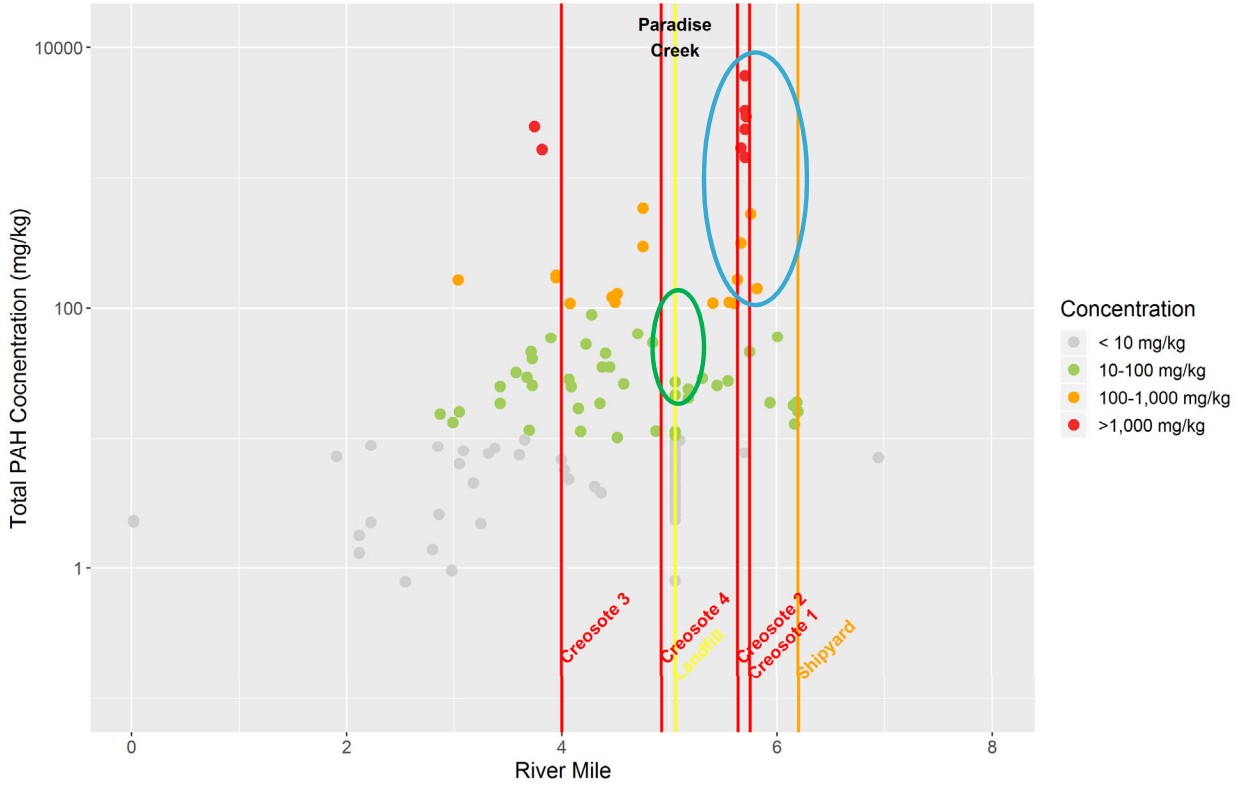
Larger Number of Analytes Results in Higher Total PAH Concentration

- Total PAHs calculated using all PAH analytes
- Often the larger the number of analytes measured, the larger the concentration of total PAHs



Standardization of Analytes Reduces Total PAH Concentration in Certain Areas

- Calculated total PAHs from U.S. Environmental Protection Agency's (EPA's) 16 priority pollutant PAHs
- Includes only samples analyzed for all 16 PAHs
- Elevated concentrations in Paradise Creek no longer present
- Samples near Creosote 1 and Creosote 2 sites with elevated concentrations still present

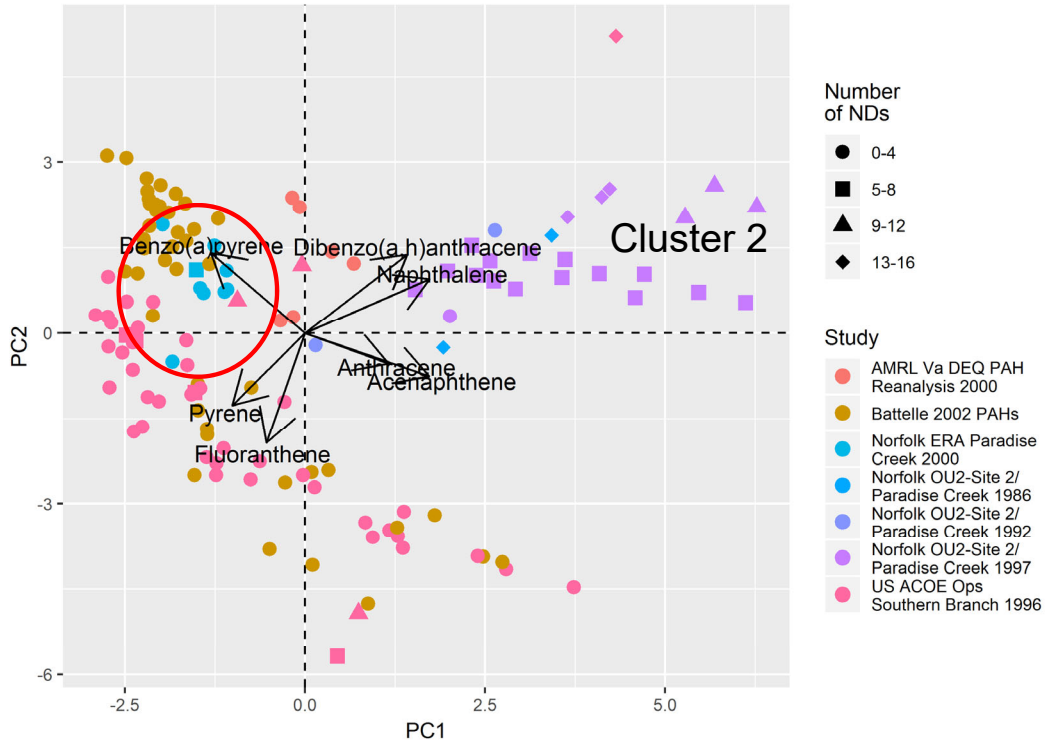


Highly Censored Samples Result in Samples Clustering Based on Number of Non-Detects (NDs)

- Principal component analysis (PCA):
  - 16 priority pollutant PAHs
  - Used half the MDL to represent NDs
  - Normalized by total PAH
- Clusters were identified using K-means clustering and the average silhouette method
- K-means analysis identified four clusters
- Results: Cluster 2 is mostly samples with high number of censored values

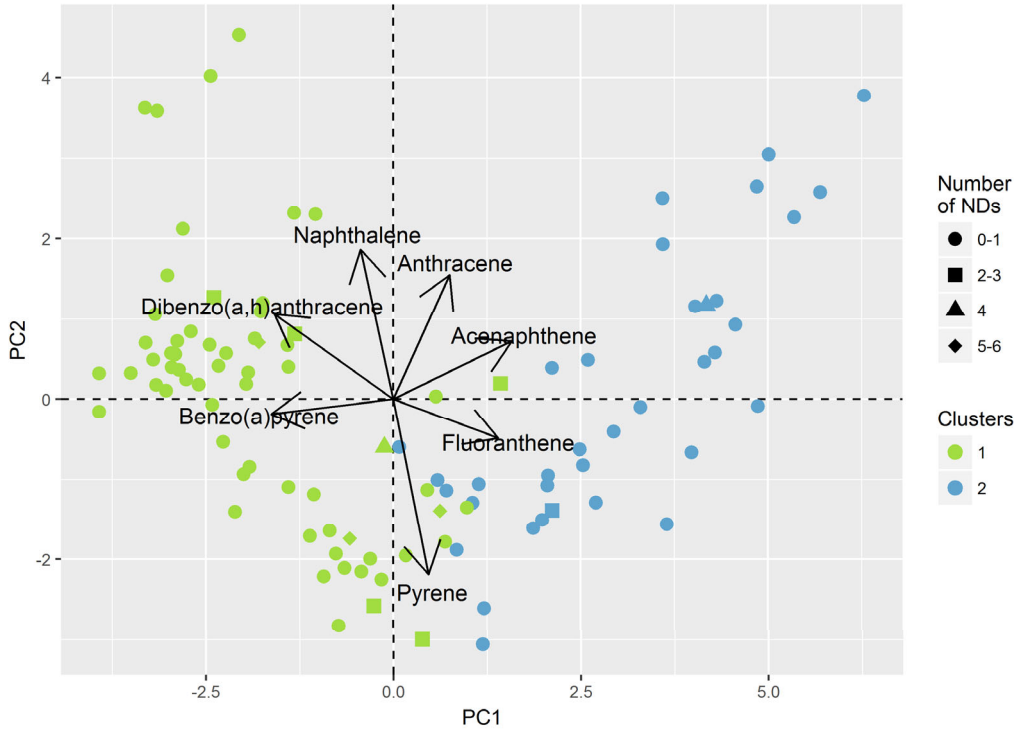
Cluster of Highly Censored Samples is Study Specific

- Cluster 2 is composed of 1986, 1992, and 1997 Paradise Creek studies
- 2000 Paradise Creek study doesn't cluster with other Paradise Creek studies
- 1986, 1992, and 1997 studies have high detection limits
- Cluster 2 likely represents differences in analytical methods and/or study design



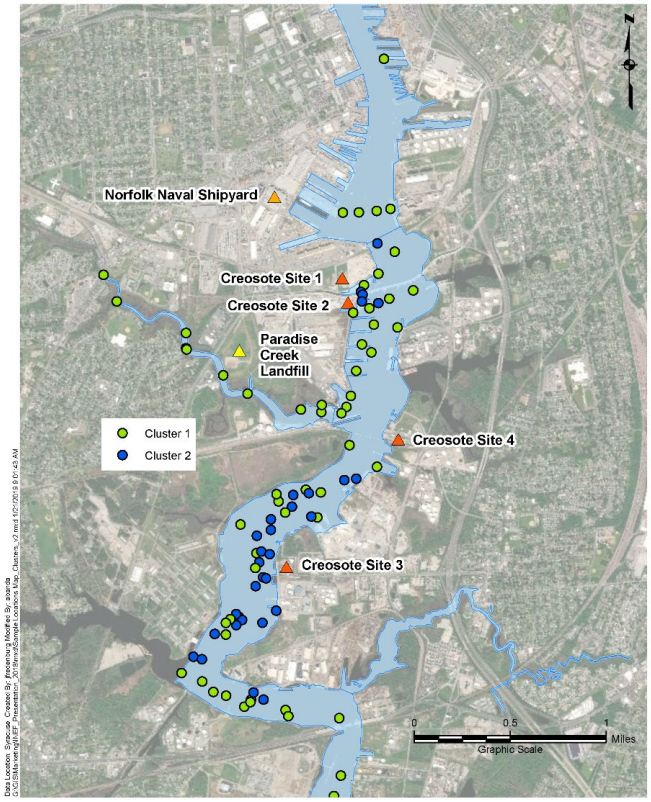
PCA and K-means analysis with Cleaned Data Set Identifies Two Clusters

- Updated PCA and K-means analysis use cleaned data
  - Excludes studies with high detection limits
  - Excludes samples with more than 7 analytes ND
- Results: Two clusters separated primarily by principal component (PC) 1



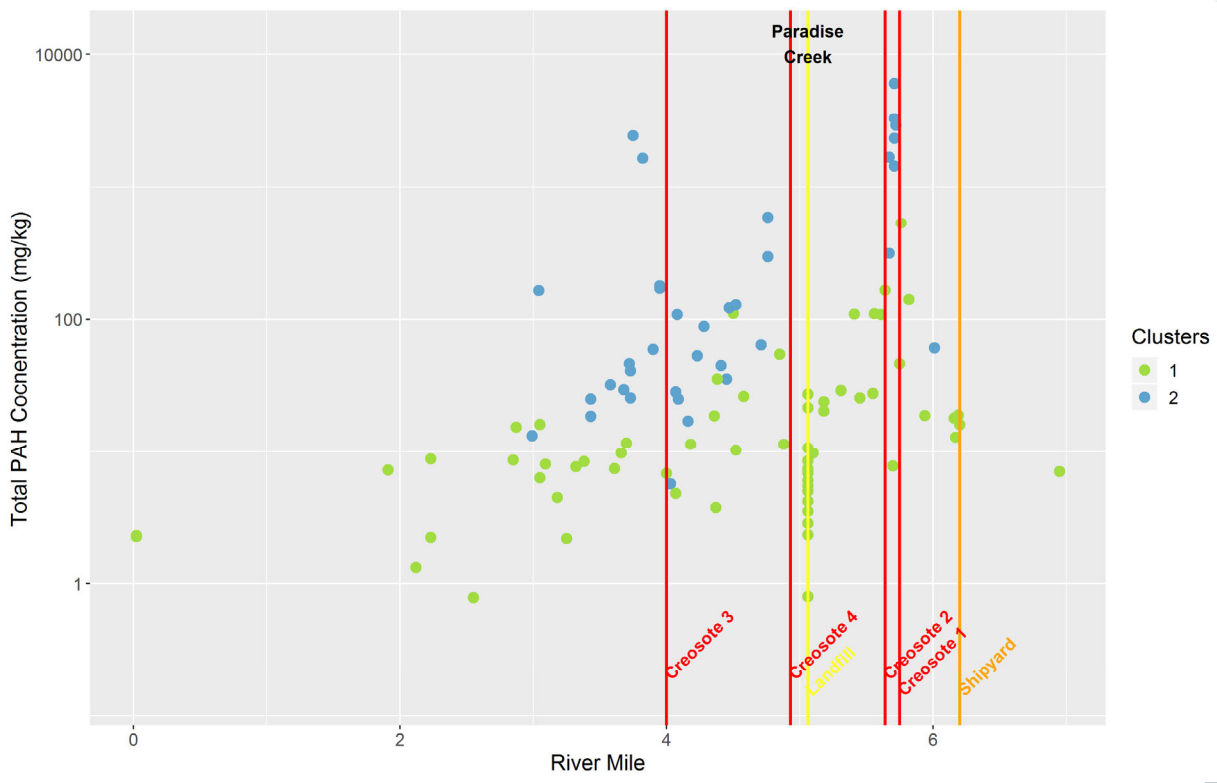
Samples in Cluster 2 Adjacent to Creosote Sites

- Cluster 1 samples in Paradise Creek are located near landfills
- Cluster 2 samples are often located near creosote treatment facilities
- PAHs in sediments near landfills appear distinct from PAHs in sediments near creosote treatment facilities



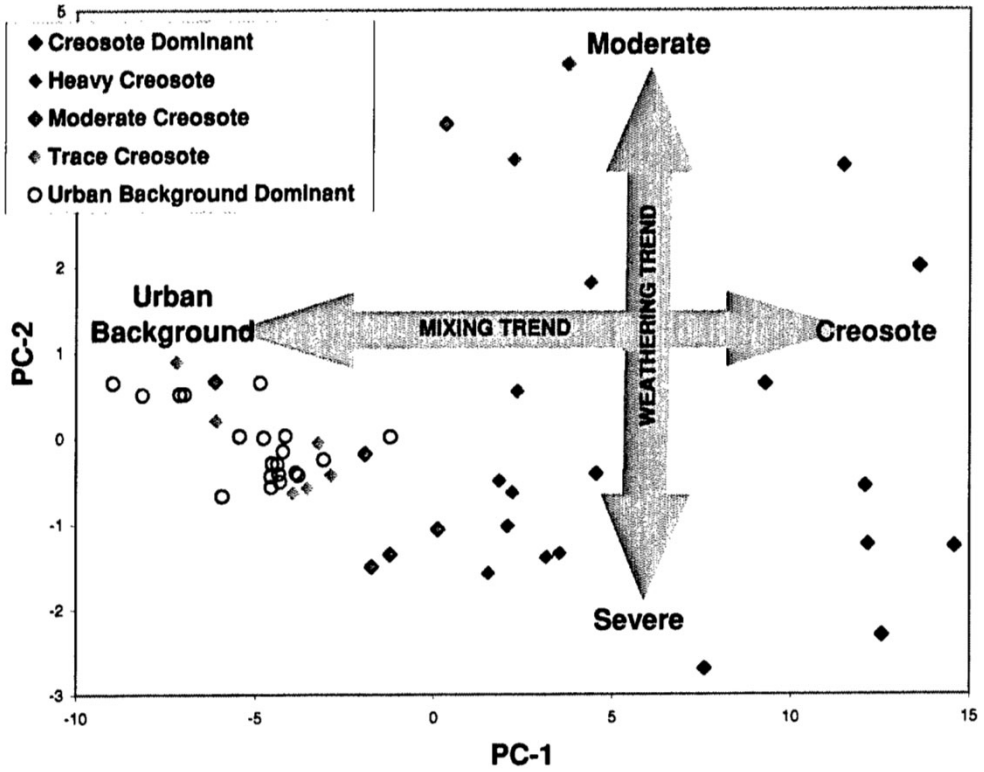
Cluster 2 Associated with Higher Total PAH Concentrations

- Highest total PAH concentrations are in Cluster 2
- Highest concentrations located near creosote sites
- Samples in Paradise Creek near landfill have low concentrations and are all in Cluster 1
- The landfill is likely not a major source of PAHs



Battelle Forensic Study also Identified Two Sources of PAHs

- Study focused on sources near Norfolk Naval Shipyard
- Identified creosote and urban background as primary inputs
- PCA of alkylated and non-alkylated PAHs
  - Background compared to creosote inputs
  - Weathering



Conclusions

- There are advantages to combining existing data sets when investigating sources and/or conducting allocation based on source identification:
  - Captures historical sources
  - Provides larger data set with more coverage
  - Cost of additional studies/analysis are prohibitive
- However, careful consideration must be taken to evaluate usability and ensure harmonization, including evaluating the following:
  - Issues arising from analysis of varying contaminants
  - Censoring of data sets
  - Variations in detection limits
  - Outliers

Thank You

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