SPATIAL ANALYSIS OF PCDD, PCDF, AND PCB SOIL CONCENTRATIONS FROM A COMMUNITY IN MICHIGAN, USA

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Introduction

The University of Michigan Dioxin Exposure Study (UMDES) was undertaken in response to concerns among the population of Midland and Saginaw Counties that the discharge of dioxin-like compounds from the Dow Chemical Company facilities in Midland has resulted in contamination of soils in the Tittabawassee River flood plain and areas of the City of Midland. There is concern that people's body burdens of polychlorinated dibenzodioxins (PCDDs), polychlorinated dibenzofurans (PCDFs), and polychlorinated biphenyls (PCBs) may be elevated because of the environmental contamination. A central goal of the UMDES was to determine the factors that explain variation in serum congener levels of PCDDs, PCDFs, and PCBs, and to quantify how much variation each factor explains.

Residential soil concentrations of PCDDs, PCDFs, and PCBs were included as one of the potentially explanatory factors. Due to respondent ineligibility and non-consent, not all UMDES respondents had their soil sampled and analyzed. Missing values in UMDES were addressed using an imputation process described elsewhere.[1] This report serves to: describe the process that was used to create spatially-based soil concentration predictions for use as an input to the imputation process; to describe elements of the spatial structure of the soil data; and to compare the spatial structure of the data both by congener and by region. Overall study results are described elsewhere.[2]

Materials and Methods

Respondent Selection: Five populations in Midland, Saginaw, Bay, Jackson, and Calhoun Counties, Michigan, USA were sampled using a two-stage area probability household sample design. In order to be eligible for participation in the soil and vegetation sampling portion of the UMDES, subjects had to have lived in their residence at least five years and had to be the owner of their residence and property. A more detailed description of the populations and respondent selection methodology is reported elsewhere.[3]

Soil Sampling and Compositing: Each selected property was sampled in multiple locations from the surface to a depth of 6 inches. Selection of locations for sampling followed a protocol that identified the house perimeter, property areas where direct contact with the soil was likely (gardens), and areas in the flood plain of the Tittabawassee River. Each sampling station was defined by laying out a 3-foot diameter sampling ring. Three cores within the ring were collected using single-use polycarbonate tubes. The exact sampling location was recorded using a handheld global positioning system (GPS). In the laboratory at the University of Michigan, soils were extruded from the sealed polycarbonate tubes and the soil cores were separated into three strata: the 0-1 inch (2.5cm) and bottom 5 inches (12.5 cm), and vegetation. The three strata of each soil set (residence zone, soil contact, or flood plain) were combined and homogenized. Detailed soil and vegetation sampling procedures can be found elsewhere.[4,5]

Analytic Sequence: The complete decision sequence of which soil and vegetation samples were analyzed is shown elsewhere[3]. Briefly, the 0-1 inch house perimeter composite samples were analyzed for all properties. If any part of the property was in the flood plain, then all remaining composites (1-6 inch and vegetation house perimeter; 0-1 inch, 1-6 inch and vegetation flood plain; and 0-6 inch and vegetation soil contact) were also submitted for analysis. If the respondent did not live in the flood plain, but had a vegetable garden or worked in a flower garden, the 0-6 inch and vegetation composites for the soil contact set were analyzed. If the TEQ of the 0-1 inch house perimeter composite for any property outside the floodplain was > 8 pg/g, then the 1-6 inch and vegetation house perimeter composites were subsequently analyzed.

Analysis of Samples: All soil and vegetation samples were analyzed for the WHO designated 29 PCDD, PCDF and PCB[6] Congeners performed by Alta Analytical Laboratory, Inc. (El Dorado Hills, California, USA) by following the US EPA Method 1688A[7]and US EPA Method 8290.[8] Congeners were extracted from soil samples and quantified using high-resolution gas chromatography/high-resolution mass spectrometry (HRGC/HRMS).

Determination of Appropriate Sample Groupings for the Creation of Prediction Maps: Five populations (flood plain, near flood plain, plume, Midland/Saginaw general, and Jackson/Calhoun) in two distinct geographic regions were sampled. The population in Jackson and Calhoun counties was separated geographically from the other populations in the study, and was therefore treated separately in the geostatistical prediction process. The remaining four populations were all located in the same geographic region. However, it was assumed that the deposition mechanism, and therefore the spatial structure, of PCDD, PCDF, and PCB concentrations was different for the flood plain population than for the remaining Midland/Saginaw/Bay county populations. Therefore, the flood plain population was also treated separately. The remaining three populations were all treated together.

Ordinary Kriging: Ordinary kriging is a member of the kriging family of generalized least squares algorithms commonly used for interpolating spatial data. The system of equations for ordinary kriging algorithm can be found elsewhere.[9] Ordinary kriging was used to produce a prediction map for each of the WHO designated PCDD, PCDF, and PCB congeners for each of the sample groupings described above. Due to the large number of prediction maps that needed to be created and the large number of input parameters that may be used to create a prediction map using ordinary kriging, an efficient optimization procedure was developed for the determining the appropriate input parameters for use with the Geostatistical Analyst Extension for ArcMAP 9.1.[10] Using TEQ as an indicator parameter, exploratory analysis indicated the five parameters that most substantially affected the predictive capability for each region. Table 1 presents the parameters and the value range for which they were tested in the optimization procedure for each congener for each region. The goal of the optimization procedure was to minimize the root mean square error, a commonly used measure of prediction accuracy[9], of the predictions as measured by cross-validation. All other input parameters were left as the ArcMAP default values.

Parameter	**Parameter values tested**
Anisotropy	None or ArcMAP calculated default
Number of lags	n/15 to n/25
Semivariogram model type	Spherical, Gaussian, Exponential
Neighbors to include	5 to n/2
Neighborhood shape	Single cell, 4 cell diagonal spokes, 4 cell straight spoke, 8 cell

Table 1: Parameters and parameter values used in ordinary kriging optimization procedure. Parameters were tested in the order listed. n=number of samples in data set being used to create prediction map.

From the optimized prediction map for each congener, the predicted house perimeter 0-1 inch value was generated for all study respondents. Additionally, for respondents in the flood plain population, the congener-specific predicted flood plain 0-1 inch and flood plain 1-5 inch concentrations were generated. For study respondents who had soil samples, the locations recorded using GPS were used. For the locations of the respondents who were missing soil samples, locations were created from the geo-coded addresses using ArcMAP.

Inter-property Correlations: A separate scatter-plot of the relationship of the house perimeter 0-1 inch concentrations and the concentrations for each other sample set and stratum (house perimeter 1-5 inch, house perimeter vegetation, soil contact 1-6 inch, and soil contact vegetation) was created for each congener. A linear regression was fit to each plot. Using the equation for the linear regression, a predicted value for each sample type was created from the predicted house perimeter 0-1 inch sample for each of the other sample set and stratum.

Results and Discussion

The predictive capability of both the ordinary kriging and the inter-property correlation procedures was dependent both on region and congener. Complete results and discussion will be available after study results have been presented to the affected communities in August of 2006.

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