



Use of Receptor Models to Evaluate Sources of PAHs in Sediment

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Key Messages

- Receptor models are being increasingly used in PAH source evaluations
- They are powerful tools, but have important limitations
- Model complexity cannot eliminate uncertainty
- When applying:
 - Present multiple lines of evidences
 - Utilize negative controls where appropriate

Receptor Models

▪ **Mixing Models**

- **Example:** EPA Chemical Mass Balance (CMB)
 - Modeler pre-identifies sources and inputs profiles
 - Model calculates best fit to the receptor (sediment) data to estimate relative contributions

▪ **Unmixing Models**

- **Example:** EPA UNMIX, PMF
 - Model uses receptor data to identify potential source profiles
 - Model calculates best fit to the receptor data to estimate relative contributions
 - Modeler compares identified source profiles to potential sources

Two Typical Uses for Receptor Models

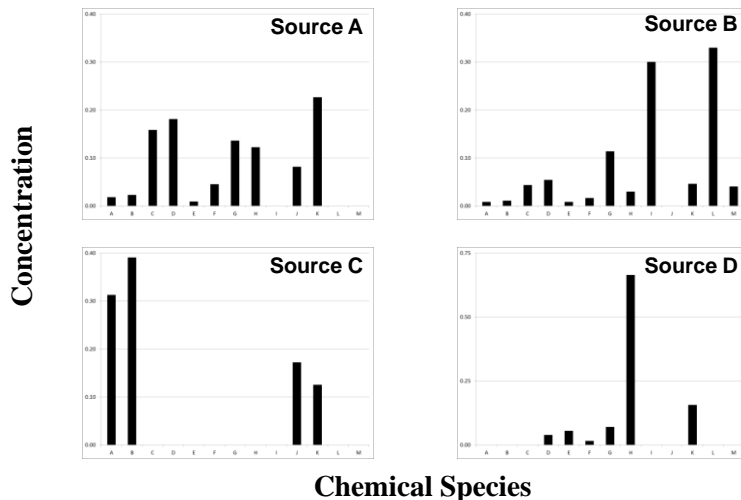
- **What are the fractional contributions of potential sources?**
- **What is the contributions of a release with a known source profile?**

General Assumptions of Receptor Models

1. All sources with a potential for contributing to the receptor have been identified
2. Source profiles are constant
3. Source profiles are linearly independent of each other
4. Chemical species are stable
5. Measurement uncertainties are random, uncorrelated, and normally distributed

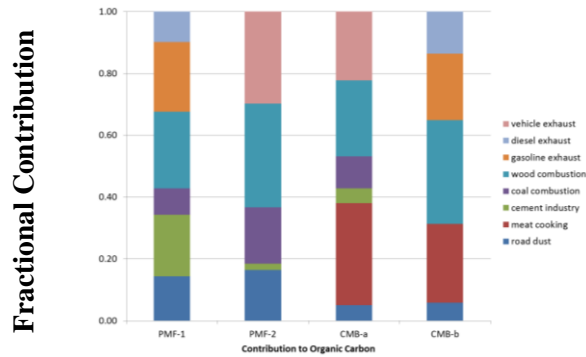
Source: Galarneau 2008

EPA's CMB and UNMIX were Developed for Evaluating Atmospheric Sources with Distinct Chemical Profiles



Source: Gordon 1988

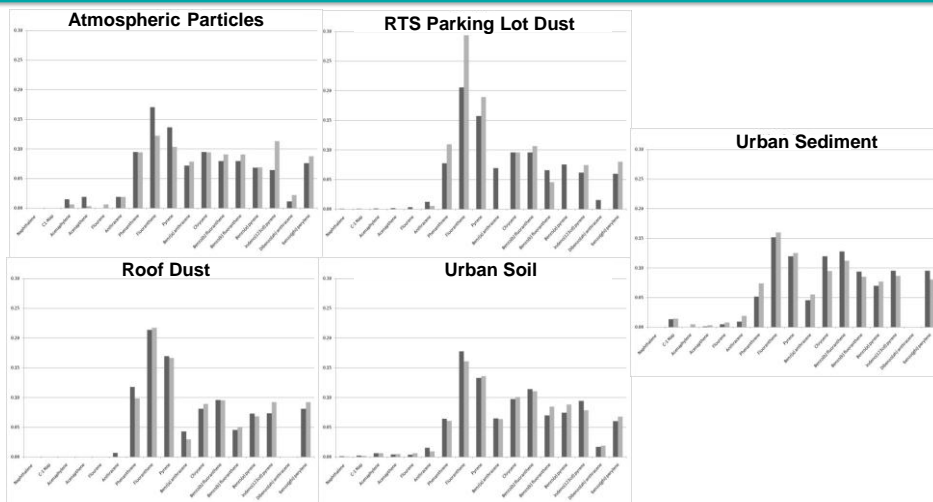
Even for “Simple” Systems, Receptor Model Results can be Highly Sensitive to Model Inputs



The calculated source contributions of organic carbon in atmospheric PM_{2.5} differs by model type and inputs.

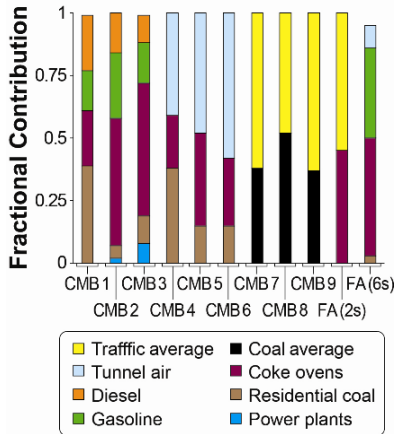
Data from Ke et al 2008

Similarity Between and Variability Within Pyrogenic PAH Source Profiles can Limit Models



From O'Reilly et al 2012

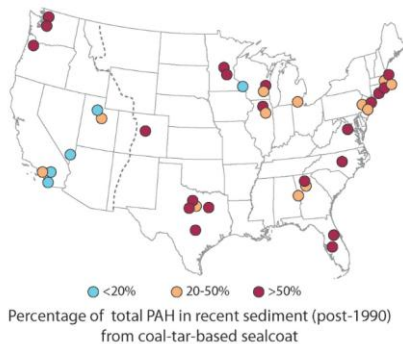
Providing the Results of Different Models with Various Source Inputs Should be Considered



- An evaluation of sources of PAH in sediments to a lake in Chicago used a range of source profiles.
- Applied a mixing (CMB) and unmixing (Factor Analysis) model

From: Li et al (2003) and Bzdusek et al (2004)

Case Study: Use of CMB to Evaluate of the Role of Refined Tar Pavement Sealers (RTS) in Urban Lake Sediments



- USGS researchers used CMB to test the hypothesis that RTS is a significant PAH source (Van Metre and Mahler, 2010)
- Results being used to advocate product bans
- Lack of negative controls limited value for hypothesis testing

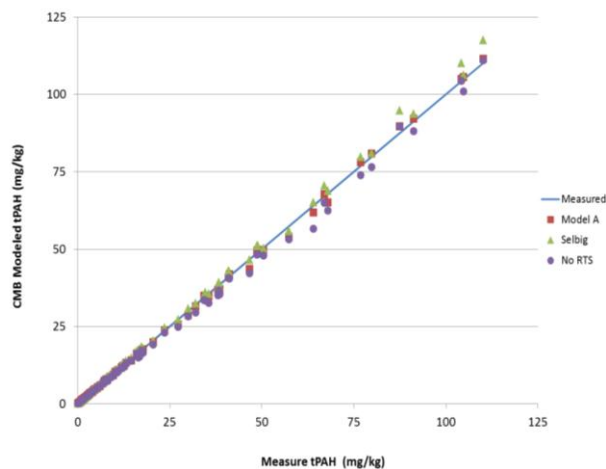
http://water.usgs.gov/nawqa/home_maps/sealcoat.html

Hypothesis Testing Requires a Negative Control

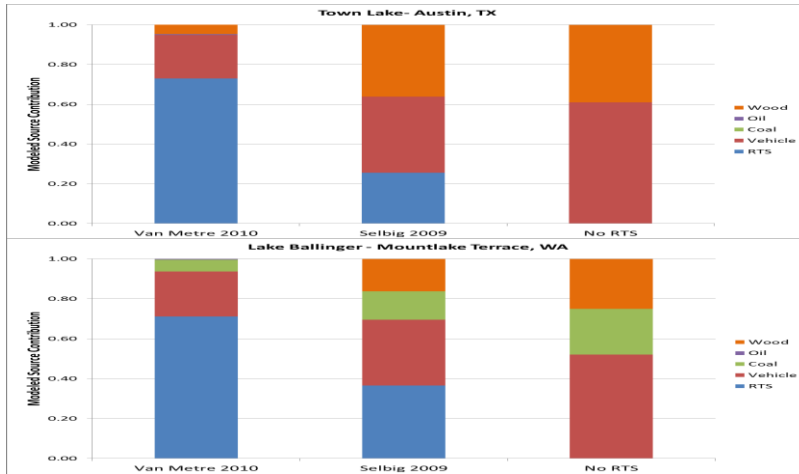
- **Comparison of three CMB Model runs**
 - **Published Results:** Model A from Van Metre et al. 2010. RTS source profile is the mean of dust from six sealed lots.
 - **Negative Control:** Did not include RTS as a source profile. Remaining sources from Van Metre et al. 2010.
 - **Different RTS Source Profile:** Replaced Van Metre RTS with Selbig (2009) mean of 9 RTS lot runoff samples. Remaining sources from Van Metre et al. 2010.

Excellent Match Between Measured and Modeled Concentrations Without RTS as a Source Input

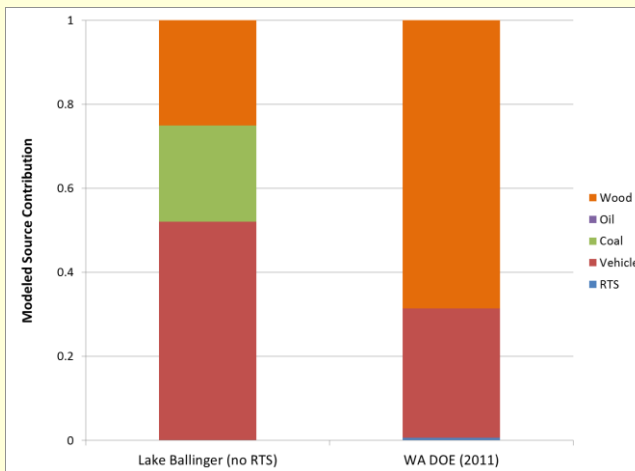
$R^2 > 0.996$ for each method



The PAH Profile of Lake Sediments can be Modeled Without Any RTS Contribution

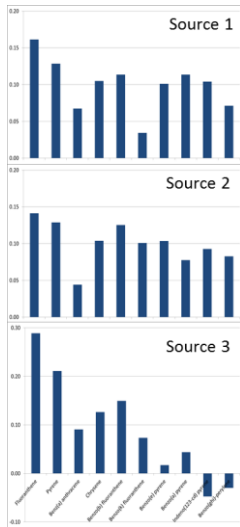


Multiple Lines of Evidence: Comparison of RTS Free Model Output with Regional Emission Source Study



WA DOE (2011) Assessment of Selected Toxic Chemicals in the Puget Sound Basin

Multiple Lines of Evidence: PAH Source Profiles Identified by UNMIX are More Similar to Sources Other Than RTS



	Source 1	Source 2	Source 3
Coal-related	0.65	0.53	0.91
Traffic-related	0.70	0.70	0.76
Wood	0.68	0.62	0.86
Fuel oil	0.68	0.54	0.33
Soil	0.82	0.89	0.89
Highway	0.86	0.83	0.73
Roof dust	0.84	0.78	0.75
RT lot dust	0.82	0.84	0.86
RT sealer	0.76	0.59	0.86

Van Metre and Mahler (2010) extended 8 lake data set used as input to UNMIX. Results support that sediments are impacted by a mix of pyrogenic sources. They are not more similar to sealer than other sources.

From O'Reilly et al 2012

RTS Evaluation Summary

- **Receptor models do not support the hypothesis that RTS is a significant source of pahs in sediments**
 - The correlation between modeled and measured total PAH concentrations were similar with or without RTS
 - The PAH profile of sediment from all 40 lakes can be characterized without any contribution of RTS
 - UNMIX suggests potential source types that are more similar to other sources than they are to RTS

Key Messages

- **Receptor models are powerful tools, but have important limitations**
- **Model complexity cannot eliminate uncertainty**
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 - Present multiple lines of evidences
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References

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