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Using multivariate statistical tools to evaluate dioxin/furan congener profiles and inform policy decisions

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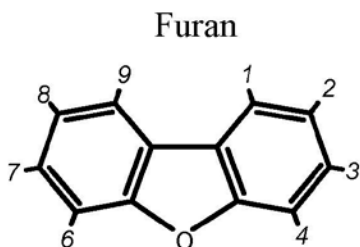


 **NewFields**

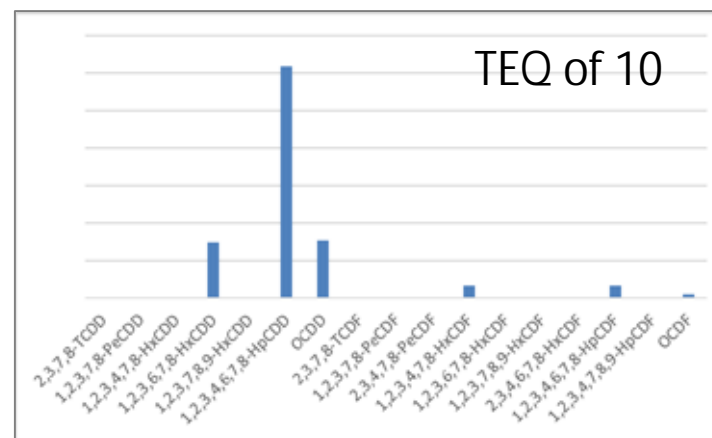
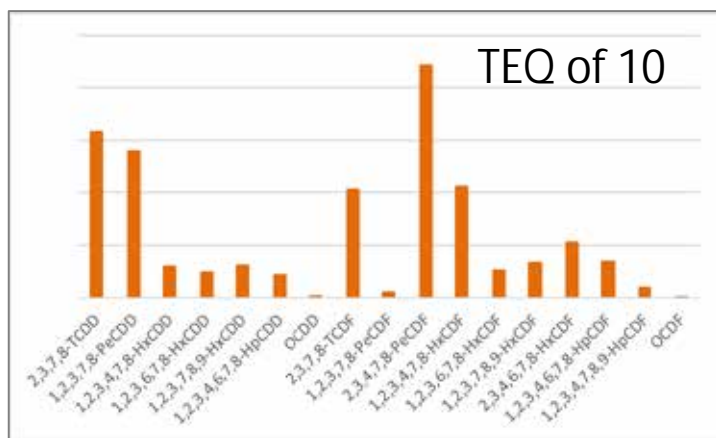
Using Multivariate Statistical Tools to Evaluate Dioxin/Furan
Congener Profiles and Inform Policy Decisions
April 5, 2018

Dioxin/Furan Congeners

17 most toxic congeners are typically evaluated.
Each congener is assigned a certain toxicity factor.
Total toxicity referred to as toxic equivalency (TEQ).



It is possible for two samples to have the same toxicity, but include a completely different mix of congeners.



Environmental Forensics and Chemometrics

Chemometrics is a subset of environmental forensics that incorporates multivariate statistics geographic information systems to identify:



Unique chemical signatures (fingerprints)



Map the spatial distribution (footprints) of each signature

The method also applies to:

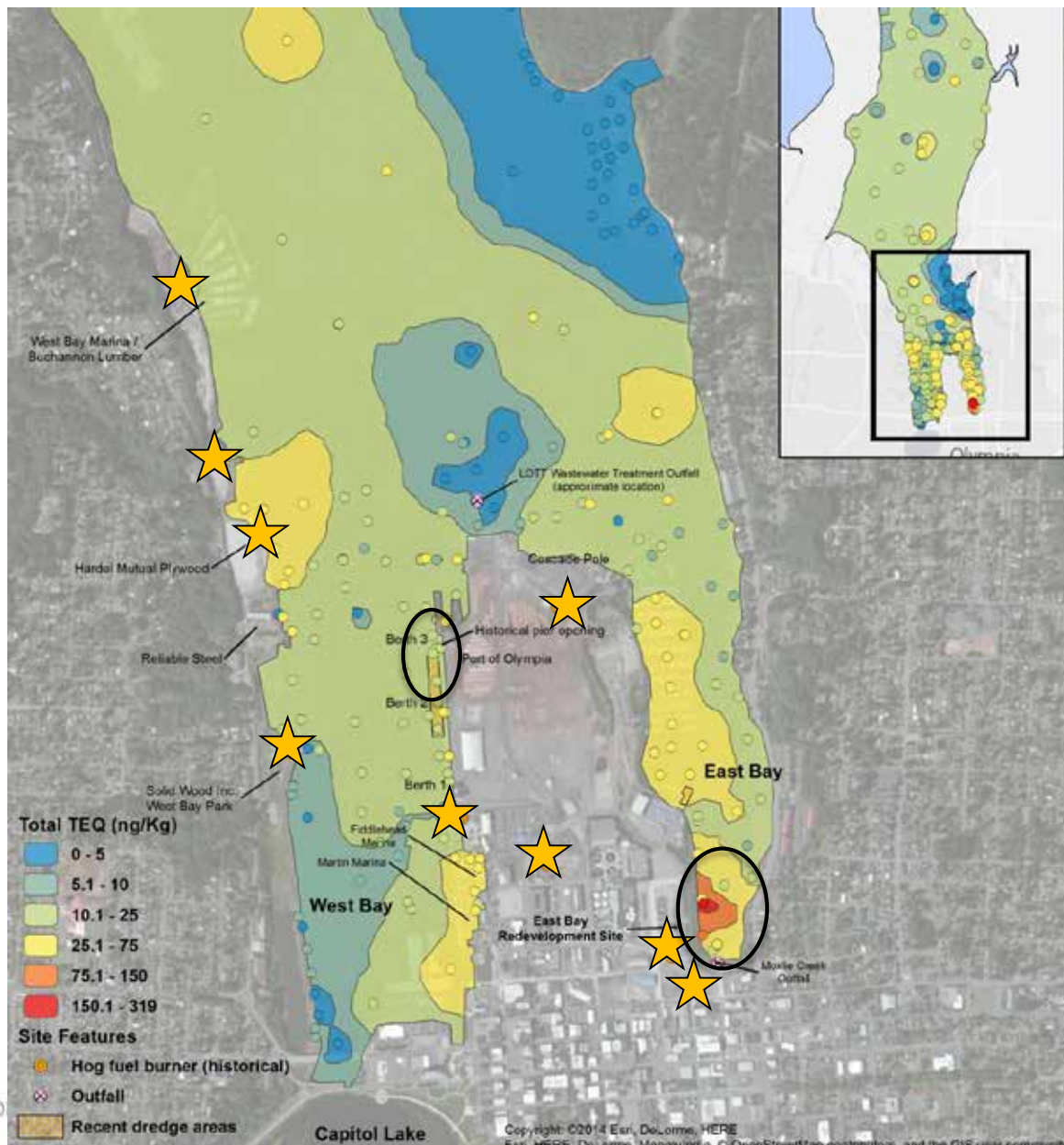
- PCB congeners
- Alkylated PAH
- Polybrominated biphenyl ethers (PBDEs)
- Pharmaceuticals and personal care products (PPP)

Study Objectives

NewFields was tasked by Ecology to characterize the dioxin/furan concentrations in sediments in Budd Inlet to better:

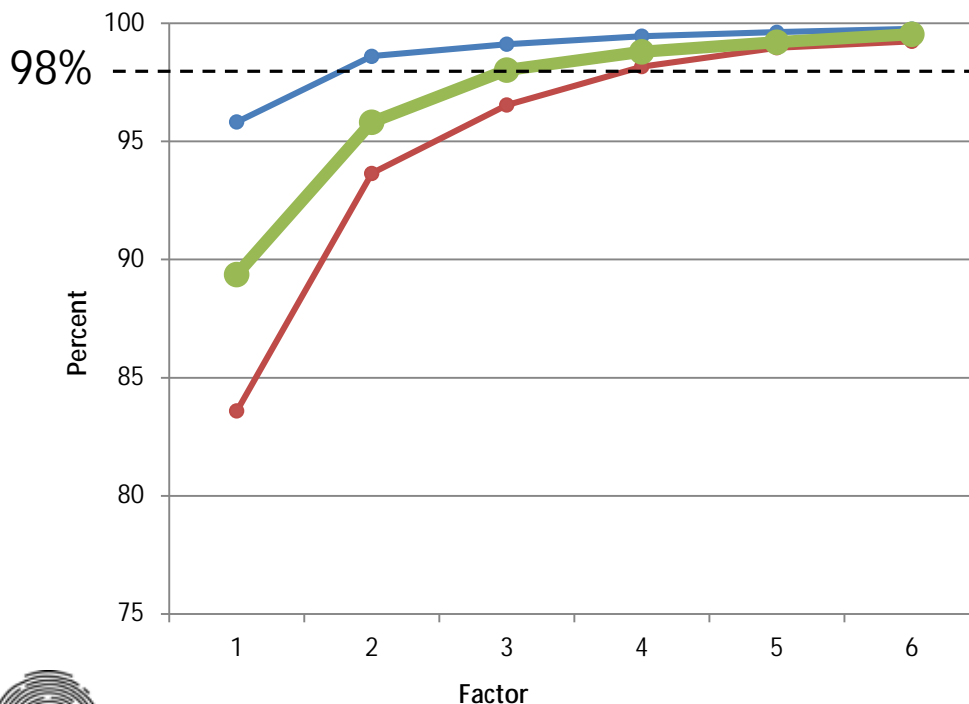
1. Identify distinct chemical signatures in sediments;
2. Determine the relative contribution of these signatures to bay-wide dioxin/furan concentrations; and
3. Identify potential upland point source locations.

Budd Inlet – Surface Conc.



Step 1 - Data Screening - PCA

Principal components analysis (PCA) is the first step in reducing the number of variables (unique fingerprints) in the data set.



The goal is to select the fewest factors that contain the most variability. The number of factors is dependent on the complexity of the data set.

Bay 1 – Oakland Bay – two factors

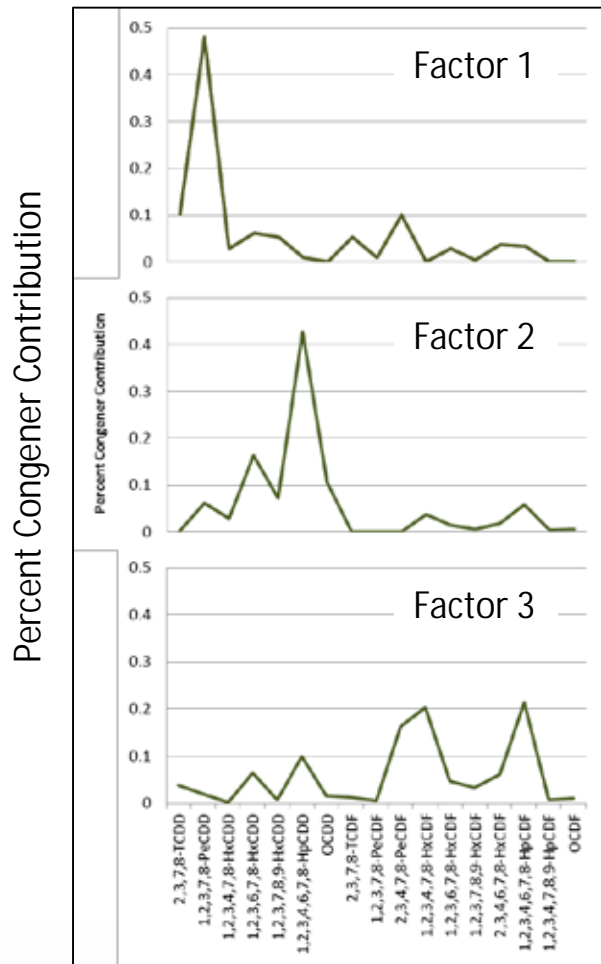
Bay 2 – Budd Inlet – three factors

Bay 3 – Port Angeles – four factors

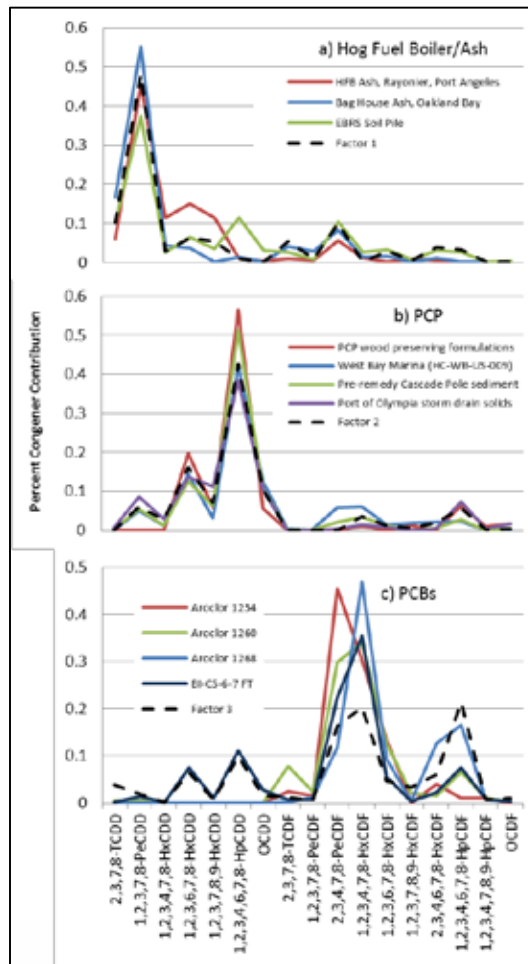


Step 2 - Unmixing Analysis and Source Matching

The unmixing model provides the modeled congener profile for each of the factors. Factor profiles are compared to the NewFields source library.



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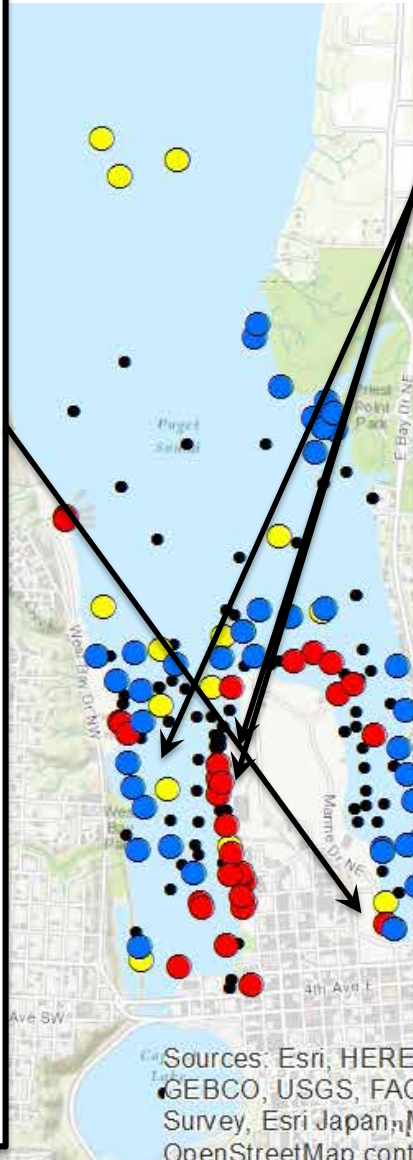
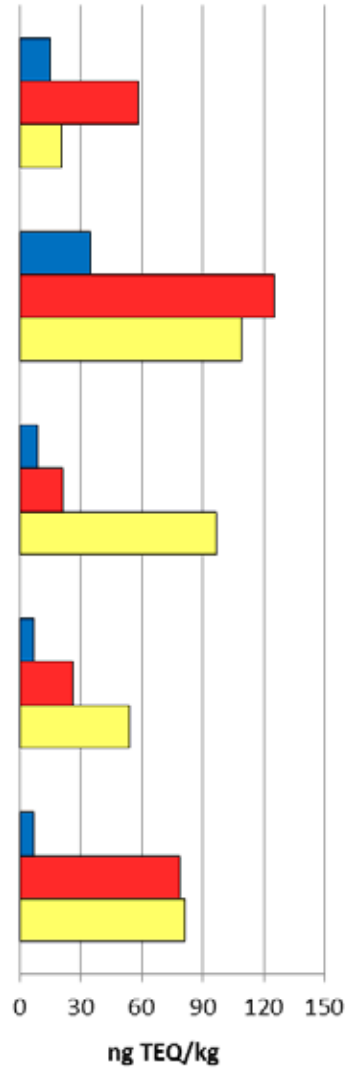
Surface and Subsurface Contributions



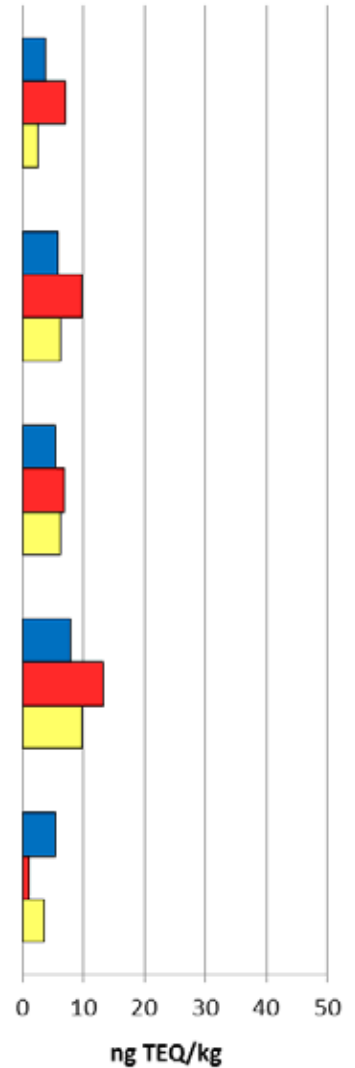
Legend

- Factor
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d. Southern East Bay



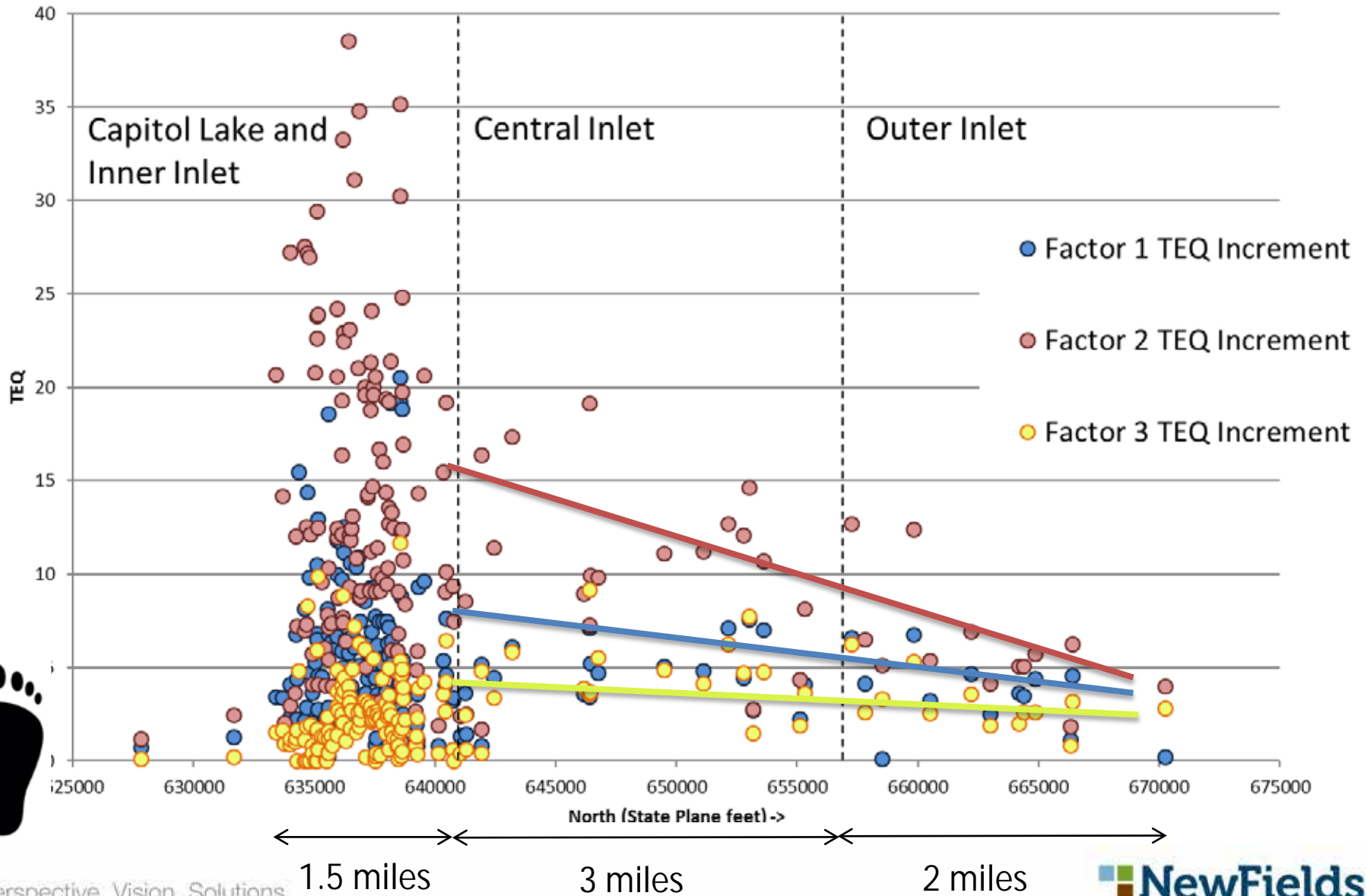
c. Central West Bay



Sources: Esri, HERE, GEBCO, USGS, FAO, Survey, Esri Japan, N, OpenStreetMap contributors, and the GIS User, Cor



Surface Sediment Fractional Contribution



Summary

- Chemometric methods can be used to differentiate dioxin/furan signatures in sediments.
- Three distinct signatures were identified, and each could be traced to a historical source or process.
- Identified profiles have a distinct spatial footprint within surface sediments, which can be used to approximate the extent of point source contributions.

Report available at:

<https://fortress.wa.gov/ecy/publications/documents/1609101.pdf>

Thanks

Tim Hammermeister – NewFields

Jon Nuwer – NewFields

Pete Striplin – WA Dept. of Ecology

Chance Asher – WA Dept. of Ecology

Budd Inlet Circulation

