

A Knowledge-Based Reasoning for the Interpretation of PAH Data

Progress Report for the Period: 12 April to Sept 15th, 2007

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Introduction/Abstract

PAHs have multiple sources, but in aquatic urban environments, they are essentially always encountered as a composite mixture. An understanding of the localized inputs of PAHs observed in a given area of interest is a crucial foundation for any management decision: appropriate control or remedial actions cannot be evaluated until there is a thorough understanding of where the PAHs observed actually came from.

This project is to develop a knowledge-based model for the attribution of PAH source types. The overall model analyses available PAH data against multiple sub-models for indicating PAH source types. Each sub-model generates an estimate of the likelihood that the set of PAH observations came from that type of PAH source. The primary sources are either petrogenic or pyrogenic ones. The two preferred sub-models for these major source types relies on a full suite of PAH data that would include alkylated PAHs. It is based on the observation that crude oil sources have a progression of increasing concentration within five different homologue series.

Accomplishments

Scheduled Tasks

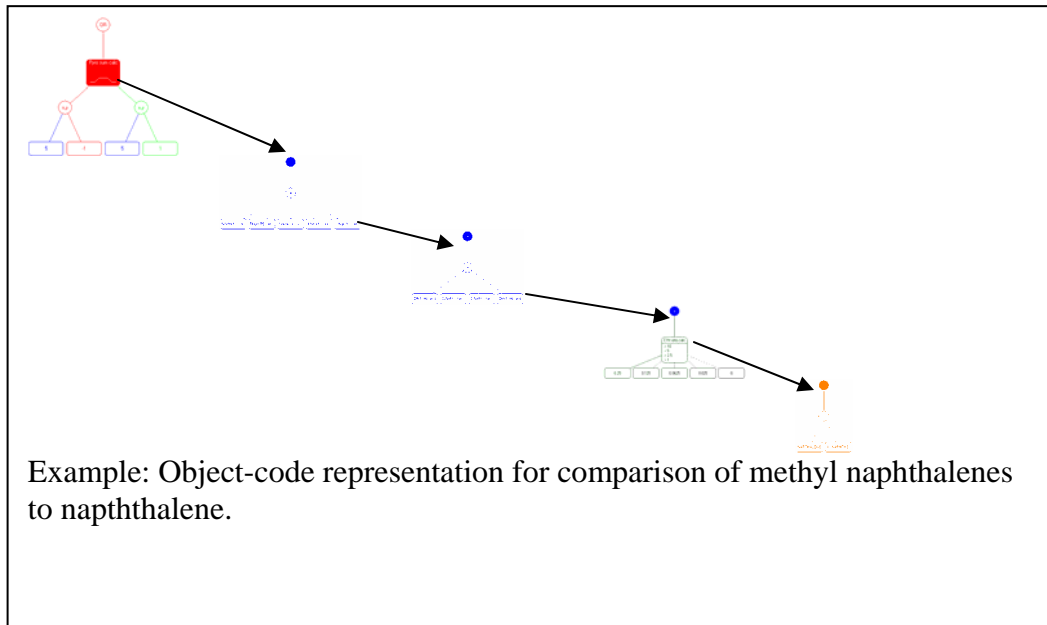
- 1 - Secure training on software
- 2 - Conduct literature search on indices
- 3 - Build draft model
- 4 - Test model against PAH data sets
- 5 - Refine model as appropriate

Progress on These Tasks

- 1 – Training was arranged for the last week of June
- 2 – Numerous additional references were collected on indices during July/August
- 3 – The preferred model using full PAH chemistry for both pyrogenic and crude oil source types has been drafted. Also, numerous sub-models using censored data have been drafted. These models assign the likelihood that the PAHs observed belong to petrogenic sources and also to pyrogenic sources.

The overall model potentially makes calls to over 60 analytes and makes over 80 calculations.

The following illustration displays just one small portion of the object-level programming which conducts one of the 15 homologue comparisons performed by the sub-model for pyrogenic sources; assigns an index value for that homologue according to the degree of its presence, and then ranks the sum of the 15 individual indices for their likelihood of representing a pyrogenic source.



If the available PAH data is censored (ie, includes only priority pollutant PAHs), the overall model defers to other sub-models which calculate a variety of indicator indices.

Tasks for the next Reporting Period

The model will next be tested by analyzing several data sets associated with known or suspected source types to determine model performance.