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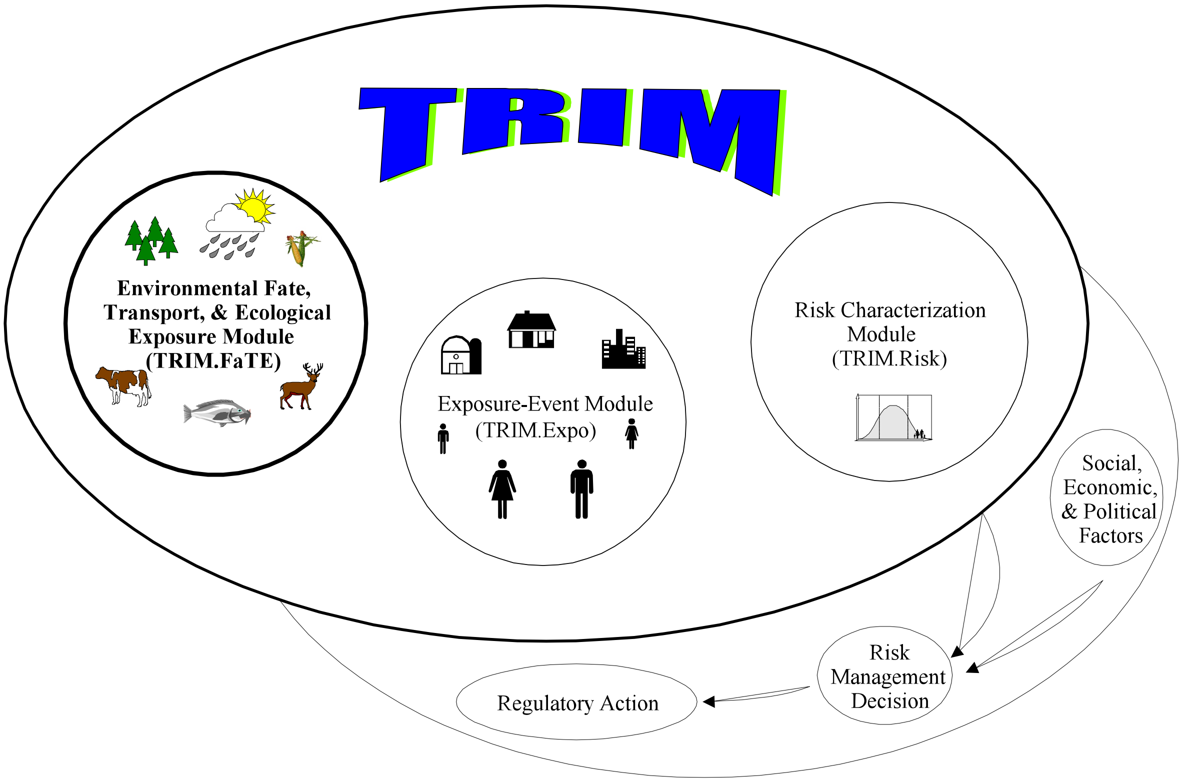
Evaluation of TRIM.FaTE

Volume III: Model Comparison Focusing on Dioxin Test Case



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Volume III: Model Comparison Focusing on Dioxin Test Case

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EXECUTIVE SUMMARY

This report is the first of two detailed reports describing the application of the TRIM.FaTE model to the emissions of dioxin-like compounds from a municipal solid waste combustion facility in Columbus, Ohio. This first report (Volume III of the Evaluation of TRIM.FaTE) describes in detail the comparison of TRIM.FaTE results to the dioxin monitoring data and modeling results presented in an earlier assessment conducted by EPA's Office of Research and Development (ORD). The second report (Volume IV) evaluates the sensitivity of TRIM.FaTE in this application to changes in emission rates and spatial resolution and to the inclusion of biotic compartments. These analyses are part of the continuing efforts to evaluate the TRIM.FaTE model and will help in guiding its further development and refinement.

The three TRIM.FaTE simulations selected for this report used different combinations of temporal resolution, emissions data, and meteorological data to facilitate comparison with the modeled and measured data presented in Lorber et al. (2000), which describes a model-to-monitor comparison of dioxin and furan concentrations in air and soil near the Columbus Municipal Solid Waste-to-Energy (CMSWTE) facility. For the comparison of air concentrations, the modeled and measured concentrations from Lorber et al. (2000) are compared to TRIM.FaTE results for a 48-hour period in March 1994. For the comparison of soil concentrations, the modeled and measured concentrations from Lorber et al. (2000) for the 1992 and 1994 emission scenarios at the 11.5 year mark are compared to TRIM.FaTE results for the same two emission scenarios and point in time. Table ES-1 presents a summary of the measured and modeled data used for the comparisons in this report.

Table ES-1. Overview of Measured and Modeled Data

Media	Measured		Modeled (TRIM.FaTE and Lorber et al. 2000)		
	Sampling Dates	Samples Collected	Emissions	Meteorological Data Used	Modeling Period Used for Comparison
Air	Mar 15-17, 1994	4	1994 stack test	1994	48-period corresponding to the sampling period
Soil	Dec 1995	32	1992 stack test	1989	Results at 11.5 years
			1994 stack test	1989	Results at 11.5 years

Each of the TRIM.FaTE simulations included in this analysis modeled the fate and transport of the same 17 individual dioxin and furan congeners addressed in Lorber et al. (2000). Emissions from the stack tests conducted at the CMSWTE facility in 1992 (Ohio EPA 1994) and 1994 (SWACO 1994) were used as the basis for chemical-specific emission rates for this analysis. The overall size and extent of the area for which pollutant fate and transport were modeled (i.e., the modeling region) were determined based on the location of the emission source, expected mobility of the chemicals of primary interest, locations of receptors of interest (e.g., monitoring stations), and watershed boundaries for the water bodies of interest. Results were presented for the group of congeners, in terms of dioxin toxic equivalents (TEQs), as well as for some congeners individually.

Overall, the TRIM.FaTE-estimated air and soil concentrations compared well with the measured and predicted concentrations presented in Lorber et al. (2000). For the air comparison, TRIM.FaTE-predicted air concentrations were compared to predicted and measured concentrations reported in Lorber et al. (2000) for four locations around the facility. A summary of these comparisons is provided in Table ES-2. The 48-hour air concentrations for dioxin TEQs from Lorber et al. (2000) and those estimated using TRIM.FaTE generally have similar magnitudes, but slightly different spatial patterns. For dioxin TEQ concentrations in air, the spatial differences in the modeling results are likely due in part to the comparison between point concentrations (from Lorber et al. 2000) and compartment concentrations (from TRIM.FaTE). The TEQ air concentrations predicted with TRIM.FaTE are generally more similar to the measured concentrations than the Lorber et al. (2000) modeling results both in magnitude and spatial pattern.

Table ES-2. Comparison of Average Air Concentrations: Measured and Modeled

Comparison Location	Pollutant	Range of Air Concentrations (pg/m^3)		
		Lorber et al. (2000)		TRIM.FaTE
		Measured Concentrations[a]	Modeled Concentrations[b]	Modeled Concentrations
1	TEQ	0.12	0.15 - 0.30	0.12 - 0.33
	OCDD	0.4	1.2 - 2.4	1.1 - 3.0
2	TEQ	0.01	0.15 - 0.30	0.0018 - 0.0081
	OCDD	0.5	2.4 - 3.6	0.016 - 0.073
3	TEQ	0	0.00 - 0.15	0.0023 - 0.0081
	OCDD	0	0.0 - 1.2	0.021 - 0.073
4	TEQ	0	0	0.00038 - 0.0026
	OCDD	0	0	0.0034 - 0.024

[a] The measured concentrations reported here are as presented in Figure 2 of Lorber et al. (2000) and, as described there, are intended to represent the TEQ concentration pertinent to the source that was modeled, taking into account a "background concentration." For example, the "0.00" entries indicate instances where the adjustment (i.e., measured concentrations minus an estimated background concentration) produced a concentration less than or equal to zero.

[b] Values were estimated from isolines (based on Figure 2, Lorber et al. 2000); ranges are presented if exact values could not be determined from the isolines.

Estimated 48-hour average air concentrations for 1,2,3,4,6,7,8,9-octachloro-dibenzo(p)-dioxin (OCDD) were also evaluated in this analysis because results for this congener were reported by Lorber et al. (2000) for these four locations. Overall, most TRIM.FaTE concentrations were similar in magnitude to the results reported by Lorber et al. (2000), with non-zero measured and modeled concentrations reported by Lorber et al. (2000) generally within an order of magnitude of the TRIM.FaTE results for corresponding locations (see Table ES-2). Zero values reported by Lorber et al. 2000 (indicating background levels) also generally corresponded to lower TRIM.FaTE results. As with the dioxin TEQ results, differences between TRIM.FaTE values and those reported by Lorber et al. (2000) may be due in part to differences in what the values represent (i.e., TRIM.FaTE average concentrations for a compartment versus measured and predicted concentrations for a discrete point from Lorber et al. 2000). However, the spatial pattern of the TRIM.FaTE results was somewhat different from those in Lorber et al. (2000). TRIM.FaTE air concentrations for OCDD were highest to the southeast of the source, which is consistent with the predominant wind direction for this time period. Both the measured and modeled concentrations reported by Lorber et al. (2000), however, were highest for the monitoring station located northeast of the source. TRIM.FaTE results corresponding to this northeast location were at least one to two orders of magnitude lower than the concentrations reported by Lorber et al. (2000), with the greatest differences apparent for the model to model comparison. It is noted that the spatial pattern of measured concentrations for OCDD – especially for the station northeast of the source – was not consistent with the pattern of measured concentrations for dioxin TEQs. It is unclear why this difference in spatial pattern occurred.

TRIM.FaTE-estimated soil concentrations were compared to predicted and measured soil concentrations reported by Lorber et al. (2000) for three spatially averaged regions. A summary of these comparisons is provided in Table ES-3. Results were generally similar, with concentrations decreasing with distance from the source and most results for comparable locations within about an order of magnitude, although some differences greater than an order of magnitude were noted. For the region closest to the source, TRIM.FaTE dioxin TEQ results were within the ranges of model-predicted and measured concentrations from Lorber et al. (2000). OCDD results were less similar within this region, with TRIM.FaTE concentration ranges roughly a factor of two higher than the modeled-predicted concentrations from Lorber et al. (2000) and a factor of three less than the measured concentrations. In areas farther from the source, TRIM.FaTE soil concentrations for both dioxin TEQs and OCDD were slightly lower than the Lorber et al. (2000) model-predicted concentrations; this trend may result from the longer soil dioxin dissipation half-life used in the modeling by Lorber et al. (2000). The TRIM.FaTE-predicted dioxin TEQ soil concentrations in these regions were slightly higher than the measured dioxin TEQ concentrations. Conversely, the TRIM.FaTE-predicted OCDD concentrations in soil in these regions were approximately an order of magnitude lower than the measured OCDD concentrations. The model-predicted TEQ concentrations in soil from TRIM.FaTE and Lorber et al. (2000) are somewhat different in their spatial patterns, with TRIM.FaTE concentrations highest to the west and north and concentrations estimated by Lorber et al. (2000) highest directly to the north. Interpretations of the results of these comparisons of regional estimates are notably limited by the fact that the locations of the soil sampling/modeling results (Lorber et al. 2000) used in this analysis to estimate the regional values were not distributed evenly throughout the regions and by the inexact spatial match-up of the regions with the TRIM.FaTE parcels.

Table ES-3. Comparison of Average Soil Concentrations Measured and Modeled

Comparison Location	Range of Soil Concentrations (pg/g dry weight)					
	Pollutant	Lorber et al. (2000)			TRIM.FaTE	
		Measured[a]	Modeled[a] (1992 Emissions)	Modeled[a] (1994 Emissions)	Modeled (1992 Emissions)	Modeled (1994 Emissions)
< 0.5km from source	TEQ	45 - 466	83 - 236	24 - 69	210 - 220	37 - 38
	OCDD	1,431 - 2,901	156 - 445	243 - 696	600 - 610	890 - 900
0.5km - 3km from source	TEQ	9	34	10	21 - 23	4
	OCDD	613	64	100	51	58
3km - 8km from source	TEQ	< 1	8	2	6	1
	OCDD	150	16	25	13	19

[a] All measured and modeled concentrations corresponding to the on-site and off-site values as reported in Lorber et al. (2000).

1.0 INTRODUCTION

This report is the first of two detailed reports describing the application of the TRIM.FaTE model to the emissions of dioxin-like compounds from a municipal solid waste combustion facility in Columbus, Ohio. This first report describes in detail the comparison of TRIM.FaTE results to the monitoring data and modeling results presented in an assessment conducted by EPA's Office of Research and Development (ORD). The second report evaluates the sensitivity of TRIM.FaTE in this application to changes in emission rates and spatial resolution and to the inclusion of biotic compartments. These analyses are part of the continuing efforts to evaluate the TRIM.FaTE model and will help in guiding its further development and refinement.

1.1 Objective

The goal of this analysis is to evaluate how TRIM.FaTE performs in modeling the multimedia fate and transport of dioxins through comparisons with monitoring data and results from previous modeling analyses. Specifically, this analysis compares TRIM.FaTE results in key compartments (i.e., air and soil) with monitoring data and results from multimedia modeling of this facility performed as part of EPA's Dioxin Reassessment (EPA 2000).

1.2 Description of Facility

The Columbus Municipal Solid Waste-to-Energy (CMSWTE) facility in Columbus, Ohio, started operations in June 1983 and processed an average of 1,600 metric tons of solid waste per day. During its operation, this facility was one of the highest single emitters of dioxin-like compounds in the United States (Lorber et al. 2000). In 1994, combustion improvements were made to reduce dioxin emissions at the facility, resulting in an approximately 75 percent reduction in emissions of dioxin-like compounds. The facility subsequently ceased operation in December 1994.

1.3 Previous Analysis of the Facility

In this report, TRIM.FaTE results are compared to monitoring data and modeling results from a previous analysis performed for the CMSWTE facility presented in Lorber et al. (2000). The Lorber et al. (2000) study used for comparison to TRIM.FaTE describes a model-to-monitor comparison of dioxin and furan concentrations in air and soil near the CMSWTE facility.

In their analysis, Lorber et al. (2000) used site-specific information to predict average ground-level air concentrations and deposition rates and soil concentrations of individual congeners and dioxin toxic equivalents (TEQs) for dioxin-like compounds. The stack parameter and emission rate data used in this analysis were based on information from stack tests conducted at the facility in 1992 and 1994 (Ohio EPA 1994). The meteorological data used were based on wind speed and direction data collected for 1989 and 1994. The 1989 data were gathered from nearby airport locations and were used for the soil modeling and the 1994 data were from both nearby airport locations and on-site sources and were used for the air dispersion modeling (M. Lorber, personal communication, January 2, 2004).

Air concentrations were modeled using the Industrial Source Complex Short Term model (ISCST3)and 1994 meteorological data sets and emission rates based on the 1994 stack tests. The modeled air concentrations were compared to air samples taken during 48-hour periods in March 1994 and April 1994 at monitoring stations between 1.8 and 3.0 kilometers from the site, mostly in the historical downwind direction (i.e., northeast).

Deposition rates were modeled using ISCST3 and 1989 meteorological data for two different emission scenarios, one based on the 1992 stack tests and the other based on the 1994 stack tests. Predicted annual average dry and wet deposition rates of particle-bound dioxins were estimated for these emission scenarios and input into a simple soil reservoir model to predict soil concentrations at a depth of 7.5 cm after 11.5 years of emissions (corresponding to the time the facility was operational). The resulting soil concentrations were compared to measured concentrations at this same depth collected in several regions at varying distances from the facility.

1.4 Comparison of Models

Because this report includes a model-to-model comparison of results at the CMSWTE facility, a brief summary of the similarities and differences in the models used in Lorber et al. (2000) and TRIM.FaTE is presented in Table 1. All of the air dispersion and deposition modeling in Lorber et al. (2000) was conducted using ISCST3. Deposition rates of dioxins predicted by ISCST3 were input to a simple soil reservoir mixing model to estimate soil concentrations. These outputs are compared in this report to air and soil concentrations estimated using TRIM.FaTE.

Table 1. Air and Soil Model Comparison

Media Modeled	Lorber et al. (2000)		TRIM.FaTE
	ISCST3	Simple Reservoir Mixing Model	
Air	• Air dispersion only (i.e., no plume depletion) • All emissions and their subsequent fate and transport were modeled in the form of a single conservative pollutant, with no differentiation in the fate of the 17 individual congeners	N/A	• Air advection and diffusion, particle and vapor-phase deposition, atmospheric degradation, and resuspension and diffusion from surface soil to air • The emissions and subsequent fate and transport of all 17 congeners were modeled individually
Soil	• Deposition was estimated for a single conservative pollutant, with no differentiation between the 17 individual congeners • Air dispersion and particle-phase deposition • Wet and dry deposition from air input into soil model as an annual average	• Dissipation half-life in soil of 25 years for all modeled chemicals, accounting for dioxin removal from the soil by both chemical degradation and physical removal processes	• The fate and transport of all 17 congeners were modeled individually • Air advection and diffusion, particle and vapor-phase deposition, atmospheric degradation, and resuspension and diffusion from surface soil to air • Wet and dry deposition from air (varies with time during modeling period; e.g., wet deposition is dependent on rainfall) • Degradation half-life in surface and root zone soil of 10 years for all modeled chemicals • Physical removal processes (e.g., erosion, runoff) modeled separately

2.0 METHODOLOGY

This chapter describes the methodology used to compare TRIM.FaTE results with results from Lorber et al. (2000). Section 2.1 describes the three TRIM.FaTE model simulations performed. The methods used to compare the results from these TRIM.FaTE simulations to those presented in Lorber et al. (2000) are summarized in Section 2.2. A detailed description of the specifications for the TRIM.FaTE simulations used in the comparison is presented in Chapter 3.

2.1 Overview of TRIM.FaTE Simulations

The three TRIM.FaTE simulations selected for this analysis used different combinations of temporal resolution, emissions data, and meteorological data to facilitate comparison with the modeled and measured data presented in Lorber et al. (2000). Table 2 provides the stack test emissions scenario and meteorological data used for these three simulations and gives a brief description of the results from each TRIM.FaTE simulation that were used in the comparison.

Table 2. TRIM.FaTE Simulations used for Comparison to Lorber et al. (2000)

Emissions	Meteorological Data	TRIM.FaTE Concentrations Used for Comparison
1994 stack test	1994[a]	Air results corresponding to locations modeled and monitored, averaged over the 48-hour period in March 1994 corresponding to the sampling dates
1992 stack test	1989[b]	Surface and root zone soil results at 11.5 years, averaged over three regions around the source corresponding to locations modeled and monitored
1994 stack test	1989[b]	Surface and root zone soil results at 11.5 years, averaged over three regions around the source corresponding to locations modeled and monitored

[a] On-site meteorological data from 1994, which were also used in the Lorber et al. (2000) analysis, could not be obtained for this report; only meteorological data from local airports were modeled and corresponding results presented in this report.

[b] Meteorological data from 1989, used for soil deposition modeling in Lorber et al. (2000), were repeated for each year of the simulation.

For the comparison of air concentrations, the modeled and measured concentrations from Lorber et al. (2000) are compared to TRIM.FaTE results for a 48-hour period in March 1994. The TRIM.FaTE simulation used 1994 meteorological data and the 1994 stack test emissions (i.e., the same meteorological and emissions data used in the Lorber et al. (2000) modeling) to generate air concentrations for the same 48-hour modeling period.

For the comparison of soil concentrations, the modeled and measured concentrations from Lorber et al. (2000) for the 1992 and 1994 emission scenarios at the 11.5 year mark are compared to TRIM.FaTE results for the same two emission scenarios and point in time. Two

TRIM.FaTE simulations were performed (one with each emission scenario), both using 1989 meteorological data to correspond to the meteorological data used in the Lorber et al. (2000) analysis.

2.2 Comparisons to Lorber et al. (2000)

This section describes the approach taken to process the air and soil concentrations from the TRIM.FaTE simulations for comparison with the results in Lorber et al. (2000). In addition to the comparisons described below, results for all TRIM.FaTE simulations were analyzed to confirm that the results seemed reasonable and internally consistent.

The TRIM.FaTE and Lorber et al. (2000) approaches differ in how they estimate air and soil concentrations for each modeled chemical. In the TRIM.FaTE analysis, emission rates were input for each chemical and air and soil concentrations were generated for each modeled chemical individually. The Lorber et al. (2000) analysis estimated the fate and transport of the modeled chemicals in the form of a single conservative pollutant, with no differentiation in fate of the individual compounds. Air and soil concentrations were then calculated using the results for this single pollutant and the emission rate for each chemical of interest.

The approaches also differ in the spatial and temporal resolution of their results. TRIM.FaTE is a "dynamic" model designed to enable the user to model temporal and spatial heterogeneity for all media included in the user-constructed modeling scenario. TRIM.FaTE results are generated for each modeled compartment and location at frequencies specified by the user. These outputs represent the results for that time point (i.e., a "snapshot" or instantaneous value) and are not an average over any time period. In contrast, the results presented in Lorber et al. (2000) are temporally-averaged air concentrations and spatially-averaged soil concentrations.

Temporal averaging of the TRIM.FaTE air results was performed to obtain values that were comparable to the temporal resolution of the Lorber et al. (2000) concentration results (i.e., 48-hour average air concentrations). Spatial averaging of the TRIM.FaTE soil results was performed when more than one TRIM.FaTE soil compartment was located within a region corresponding to a single, spatially-averaged result from Lorber et al. (2000). The following sections describe specifically how the TRIM.FaTE results were averaged temporally and spatially for comparison to the results in Lorber et al. (2000).

2.2.1 Comparisons to Air Concentrations

For comparison with air concentrations from Lorber et al. (2000), the estimated hourly air concentrations from the TRIM.FaTE simulation using the 1994 meteorological data and stack test emissions were averaged for each air compartment and chemical over the 48-hour period from noon on March 15 until noon on March 17, corresponding to the period of air sampling at the site. These 48-hour concentrations were then converted into TEQ concentrations for each air compartment.

The resulting TRIM.FaTE TEQ concentrations, as well as the 1,2,3,4,6,7,8,9-octachlorodibenzo(p)-dioxin (OCDD) concentrations, were compared to the TEQ and OCDD measured and modeled estimates in the Lorber et al. (2000) analysis.[1] In Lorber et al. (2000), the TEQ and OCDD results are presented on maps with the measured concentrations listed as values at the corresponding monitoring locations and the modeled results shown as isolines. The measured values were compared to the estimated TRIM.FaTE air concentrations from the air compartments where the monitors were located. As the original predicted concentrations from Lorber et al. (2000) were no longer available, the concentrations were estimated from the isolines for all of the locations. In light of this, most of the modeled concentrations are presented as ranges because exact values could not be determined from the isolines. In addition, the overall TRIM.FaTE spatial distributions of pollutant concentrations over the 48-hour period in the simulation were compared to the corresponding TEQ spatial distributions (presented as isoline figures) in Lorber et al. (2000).

2.2.2 Comparisons to Soil Concentrations

The estimated soil concentrations from TRIM.FaTE using both the 1992 and 1994 stack test emissions with 1989 meteorological data were compared to the corresponding measured and modeled concentrations from Lorber et al. (2000). The surface soil and root zone soil concentrations from the TRIM.FaTE simulations were modeled to depths of 1 cm and 82 cm, respectively, whereas Lorber et al. (2000) presented measured and modeled results for a depth of 7.5 cm for surface soil.[2] Therefore, in order to compare the results at a depth of 7.5 cm, the lower and upper bounds of the TRIM.FaTE soil concentrations within the top 7.5 cm of soil were estimated. The lower bound concentration in each compartment was calculated for each chemical by dividing the total chemical mass in each surface soil compartment by the volume of soil equal to the parcel area down to 7.5 cm from the surface. The upper bound concentration in each compartment was calculated for each chemical by dividing the total chemical mass in each pair of surface soil and root zone soil compartments by the volume of soil equal to the parcel area down to 7.5 cm from the surface.

The instantaneous surface soil and root zone soil concentrations at the midpoint of the 12th year were used for comparison to Lorber et al. (2000), which modeled the soil concentrations associated with 11.5 years of deposition. The TRIM.FaTE chemical-specific soil concentrations were converted to TEQ concentrations, and then the resulting TEQ concentrations, as well as the OCDD concentrations, were averaged spatially across the soil compartments corresponding to

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[1] Only dioxin TEQ and OCDD concentrations were compared in this report because Lorber et al. (2000) focused on TEQ concentrations and homolog group concentrations, only presenting results for a single compound in the case of OCDD. Lorber et al. (2000) also included 25 compounds in the calculation of homolog group concentrations. The TRIM.FaTE simulation was limited to the compounds which comprise the dioxin TEQ and thus only included 17 of the 25 compounds in the homolog group. Therefore, no comparison was made to the homolog group concentrations calculated in Lorber et al. (2000).

[2] It is important to note that TRIM.FaTE is very flexible with respect to assigning the depths of different compartments, including surface soil. The algorithms associated with the surface soil compartments have been evaluated and shown to be valid to depths of up to one meter (McKone and Bennett 2003). The soil depths in TRIM.FaTE for this application were selected based on configurations used in previous TRIM.FaTE applications and the fact that dioxins have a tendency to accumulate in the very top layer of the soil and they leach sparingly; thus a shallow surface soil depth was modeled to capture this expected sharp gradient from surface to root zone soil.

the monitoring regions described in Lorber et al. (2000). In the Lorber et al. (2000), the sampling locations were broken down into four regions:

- On-site (within the facility's fenceline)
- Off-site (just outside property, downwind within 500 meters)
- Urban (all directions within approximately three kilometers)
- Urban background (all directions from three to eight kilometers)

For this comparison, samples collected within the "on-site" region are compared to TRIM.FaTE results only for informational purposes because Lorber et al. (2000) states that the concentrations for the on-site samples were quite high and likely due to sources other than deposition from the facility emissions. Also, modeled results within the on-site and off-site regions were presented together (i.e., as a range) because the distance to the facility's fenceline was not specified in Lorber et al. (2000). Thus, the comparison is based on three spatially averaged regions as follows:

- Region 1 - Close to the source (within 500 meters)
- Region 2 - Urban (between 500 meters and three kilometers)
- Region 3 - Urban background (between three and eight kilometers)

The resulting TEQ and OCDD concentrations in each region were compared to both the monitoring data for the corresponding locations and modeling results for the corresponding combinations of location and emission scenario (i.e., 1992 and 1994 stack tests) from Lorber et al. (2000). In addition, the overall TRIM.FaTE spatial distributions of pollutant concentrations, averaged over the last year of the modeling period, were compared to the corresponding TEQ spatial distributions (presented as isoline figures) in Lorber et al. (2000).

3.0 SPECIFICATIONS OF TRIM.FaTE SIMULATIONS

This chapter briefly summarizes the specifications of the three TRIM.FaTE simulations described in Section 2.1. This information is supplemented by Appendix A, which provides detailed documentation of the specifications of these TRIM.FaTE simulations. The modeling concepts, approaches, algorithms, and assumptions used in TRIM.FaTE are documented in detail in the two-volume TRIM.FaTE Technical Support Document (EPA 2002a and b) and are not discussed at length here.

3.1 Modeled Chemicals and Emission Rates

Each of the TRIM.FaTE simulations included in this analysis modeled the fate and transport of the same 17 individual dioxin and furan congeners addressed in Lorber et al. (2000).[3] These congeners are listed in Table 3 along with the abbreviations that are commonly used for them. The chemical properties used in TRIM.FaTE for the these congeners are documented in Appendix B.

Emissions from the stack tests conducted at the CMSWTE facility in 1992 (Ohio EPA 1994) and in 1994 (SWACO 1994) were used as the basis for chemical-specific emission rates for this analysis, just as they were in Lorber et al. (2000). The detailed calculations of the chemical-specific emission rates used in both the TRIM.FaTE simulations and in Lorber et al. (2000) are included in Appendix C.

3.2 Spatial Layout

For this analysis, the overall size and extent of the area for which pollutant fate and transport were modeled (i.e., the modeling region) were determined based on the location of the emissions source, expected mobility of the chemicals of primary interest, locations of receptors of interest (e.g., monitoring stations), and watershed boundaries for the water bodies of interest. The vertical dimension of the lower air layer was set to the mixing height, which varied temporally as a function of the meteorological conditions. Additional detail on the creation of the modeling region, air layout, and surface layout is provided in Appendix A.

The modeling region was centered on the source location because the locations of interest (primarily the air and soil monitoring locations discussed in Lorber et al. 2000) are scattered around the facility, rather than on one side, and the wind direction in the Columbus area varies widely over the meteorological periods modeled. Wind roses generated using the meteorological data for the site are provided in Appendix D.

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[3] Note that in the TRIM.FaTE analysis, emission rates were input for each chemical and air and soil concentrations were generated for each modeled chemical individually. In contrast, the Lorber et al. (2000) analysis estimated the fate and transport of the modeled chemicals in the form of a single conservative pollutant, with no differentiation in fate of the individual compounds. Air and soil concentrations were then calculated using the results for this single pollutant and the emission rate for each chemical of interest.

Table 3. Dioxin and Furan Congeners Used for Comparison

CONGENER	ABBREVIATION
Dioxins	
2,3,7,8-Tetrachlorodibenzo(p)dioxin	TCDD
1,2,3,7,8-Pentachlorodibenzo(p)dioxin	PeCDD
1,2,3,4,7,8-Hexachlorodibenzo(p)dioxin	1,2,3,4,7,8-HxCDD
1,2,3,6,7,8-Hexachlorodibenzo(p)dioxin	1,2,3,6,7,8-HxCDD
1,2,3,7,8,9-Hexachlorodibenzo(p)dioxin	1,2,3,7,8,9-HxCDD
1,2,3,4,6,7,8-Heptachlorodibenzo(p)dioxin	HpCDD
1,2,3,4,6,7,8,9-Octachlorodibenzo(p)dioxin	OCDD
Furans	
2,3,7,8-Tetrachlorodibenzo(p)furan	TCDF
1,2,3,7,8-Pentachlorodibenzo(p)furan	1,2,3,7,8-PeCDF
2,3,4,7,8-Pentachlorodibenzo(p)furan	2,3,4,7,8-PeCDF
1,2,3,4,7,8-Hexachlorodibenzo(p)furan	1,2,3,4,7,8-HxCDF
1,2,3,6,7,8-Hexachlorodibenzo(p)furan	1,2,3,6,7,8-HxCDF
1,2,3,7,8,9-Hexachlorodibenzo(p)furan	1,2,3,7,8,9-HxCDF
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1,2,3,4,6,7,8-Heptachlorodibenzo(p)furan	1,2,3,4,6,7,8-HpCDF
1,2,3,4,7,8,9-Heptachlorodibenzo(p)furan	1,2,3,4,7,8,9-HpCDF
1,2,3,4,6,7,8,9-Octachlorodibenzo(p)furan	OCDF

The configuration of the air layout presented in Figure 1 shows the 33 individual air parcels (i.e., two-dimensional areas used to subdivide the modeling region) in the lower air layer. The vertical dimension of the lower air layer (i.e., the upper boundary) was set to the mixing height, which varied temporally as a function of the meteorological conditions. A single upper air layer (not shown on the figure) was also included to track emissions released above the mixing height (i.e., during times when the mixing height is lower than the source elevation). This upper air layer is considered a sink for the purposes of this report because the mass released to this upper layer was not further simulated (e.g., in terms of any transport or transformation processes).

The surface layout presented in Figure 2 consists of 27 soil parcels (e.g., N1, W1), including a small source parcel centered on the emission source, and three surface water parcels (i.e., Scioto, Olentangy, and Combined). The individual parcels in the surface layout, which were designed with consideration of watershed boundaries, do not line up exactly with the air layout, although the outer boundaries of the regions are the same.

Figure 1. Layout of TRIM.FaTE Air Parcels

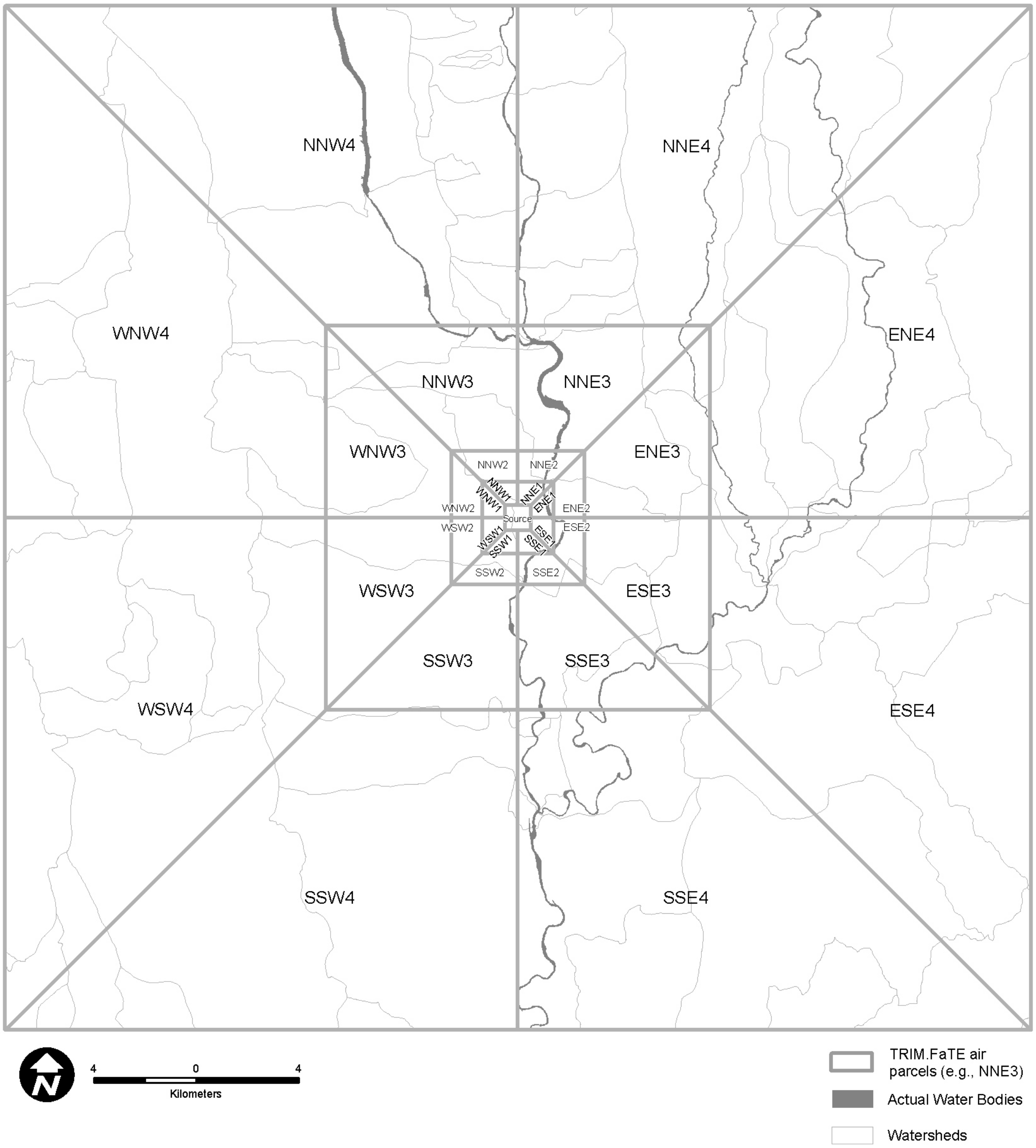
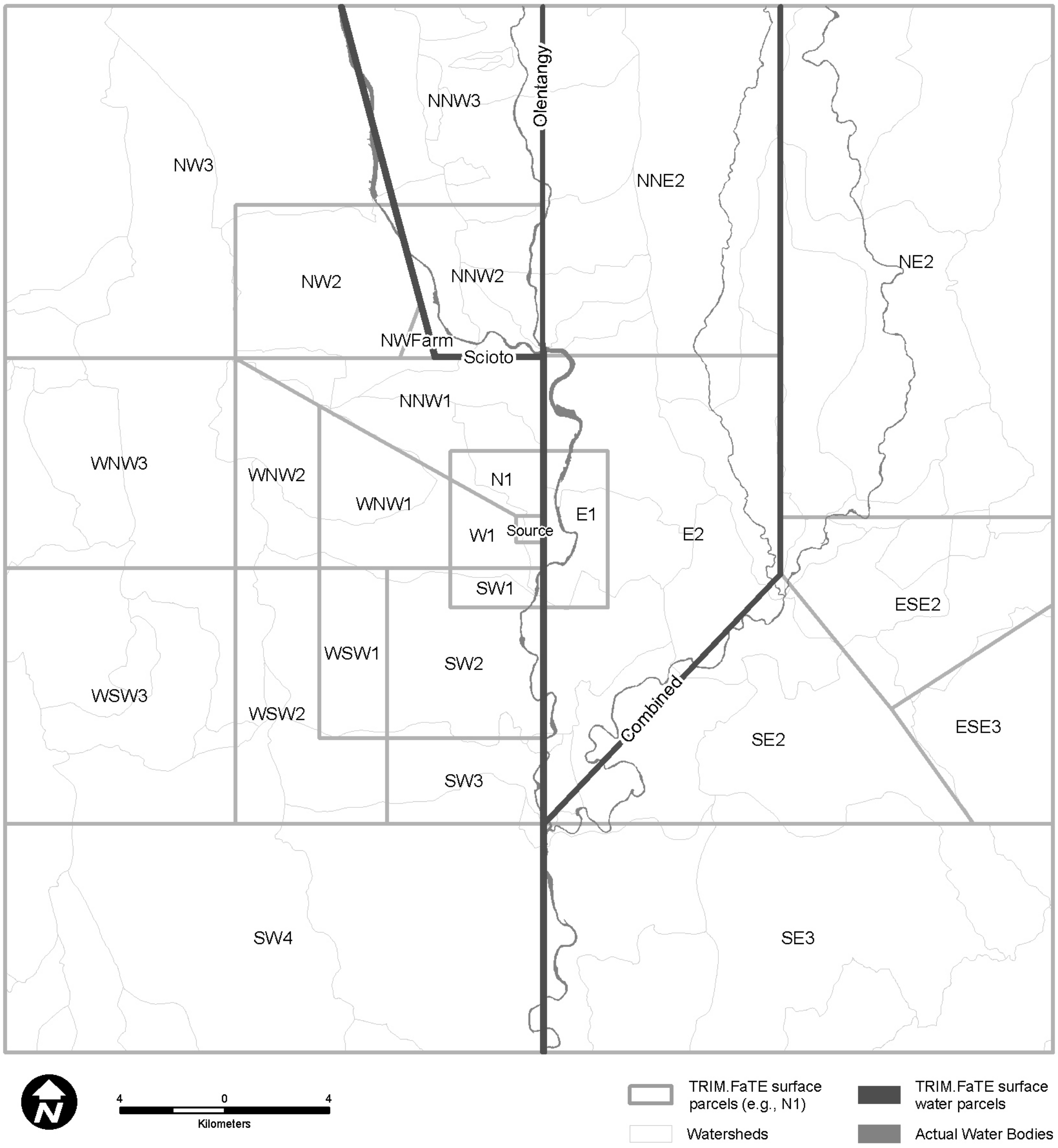


Figure 2. Layout of TRIM.FaTE Surface Parcels



3.3 Meteorological Data

The meteorological data used in this analysis are the local airport data from 1989 (for the soil analyses) and 1994 (for the air analyses) used in Lorber et al. (2000) (M. Lorber, personal communication, January 2, 2004). Overall, the 1989 and 1994 meteorological data were similar. For instance, the wind direction at the site blows predominantly towards the northeast (approximately 30 percent of the time) for both sets of meteorological data. Appendix D contains wind roses illustrating the frequencies of different wind speeds and directions during the 1989 and 1994 meteorological data sets, as well as during the 48-hour period between March 15-17, 1994, which corresponds to the period of air monitoring and modeling described in Lorber et al. (2000).

3.4 Abiotic and Biotic Compartment Data

Lorber et al. (2000) only estimated dioxin and furan concentrations in air and soil and thus, for the purposes of this comparison, the TRIM.FaTE simulations only needed to include air, surface soil, and root zone soil compartments, as well as any other compartment types that significantly impact the overall mass balance. Abiotic media included in these TRIM.FaTE simulations were air, soil (surface, root zone, and vadose zone), groundwater, surface water, and sediment. Previous TRIM.FaTE analyses indicate that no biotic medium other than vegetation significantly impacts the overall mass balance and thus only vegetation compartment types (i.e., grasses/herbs, agricultural vegetation, and deciduous forests) were included in these simulations. Appendix B documents the inputs for all abiotic and biotic compartments included in these simulations.

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4.0 ANALYSIS OF TRIM.FaTE RESULTS

This chapter presents the results from the TRIM.FaTE simulations and describes the temporal patterns of pollutant mass, variations in results across modeled chemicals, and spatial distributions of pollutant concentrations, focusing on the air and soil compartments that are relevant to the comparisons to Lorber et al. (2000). The results presented in this section are provided to give a sense of the overall patterns and trends of the TRIM.FaTE outputs for the different simulations.

4.1 Temporal Patterns

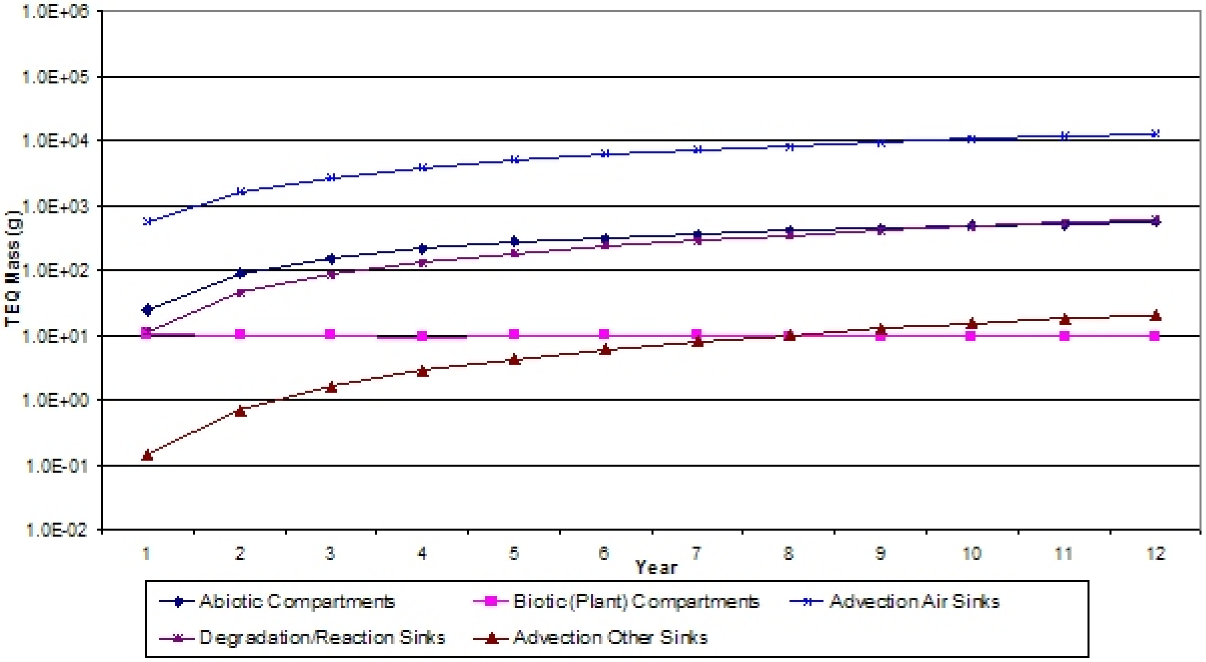
This section describes the mass accumulation of the modeled dioxin-like compounds over time. Results are presented as annual averages for the simulation using 1989 meteorological data and 1992 stack test emissions. The overall trends from the TRIM.FaTE simulation using 1994 stack test emissions are similar to the results presented in this section. All results in this chapter are shown as TEQ, which represents the toxicity-weighted total mass of all 17 dioxins and furans.

4.1.1 Overall Mass Distribution

Figure 3 illustrates the accumulation and loss of dioxin mass from the modeling region during the 12-year modeling period. Most of the mass (approximately 90 percent) ends up in the air advection sinks, the majority of which is transported via horizontal air advection beyond the modeling region boundaries. After the pollutant mass reaches the air advection sinks, its fate and transport is no longer modeled. These results are consistent with results from other TRIM applications and are reasonable because the dioxin emissions are released in the air, where transport between compartments occurs rapidly, degradation is relatively slow, and the size of the modeling region is relatively small (the source to boundary distance ranges from 12 to 14.5 miles or approximately 19 to 23 kilometers). Both the other types of advection sinks (i.e., erosion/runoff sinks for surface soil and flush rate sinks for surface water) and the degradation/reaction sinks (associated with all of the compartments) contain more than an order of magnitude less dioxin mass than the air advection sinks. Overall, the total dioxin mass in the sink compartments accounts for 94 percent of the total mass in the system at the end of the first year of the simulation and 96 percent by the end of the modeling period (i.e., end of year 12).

Most of the dioxin mass remaining in the modeling region (i.e., not in the sinks) at any time is in the abiotic compartments. The dioxin mass in the abiotic compartments increases over time until the end of the simulation, at which time it accounts for approximately 4 to 5 percent of the total dioxin mass in the system (including sinks). The mass of dioxin in the biotic (i.e., vegetation) compartments stays relatively constant across years of the simulation. This is primarily because all of the dioxin mass in the leaf and particle-on-leaf compartments is transferred to surface soil during litter fall each year for the vegetation types modeled in this simulation and thus does not accumulate in these compartments over time. Although root and stem compartments are also included as part of the modeled vegetation, the accumulation that occurs in these compartments is substantially less than that in the leaf and leaf particle compartments. The dioxin mass in the vegetation compartments ranges from 1.7 percent of the total mass after the first year of the simulation to 0.1 percent at the end. As seen on Figure 3, mass in the sinks and abiotic media continues to increase while mass in the biotic compartments stays relatively constant, resulting in decreasing percentage of the total mass in the plants over time.

Figure 3. Dioxin TEQ Mass - Log Scale
Overall Distribution in All Compartments and Sinks[a]



[a] Air advection sinks include the mass lost due to horizontal advection and vertical loss to the upper air layer.

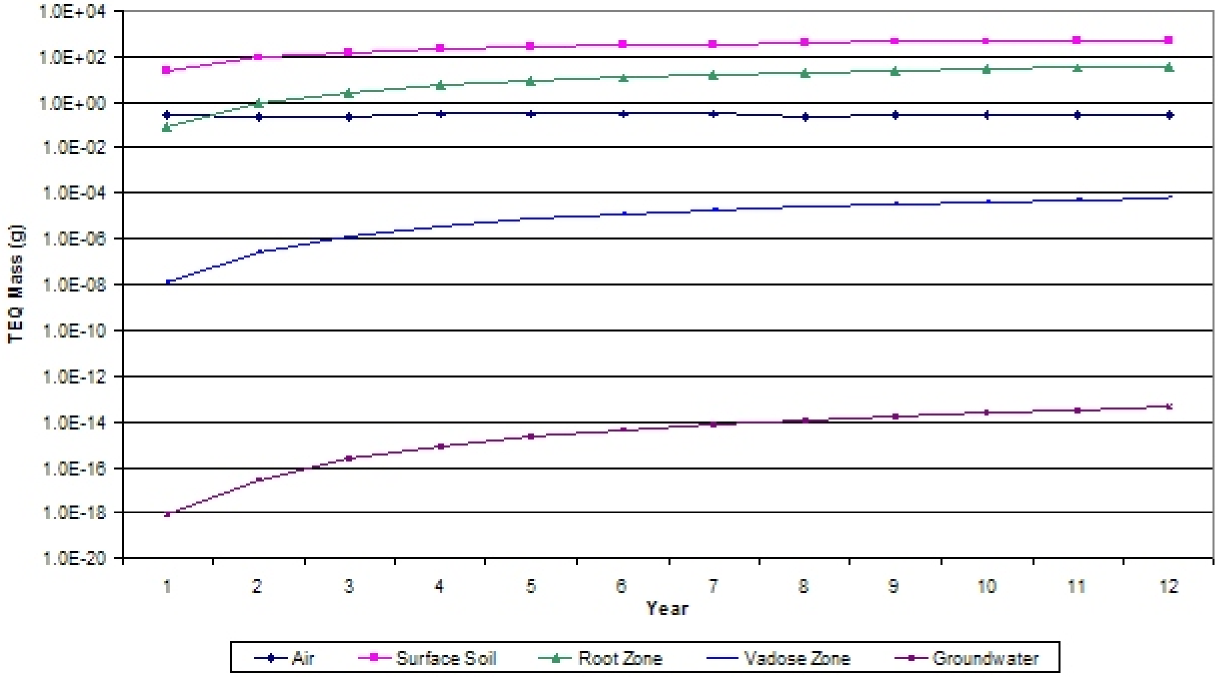
4.1.2 Mass Distribution in Abiotic Compartments

The patterns of accumulation of dioxin mass in the abiotic compartment types of interest for this analysis (i.e., air and soil) are shown in Figure 4. This figure shows that all of the soil compartments accumulate mass steadily, whereas the mass in air compartments is relatively constant over the course of the simulation. Among the abiotic compartment types, the surface soil compartments contain the most dioxin mass during the entire modeling period, although the mass in the root zone soil compartments steadily increases from year to year and begins to approach the surface soil mass towards the end of the simulation.

4.2 Variations Across Modeled Chemicals

Results for the 17 individual dioxin congeners are presented in Appendix E as annual averages for the simulation using 1989 meteorological data and 1992 stack test emissions. The overall trends from the TRIM.FaTE simulation using 1994 stack test emissions are similar to the results presented in this section. Charts similar to Figures 3 and 4 showing the overall mass distribution and the mass distributions in the air and soil compartments are presented in Appendix E for each congener.

Figure 4. Dioxin TEQ Mass - Log Scale Distribution in Abiotic Compartments



Generally, the mass distribution patterns are similar for the 17 congeners (see Figures E-1 through E-17). Throughout the simulation, the amount of mass in each compartment and sink ranges over approximately two orders of magnitude across all of the congeners. In the abiotic compartments, the mass in the air and root zone soil compartments ranges less than two orders of magnitude across congeners and slightly more than two orders of magnitude for the surface soil compartments. The congeners with the shortest half-lives in air (e.g., TCDD and TCDF) generally have less mass in the abiotic and biotic compartments and advection sinks and slightly more in the degradation/reaction sinks, and those with longer half-lives in air (e.g., 1,2,3,4,6,7,8-HpCDF and OCDD) generally have more mass in each of the abiotic and biotic compartments and advection sinks and slightly less in the degradation/ reaction sinks.

The relative distribution of mass among the soil compartment types and vegetation is similar for most of the congeners (see Figures E-18 through E-34). One difference occurs for 2,3,7,8-TCDF (and to a lesser extent, 1,2,3,7,8 PeCDD), for which the root zone soil compartment contains similar mass as the surface soil compartment by year 12; for all the other congeners, mass in root zone soil remains less than that in surface soil throughout the simulation. This difference may be explained by the octanol-water partition coefficient (K_{ow}) for 2,3,7,8-TCDF, which is the lowest of the modeled chemicals (1,2,3,7,8 PeCDD is the second lowest). In TRIM.FaTE, a lower K_{ow} results in increased percolation from surface soil to root zone soil and thus more mass in the root zone soil compartments.

4.3 Spatial Patterns

This section examines the spatial variations in dioxin concentrations in the air, surface soil, and root zone soil compartment types. Air results are presented as the annual average for the one-year simulation using 1994 meteorological data and 1994 stack test emissions. Soil results are presented as the annual average for the final year (i.e., year 12) of the simulation using 1989 meteorological data and 1992 stack test emissions. Both air and soil results are presented as TEQ concentrations of dioxins.

4.3.1 Air Concentrations

The spatial variation of dioxin concentrations across the air compartments is presented in Figure 5 for the annual TEQ concentration. The annual average air concentrations displayed in this figure are presented in tabular form in Appendix F. The spatial patterns of the results for the 48-hr period used for comparison to Lorber et al. (2000) are presented in Section 5.1. As seen in Figure 5, air concentrations consistently decrease with distance from the source, with the highest concentration in the source compartment. The lowest concentrations (which are found in the outer ring of parcels) are less than one percent of the concentration in the air compartment associated with the source parcel (i.e., they differ by more than two orders of magnitude). However, the differences among the concentrations within each ring are typically less than a factor of two, and the differences between rings are typically between a factor of two to three. Although Figure 5 shows concentrations in the north (i.e., the second ring) to be higher than the other concentrations in that ring, the differences were only about 25 percent different. It was not surprising that the concentrations do not vary substantially within and between the rings because, as the wind rose for 1994 shows (see Appendix D), the wind blows in many different directions and thus there is no strong directional pattern in the results.

4.3.2 Soil Concentrations

The spatial variation of annual average dioxin TEQ concentrations across the surface soil compartments is shown in Figure 6. As expected based on its relationship with surface soil, the distribution of concentrations in root zone soil is similar and therefore is not presented. The annual average surface and root zone soil concentrations for the final year of the modeling period (year 12) are presented in tabular form in Appendix F. As expected, the surface and root zone soil concentrations are highest at the source. In general, the concentrations tend to decrease with distance from the source and are somewhat higher in the compartments closest to the source in the west and north directions, which is to be expected based on the erosion and runoff patterns (see Appendix B) and the predominant wind speeds and directions (see Appendix D for the annual wind rose plot for 1989).

Figure 5. Spatial Variation in Dioxin TEQ Concentration (Annual Average) (1994 Emissions): Air Compartments

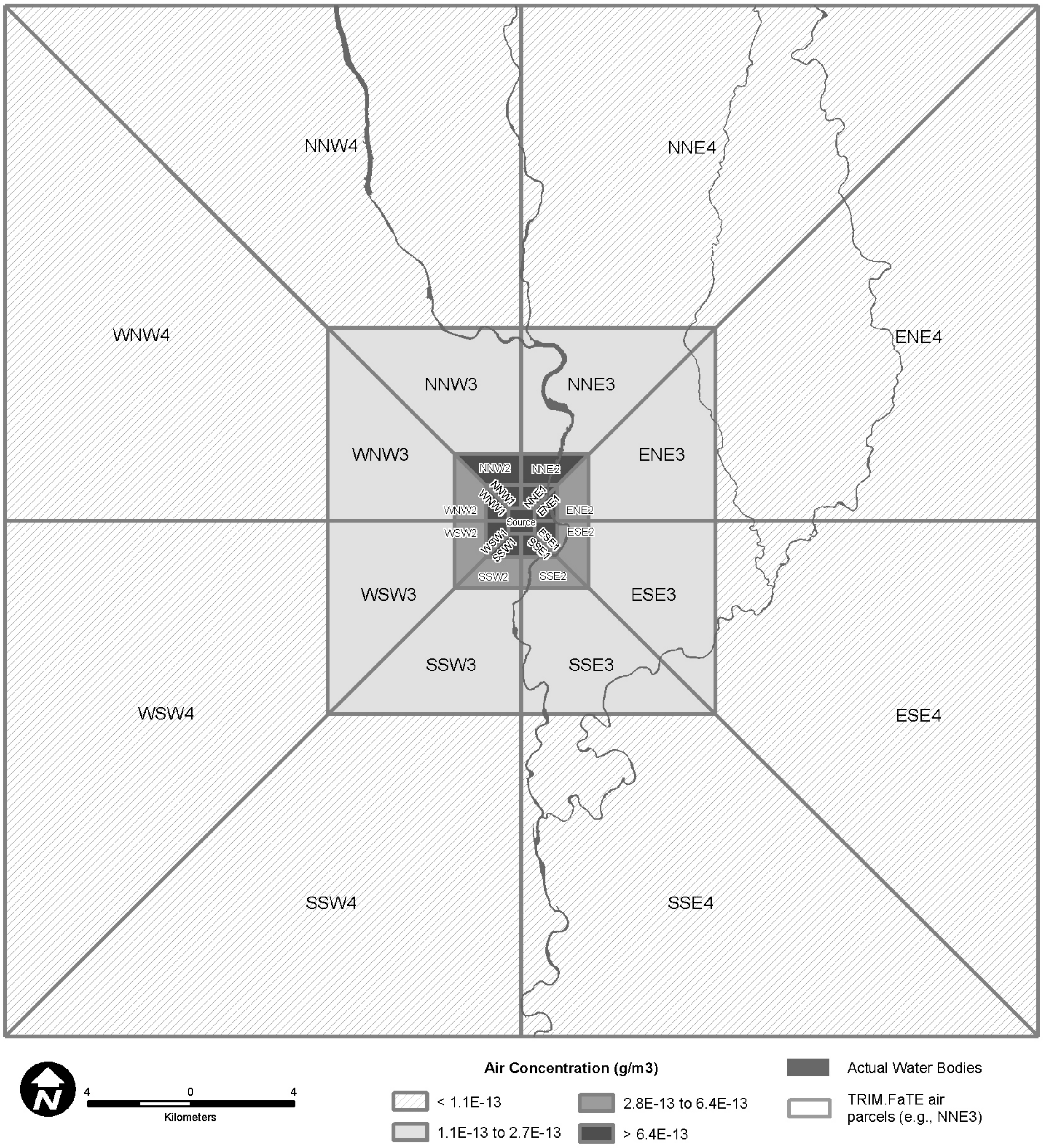
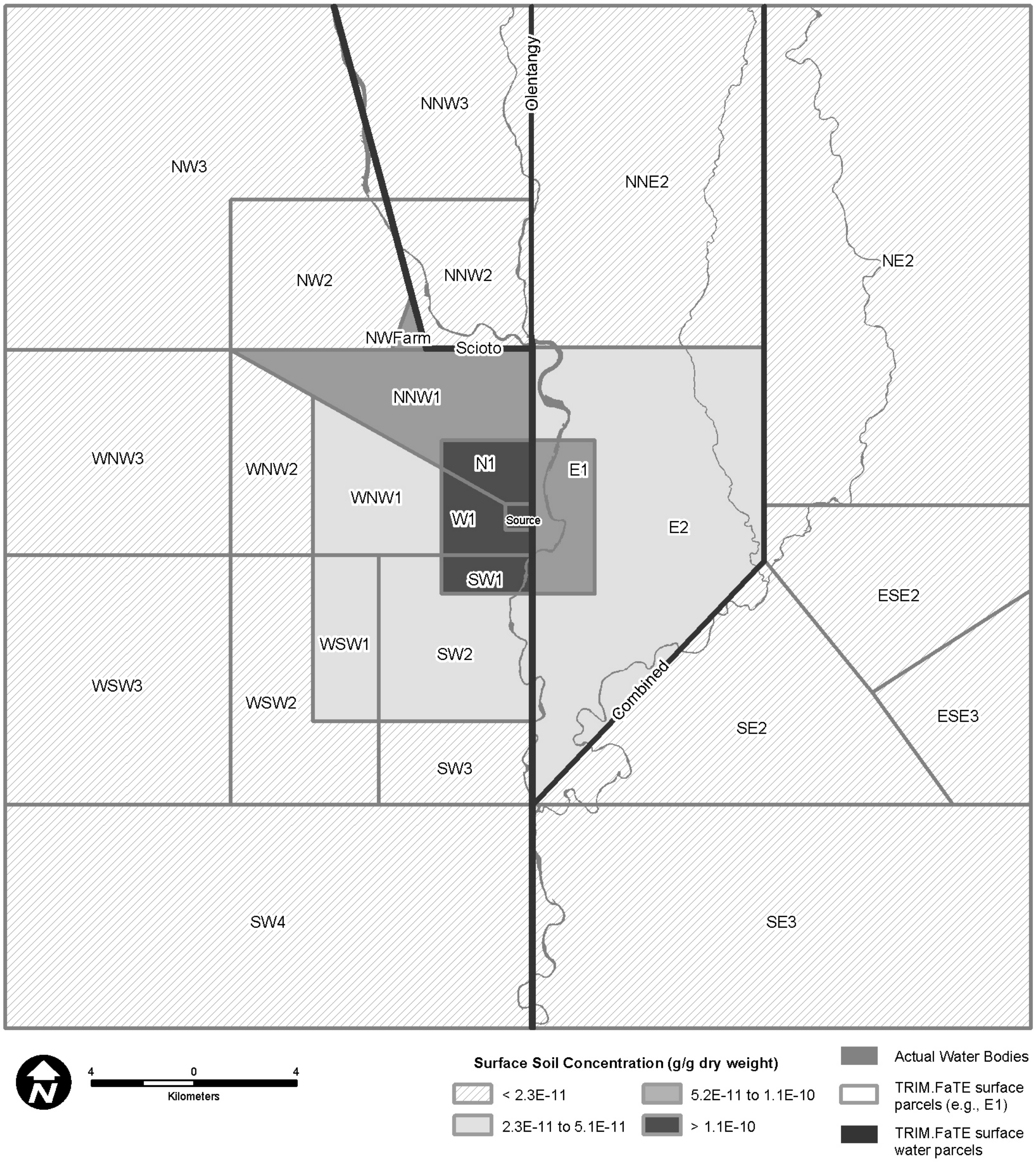


Figure 6. Spatial Variation in Annual Average Dioxin TEQ Concentrations for Year 12 (1992 Emissions): Surface Soil Compartments



5.0 COMPARISON TO LORBER et al. (2000) RESULTS

This chapter compares the results from the TRIM.FaTE simulations to the measured and modeled air and soil results presented in Lorber et al. (2000).

5.1 Air Concentration Comparisons

As described in Chapter 2, hourly air concentrations of dioxin TEQ and OCDD from the simulation using meteorological data and stack test emissions from 1994 were averaged over the period from noon on March 15th until noon on March 17th and compared to corresponding measured and modeled air concentrations presented in Lorber et al. (2000). The wind rose for March 15-17, 1994, provided in Appendix D, shows the wind blowing almost exclusively towards the southeast during this period. Figure 7 presents the TRIM.FaTE concentration results spatially for this period along with locations of the air monitoring stations relative to the TRIM.FaTE air layout. The 48-hour average TEQ air concentrations displayed in this figure, as well as the individual congener results, are presented in tabular form in Appendix F.

Table 4 shows the results from the dioxin TEQ air concentration comparison. Note that in all cases, the air monitoring locations fell on or very close to TRIM.FaTE parcel boundaries; therefore, TRIM.FaTE concentrations for the air compartments associated with both parcels are used for the comparison. It is noted that, unlike the annual average results (see Section 4.3.1), the 48-hour average concentrations for compartments associated with a given ring of TRIM.FaTE parcels (i.e., those air compartments that end in the same number) can vary by more than an order of magnitude due to the lesser variation in wind direction during a 48-hour period.

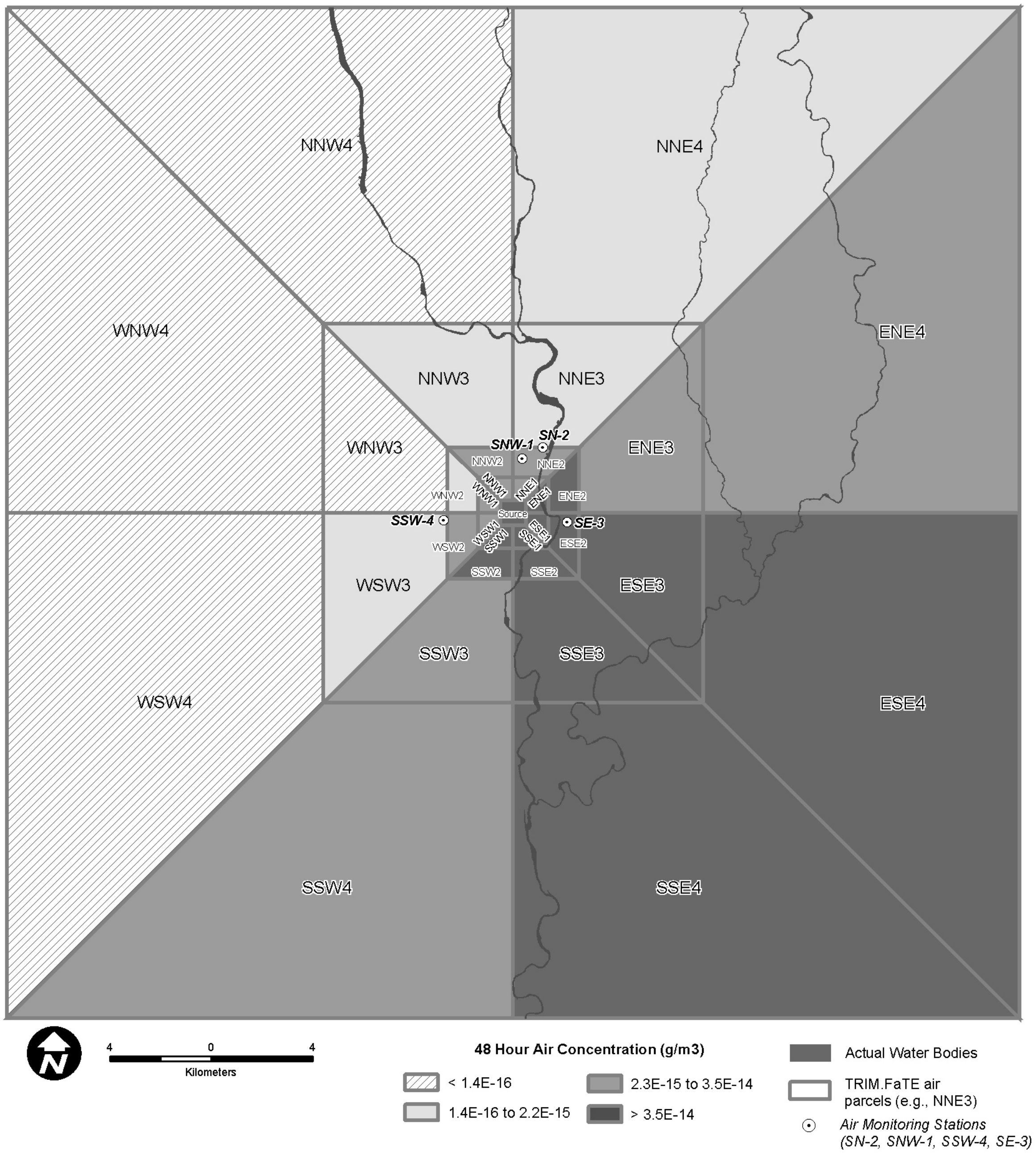
Table 4. 48-Hour Average Air Dioxin TEQ Concentration Comparison

Comparison Location	Lorber et al. (2000)			TRIM.FaTE	
	Air Monitoring Station	Measured TEQ concentration (pg/m^3)[a]	Modeled TEQ concentration (pg/m^3)[b]	Corresponding Air Compartment(s)	Modeled TEQ concentration (pg/m^3)
1	SE-3	0.12	0.15 - 0.30	ESE2 ENE2	0.33 0.12
2	SN-2	0.01	0.15 - 0.30	NNE2 NNE3	0.0081 0.0018
3	SNW-1	0	0.00 - 0.15	NNE2 NNW2	0.0081 0.0023
4	SSW-4	0	0	WSW3 WSW2	0.00038 0.0026

[a] The measured concentrations reported here are as presented in Figure 2 of Lorber et al. (2000) and, as described there, are intended to represent the TEQ concentration pertinent to the source that was modeled, taking into account a "background concentration." For example, the "0.00" entries indicate instances where the adjustment (i.e., measured concentrations minus an estimated background concentration) produced a concentration less than or equal to zero.

[b] Values were estimated from isolines (based on Figure 2, Lorber et al. 2000); ranges are presented if exact values could not be determined from the isolines.

Figure 7. Spatial Variation in 48-hr Average Dioxin TEQ Concentrations (1994 Emissions): Air Compartments and Monitors



The air concentrations estimated by TRIM.FaTE are highest in the southeast, which corresponds to the highest measured concentration (at monitoring station SE-3) as well as the predominant wind direction during the 48-hour sampling period. The SE-3 monitor is located within the ESE2 air compartment in TRIM.FaTE, near its boundary with the ENE2 air compartment. The measured and modeled TEQ air concentrations at the SE-3 monitor from Lorber et al. (2000) fall between the TRIM.FaTE-estimated concentrations in the ESE2 and ENE2 compartments, although they are closer to the concentration in the ENE2 compartment. Given the assumed homogeneity within TRIM.FaTE compartments and the location of the monitor relative to the TRIM.FaTE compartments, the TRIM.FaTE results for this monitor location compare reasonably well with both the measured and modeled concentrations from Lorber et al. (2000).

The SN-2 monitor is located on the boundary between the NNE2 and NNE3 air compartments in the TRIM.FaTE simulation. The TRIM.FaTE air concentration in NNE2 is very close (identical to two significant figures) to the measured concentration at SN-2. The TRIM.FaTE-estimated concentration in NNE3 is slightly lower than the concentrations at NNE2 and monitor SN-2, which is reasonable considering that the concentration in NNE3 represents a much larger area farther from the source than NNE2 and SN-2. The modeled concentration at SN-2 in Lorber et al. (2000) is more than an order of magnitude higher than the measured and TRIM.FaTE modeled concentrations at this location. Both the TRIM.FaTE results and measured values at this location are consistent with the meteorological data (see Appendix D), which shows that the wind blew towards the northeast only about five percent of the time during this period. Lorber et al. (2000) suggested that the much higher results in their analysis are perhaps due to the fact that the plume depletion option was not used for the air modeling with ISCST3.

The TRIM.FaTE concentrations in air compartments associated with the monitoring stations SNW-1 and SSW-4 are very close to the measured concentrations at these locations. It should be noted, however, that a detailed comparison of the TRIM.FaTE concentrations with the measured data is difficult at the monitoring locations with concentrations of zero (i.e., SNW-1 and SSW-4) because the detection limits for the air samples are not reported in Lorber et al. (2000) and the measured values were only reported out to two decimal places.

Table 5 presents the comparison between TRIM.FaTE 48-hour average concentrations of OCDD and the corresponding measured and modeled values from Lorber et al. (2000), using the same degree of precision. The TRIM.FaTE concentrations for OCDD follow the same pattern seen in Table 4 for the TEQ concentrations, with the highest concentration in the southeast and lowest in the southwest. Similarly, the OCDD results presented in Lorber et al. (2000) are consistent with the pattern for TEQ (see Table 4), although the pattern is not the same as the pattern of TRIM.FaTE results. However, the measured values show a different pattern than for TEQ, with OCDD concentrations highest at monitor SN-2 (located to the north), which is somewhat surprising based on the wind rose for this period (Appendix D). In addition, both the TRIM.FaTE and Lorber et al. (2000) modeled OCDD concentrations are significantly higher than the measured values at SE-3 (the monitor in the southeast). The TRIM.FaTE concentrations at the other two monitoring locations are very close to the measured values (identical to two decimal places for all but one of the values).

Table 5. 48-Hour Average Air OCDD Concentration Comparison

Lorber et al. (2000)			TRIM.FaTE	
Air Monitoring Station	**Measured concentration (pg/m^3)[a]**	**Modeled concentration (pg/m^3)[b]**	**Corresponding Air Compartment(s)**	**Modeled concentration (pg/m^3)**
SE-3	0.4	1.2 - 2.4	ESE2 ENE2	3.0 1.1
SN-2	0.5	2.4 - 3.6	NNE2 NNE3	0.073 0.016
SNW-1	0	0.0 - 1.2	NNE2 NNW2	0.073 0.021
SSW-4	0	0	WSW3 WSW2	0.0034 0.024

[a] The measured concentrations reported here are as presented in Figure 2 of Lorber et al. (2000) and, as described there, are intended to represent the TEQ concentration pertinent to the source that was modeled, taking into account a "background concentration." For example, the "0.0" entries indicate instances where the adjustment (i.e., measured concentrations minus an estimated background concentration) produced a concentration less than or equal to zero.

[b] Values were estimated from isolines (based on Figure 2, Lorber et al. 2000); ranges are presented if exact values could not be determined from the isolines.

When comparing the spatial distributions, the TEQ air concentrations are similar for the TRIM.FaTE and Lorber et al. (2000) results. As shown in Figure 7, the dioxin TEQ air concentrations for TRIM.FaTE over the 48-hour period decrease with distance from the source with the highest concentrations in the southeast, similar to what is expected based on the wind rose for that period (see Appendix D). The results in Lorber et al. (2000) show more directional variability (for both TEQ and OCDD concentrations) with the highest air concentrations in both the southeast (near monitor SE-3) and northeast (near monitor SN-2) and zero air concentrations in the southwest (near monitor SSW-4). As described above, the large size of the TRIM.FaTE air parcels may contribute to this difference in spatial distribution of air concentrations. Averaging over the parcel area likely results in the loss of information about very low and high point values. However, the TRIM.FaTE results are consistent with the meteorological data and the TEQ measured concentrations for the period.

5.2 Soil Concentration Comparisons

Concentrations of dioxins in surface and root zone soil from the TRIM.FaTE simulations using emissions from 1992 and 1994 stack tests were compared to both measured and modeled soil concentrations reported in Lorber et al. (2000) for the regions described in Section 2.2.2. The number of samples taken in each region and the corresponding TRIM.FaTE parcels are summarized in Table 6 and shown in Figure 8. Note that Figure 8 does not show the complete extent of the modeling region; only the TRIM.FaTE parcels and sampling locations corresponding to the regions described in Lorber et al. (2000) are shown for the purposes of the soil comparison. It should also be noted that the Lorber et al. (2000) soil samples were collected

Table 6. Lorber et al. (2000) Monitoring Regions and Sampling Locations and Corresponding TRIM.FaTE Parcels Used for Comparison

Region	Description of region	Lorber et al. (2000) Monitoring Region (Associated Number of Samples)	Corresponding TRIM.FaTE Parcels
1	Within 500 meters of source	Off-site (5)	Source
2	Between 500 m to 3 km of source	Urban (14)	N1, E1, W1, SW1
3	Between 3 km to 8 km of source	Urban background (13)	E2, NNW1, WNW1, SW2, WSW1

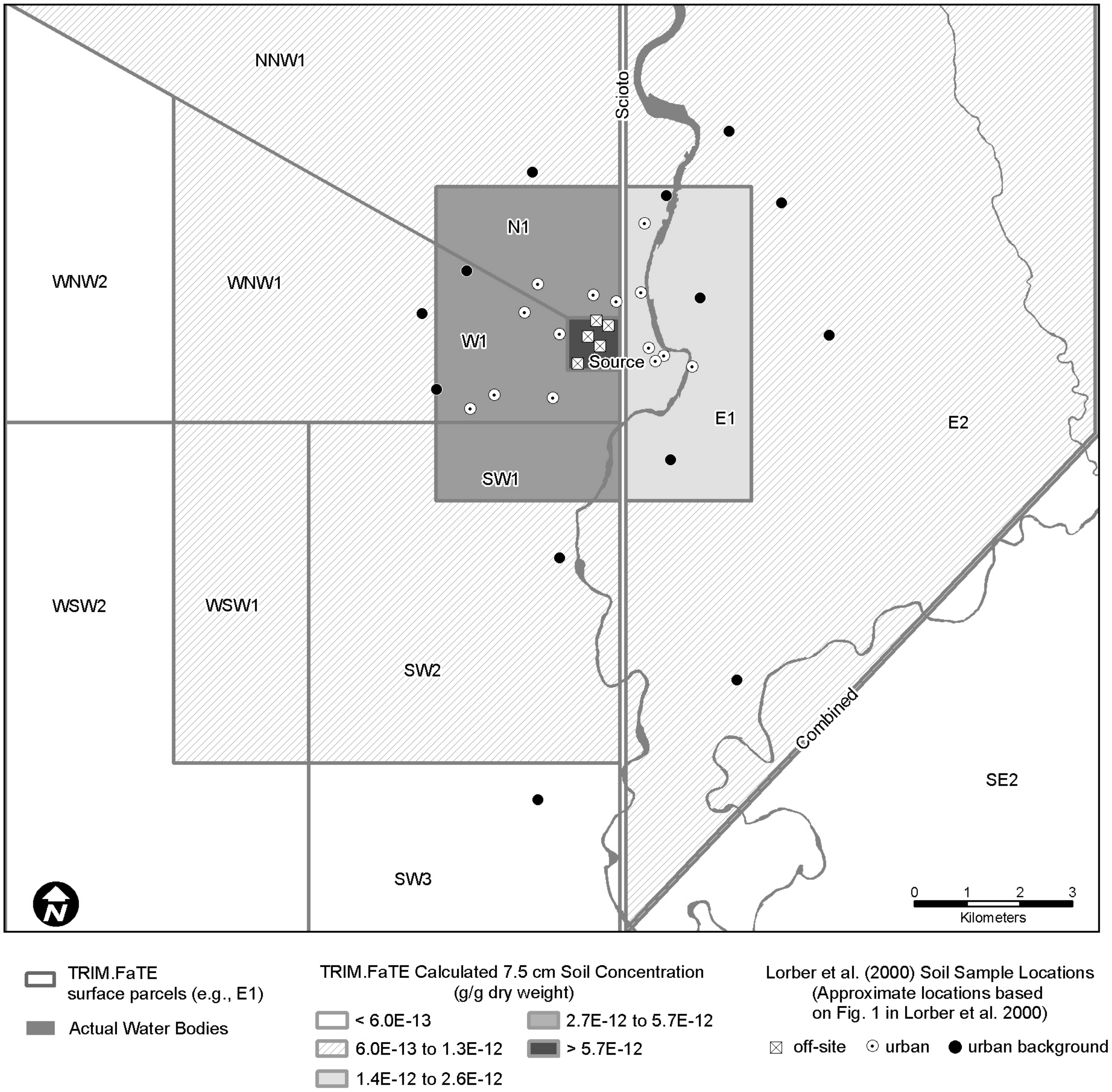
in regions well within the boundaries of the TRIM.FaTE modeling region, which extends approximately 10 km beyond the Region 3 sampling locations.

The measured and modeled soil estimates presented in Lorber et al. (2000) were averaged using a simple mean for all of the sampling locations in each of the regions. The soil sampling locations in Lorber et al. (2000) were not distributed evenly throughout the regions and in some cases were not within the boundaries of the region as described in the study; thus, the resulting averages across each region are not necessarily representative of the concentrations throughout the region. For Regions 2 and 3, which contain multiple TRIM.FaTE parcels, the concentrations for the corresponding compartments were area-weighted and averaged to obtain a single value for each region.

In Tables 7 and 8, TRIM.FaTE soil concentrations for TEQ and OCDD, respectively, are compared with measured and modeled results from Lorber et al. (2000). The measured concentrations were collected at the end of 1995. Two sets of modeled results are presented in Lorber et al. (2000), one based on 1992 stack test emissions and the other based on 1994 stack test emissions. For the TRIM.FaTE results, the surface soil and root zone soil concentrations were used to calculate the upper and lower bound of soil concentrations at a depth of 7.5 cm, using the methods described in Section 2.2.2, for both emissions scenarios. In cases where the upper and lower bound concentrations were different, both concentrations are provided in the comparison tables.

Figure 8 presents the TEQ concentrations spatially for the three regions using the 1994 stack test emissions and the upper bound of the TRIM.FaTE concentrations at a depth of 7.5 cm. The TRIM.FaTE calculated upper and lower bounds for the soil TEQ concentrations at a depth of 7.5 cm are presented for all compartments in tabular form in Appendix F. The TRIM.FaTE calculated soil concentrations were also compared to the local background concentration of 4.0E-12 g/g TEQ cited in Lorber et al. (2000). The TRIM.FaTE concentrations were below this background level at all locations except the Source, N1, and W1 compartments. This is consistent with Lorber et al. (2000), which states that local soil background concentration was reached at a distance of approximately three kilometers from the source.

Figure 8. Spatial Variation in Calculated 7.5 cm Soil Dioxin TEQ Concentrations at 11.5 Years (1994 Emissions): Soil Compartments and Corresponding Sampling Locations



As shown in Table 7, the measured results are generally closer to the modeled concentrations using the 1994 stack test emissions for both the TRIM.FaTE simulations and the Lorber et al. (2000) modeling simulations. Because the soil measurements were taken in December 1995 after the facility was no longer operating, the concentrations in soil were likely influenced by a range of emission rates (from before and after emission controls were implemented) and thus neither rate is likely to be truly representative of the actual emissions affecting these soil samples. The variations in emissions over the 11.5 year period of operation are likely to contribute to differences in measured and modeled results. In general, the modeled TRIM.FaTE results from both stack test emissions scenarios for both models are within the same order of magnitude as the measured concentrations, with the measured concentrations falling

Table 7. Comparison of Soil Dioxin TEQ Concentrations

	Lorber et al. (2000)			TRIM.FaTE	
Region	Measured (mean, Dec 1995)	Modeled (1992 Stack Test Emissions)[a]	Modeled (1994 Stack Test Emissions)[a]	Modeled (1992 Stack Test Emissions)[b]	Modeled (1994 Stack Test Emissions)[b]
	pg/g dry weight	pg/g dry weight	pg/g dry weight	pg/g dry weight	pg/g dry weight
1 (within 500 m of source)	45 - 466[c]	83 - 236	24 - 69	210-220	37-38
2 (500 m to 3 km from source)	9	34	10	21-23	4
3 (3 km to 8 km from source)	< 1	8	2	6	1

[a] A range is presented for the Lorber et al. (2000) measured and modeled concentrations in Region 1, corresponding to the on-site and off-site values as reported in Lorber et al. (2000).

[b] A range is presented if the estimated upper and lower bounds of the soil concentrations differed based on the methods used to calculate soil concentrations at a depth of 7.5 cm.

[c] On-site value for presentation purposes only (see Section 2.2.2).

between the modeled concentrations for 1992 and 1994 emission scenarios. The TRIM.FaTE results show a sharper decrease in concentrations closer to the source than the measured or modeled results presented in Lorber et al. (2000), with the concentrations decreasing by approximately an order of magnitude between Regions 1 and 2.

In Region 1, the TRIM.FaTE TEQ soil concentrations fall between the modeled concentrations from Lorber et al. (2000) for both emissions scenarios. For the outer two regions, the TRIM.FaTE concentrations are between 25 and 40 percent lower than the corresponding Lorber et al. (2000) modeled results for the 1992 emission scenario and between 50 and 60 percent lower for the 1994 emission scenario. The TRIM.FaTE concentrations for the 1994 emission scenario in Regions 1 and 3 are within 20 percent of the measured concentrations, and the TRIM.FaTE results from Region 2 are approximately 60 percent lower than the measured concentrations.

In Table 8, the TRIM.FaTE soil concentrations for OCDD are compared to the corresponding modeled and measured results in Lorber et al. (2000). It is worthwhile to point out that the modeled concentrations of OCDD actually increased between the simulation using 1992 stack test emissions and the simulation using 1994 stack test emissions, despite the overall TEQ emissions being reduced in 1994 stack test simulation. This is a result of the individual congener profile changing between the scenarios and emissions actually increasing for OCDD from the 1992 emission scenario to the 1994 scenario (see Appendix C). Overall, the measured soil concentrations of OCDD are much larger than the modeled soil concentrations from both TRIM.FaTE and Lorber et al. (2000) (by approximately an order of magnitude for Regions 2 and 3), although the TRIM.FaTE concentrations for the 1994 emission scenario are closer to the measured values in Region 1 than the Lorber et al. (2000) modeled results.

Table 8. Comparison of Soil Dioxin OCDD Concentrations

Region	Lorber et al. (2000)			TRIM.FaTE	
	Measured (mean, Dec 1995)	Modeled (1992 Stack Test Emissions)[a]	Modeled (1994 Stack Test Emissions)[a]	Modeled (1992 Stack Test Emissions)[b]	Modeled (1994 Stack Test Emissions)[b]
	pg/g dry weight	pg/g dry weight	pg/g dry weight	pg/g dry weight	pg/g dry weight
1 (within 500 m of source)	1,431[c] - 2,901	156 - 445	243 - 696	600-610	890 - 900
2 (500 m to 3 km from source)	613	64	100	51	58
3 (3 km to 8 km from source)	150	16	25	13	19

[a] A range is presented for the Lorber et al. (2000) measured and modeled concentrations in Region 1, corresponding to the on-site and off-site values as reported in Lorber et al. (2000).

[b] A range is presented if the estimated upper and lower bounds of the soil concentrations differed based on the methods used to calculate soil concentrations at a depth of 7.5 cm.

[c] On-site value for presentation purposes only (see Section 2.2.2).

One possible explanation for some of the modeled differences (e.g., the lower TRIM.FaTE soil concentrations in Regions 2 and 3 presented in Tables 7 and 8) may be the different dioxin soil dissipation rates used by the two models. In Lorber et al. (2000), a dioxin dissipation half-life of 25 years was used to account for dioxin removal from the soil by both chemical degradation and physical removal processes (e.g., runoff and erosion). In TRIM.FaTE, a 10-year degradation half-life value was used to model chemical degradation in soil; however, physical removal processes were modeled separately. In order to more directly compare the dissipation rate used in Lorber et al. (2000) to that modeled in TRIM.FaTE, the “effective” dissipation half-life (taking into account both chemical and physical removal processes) was calculated empirically from TRIM.FaTE results for 2,3,7,8-TCDD and 1,2,3,4,6,7,8,9-OCDD and was found to be approximately 6.5 and nine years, respectively. Therefore, the dioxin dissipation half-life used in the Lorber et al. (2000) analysis is roughly three times longer than the effective dissipation half-life used in TRIM.FaTE for these two chemicals. Both the dissipation rate used in the Lorber et al. (2000) analysis and the effective dissipation rate modeled in TRIM.FaTE fall within the range of the values reported in the literature for dioxin-like compounds in surface and subsurface soils (Mackay et al. 2000) and thus it is not clear that one value is preferable to the other. A more detailed discussion of the differences between the dissipation rate used in Lorber et al. (2000) and half-life values used in TRIM.FaTE is included in Appendix B.

The spatial distributions of the soil concentrations were also compared for the two models. Lorber et al. (2000) presents isoline figures of TEQ and OCDD concentrations for the two emissions scenarios within approximately one kilometer of the source for modeled concentrations and within one to two kilometers of the source for the measured values (not shown here). All of the figures show the highest soil concentrations to the north of the source for the modeled results and to the northeast for the measured concentrations. Figure 8 presents the spatial distribution of TRIM.FaTE soil concentrations (calculated to a depth of 7.5 cm) within approximately three kilometers using 1994 stack test emissions; detailed results from this simulation are presented in Appendix F. The TRIM.FaTE results show the highest soil concentrations to the north and west of the source, with concentrations of similar magnitudes to the east near the source (i.e., E1). It appears that the modeled soil concentrations estimated in Lorber et al. (2000) are more similar to the pattern of air concentrations estimated by TRIM.FaTE (see Figure 5), which show higher air concentrations to the north, than the pattern of TRIM.FaTE-estimated soil concentrations. There are several possible explanations for this. First, TRIM.FaTE models runoff and erosion explicitly and requires the user to estimate runoff and erosion patterns between parcels. Second, the size and shape of the parcels in TRIM.FaTE simulations may also have contributed to the differences. For instance, surface parcel E1 covers a fairly large area (extending out to three kilometers from the source) and it appears from the measured results that the concentrations in the eastern direction are higher to the north and much lower to the south; however, this is not distinguishable when looking at the TRIM.FaTE results because of how the layout was designed (e.g., there is one large parcel versus two or more smaller ones in the same area).

5.3 Modeling Uncertainties/Limitations

As with most model-to-monitor and model-to-model comparisons, there were several uncertainties and limitations in this comparison. These include model differences, accuracy of input data, types of algorithms used, and the output format and aggregation of data. Table 1 in Section 1.4 summarizes the similarities and differences between the two models; other issues associated with the model-to-model comparisons are discussed below.

Uncertainties involving the inputs and setup of TRIM.FaTE (e.g., abiotic information, chemical properties, meteorological data, source emissions, spatial layout), which are documented in Appendices A and B, are unavoidable considering the amount of information needed to perform the simulations.[4] Site- and chemical-specific data were collected where possible, although data were not always readily available and much of the congener-specific information was based on data for TCDD from the literature. The same local airport meteorological data used in Lorber et al. (2000) were also used in TRIM.FaTE; however, meteorological data were not collected for every year of the facility's operation and thus this data set may not have captured the year-to-year variability in meteorological conditions, potentially affecting the comparison of modeled results to measurements. It is unlikely that this affected the comparison of modeled data to measurements in air because dioxins do not accumulate in air over time. However, it may have affected the comparison to soil measurements because variations in meteorological conditions over time can have an impact on the accumulation of dioxins in soil.

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[4] An analysis of the sensitivity of each user-supplied input parameter is included in the TRIM.FaTE Mercury Test Case evaluation report (EPA 2004).

Lorber et al. (2000) also noted the uncertainty of the source emissions. The stack tests may not be completely accurate due to a rain event during the 1992 test and the fact that only the two stack tests were performed during the entire period of operation. Representative input data were gathered to the extent possible for TRIM.FaTE, given its availability in the literature and the resources available for this analysis. Other sources of uncertainty in comparing TRIM.FaTE to the Lorber et al. (2000) analysis involve the actual mechanisms and algorithms of the modeling approaches as they relate to dioxin-like compounds. For example, Lorber et al. (2000) state that ISCST3 does not include an algorithm for dechlorination; in contrast, TRIM.FaTE models chemical degradation (which includes dechlorination).

Output format and data aggregation were sources of uncertainty for both the air and soil comparisons. In Lorber et al. (2000), air concentrations were modeled at the point location of the air monitors. For this TRIM.FaTE analysis, the air concentrations for the comparison were predicted for individual air compartments that represent areas ranging from 2.4 km^2 to 25 km^2. Therefore, TRIM.FaTE air concentrations are not as spatially "fine-tuned" as those estimated using ISCST3, making it more difficult to compare the results at a specific location (i.e., the air monitors).

The TRIM.FaTE soil concentrations are also predicted for individual compartments with areas for the comparison ranging from one km^2 in Region 1 (for the source compartment) to 102 km^2 in Region 3 (for the E2 compartment). Similarly, the Lorber et al. (2000) results were presented for spatially aggregated areas (i.e., measured concentrations were averaged for all samples in each of the three regions); however, not all of sampling locations fell within the specified regions (e.g., some urban background samples were taken at two kilometers, which is outside the three to eight kilometer regions specified for urban background). In addition, the samples were not distributed evenly around the source and thus concentrations in some areas were weighted more than others. Therefore, for the soil comparison, both the aggregation of data in Lorber et al. (2000) and the size and orientation of the surface parcels in TRIM.FaTE likely contributed to some of the differences in the modeled and monitored results. It should be noted that the second report for this dioxin application focuses on the effects of differences in spatial resolution in TRIM.FaTE for both air and surface compartments.

5.4 Summary of Comparisons

Overall, the TRIM.FaTE-estimated air and soil concentrations of the 17 dioxin/furan congeners compared well to the results presented in Lorber et al. (2000). The modeled air TEQ concentrations for the 48-hour period from Lorber et al. (2000) and TRIM.FaTE generally have similar magnitudes, but slightly different spatial patterns. For both TEQ and OCDD air results, the spatial differences between the Lorber et al. (2000) results and the TRIM.FaTE results are likely due to some extent to the comparison between point concentrations and compartment concentrations. TEQ air concentrations modeled in TRIM.FaTE are generally more similar to the measured concentrations both in magnitude and spatial pattern. OCDD measured air concentrations do not match as well as the TEQ concentrations for both the TRIM.FaTE and Lorber et al. (2000) modeling results. The measured concentrations are lower to the southeast (the predominant wind direction) than both TRIM.FaTE and Lorber et al. (2000) modeled concentrations. Also, the measured values are highest to the northeast, which is similar to Lorber et al. (2000) results spatially although not in magnitude. However, this pattern does not match TEQ results or TRIM.FaTE results spatially and it does not appear based on the wind rose (see Appendix D) that this location should have the highest concentration associated with the source.

For the soil comparison, the TRIM.FaTE soil concentrations are slightly lower than the Lorber et al. (2000) modeled concentrations for TEQ and OCDD, except for locations close to the source where the TRIM.FaTE values fall within the range of Lorber et al. (2000) values for TEQ and are higher than OCDD concentrations. The slightly lower TRIM.FaTE concentrations in the outer regions may be related to the longer soil dioxin dissipation half-life used in the Lorber et al. (2000) modeling than in the TRIM.FaTE modeling. The measured TEQ concentrations fall within the range of TRIM.FaTE results for the two emissions scenarios, but the measured OCDD concentrations are much higher than all of the modeled concentrations from both the TRIM.FaTE and the Lorber et al. (2000) modeling. Spatially, the TEQ soil results from the two models are somewhat different in their patterns (the TRIM.FaTE concentrations are highest to the west and north, while the Lorber et al. (2000) values are highest directly to the north). However, the Lorber et al. (2000) spatial distribution for soil concentration matches closely to the TRIM.FaTE air concentration distribution, which is reasonable because Lorber et al. (2000) used an overall dissipation rate that does not vary spatially, whereas TRIM.FaTE models other soil processes (e.g., erosion, runoff) that vary by compartment independent of air.

6.0 REFERENCES

Lorber, M., A. Eschenroeder and R. Robinson. 2000. Testing the USA EPA's ISCST-Version 3 model on dioxins: A comparison of predicted and observed air and soil concentrations. Atmospheric Environment. 34(23): 3995-4010.

Mackay, D., W.Y. Shiu and K.C. Ma. 2000. Physical-Chemical Properties and Environmental Fate Handbook. Boca Raton, FL: CRC Press LLC.

McKone T. E. and D. H. Bennett. 2003. Chemical-Specific Representation of Air-Soil Exchange and Soil Penetration in Regional Multimedia Models. Environmental Science & Technology. 37(14): 3123 - 3132.

Ohio Environmental Protection Agency (OEPA). 1994. Risk assessment of potential health effects of dioxins and dibenzofurans emitted from the Columbus solid waste authority's reduction facility. The Ohio Environmental Protection Agency, Division of Air Pollution Control. February 28, 1994.

Solid Waste Authority of Central Ohio (SWACO). 1994. Corrected Data for March 16-18, 1994 Dioxin Test Waste to Energy Facility. Memorandum to U.S. EPA Region 5. October 26, 1994.

U.S. Environmental Protection Agency (EPA). 2000. Dioxin reassessment: Exposure and human health reassessment of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) and related compounds. Draft Final Report. EPA/600/P-00/001Bb. September 2000. Exposure Assessment and Risk Characterization Group. National Center for Environmental Assessment - Washington, DC.

U.S. EPA. 2002a. Total Risk Integrated Methodology: TRIM.FaTE Technical Support Document, Volume I: Description of Module. EPA-453/R-02-011a. September 2002. Emissions Standards and Air Quality Strategies and Standards Divisions. Office of Air Quality Planning and Standards - Research Triangle Park, NC.

U.S. EPA. 2002b. Total Risk Integrated Methodology: TRIM.FaTE Technical Support Document, Volume II: Description of Chemical Transport and Transformation Algorithms. EPA-453/R-02-011b. September 2002. Emissions Standards and Air Quality Strategies and Standards Divisions. Office of Air Quality Planning and Standards - Research Triangle Park, NC.

U.S. EPA. 2004. Evaluation of TRIM.FaTE Volume II: Model Performance Focusing on Mercury Test Case. In preparation. Emissions Standards and Air Quality Strategies and Standards Divisions. Office of Air Quality Planning and Standards. Research Triangle Park, NC.

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