VALIDATON OF THE AERMOD AIR DISPERSION MODEL: APPLICATION TO CONGENER-SPECIFIC DIOXIN DEPOSITION FROM AN INCINERATOR IN MIDLAND, MICHIGAN

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Abstract

AERMOD dispersion and deposition modeling of ten priority dioxins and furans in the emission profile of the Dow Chemical Company incinerator was coupled to geostatistical modeling of soil dioxin data collected in Midland (MI) as part of the University of Michigan Dioxin Exposure study to validate the emissions model output. Wet and dry deposition fluxes explained 40-80% of the trends in soil dioxins and 25-40% of furans, based on regression analysis. By applying accuracy plots and goodness-of-fit approaches to Gaussian simulations of 100 realizations, we were able to quantify the accuracy of the model. Except for PeCDF and OCDD, the predictions of concentrations at 68 sampling locations are accurate and precise. Close to the plant, the true soil measurements fall into the upper tail (75%) of model predictions, and the model predictions were more accurate at greater distance from the incinerator. Congener-specific deposition estimates using AERMOD resulted in an increase of the total predicted TEQ of soil values relative to ISCT3 estimates based on stack TEQ emission data.

Introduction

During 2002-2004, the University of Michigan Dioxin Exposure Study (UMDES) conducted a soil sampling campaign in Midland, MI to assess whether exposure to incinerator emissions is a significant contributor to blood serum of residents living in the plume region. Our previous AERMOD modeling results[1] indicated that the dioxin deposition fluxes are dominated by the higher chlorinated compounds (HpCDD, OCDD, HpCDF and OCDF). We observed that dry deposition of gas-phase dioxins is important for the lesser-chlorinated PCDD/F congeners (tetra- and pentaCDD/F), with contributions ranging from 30 to 50% to the total deposition. Wet deposition is less important for these congeners, but this process contributes 10% of the deposition of higher chlorinated congeners (OCDD, OCDF).

Cross validation of air dispersion models such as ISCST3 and AERMOD is limited. Model validation for AERMOD is done by comparison of model predictions (air concentrations) against the available air samples. Although AERMOD or ISCST3 can predict contaminant deposition fluxes, the direct comparison of model outputs and ground level concentrations of contaminants are more difficult. Often air dispersion model is coupled with soil models or statistical models to obtain soil concentration predictions. Among these model modifications, a probabilistic approach allows assessing local uncertainties of the predictions, as we detailed in previous papers[2,3]. This paper further explores the air dispersion model and geostatiscal modeling approach to predict spatial distribution of specific dioxin congeners emitted from the incinerator in Midland.

Materials and Methods

Air dispersion modeling: The modeling area is a 261x261 grid (spacing = 50m) centered on the incinerator but excluding the plant property. Each grid node is considered as a receptor in the AERMOD model. Five year (2001-2005) meteorological data used as input files to AERMOD were provided by the Michigan Department of Environmental Quality (MDEQ) for the weather station at Midland-Bay-Saginaw (MBS). Emission rates of the 10 dioxin congeners are identified with the real emission measured in 1992 (EPA)[4] for the 830 incinerator stack and adjusted based on the new WHO-$TEF_{D/F}$ 2005 scheme. As deposition of dioxins is associated with particles, particle size distribution, particle fraction and particle diameters are important parameter inputs in the deposition algorithm (AERMOD). In addition, dioxin congeners are distributed between vapor and particulate phases; therefore vapor/particle partitioning is considered. The dioxin-bound particulate percentage, particle size characterization and real emission rates of the selected dioxin congeners were reported earlier (Trinh et al., 2008). AERMOD runs were conducted using both vapor and particle deposition using the actual emission rates for dioxin congeners from the incinerator in 1992, and TEQ emissions in 1984. Model outputs (air concentration, total deposition, wet and dry deposition fluxes) were then modified for each congener to reflect the proportion of dioxins partitioned into vapor and particulate phases[1,5].

Geostatistical modeling: The relationship between the output of the air dispersion model (dry and wet depositions) and field data (normal score transformed values of congener concentration) is modeled using linear regression. The regression function is later applied to the entire 261x261 grid, generating a spatial trend that is incorporated in Sequential Gaussian simulation (sGs). One hundred grids of simulated congener concentrations were generated by sGs using the semivariogram of regression residuals and the 68 UMDES soil data. The concentration at each receptor point is predicted as the average of 100 simulated values. Data visualization is conducted using STIS software (Space-Time Intelligence System™, TerraSeer®.)

Model validation: The validation followed the procedures previously described for accuracy plots and goodness of fit analysis[3].

Results and Discussion

Soil data: The soil concentrations of dioxins and furans in the Midland area are very skewed, as shown in Table 1. Particularly OCDD and several furans showed the presence of extreme outliers. Extreme outliers in the distribution of the true observations will likely affect the point simulation values. As required by sequential Gaussian simulation, soil data are first normal transformed to avoid the skewedness in the data distribution.

PCDD/F	Mean	Std Dev	Std. Error	C.I. of Mean	Range	Max	Min	Median	25%	75%
TCDD	21.2	23.2	2.8	5.6	116.1	117	0.9	12.9	4.1	29.7
PeCDD	10.2	8.9	1.1	2.2	41.6	42.3	0.7	8.3	3.6	14.0
HxCDD	7.9	7.4	0.9	1.8	36.1	36.9	0.8	5.9	3.2	10.0
HpCDD	350.1	300.2	36.4	72.7	1557.6	1600.0	42.4	272.0	136.5	495.5
OCDD	3241.8	2779.3	337.0	672.7	14965.0	15300.0	335.0	2655.0	1170.0	4600
TeCDF	46.5	212.6	25.8	51.5	1718.9	1720.0	1.1	6.4	2.7	19.9
PeCDF	25.2	99.9	12.1	24.2	820.7	822.0	1.3	6.3	3.1	15.2
HxCDF	26.1	85.0	10.3	20.6	682.6	684.0	1.4	9.5	4.3	19.0
HpCDF	140.9	157.0	19.0	38.0	866.6	885.0	18.4	93.9	41.4	169.5
OCDF	353.7	685.6	83.1	165.9	5471.1	5500.0	28.9	217.0	79.2	394.5

Validation study. Each of the 68 UMDES data was compared to the distribution of 100 TEQ values simulated at the closest grid node. Generally, the true soil values tend to fall within the upper tail of the simulated local distributions for locations, which are close to the source incinerator. Further from the source, the true soil values are better captured within the 25-75th quantile range. The probability interval of the global distribution (the 68 soil available data) was plotted against the empirical probability interval of the local distribution (100 simulated values at grid node that is closest to the sampling location) to quantify the accuracy of the model of uncertainty (estimated vs. measured fractions of values).

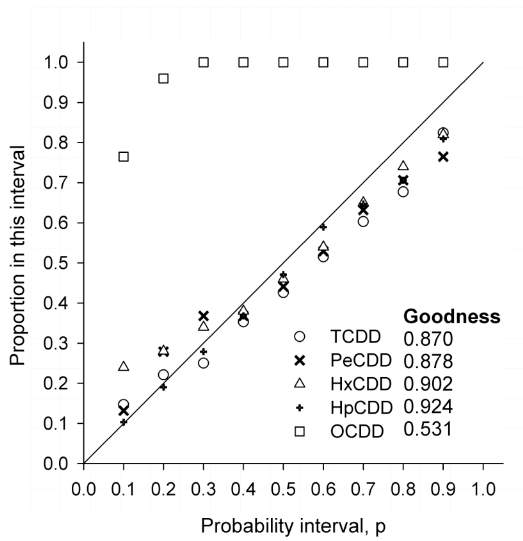

Figure 1. Accuracy plot and goodness-of-fit metrics for simulated dioxin values.

Based on the accuracy plot (Figure 1), all dioxin congeners except for OCDD are scattered around the 45° line, which indicates that the probability of simulated values to be within measured probability intervals is high. For example, at the probability interval of 0.5 (25% -75%), 45-55% of all simulated values are captured in this interval. Using this metric, OCDD simulations were highly accurate because at most probability intervals, 100% of all simulated values are captured. However, when these data are supplemented with goodness-of-fit metrics, which measures precision ('how close are the simulated values to the actual values'), simulated OCDD values are very imprecise. All other congeners concentrations are simulated with high precision (close to 1).

Geostatistical model. Dry and wet deposition fluxes of each congener were regressed against normal score transformed 68 available soil data to derive a residual trend of normal score predictions. This spatial trend and the semivariogram parameters of the normal score residuals are then incorporated in sequential Gaussian simulations. Auto correlations from the congener semivariograms are at distances of 285 m for TCDD, PeCDD, OCDF, HxCDD, HxCDF and HpCDD, at 380 m for TeCDF and 550 m for PeCDF and HxCDF; and lastly at 1700 m for OCDD. The correlation coefficients of dry deposition flux and wet deposition fluxes with normal score transformed soil data for each congener indicated that wet deposition is highly correlated (0.4-0.8) with soil congener data while dry depositions are only correlated (0.3-0.4) with the highly chlorinated congeners (HpCDD/F, OCDD/F).

These regression results based on coupled AERMOD deposition prediction and soil semivariograms were used to inform the geospatial modeling of congener-specific concentrations across the Midland region (data not shown). For comparison purposes, the TEF-weighted sum of all 10 congeners in the deposition plume was compared with the previous TEQ-based deposition using the ISCT3 model (Figure 2). A few observations can be made based on this comparison: (i) ISCT3 modeling of TEQ-based emissions results in lower soil TEQ predictions than those based on the congener-specific emissions using AERMOD; (ii) the extent of the 'soil plume' is larger based on congener-specific AERMOD models than using TEQ-ISCT3 models; (iii) generally, the extent of contamination of the highest TEQ areas around the plant is similar, indicating that the geostatistical model is robust and is not significantly influenced by the deposition models. Therefore, the differences between the prior and current soil TEQ estimates are controlled by the choice of dispersion model used, and by incorporation of congener-specific information. Lastly, considering that the correlation between wet and dry deposition and actual measured soil data was higher for congener-specific/AERMOD models (0.4-0.8) than for TEQ/ISCT3 models (<0.4), the former better predicts the soil value trends and is a better test of the hypothesis as to whether the soil contamination is driven by incinerator emissions deposition.

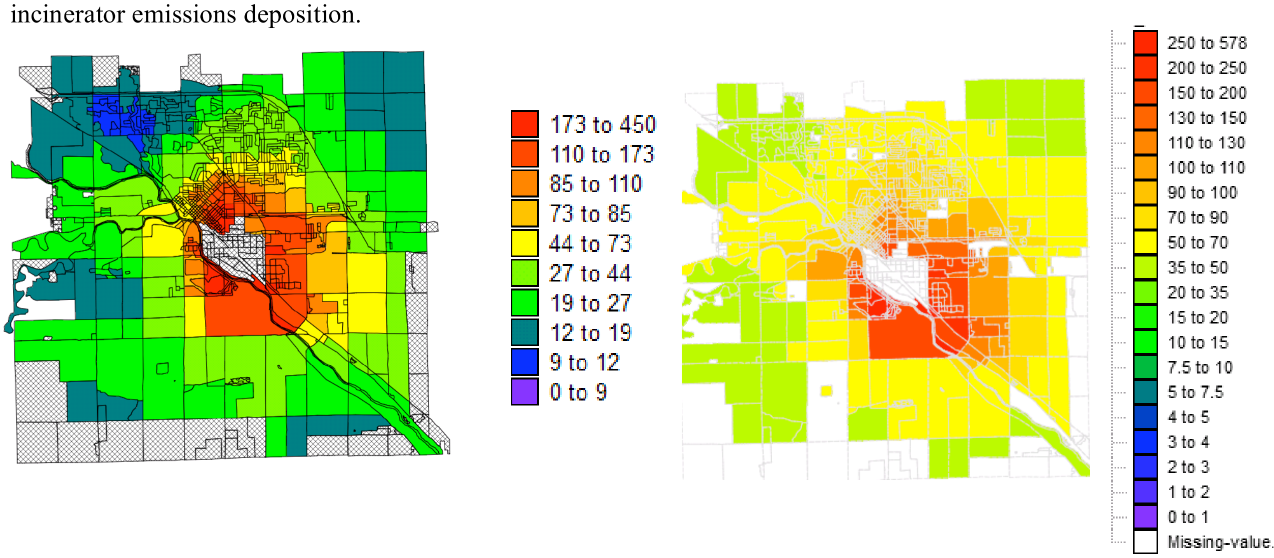

Figure 2. Mean TEQ values at the census block level (left: TEQ deposition modeled using ISCST3; right: sum of mean TEQ from 10 dioxin and furan congeners modeled using AERMOD). Scale of concentration in ng/g of soil.

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