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Tracking polychlorinated biphenyls (PCBs) congener patterns in Newark Bay surface sediment using principal component analysis (PCA) and positive matrix factorization (PMF)

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HIGHLIGHTS

• PCB congener data for Newark Bay surface sediments were obtained.

• Data analyzed using PCA and PMF.

- Five factors from PMF; all related to the PCA loading plot.
- Each PMF factor identifies source areas from which the different PCBs originate.
- PMF has the ability to provide additional interpretation over the PCA scores plot.

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ABSTRACT

PCB congener data for Newark Bay surface sediments were analyzed using PCA and PMF, and relationships between the outcomes from these two techniques were explored. The PCA scores plot separated the Lower Passaic River Mouth samples from North Newark Bay, thus indicating dissimilarity. Although PCA was able to identify subareas in the Bay system with specific PCB congener patterns (e.g., higher chlorinated congeners in Elizabeth River), further conclusions reading potential PCB source profiles or potential upland source areas were not clear for the PCA scores plot. PMF identified five source factors, and explained the Bay sample congener profiles as a mix of these Factors. This PMF solution was equivalent to (1) defining an envelope that encompasses all samples on the PCA scores plot, (2) defining source factors that plot on that envelope, and (3) explaining the congener profile for each Bay sediment sample (inside the scores plot envelope) as a mix of factors. PMF analysis allowed identifying characteristic features in the source factor congener distributions that allowed tracking of source factors to shoreline areas where PCB inputs to the Bay may have originated. The combined analysis from PCA and PMF showed that direct discharges to the Bay are likely the dominant sources of PCBs to the sediment. Review of historical upland activities and regulatory files will be needed, in addition to the PCA and PMF analysis, to fully reconstruct the history of operations and PCB releases around the Newark Bay area that impacted the Bay sediment. © 2013 Elsevier B.V. All rights reserved.

1. Introduction

Newark Bay, located in northeastern New Jersey, USA, encompasses an area roughly six-miles long and one-mile wide and it is joined with four major tributaries: Passaic River, Hackensack River, Arthur Kill, and Kill van Kull (Fig. 1). In the late 1970s, elevated levels of PCBs found in fish samples collected from Newark Bay (Bay) and its tributaries raised health concerns [1]. As a result, characterization of a wide range of pollutants in the Bay's sediments has been ongoing since 1990 [1–17]. These sediment studies, which measured PCBs as a select group of dioxin-like congeners, homologues, and conventional Aroclor quantities, provided information on the spatial and temporal distribution of PCBs in Newark Bay. (For example, Iannuzzi et al. [2] suggested that the greater portion of PCBs in Newark Bay resulted from direct discharges into the Bay. The major tributaries feeding into Newark Bay were not the primary sources.) However, the pre 2005 data sets were inadequate for a quantitative evaluation of PCB congener patterns and potential upland source areas because of a limited number of congeners being analyzed.

Starting in 2006, a more complete set of PCB congeners were analyzed for in Newark Bay sediment [18–20]. These more recent







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Fig. 1. Surface sediment sampling locations.

studies provided a robust data for identifying congener profiles of potential PCB sources and their spatial distribution. In 2011, the United States Environmental Protection Agency (USEPA), under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA; i.e., Superfund), designated Newark Bay and its confluences with the Hackensack River, Passaic River, Arthur Kill, and Kill van Kull as the Newark Bay Study Area (NBSA) [21].

In this work, the pattern of PCB congeners in sediments from Newark Bay was tracked by analyzing the surface sediment congener data generated from the recent and comprehensive CERCLA sediment studies by using principal components analysis (PCA) and positive matrix factorization (PMF). These numerical tools are well suited for identifying and separating contaminant patterns in sediments (e.g., [22,23]). The outcome from the PCA and PMF analyses were compared to one another to explore how the PMF end member sources (Factors) are derived from and related to the PCA scores analysis. Collectively, PCA and PMF enabled tracking of PCB congener patterns in the surface sediment and identifying of source areas from which these PCBs may have originated.

2. Methods - sediment sampling and laboratory analysis

PCB congener data used in this work are publically available at www.ournewarkbay.org, and includes:

- The NBSA 2005 Phase I and 2007 Phase II Remedial Investigation (RI) sediment sampling programs. The data include PCB homologue and congener data for 129 surface sediment samples.
- The 2007–2008 USEPA RI sediment sampling program at river mile (RM) 0 to RM1 of the Lower Passaic River. The data include PCB homologue and congener data for 14 surface sediment samples.

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