APPLICATION OF PRINCIPAL COMPONENTS ANALYSIS AND SEQUENTIAL GAUSSIAN SIMULATION TO A COMPREHENSIVE SOIL SAMPLING DATASET TO PREDICT PCDD/F CONCENTRATIONS IN MIDLAND, MI

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Introduction:

Dioxin and furan concentrations measured in the City of Midland, MI are believed to be primarily the result of air deposition from historic sources. To predict soil TEQ across the City of Midland, a two-part analysis was performed: 1) principal components analysis (PCA) to identify soil samples that reflected a deposition fingerprint, and 2) geostatstical modeling based on a sequential Gaussian simulation (SGS) to predict soil TEQ in areas across the City of Midland that had not been sampled.

Materials and methods:

A soil sampling dataset comprised of 516 sample was obtained from Dow Chemical. The soil samples in this dataset were collected between 1983 to 2008 by a various entities (eg, MDEQ, USEPA, Dow Chemical) from a wide range of environments (e.g., residential, commercial/industrial, agricultural, flood plain). Data believed to reflect non-deposition related sources (e.g. on-site samples, the 5-year flood plain, core samples at depth, near a haul road) were set aside. Principal components analysis (PCA) was then employed on the remaining samples using 2,3,7,8 substituted PCDD/F congeners to identify an air deposition related fingerprint in Midland. Those soil samples that were set aside were then re-evaluated using PCA, and in cases where those samples were determined to indicate a deposition fingerprint, those samples were retained in the soils dataset considered for further evaluation. This process resulted in 175 samples in the City of Midland that were believed to clearly reflect the influence of airborne PCDD/F deposition.

In our analysis, three historic PCDD/F combustion sources were modeled using AERMOD to produce estimates of TEQ deposition (wet particle, dry particle, wet vapor, dry vapor) and air concentration (particle and vapor) for two receptor sets: 1) a grid that reflects the specific soil sample locations used in the analysis, and 2) a generic grid covering the City of Midland (with 50 meter spacing, 68,121 points total). Soils data were normal score transformed (NST), and the NST data were regressed with the deposition and concentration estimates generated using AERMOD. The resulting regression model was used to generate a trend for the generic grid, and the regression residuals were modeled using a semivariogram. The residuals and the semivariogram were then included in a SGS analysis and 100 TEQ estimates were generated at each point on the generic grid.

Results and discussion:
Using the results of the SGS (100 realizations at each point on a 50 meter grid across Midland) summary statistics were generated for each point in the generic grid to represent central tendency and high-end soil concentrations. Uncertainty is modeled across the City of Midland by calculating the coefficient of variation (standard deviation divided by the mean) at each point in the generic grid. This allows for the visualization of locations where the standard deviation is high relative to the mean predicted soil TEQ. Finally, crossplots are presented in which measured concentration vs. modeled concentration (e.g., mean, 95% UCL on the mean) are plotted as X and Y for each soil sample in Midland. This allows for the identification of the extent of conservatism for different ranges of measured soil TEQ.

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References:
1. Goovaerts, P., Trinh, T., Demond, A., Franzblau, F., Garabrant, D., Gillespie, B., Lepkowski, J., Adriens, P. *Geostatistical Modeling of the Spatial Distribution of Soil Dioxin in the Vicinity of an Incinerator. 1. Theory and Application to Midland, Michigan*. Environmental Science and Technology, 2008. 42, 3655-3661.

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