

Application of Pattern Recognition Techniques to Evaluate Polychlorinated Dibenzo-*p*-dioxin and Dibenzofuran Distributions in Surficial Sediments from the Lower Passaic River and Newark Bay

RICHARD J. WENNING,*¹ MARK A. HARRIS,† BRENT FINLEY,‡
DENNIS J. PAUSTENBACH,‡ AND HADLEY BEDBURY†

**ChemRisk—A Division of McLaren/Hart, Stroudwater Crossing, 1685 Congress Street, Portland, Maine 04102*; †*ChemRisk—A Division of McLaren/Hart, 1135 Atlantic Avenue, Alameda, California 94501*; and ‡*Maxus Energy Corporation, 717 North Harwood, Dallas, Texas 75201*

Isomer-specific determinations of polychlorinated dibenzo-*p*-dioxins (PCDDs) and dibenzofurans (PCDFs) were performed in 19 surficial sediment samples collected from the lower Passaic River and Newark Bay, New Jersey. Total PCDD and PCDF concentrations ranged from 415 to 23,300 ng/kg (dry wt) and 37 to 8400 ng/kg, respectively. OCDD and OCDF were the predominant congeners in all samples, followed by the hepta-, hexa-, tetra-, and penta-chlorinated compounds. Forty-seven percent (9/19) of the sediment samples contained no detectable levels of 2, 3, 7, 8-TCDD. The concentrations of 2, 3, 7, 8-TCDD and 2, 3, 7, 8-TCDF ranged from nondetect to 510 ng/kg (geometric mean of 5 ng/kg) and from 2.8 to 480 ng/kg (geometric mean of 13 ng/kg), respectively. The composition of PCDD/Fs in sediments was evaluated using chemometric pattern recognition techniques. Principal components analysis and complete linkage:farthest neighbor cluster analysis revealed the presence of at least five distinctive fingerprint patterns in surficial sediments collected from different locations in the Newark Bay estuary. Differences among PCDD/F patterns were attributable to the relative presence or absence of 1, 2, 3, 4, 6, 7, 8-HpCDF and the hepta-, hexa-, and octa-chlorinated congeners. To determine whether the presence of PCDD/Fs in sediments could be associated with a single source, residues in sediments were compared to those found in three soil samples and one sump sediment sample from a former 2, 4, 5-T manufacturing plant. Significant compositional differences were observed between the two data sets. Fingerprint patterns in sediments were dominated by the higher PCDD/F chlorinated congeners and contained significantly lower levels of the tetra-chlorinated congeners, particularly 2, 3, 7, 8-TCDD, than soils from the former 2, 4, 5-T plant. These differences, as well as those observed among surficial sediments from different locations, indicate that there are clearly several different sources of 2, 3, 7, 8-TCDD and other PCDD/Fs to the estuary.