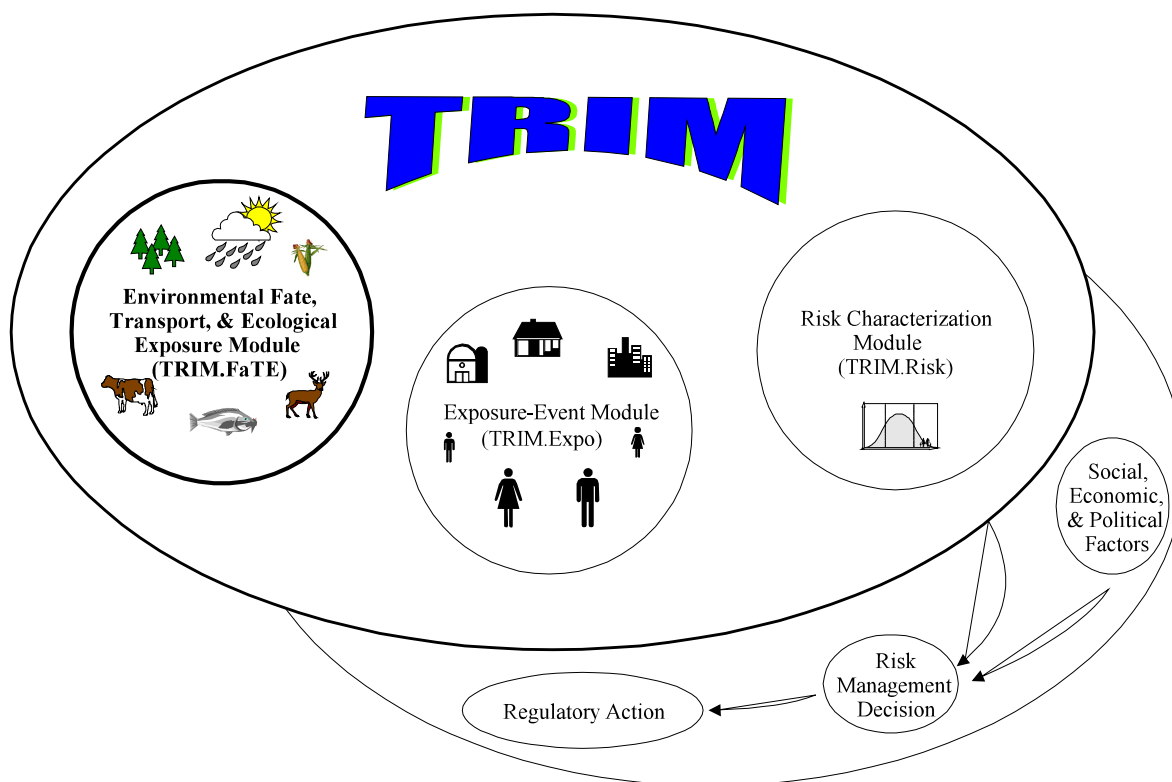




# Evaluation of TRIM.FaTE

## 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	Range of Air Concentrations (pg/m <sup>3</sup> )			
	Pollutant	Lorber et al. (2000)		TRIM.FaTE
		Measured Concentrations <sup>a</sup>	Modeled Concentrations <sup>b</sup>	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

<sup>a</sup>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.

<sup>b</sup>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 <sup>a</sup>	Modeled <sup>a</sup> (1992 Emissions)	Modeled <sup>a</sup> (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

<sup>a</sup> 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	<ul style="list-style-type: none"> <li>• Air dispersion only (i.e., no plume depletion)</li> <li>• 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</li> </ul>	N/A	<ul style="list-style-type: none"> <li>• Air advection and diffusion, particle and vapor-phase deposition, atmospheric degradation, and resuspension and diffusion from surface soil to air</li> <li>• The emissions and subsequent fate and transport of all 17 congeners were modeled individually</li> </ul>
Soil	<ul style="list-style-type: none"> <li>• Deposition was estimated for a single conservative pollutant, with no differentiation between the 17 individual congeners</li> <li>• Air dispersion and particle-phase deposition</li> <li>• Wet and dry deposition from air input into soil model as an annual average</li> </ul>	<ul style="list-style-type: none"> <li>• 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</li> </ul>	<ul style="list-style-type: none"> <li>• The fate and transport of all 17 congeners were modeled individually</li> <li>• Air advection and diffusion, particle and vapor-phase deposition, atmospheric degradation, and resuspension and diffusion from surface soil to air</li> <li>• Wet and dry deposition from air (varies with time during modeling period; e.g., wet deposition is dependent on rainfall)</li> <li>• Degradation half-life in surface and root zone soil of 10 years for all modeled chemicals</li> <li>• Physical removal processes (e.g., erosion, runoff) modeled separately</li> </ul>

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## 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 <sup>a</sup>	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 <sup>b</sup>	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 <sup>b</sup>	Surface and root zone soil results at 11.5 years, averaged over three regions around the source corresponding to locations modeled and monitored

<sup>a</sup>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.

<sup>b</sup>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-octachloro-dibenzo(p)-dioxin (OCDD) concentrations, were compared to the TEQ and OCDD measured and



modeled estimates in the Lorber et al. (2000) analysis.<sup>1</sup> 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.<sup>2</sup> 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 12<sup>th</sup> 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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<sup>1</sup> 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).

<sup>2</sup> 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).<sup>3</sup> 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 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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<sup>3</sup> 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.

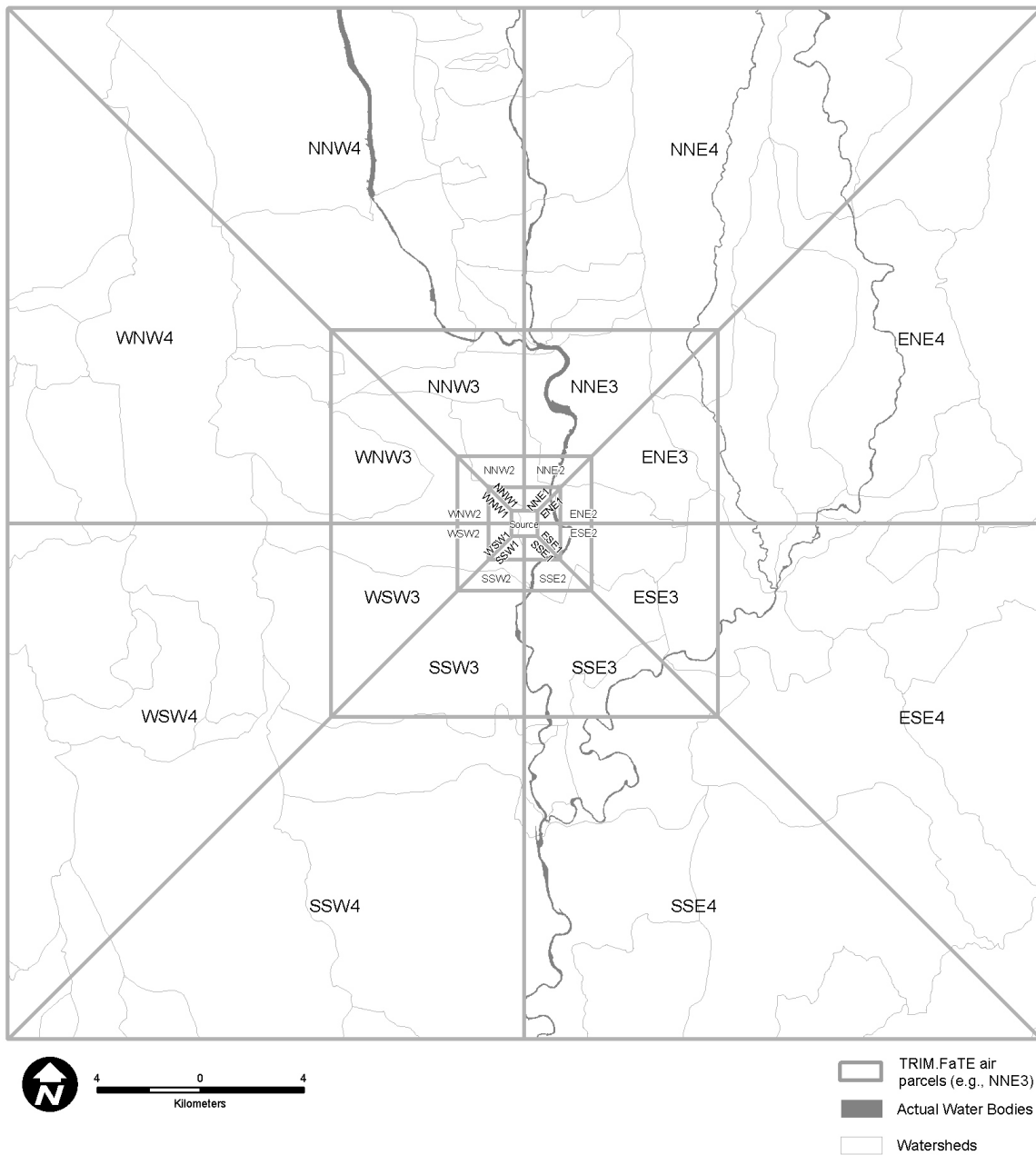
**Table 3. Dioxin and Furan Congeners Used for Comparison**

CONGENER	ABBREVIATION
<b>Dioxins</b>	
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
<b>Furans</b>	
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
2,3,4,6,7,8-Hexachlorodibenzo(p)furan	2,3,4,6,7,8-HxCDF
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

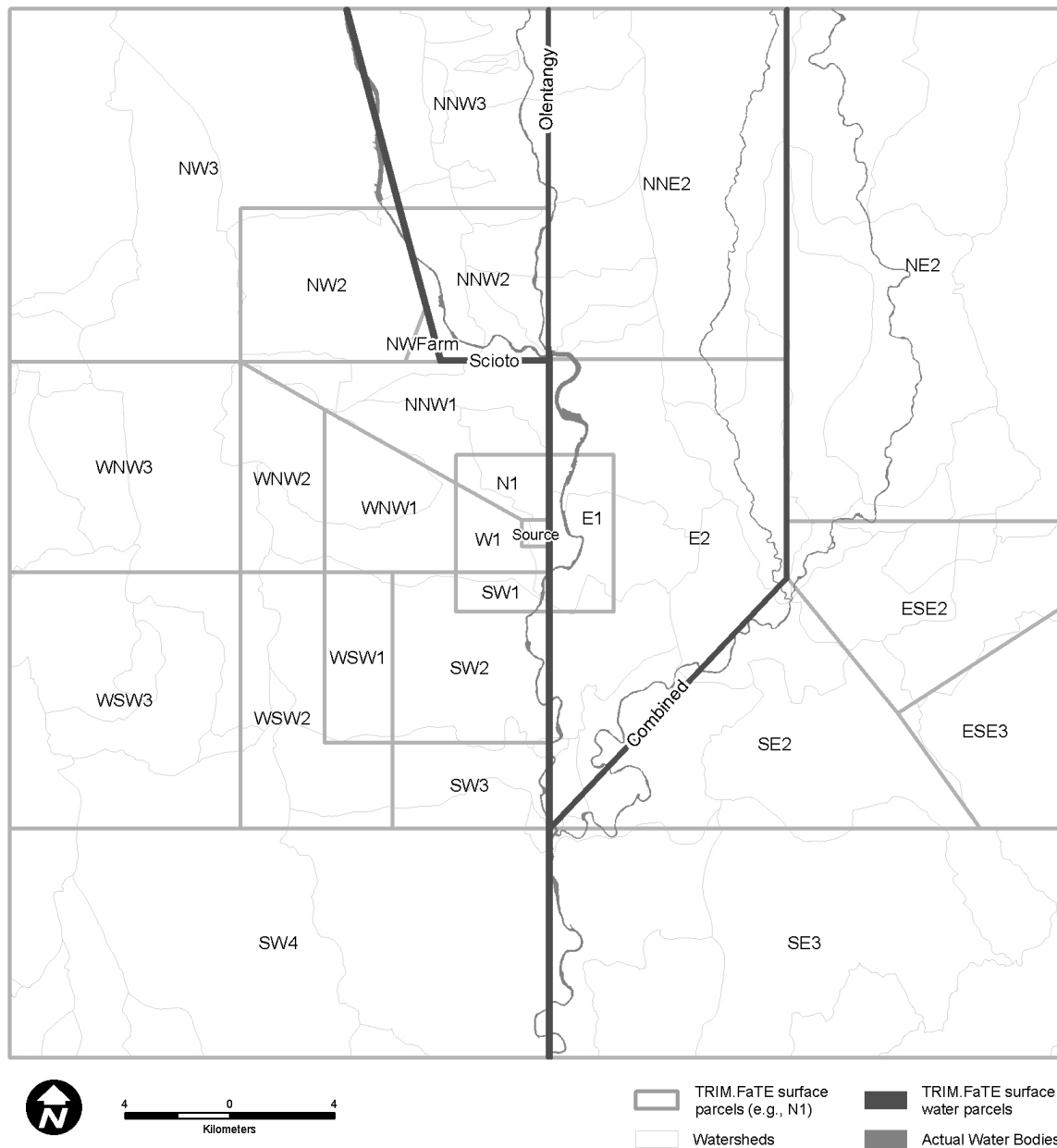
The configuration of the air layout presented in Figure 1 shows the 33 individual air parcels (i.e., two-dimensional areas used to subdivide the modeling region) in the lower air layer. The vertical dimension of the lower air layer (i.e., the upper boundary) was set to the mixing height, which varied 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.

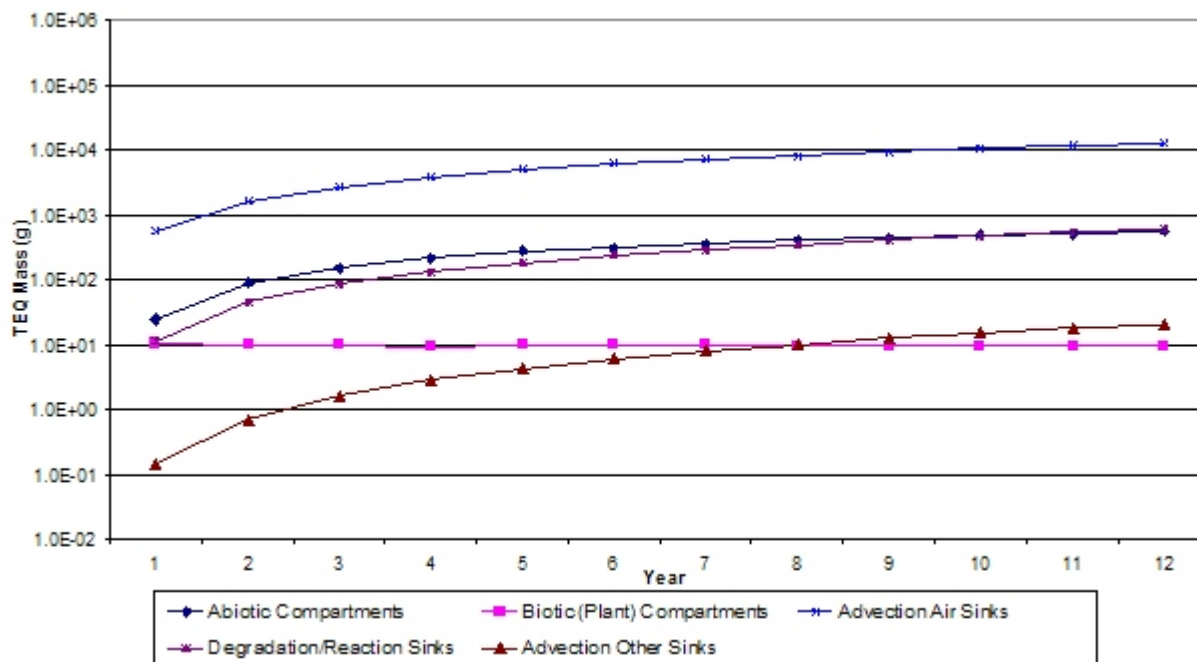
#### 4.1.1 Overall Mass Distribution

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<sup>a</sup>**



<sup>a</sup>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

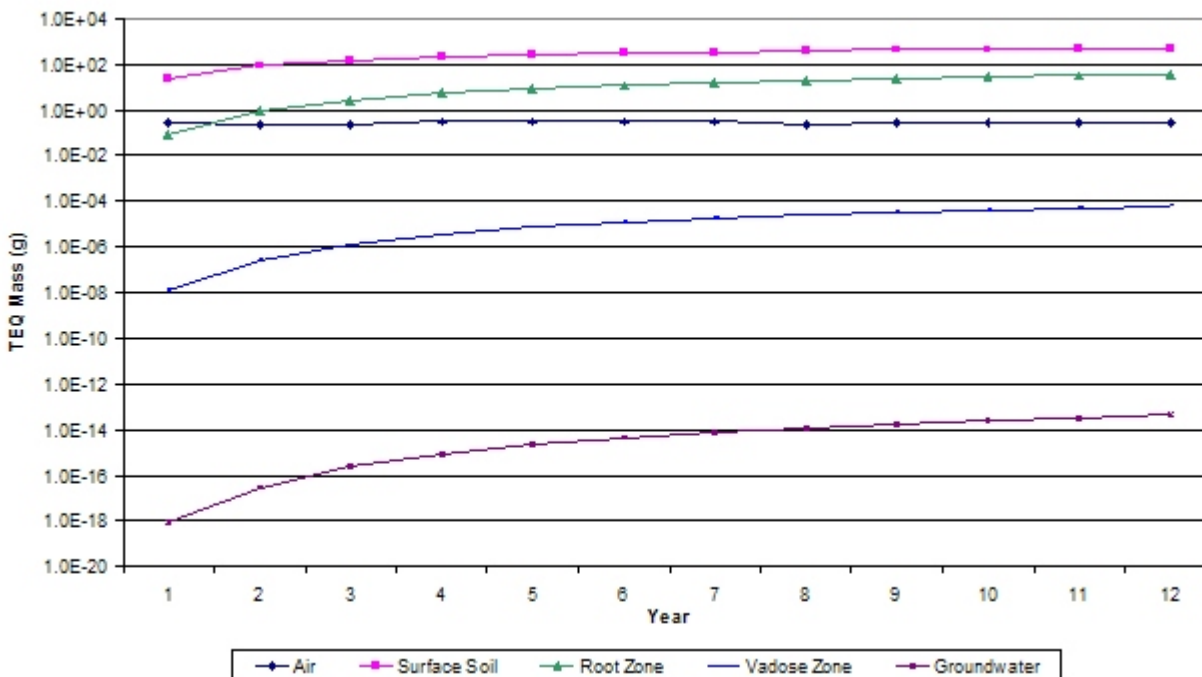
The patterns of accumulation of dioxin mass in the abiotic compartment types of interest for this analysis (i.e., air and soil) are shown in Figure 4. This figure shows that all of the soil compartments accumulate mass steadily, whereas the mass in air compartments is relatively constant over the course 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.

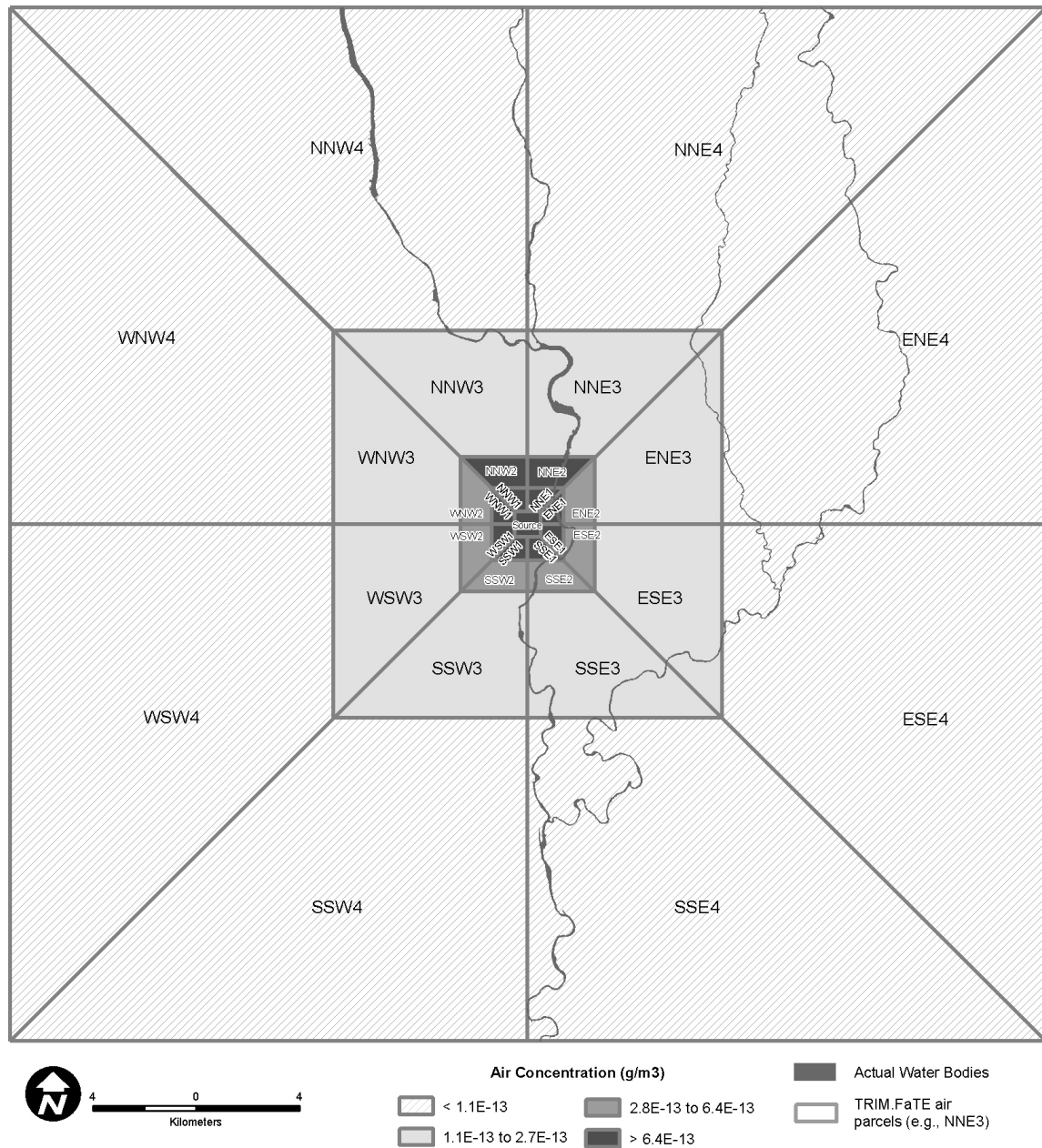
#### 4.3.1 Air Concentrations

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.

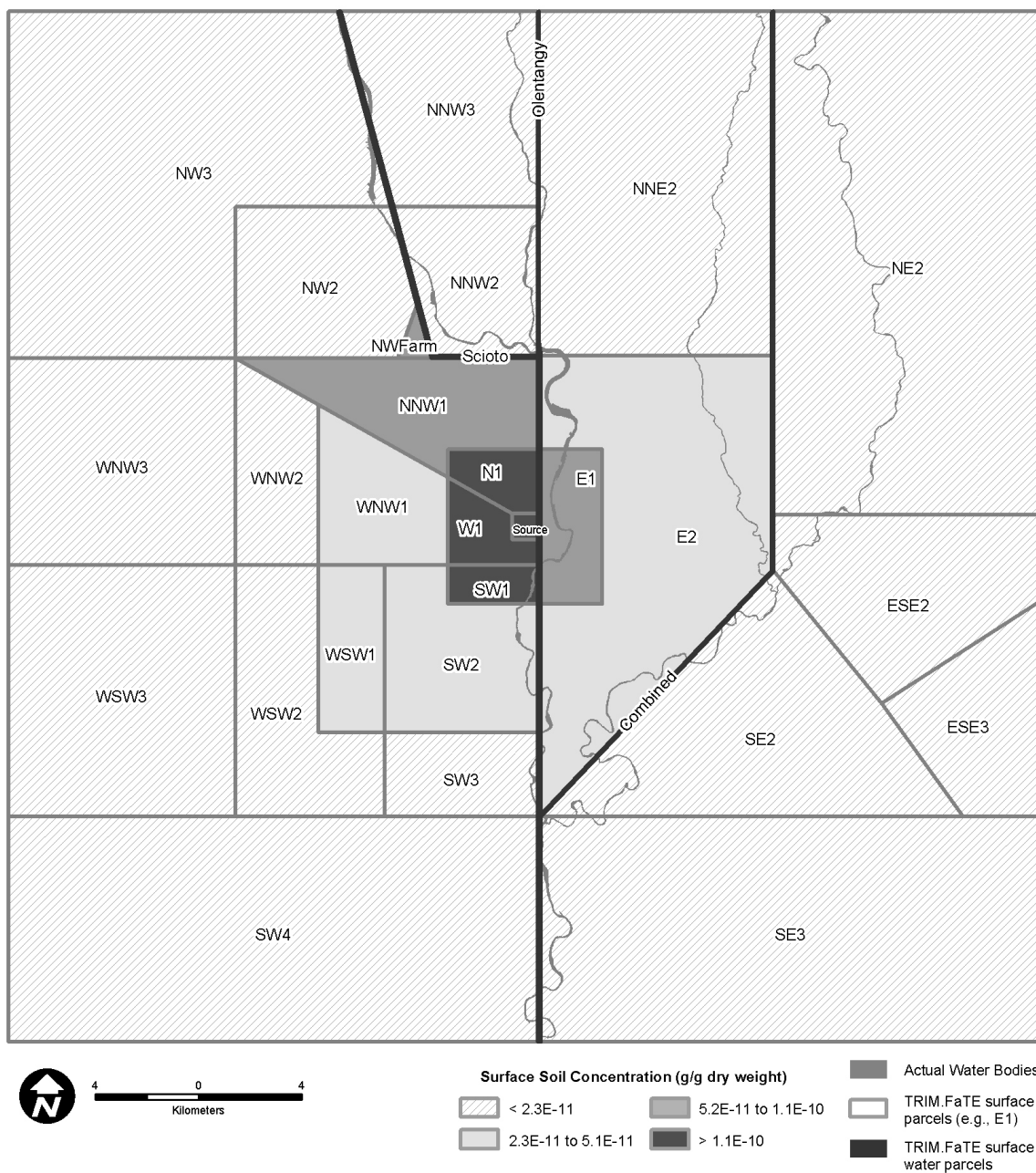
#### 4.3.2 Soil Concentrations

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 15<sup>th</sup> until noon on March 17<sup>th</sup> 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.

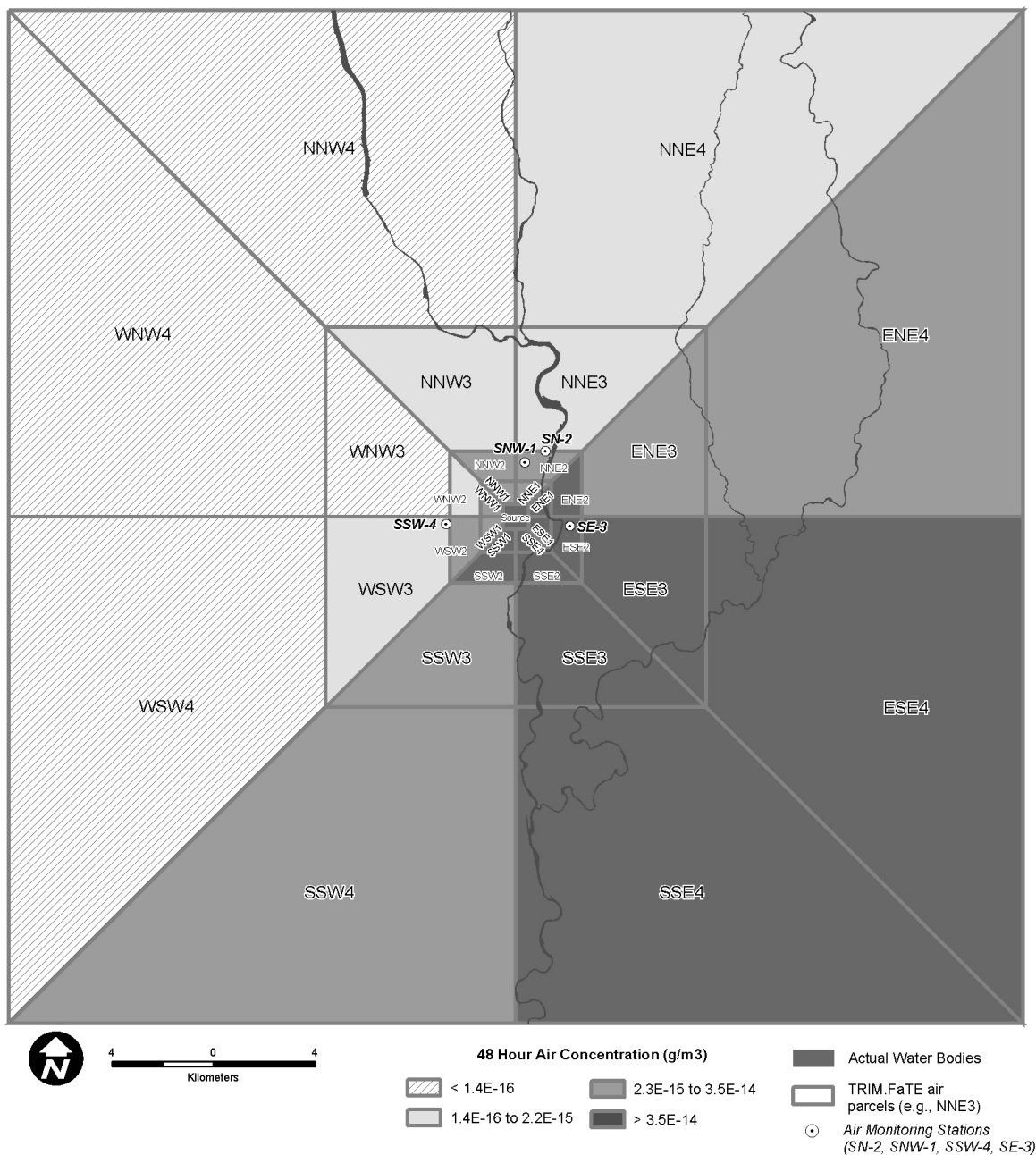
**Table 4. 48-Hour Average Air Dioxin TEQ Concentration Comparison**

Comparison Location	Lorber et al. (2000)			TRIM.FaTE	
	Air Monitoring Station	Measured TEQ concentration (pg/m <sup>3</sup> ) <sup>a</sup>	Modeled TEQ concentration (pg/m <sup>3</sup> ) <sup>b</sup>	Corresponding Air Compartment(s)	Modeled TEQ concentration (pg/m <sup>3</sup> )
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

<sup>a</sup>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.

<sup>b</sup>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 <sup>3</sup> ) <sup>a</sup>	Modeled concentration (pg/m <sup>3</sup> ) <sup>b</sup>	Corresponding Air Compartment(s)	Modeled concentration (pg/m <sup>3</sup> )
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

<sup>a</sup>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.

<sup>b</sup>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

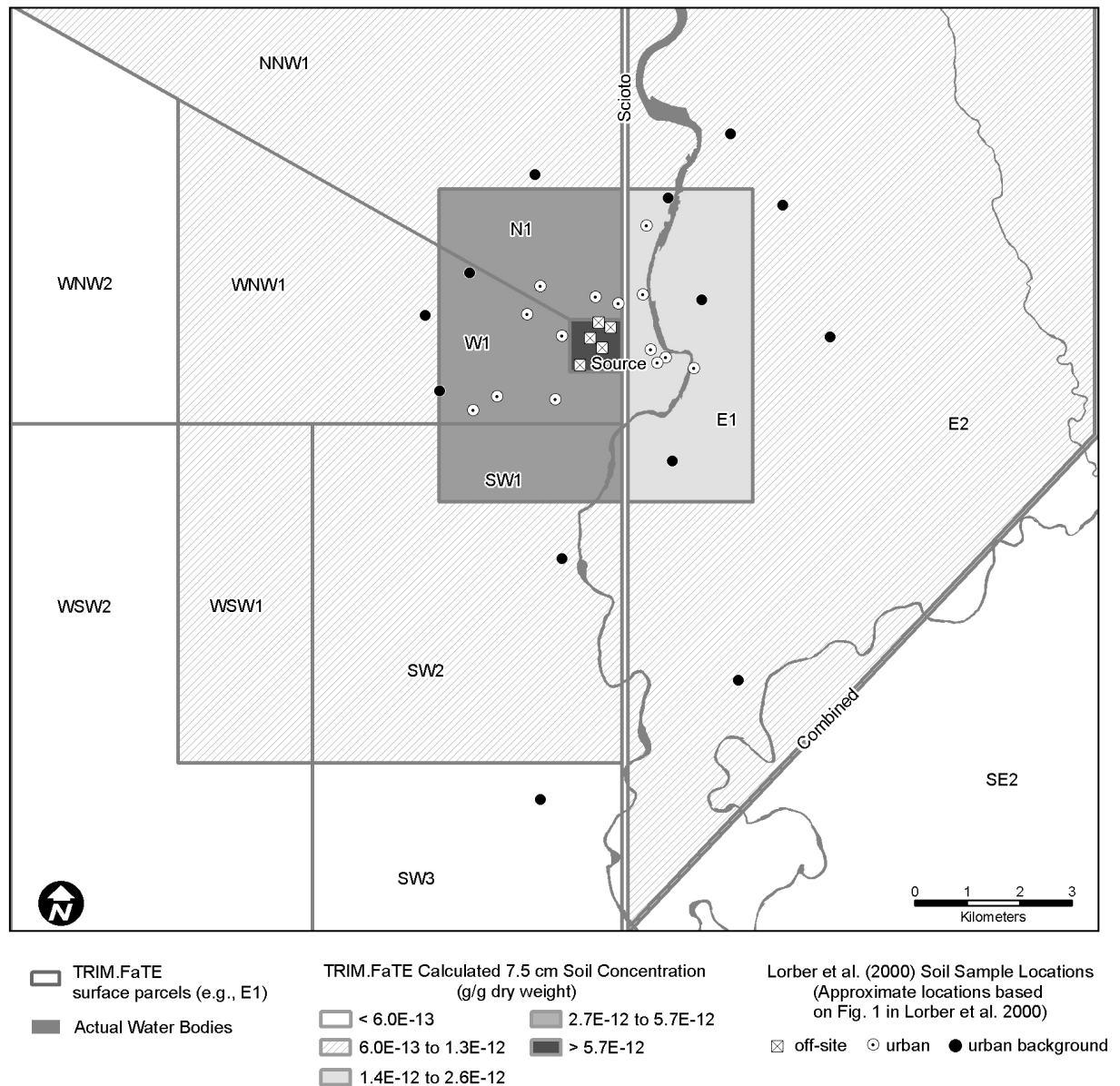
in regions well within the boundaries of the TRIM.FaTE modeling region, which extends approximately 10 km beyond the Region 3 sampling locations.

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**

Region	Lorber et al. (2000)			TRIM.FaTE	
	Measured (mean, Dec 1995)	Modeled (1992 Stack Test Emissions) <sup>a</sup>	Modeled (1994 Stack Test Emissions) <sup>a</sup>	Modeled (1992 Stack Test Emissions) <sup>b</sup>	Modeled (1994 Stack Test Emissions) <sup>b</sup>
	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 <sup>c</sup>	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

<sup>a</sup> 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).

<sup>b</sup> 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.

<sup>c</sup> 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) <sup>a</sup>	Modeled (1994 Stack Test Emissions) <sup>a</sup>	Modeled (1992 Stack Test Emissions) <sup>b</sup>	Modeled (1994 Stack Test Emissions) <sup>b</sup>
	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 <sup>c</sup> - 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

<sup>a</sup> 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).

<sup>b</sup> 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.

<sup>c</sup> 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.<sup>4</sup> 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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<sup>4</sup> 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<sup>2</sup> to 25 km<sup>2</sup>. 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<sup>2</sup> in Region 1 (for the source compartment) to 102 km<sup>2</sup> 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.

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## **Appendix A.**

### **SPECIFICATIONS OF TRIM.FaTE SIMULATIONS**

This appendix summarizes the specifications of the TRIM.FaTE simulations.

- Section A.1 lists the chemicals modeled in these simulations and describes how the chemical-specific emission rates were calculated.
- The spatial layout and the methodology used to develop the layout are described in Section A.2.
- Sections A.3, A.4, and A.5, describe the meteorological, environmental setting, and biotic data used in the simulations.
- The overall simulation settings – including the data, simulation, and output time steps and output data export settings – are described in Section A.6.

References are included at the end of the appendix.

This information is supplemented by Appendices B and C, which provide detailed documentation of the values and references for all the input parameters used in the TRIM.FaTE simulations for this analysis. The modeling concepts, approaches, algorithms, equations, and assumptions used in TRIM.FaTE (including the TRIM.FaTE library used in this analysis) are documented in detail in a two-volume Technical Support Document (EPA 2002a and b) and are not discussed at length here.

## **A.1 Modeled Chemicals and Emission Rates**

### **A.1.1 Chemical Data**

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 the Lorber et al. 2000 report. These congeners are listed in Table 2 of the report along with the abbreviations that are commonly used for them. The chemical properties used in TRIM.FaTE for these congeners are documented in Appendix B.

The fate and transport of these 17 congeners were modeled in TRIM.FaTE individually. To facilitate comparison with the results presented in the Lorber et al. reports, the individual results for these chemicals were subsequently combined into toxic equivalent (TEQ) concentrations. These TEQ concentrations were calculated by multiplying the compartment concentrations of each congener by its corresponding toxicity equivalent factor (TEF), which were the exact same as used by Lorber et al. (2000) and described in Appendix C, and then summing the resulting products across all of the congeners. In addition, congener-specific compartment results for TCDD and OCDD from TRIM.FaTE are compared to the corresponding results from the Lorber et al. 2000 report. These congeners were chosen because they were the only two congeners in the Lorber et al. 2000 report for which individual results are presented both on tables and in spatial plots.

### **A.1.2 Calculating Chemical-specific Emission Rates**

Emissions from stack tests conducted at the CMSWTE facility in 1992 (Ohio EPA 1994) and 1994 (SWA 1994) that were used in the Lorber et al. 2000 report were also used as the basis for chemical-specific emission rates for this analysis. The detailed calculations using the stack test data to obtain chemical-specific emission rates for TRIM.FaTE are included in Appendix C. In these calculations, the 1992 and 1994 stack test data were converted to the correct units for TRIM.FaTE (grams of chemical emitted per day) and adjusted for usage based on the assumption that on average 4.22 boilers were used continuously at the facility. This same methodology was used to calculate the emissions used in the Lorber report as well. Appendix C summarizes the chemical-specific emission rates that were modeled using the 1992 and 1994 stack tests.

### **A.1.3 Calculating Specific Emission Rates for each Stack Test**

The Lorber et al. 2000 analysis reported emission rates in terms of TEQ emissions. Because TRIM.FaTE modeled each congener individually, instead of as TEQ emissions, congener-specific emission rates needed to be developed. Using the stack tests referenced as the source of emissions data for the Lorber et al. 2000 report, emission rates were calculated for each congener (these calculations are described in detail in Appendix C).

The 1994 emissions reflected a combustion improvements at the facility that reduced emissions by approximately 73 percent in terms of TEQ concentration. The congener-specific emission rates for 1994 are not all reduced by 73 percent, this only refers to the TEQ concentration; in fact, some of the congener (e.g., OCDD) concentrations increase from 1992 to 1994.

To confirm the calculations were correct, the congener-specific emission rates from the 1992 and 1994 stack test were converted into TEQ emission rates (in grams per second) and compared to the emission rates reported in two Lorber et al. reports (1996 and 2000). This comparison showed that the emission rates used in the TRIM.FaTE simulations were consistent with emissions used by Lorber et al. Appendix C summarizes the emissions in TEQ modeled for each stack test.

## A.2 Spatial Layout

The spatial layout of parcels provides the underlying framework for a TRIM.FaTE simulation. Thus, it is important to create a layout that is representative of the area being modeled and, in this application, similar to the areas outlined in the reports to which these results were to be compared. The process of designing the spatial layout for this TRIM.FaTE analysis involved defining the modeling region (Section A.2.1) and delineating this region into surface parcels (Section A.2.2) and air parcels (Section A.2.3). Definitions for important spatial terms used in this section are summarized in the text box below.

A **parcel** is a planar (i.e., two-dimensional), horizontal geographical area used to subdivide the modeling region. Parcels, which are polygons of virtually any size or shape, are the basis for defining volume elements and do not change for a given scenario. There can be separate parcels for air and for the land surface (soil or surface water).

A **volume element** is a bounded three-dimensional space that defines the location of one or more compartments.

A **compartment** is defined as a unit of space characterized by its homogeneous physical composition and within which it is assumed, for modeling purposes, that all chemical mass is homogeneously distributed and is in phase equilibrium.

### A.2.1 Modeling Region

For this analysis, the overall size and extent of the area for which pollutant fate and transport were modeled (i.e., the modeling region) was determined based on the location of the emissions source, expected mobility of the chemicals of primary interest (i.e., chemicals listed in Table A.1), locations or receptors of interest (e.g., dairy farms, monitoring stations), and watershed boundaries for the water bodies of interest. The size and extent of the modeling region was determined by identifying the location of interest farthest from the source and

creating a square centered on the source that captured this location<sup>1</sup>. A square shape was selected to allow for an equal number of air parcels in each direction. The modeling region was centered on the source location because the locations of interest (primarily the monitoring locations discussed in the Lorber et al. 2000 report) are scattered around the facility, rather than on one side, and the wind direction in the Columbus area (based on the available meteorological data) varies across the site.

### **A.2.2 Surface Layout**

The surface parcels were designed based on the source location, locations of water bodies, watershed boundaries for these water bodies, and locations and receptors of interest. The layout is centered on a square source parcel that approximates the surface area of the facility. Surface parcels included either soil or water parcels.

Four primary water bodies were identified within the modeling region: Scioto River, Olentangy River, Walnut Creek, and Alum Creek. Surface parcels were created for the Scioto River and Olentangy River based on the path and average width of these water bodies. Walnut Creek and Alum Creek were combined into a single surface parcel because they run together for nearly half of their distance within the modeling region. The remaining surface parcels were delineated based on the monitoring and modeling locations in the Lorber et al. 2000 report, as well as the watershed boundaries within the modeling region.

The resulting surface parcel layout, presented in Figure 1 in the main body of this report, consists of 27 soil parcels (including a small source parcel centered on the emission source) and three surface water parcels, for a total of 30 surface parcels.

For each soil parcel, four volume elements were defined (i.e., surface soil, root soil, vadose soil, and groundwater) that correspond to soil layers. The depths for these volume elements were 1 cm, 81 cm, 153 cm, and 3 m, respectively<sup>2</sup>. Associated with each surface water parcels is a surface water volume element above a sediment volume element. The depths of the surface water and sediment volume elements were based on site-specific or regional data and professional judgment, and are presented in Appendix B.

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<sup>1</sup>See TRIM.FaTE User's Guide (EPA 2003) for more information on TRIM.FaTE parcel designs.

<sup>2</sup>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 at depths of up to one meter. The soil depths in TRIM.FaTE for this application were selected based on site-specific data and configurations used in previous TRIM.FaTE applications.

### **A.2.3 Air Layout**

The air parcels were designed based on the source location, the degradation rates of the modeled chemicals, the locations and receptors of interest, and the desire to maintain a regular, symmetric layout in an “approximated radial grid” shape. The air portion of the modeling region was divided into two vertical layers of volume elements. The boundary between the two layers corresponds to the atmospheric mixing height and varies with time. The air layer closest to the ground was divided into individual parcels (and associated volume elements) designed to provide higher spatial resolution near the facility (where the gradient of concentrations is greater) and less resolution further from the facility (where the gradient of concentrations is smaller). This bottom air layer was centered on a source parcel that matches exactly with the source parcel in the surface parcel layout. The remaining air parcels in the bottom layer were arranged in a grid of polygons designed to approximate a polar grid originating from the source parcel. The radial distances between the parcels were selected to maintain a consistent relative decrease in estimated air concentrations with distance from the source. The upper air layer was designed as a single air volume element covering the entire modeling region with the top of the layer set to 4.0 kilometers, which is approximately 1.0 kilometer above the maximum mixing height for the meteorological data used at the site. This upper air layer was included to track emissions released above the mixing height (i.e., during times when the mixing height is lower than the source elevation) and is considered a sink for the purposes of this report since the mass released to the upper layer remains there and is no longer available.

The resulting air configuration is presented in Figure 2 in the Report. This figure shows the 33 individual air parcels in the bottom layer. The top layer consists of a single volume element with the same outer boundary as the outer boundary of the bottom layer. The air parcels do not line up exactly with the surface parcels, although the outer boundaries of both parcel sets are the same. Figure 2 also shows the air monitoring locations from the Lorber et al. 2000 report.

### **A.3 Meteorological Data**

The meteorological data used in this analysis correspond exactly to the 1989 data used in the Lorber et al. 2000 report for the soil analyses, and the 1994 local airport data for the air analyses. The surface air data were from Columbus, Ohio, and the upper air data are from Dayton, Ohio. These data were downloaded from EPA's Support Center for Regulatory Air Models web site (see <http://www.epa.gov/ttn/scram/>). All meteorological data required by TRIM.FaTE were presented in one-hour time steps.

The soil results from the Lorber et al. 2000 report were modeled using only one year of meteorological data (1989) and assumed that deposition in subsequent years was identical to the modeled year; therefore, in the two 12-year TRIM.FaTE simulations used for the soil comparisons, the 1989 meteorological data were repeated for all of the years over the course of the simulation.



#### **A.4 Abiotic Compartment Data**

For this report, the results from the TRIM.FaTE model simulations were compared only to the air and soil concentrations in the Lorber et al. 2000 report. Therefore, only air, surface soil, and root zone soil compartments, as well as the other compartment types that significantly impact the overall mass balance, were needed in the simulations. Abiotic media included in these TRIM.FaTE simulations were air, soil (surface, root zone, and vadose zone), groundwater, surface water, and sediment.

For the environmental setting (i.e., abiotic) input data, site-specific values were obtained or calculated, when possible, using U.S. Geological Survey data, topographic maps, and other resources with local or regional information. The representativeness of the data was evaluated, if possible, based on the purpose of the simulation and resources available. Appendix B contains the documentation of values for all environmental setting data. Chemical-specific input data for the abiotic compartments were obtained for the 17 dioxin-like compounds and are also documented in Appendix B. Calculations and assumptions for the surface water data are detailed at the end of Appendix B for the three surface water bodies included in the TRIM.FaTE simulations.

#### **A.5 Biotic Compartment Data**

There are no comparison data for biota in the Lorber et al. 2000 report. Based on results from previous TRIM.FaTE analyses, the presence of vegetation has the potential to affect the mass balance in other compartments, such as air (e.g., via the intake of chemicals to leaves through the stomata) and soil (via transfer of the chemical to soil during litter fall); therefore, plant compartments were included wherever appropriate. Other biotic compartments, such as terrestrial and aquatic animals, are not expected to significantly impact air or soil concentrations and, thus, were not considered in this analysis.

Terrestrial vegetation types (i.e., grasses/herbs, agriculture, and deciduous forests) were assigned to all surface parcels based on land use information from the National Land Cover Data database. Based on these data, most of the surface parcels were assigned grasses/herbs. One of the surface parcels was assigned the deciduous forest vegetation type, and two were assigned agricultural vegetation. The remaining surface parcel corresponded to the source location and was not assigned any vegetation. Documentation of the vegetation types of each plant compartment, as well as the corresponding input data are included in Appendix B.

#### **A.6 Simulation Settings**

This section describes the settings for the TRIM.FaTE simulations included in the analysis. Section A.6.1 describes the details of the scenario setup, Section A.6.2 describes the time-varying inputs used in the analysis, Section A.6.3 describes the selected simulation and output time steps, and Section A.6.4 describes the selected options for exporting results from TRIM.FaTE.

### A.6.1 Scenario Setup

Table A-2 lists the three simulations modeled for this comparison report with the details of the setup. The emissions, summarized in Section A.1, refer to the stack tests upon which they are based. The modeling period used for this comparison report lists the time period that was chosen to correspond to the those used in the Lorber et al. 2000 report. All of the simulations were set up using only plants for biota, all 17 dioxins/furans used in the Lorber report, a meteorological data time step of one hour (the smallest increment that the data are reported), a simulation time step of one hour (see Section A.6.2), and an output time step of monthly or hourly (see Section A.6.2).

**Table A-2. Detailed List of TRIM.FaTE Simulations**

Emissions	Modeling Period Used for Comparison	Biota	Chemicals	Met Data Time Step	Sim Time Step	Output Time Step	Compartments Used for Comparison
1994 stack test	1 year	Vegetation only	17 dioxin/ furans	1hr	1hr	1hr	Air
1992 stack test	12 years	Vegetation only	17 dioxin/ furans	1hr	1hr	Monthly (i.e., 730 hrs)	Surface and root zone soil
1994 stack test	12 years	Vegetation only	17 dioxin/ furans	1hr	1hr	Monthly (i.e., 730 hrs)	Surface and root zone soil

### A.6.2 Time-varying Inputs

Some of the inputs to the TRIM.FaTE simulations described in this report varied with time: meteorological data and vegetation data (i.e., AllowExchange and litter fall rate). The AllowExchange property is a Boolean property that indicates whether it is the growing season for each vegetation type. For this application, the grasses/herbs, agriculture, and deciduous forest compartments had a growing season starting on April 15<sup>th</sup> (the local spring thaw) and ending on November 5<sup>th</sup> (the local fall freeze) of each year modeled. The litter fall rate property is a seasonal property used to model the loss of plant leaves (and particles on leaves) to soil. For all three vegetation types modeled, litter fall was set to begin at this site with the first frost on November 5<sup>th</sup> of every year, and ended December 4<sup>th</sup>, and assumed that 99 percent of leaves fall at a constant rate over these 30 days.

### A.6.3 Simulation and Output Time Steps

The simulation and output time steps are simulation settings used to specify how often the model will calculate the mass and concentration in each compartment and how often these data will be output. The simulation time step specifies the frequency at which the model will calculate transfer factors and chemical mass exchange between compartments. For all simulations associated with this analysis, the simulation time step was set to one hour,

corresponding to the smallest input data time step (i.e., the time-varying data that changes most frequently).

The output time step specifies how often the model outputs (e.g., mass and concentrations in each compartment, deposition rates to surface soil compartments) will be reported. The output time step was either monthly<sup>3</sup> (for the simulations used for comparison to soil concentrations) or hourly (for the simulation used for comparison to air concentrations). Because soil concentrations change more gradually over time than air concentrations and thus do not need to be output as frequently, monthly time steps were used for the simulations used in the surface soil comparisons to reduce the volume of output data generated by TRIM.FaTE. Conversely, air concentrations can change significantly from hour to hour based on changes in the meteorological conditions and thus the simulations used in the air comparisons used hourly output time steps.

#### **A.6.4 Output Data Export Settings**

For each TRIM.FaTE simulation included in this analysis, the following types of outputs were selected:

- Moles of each modeled chemical in each compartment at each output time step;
- Mass of each modeled chemical in each compartment at each output time step;
- Concentration of each modeled chemical in each compartment at each output time step; and
- Wet and dry particle and vapor deposition rates to each surface soil compartment at each output time step.

In addition to these outputs, several diagnostic outputs (e.g., HTML export) were generated to provide additional insight into how the model is working. Although the comparisons focused on the concentration outputs, the additional outputs were useful for interpreting results.

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<sup>3</sup> The monthly output time step outputs the results every 730 hours to approximate the average number of hours in a month.

## References

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## **Appendix B**

### **DOCUMENTATION OF TRIM.FaTE INPUT PARAMETERS**

This appendix contains the following sets of tables, including supplemental tables with calculations and discussion where appropriate, listing and describing the input parameters used in TRIM.FaTE:

- chemical-independent parameters for abiotic and biotic (i.e., plant) compartment types;
- chemical-dependent (i.e., value varies by chemical) parameters independent of compartment type;
- chemical-dependent parameters for abiotic and biotic (i.e., plant) compartment types.

For each parameter listed, the parameter name, input units, value used, and a reference are given. Full citations for each reference are provided at the end. Several attachments, referred to in the tables, provide additional detailed documentation.

Within the framework of the TRIM.FaTE computer model, several different kinds of “properties” are defined and used. The input parameters listed in this appendix fall into the following categories of TRIM.FaTE properties:

- compartment properties (includes by far the largest number of input parameters);
- volume element (VE) properties;
- link properties;
- chemical properties;
- source properties; and
- scenario properties.

In the following tables, the property type is identified for all input parameters that are not compartment properties.

Note that the units listed in these tables are the units in which model input values need to be expressed. In a few cases, these computer model input units do not match the units used for the same parameter in equations and derivations in TRIM.FaTE Technical Support Document Volume II. In such cases, there are internal units conversions in the computer model that account for the differences.

**Chemical-Independent/Abiotic -- Documentation for OH WTE Dioxin Test Case**  
**(same values used for all air compartments)**

**Air Compartment Type**

Parameter Name	Units	Value Used	Reference
Atmospheric dust load	kg[dust]/m <sup>3</sup> [air]	7.80E-08	Bidleman 1988
Density of air	g/cm <sup>3</sup>	0.0012	U.S. EPA 1997
Dust density	kg[dust]/m <sup>3</sup> [dust]	1,400	Bidleman 1988
Fraction organic matter on particulates	unitless	0.2	Harner and Bidleman 1998
Height [VE property] <sup>a</sup>	m	mixing height (varies hourly)	Local airport meteorological data, 1989 and 1994
Washout ratio	[mass chem/volume rain]/[ mass chem/volume air]	33,495	Vulykh and Shatalov 2001

<sup>a</sup>Height of air volume elements is set in TRIM.FaTE using two properties, the bottom of the volume element (set at 0 meters) and the top of the volume element (set to the mixing height, which varies hourly).

**Chemical-Independent/Abiotic -- Documentation for OH WTE Dioxin Test Case**  
**(same values used for all soil compartments of each type, except where noted)**

**Soil Compartment Types**

Parameter Name	Units	Value Used	Reference
<b>Surface Soil Compartment Type</b>			
Air content	volume[air]/volume[compartment]	0.25	McKone et al. 2001 (Table A-2)
Average vertical velocity of water (percolation)	m/day	7.00E-02	Professional judgment, based on water balance calculations
Density of soil solids (dry weight)	kg[soil]/m <sup>3</sup> [soil]	2600	McKone et al. 2001 (Table 3)
Depth [VE property] <sup>a</sup>	m	0.01	Professional judgment, based on McKone et al. 2001 (p. 30)
Erosion fraction [Link property]	unitless	compartment boundary-specific <sup>a</sup>	See "Erosion and Runoff Fractions" table
Fraction of area available for erosion	m <sup>2</sup> [area available]/m <sup>2</sup> [total]	varies by parcel	Calculated based on the percentage of parcel area covered by roads and based on the estimated density of development; see "Fraction of Area Available for Erosion and Runoff" table
Fraction of area available for runoff	m <sup>2</sup> [area available]/m <sup>2</sup> [total]	1	Professional judgment; all area assumed to be available for runoff
Fraction of area available for vertical diffusion	m <sup>2</sup> [area available]/m <sup>2</sup> [total]	varies by parcel	Calculated based on the percentage of parcel area covered by roads and based on the estimated density of development; see "Fraction of Area Available for Erosion and Runoff" table
Organic carbon fraction	unitless	0.02	Lorber et al. 1996 (Table 1)
Water content	volume[water]/volume[compartment]	0.22	McKone et al. 2001 (Table A-2)
Boundary layer thickness above surface soil	m	0.005	Thibodeaux 1996; McKone et al. 2001 (Table 3)
Total erosion rate	kg [soil]/m <sup>2</sup> /day	5.50E-04	van der Leeden et al. 1991, as cited in McKone et al. 2001, p.23
Total runoff rate	m <sup>3</sup> [water]/m <sup>2</sup> /day	0.0011	van der Leeden et al. 1991, as cited in McKone et al. 2001, p.18
<b>Root Zone Soil Compartment Type</b>			
Air content	volume[air]/volume[compartment]	0.19	McKone et al. 2001 (Table A-3)
Average vertical velocity of water (percolation)	m/day	7.00E-02	Professional judgment, based on water balance calculations
Density of soil solids (dry weight)	kg[soil]/m <sup>3</sup> [soil]	2,600	McKone et al. 2001 (Table 3)

**Chemical-Independent/Abiotic -- Documentation for OH WTE Dioxin Test Case**  
**(same values used for all soil compartments of each type, except where noted)**

**Soil Compartment Types**

Parameter Name	Units	Value Used	Reference
Depth [VE property] <sup>a</sup>	m	0.81	McKone et al. 2001 (Table A-3)
Organic carbon fraction	unitless	0.007	McKone et al. 2001 (Table A-3)
Water content	volume[water]/volume[compartment]	0.24	McKone et al. 2001 (Table A-3)
<b>Vadose Zone Soil Compartment Type</b>			
Air content	volume[air]/volume[compartment]	0.16	McKone et al. 2001 (Table A-4)
Average vertical velocity of water (percolation)	m/day	7.00E-02	Professional judgment, based on water balance calculations
Density of soil solids (dry weight)	kg[soil]/m <sup>3</sup> [soil]	2,600	McKone et al. 2001 (Table 3)
Depth [VE property] <sup>a</sup>	m	1.53	McKone et al. 2001 (Table A-4)
Organic carbon fraction	unitless	0.002	McKone et al. 2001 (Table A-4)
Water content	volume[water]/volume[compartment]	0.23	McKone et al. 2001 (Table A-4)
<b>Ground Water Compartment Type</b>			
Depth [VE property] <sup>a</sup>	m	3	McKone et al. 2001 (Table 3)
Organic carbon fraction	unitless	0.002	McKone et al. 2001 (Table A-4)
Porosity	volume[total pore space]/volume[compartment]	0.2	McKone et al. 2001 (Table 3)
Solid material density in aquifer	kg[soil]/m <sup>3</sup> [soil]	2,600	McKone et al. 2001 (Table 3)

<sup>a</sup>Set using the volume element properties named "top" and "bottom."

<sup>b</sup>See separate erosion/runoff fraction table.



**Chemical-Independent/Abiotic -- Documentation for OH WTE Dioxin Test Case**  
**Fraction of Area Available for Erosion and Runoff**

<b>Compartment</b>	<b>Percentage of Total Area Covered by Roads</b>	<b>Urban?</b>	<b>Fraction of Area Available for Erosion</b>	<b>Fraction of Area Available for Vertical Diffusion (Runoff)</b>
SurfSoil_E1	10.64%	Y	0.79	0.79
SurfSoil_E2	10.64%	Y	0.79	0.79
SurfSoil_ESE2	4.56%	N	0.95	0.95
SurfSoil_ESE3	3.54%	N	0.96	0.96
SurfSoil_N1	14.98%	Y	0.70	0.70
SurfSoil_NE2	8.08%	N	0.92	0.92
SurfSoil_NNE2	14.31%	Y	0.71	0.71
SurfSoil_NNW1	14.98%	Y	0.70	0.70
SurfSoil_NNW2	13.16%	Y	0.74	0.74
SurfSoil_NNW3	11.99%	Y	0.76	0.76
SurfSoil_NW2	7.55%	N	0.92	0.92
SurfSoil_NW3	3.52%	N	0.96	0.96
SurfSoil_NWFarm	13.61%	N	0.86	0.86
SurfSoil_SE2	3.72%	N	0.96	0.96
SurfSoil_SE3	2.25%	N	0.98	0.98
SurfSoil_Source	8.71%	Y	0.83	0.83
SurfSoil_SW1	3.85%	N	0.96	0.96
SurfSoil_SW2	3.85%	N	0.96	0.96

**Chemical-Independent/Abiotic -- Documentation for OH WTE Dioxin Test Case**  
**Fraction of Area Available for Erosion and Runoff**

Compartment	Percentage of Total Area Covered by Roads	Urban?	Fraction of Area Available for Erosion	Fraction of Area Available for Vertical Diffusion (Runoff)
SurfSoil_SW3	3.85%	N	0.96	0.96
SurfSoil_SW4	2.32%	N	0.98	0.98
SurfSoil_W1	8.21%	Y	0.84	0.84
SurfSoil_WNW1	8.21%	Y	0.84	0.84
SurfSoil_WNW2	8.21%	Y	0.84	0.84
SurfSoil_WNW3	3.42%	N	0.97	0.97
SurfSoil_WSW1	3.66%	N	0.96	0.96
SurfSoil_WSW2	3.66%	N	0.96	0.96
SurfSoil_WSW3	2.87%	N	0.97	0.97

**Methodology:** First, we calculated the percentage of each parcel covered by roads using GIS. We assumed each road was 25 feet wide, based on the assumption that each lane is, on average, 8 feet wide and there is a mixture of different numbers of lanes throughout the study area. We then identified which parcels appeared to be highly developed (using USGS quad maps) (these are indicated by a "Y" in the "Urban?" column) and assumed that the percentage of area available for erosion and vertical diffusion in these parcels was twice the area covered by roads (to account for buildings, sidewalks, parking lots, etc.). For the remaining parcels, we assumed the percentage of area available for erosion and vertical diffusion was equal to the percentage of area covered by roads.

## Erosion and Runoff Fractions -- Documentation for OH WTE Dioxin Test Case

### Surface Soil Compartment Type

Originating Compartment	Destination Compartment	Runoff/Erosion Fraction <sup>a</sup>
SurfSoil_Source	SurfSoil_N1	0.00
	SurfSoil_W1	0.00
	SW_Scioto	1.00
SurfSoil_N1	SurfSoil_Source	0.30
	SurfSoil_W1	0.20
	SurfSoil_NNW1	0.00
	SW_Scioto	0.50
SurfSoil_NNW1	SW_Scioto	0.30
	SurfSoil_Source	0.15
	SurfSoil_WNW1	0.30
	SurfSoil_NWFarm	0.25
	SurfSoil_NW2	0.00
SurfSoil_NWFarm	SW_Scioto	1.00
	SurfSoil_NNW1	0.00
	SurfSoil_NW2	0.00
SurfSoil_NW2	SW_Scioto	0.69
	SurfSoil_NWFarm	0.29
	SurfSoil_NNW1	0.02
	SurfSoil_NW3	0.00
SurfSoil_NW3	SW_Scioto	0.34
	SurfSoil_NW2	0.00
	SurfSoil_WNW2	0.36
	out	0.30
SurfSoil_NNW2	SW_Scioto	0.55
	SW_Olentangy	0.45
	SurfSoil_NNW3	0.00
SurfSoil_NNW3	SW_Scioto	0.30
	SW_Olentangy	0.67
	SurfSoil_NNW2	0.03
SurfSoil_W1	SurfSoil_Source	0.00
	SW_Scioto	0.90
	SurfSoil_SW1	0.10
	SurfSoil_WNW1	0.00
	SurfSoil_N1	0.00
SurfSoil_WNW1	SurfSoil_W1	0.98
	SurfSoil_SW2	0.00
	SurfSoil_WSW1	0.02
	SurfSoil_WNW2	0.00
	SurfSoil_NNW1	0.00

## Erosion and Runoff Fractions -- Documentation for OH WTE Dioxin Test Case

### Surface Soil Compartment Type

Originating Compartment	Destination Compartment	Runoff/Erosion Fraction <sup>a</sup>
SurfSoil_WNW2	SurfSoil_WNW3	0.17
	SurfSoil_WNW1	0.77
	SurfSoil_WSW2	0.06
	SurfSoil_NNW1	0.00
SurfSoil_WNW3	SurfSoil_WNW2	0.03
	SurfSoil_WSW3	0.97
	SurfSoil_NW3	0.00
	out	0.00
SurfSoil_SW1	SurfSoil_W1	0.00
	SurfSoil_SW2	0.00
	SW_Scioto	1.00
SurfSoil_SW2	SurfSoil_SW3	0.10
	SurfSoil_WSW1	0.00
	SurfSoil_WNW1	0.00
	SurfSoil_SW1	0.00
	SW_Scioto	0.90
SurfSoil_SW3	SW_Scioto	0.55
	SurfSoil_SW4	0.45
	SurfSoil_WSW2	0.00
	SurfSoil_SW2	0.00
SurfSoil_WSW1	SurfSoil_SW2	1.00
	SurfSoil_WSW2	0.00
	SurfSoil_WNW1	0.00
SurfSoil_WSW2	SurfSoil_WSW3	0.40
	SurfSoil_WSW1	0.25
	SurfSoil_WNW2	0.30
	SurfSoil_SW3	0.00
	SurfSoil_SW4	0.05
SurfSoil_WSW3	SurfSoil_WSW2	0.00
	SurfSoil_WNW3	0.00
	SurfSoil_SW4	1.00
	out	0.00
SurfSoil_SW4	SW_Scioto	0.39
	SurfSoil_SW3	0.00
	SurfSoil_WSW2	0.00
	SurfSoil_WSW3	0.00
	out	0.61
SurfSoil_E1	SurfSoil_E2	0.00
	SW_Scioto	1.00

## Erosion and Runoff Fractions -- Documentation for OH WTE Dioxin Test Case

### Surface Soil Compartment Type

Originating Compartment	Destination Compartment	Runoff/Erosion Fraction <sup>a</sup>
SurfSoil_E2	SurfSoil_E1	0.10
	SurfSoil_NNE2	0.00
	SW_Combined	0.50
	SW_Scioto	0.40
SurfSoil_NNE2	SurfSoil_E2	0.55
	SW_Olentangy	0.39
	SW_Combined	0.06
	out	0.00
SurfSoil_NE2	SurfSoil_ESE2	0.99
	SW_Combined	0.01
	out	0.00
SurfSoil_SE2	SurfSoil_ESE2	0.00
	SurfSoil_ESE3	0.00
	SurfSoil_SE3	0.56
	SW_Combined	0.44
SurfSoil_ESE2	SurfSoil_NE2	0.01
	SurfSoil_ESE3	0.39
	SurfSoil_SE2	0.58
	SW_Combined	0.02
	out	0.00
SurfSoil_ESE3	SurfSoil_ESE2	0.00
	SurfSoil_SE2	1.00
	SurfSoil_SE3	0.00
	out	0.00
SurfSoil_SE3	SurfSoil_SE2	0.08
	SurfSoil_ESE3	0.00
	SW_Scioto	0.32
	out	0.60

<sup>a</sup>Link properties - all values estimated using site watershed and topographic maps.

## Chemical-Independent Properties -- Documentation for OH WTE Dioxin Site Scioto River

Parameter Name	Units	Value Used	Reference
Algae carbon content (fraction)	unitless	0.465	APHA 1995
Algae density in water column	g[algae]/L[water]	0.0025	Derived from Millard et al. 1996
Algae growth rate	1/day	0.7	Hudson et al. 1994 as cited in Mason et al. 1995
Algae radius	um	2.5	Mason et al. 1995
Algae water content (fraction)	unitless	0.9	APHA 1995
Average algae cell density (per vol cell, not water)	g[algae]/m <sup>3</sup> [algae]	1,000,000	Mason et al. 1995, Mason et al. 1996
Boundary layer thickness above sediment	m	0.02	Cal EPA 1993
Chloride concentration	mg/L	42.1	USGS 2003a <sup>d</sup>
Chlorophyll concentration	mg/L	1.48E-02	U.S. EPA 2003a <sup>d</sup>
Current velocity <sup>a</sup>	m/s	5.30E-01	USGS 2003a <sup>d</sup>
Depth [VE property]	m	0.67	Professional judgment, based on maps, stream orders, and Keup 1985
Diffusive exchange coefficient [Link property] <sup>b</sup>	m <sup>2</sup> /day	2.25E-04	Ambrose et al. 1995
Dimensionless viscous sublayer thickness	unitless	4	Ambrose et al. 1995
Drag coefficient for water body	unitless	0.0011	Ambrose et al. 1995
Flush rate <sup>c</sup>	1/year	5.64E+02	USGS 2003a, professional judgement <sup>d</sup>
Organic carbon fraction in suspended sediments	unitless	0.02	McKone et al. 2001 (Table 3)
pH	unitless	7.72	USGS 2003a <sup>d</sup>
Suspended sediment density	kg[sediment]/m <sup>3</sup> [sediment]	2.65E+03	U.S. EPA 1998
Suspended sediment deposition velocity	m/day	2	U.S. EPA 1997
Total suspended sediment concentration	kg[sediment]/m <sup>3</sup> [water column]	2.63E-01	USGS 2003c <sup>d</sup>
Water temperature [VE property]	degrees K	289.3	USGS 2003a <sup>d</sup>

<sup>a</sup>Flowing water bodies only (i.e., rivers, streams).

<sup>b</sup>For all surface water compartments connected to other surface water compartments.

<sup>c</sup>For all surface water compartments connected to a flush rate sink (i.e., all or part of discharge modeled to a sink).

<sup>d</sup>See following sections, "Surface Water Calculations" and "Surface Water Properties" for a detailed description of calculations.

## Chemical-Independent Properties -- Documentation for OH WTE Dioxin Site Olentangy River

Parameter Name	Units	Value Used	Reference
Algae carbon content (fraction)	unitless	0.465	APHA 1995
Algae density in water column	g[algae]/L[water]	0.0025	Derived from Millard et al. 1996
Algae growth rate	1/day	0.7	Hudson et al. 1994 as cited in Mason et al. 1995
Algae radius	um	2.5	Mason et al. 1995
Algae water content (fraction)	unitless	0.9	APHA 1995
Average algae cell density (per vol cell, not water)	g[algae]/m <sup>3</sup> [algae]	1,000,000	Mason et al. 1995, Mason et al. 1996
Boundary layer thickness above sediment	m	0.02	Cal EPA 1993
Chloride concentration	mg/L	48.2	USGS 2003b <sup>c</sup>
Chlorophyll concentration	mg/L	1.48E-02	U.S. EPA 2003a <sup>c</sup>
Current velocity <sup>a</sup>	m/s	8.30E-01	USGS 2003b <sup>c</sup>
Depth [VE property]	m	0.33	Professional judgment, based on maps, stream orders, and Keup 1985
Diffusive exchange coefficient [Link property] <sup>b</sup>	m <sup>2</sup> /day	2.25E-04	Ambrose et al. 1995
Dimensionless viscous sublayer thickness	unitless	4	Ambrose et al. 1995
Drag coefficient for water body	unitless	0.0011	Ambrose et al. 1995
Organic carbon fraction in suspended sediments	unitless	0.02	McKone et al. 2001 (Table 3)
pH	unitless	7.87	USGS 2003b <sup>c</sup>
Suspended sediment density	kg[sediment]/m <sup>3</sup> [sediment]	2.65E+03	U.S. EPA 1998
Suspended sediment deposition velocity	m/day	2	U.S. EPA 1997
Total suspended sediment concentration	kg[sediment]/m <sup>3</sup> [water column]	4.50E-02	USGS 2003b <sup>c</sup>
Water temperature [VE property]	degrees K	289.9	USGS 2003b <sup>c</sup>

<sup>a</sup>Flowing water bodies only (i.e., rivers, streams).

<sup>b</sup>For all surface water compartments connected to other surface water compartments.

<sup>c</sup>See following sections, "Surface Water Calculations" and "Surface Water Properties" for a detailed description of calculations.

## Chemical-Independent Properties -- Documentation for OH WTE Dioxin Site Combined Water Body

Parameter Name	Units	Value Used	Reference
Algae carbon content (fraction)	unitless	0.465	APHA 1995
Algae density in water column	g[algae]/L[water]	0.0025	Derived from Millard et al. 1996
Algae growth rate	1/day	0.7	Hudson et al. 1994 as cited in Mason et al. 1995
Algae radius	um	2.5	Mason et al. 1995
Algae water content (fraction)	unitless	0.9	APHA 1995
Average algae cell density (per vol cell, not water)	g[algae]/m <sup>3</sup> [algae]	1,000,000	Mason et al. 1995, Mason et al. 1996
Boundary layer thickness above sediment	m	0.02	Cal EPA 1993
Chloride concentration	mg/L	39.0	USGS 2003c,d <sup>c</sup>
Chlorophyll concentration	mg/L	1.83E-02	U.S. EPA 2003a <sup>c</sup>
Current velocity <sup>a</sup>	m/s	3.60E-01	USGS 2003c,d <sup>c</sup>
Depth [VE property]	m	0.31	Professional judgment, based on maps, stream orders, and Keup 1985
Diffusive exchange coefficient [Link property] <sup>b</sup>	m <sup>2</sup> /day	2.25E-04	Ambrose et al. 1995
Dimensionless viscous sublayer thickness	unitless	4	Ambrose et al. 1995
Drag coefficient for water body	unitless	0.0011	Ambrose et al. 1995
Organic carbon fraction in suspended sediments	unitless	0.02	McKone et al. 2001 (Table 3)
pH	unitless	7.88	USGS 2003c,d <sup>c</sup>
Suspended sediment density	kg[sediment]/m <sup>3</sup> [sediment]	2.65E+03	U.S. EPA 1998
Sediment deposition velocity	m/day	2	U.S. EPA 1997
Total suspended sediment concentration	kg[sediment]/m <sup>3</sup> [water column]	2.63E-01	USGS 2003c <sup>c</sup>
Water temperature [VE property]	degrees K	286.2	USGS 2003c,d <sup>c</sup>

<sup>a</sup>Flowing water bodies only (i.e., rivers, streams).

<sup>b</sup>For all surface water compartments connected to other surface water compartments.

<sup>c</sup>See following sections, "Surface Water Calculations" and "Surface Water Properties" for a detailed description of calculations.



## Link Properties for Surface Water Compartments -- Documentation for OH WTE Dioxin Test Case

Parameter Name	Units	Value Used	Reference
<b>Link: Surface water in Olentangy River to surface water in Scioto River</b>			
Bulk water flow [Link property]	m <sup>3</sup> [water]/-day	1.34E+06	USGS 2003b <sup>a</sup>
Distance between midpoints [Link property]	m	10725	Site-specific value; calculated using GIS.
Diffusive exchange coefficient [Link property]	m <sup>2</sup> /day	2.25E-04	Ambrose et al. 1995
<b>Link: Surface water in Combined Creek to surface water in Scioto River</b>			
Bulk water flow [Link property]	m <sup>3</sup> [water]/-day	1.22E+06	USGS 2003d <sup>a</sup>
Distance between midpoints [Link property]	m	25524	Site-specific value; calculated using GIS.
Diffusive exchange coefficient [Link property]	m <sup>2</sup> /day	2.25E-04	Ambrose et al. 1995
<b>Links: Groundwater to Surface Water</b>			
Recharge Rate [Link property]	m <sup>3</sup> [water]/m <sup>2</sup> [area]-day	-	Value not required because there is no horizontal or vertical overlap between surface water and groundwater.

<sup>a</sup>See following section, "Surface Water Calculations," for a detailed description of calculations.

**Chemical-Independent/Abiotic -- Documentation for OH WTE Dioxin Test Case**  
**(same values used for all sediment compartments)**

**Sediment Compartment Type**

Parameter Name	Units	Value Used	Reference
Depth [VE property] <sup>a</sup>	m	0.05	McKone et al. 2001 (Table 3)
Organic carbon fraction	unitless	0.02	McKone et al. 2001 (Table 3)
Porosity of the sediment zone	volume[total pore space]/volume[sediment compartment]	0.6	U.S. EPA 1998
Solid material density in sediment	kg[sediment]/m <sup>3</sup> [sediment]	2,650	U.S. EPA 1998

<sup>a</sup>Set using the volume element properties named "top" and "bottom."

# Chemical-Independent Properties -- Documentation for OH WTE Dioxin Site

## Surface Water Calculations

Three surface water bodies were modeled in the Ohio TRIM.FaTE application: the Scioto River, the Olentangy River, and a combined water body representing Alum Creek and Big Walnut Creek (denoted as Combined Water Body). The following outlines the calculations and assumptions used to develop the surface water properties for these three water bodies.

## Surface Water Flow Calculations

Properties related to surface water flow algorithms in TRIM.FaTE are:

- river current velocities;
- bulk flow rates between water bodies;
- runoff rates for the amount of precipitation that enters surface water bodies; and
- flushing rates to sinks.

The general method applied to define these properties and calculate consistent flow rates for the Ohio site involved finding measured and regional average flow data for rivers and streams near the site, gathering watershed areas and other site data, and identifying methods to maintain a water balance in the system. Specific data used were surface water flow rates from nearby USGS gages (USGS 2003a,b,c,d), watershed areas from the USGS and GIS data, surface water body properties from GIS analysis, and stream dimension data from a nation-wide study of streams and rivers (Keup 1985). The Keup data were used to help define stream physical properties (e.g., depth) in the absence of (or in conjunction with) site-specific data, and are described below in the discussion of depth. Details of the calculations are shown below, and all property values used for the Ohio TRIM.FaTE scenario are documented in the input tables included as Appendix A to this report.

**Current Velocities.** The average annual stream flow rate was divided by the reported watershed area draining to the gage site to obtain a stream flow per unit watershed area. The mean annual stream flow rate was calculated from USGS data; the watershed area is a product of average width, calculated from GIS, and depth, calculated as described in the following section on surface water properties.

• Scioto:  $0.53 \text{ m}^3/\text{m}^2\text{-s}$ , where flow rate = 1387.3 cfs =  $39.2 \text{ m}^3/\text{s}$ , based on the average of the flows at the two stations in or near the modeling region (817 cfs and 1432 cfs) and the estimated flow leaving the modeling region (2100 cfs). Average width = 110 m, and depth = 0.67 m. Current Velocity:  $39.2 \text{ m}^3/\text{s} \div 73.7 \text{ m}^2 = 0.53 \text{ m}^3/\text{m}^2\text{-s}$ .

• Olentangy:  $0.83 \text{ m}^3/\text{m}^2\text{-s}$ , where flow rate = 500 cfs =  $14.1 \text{ m}^3/\text{s}$ , based on the average of the station just north of the modeling region (450 cfs) and the estimated flow at the intersection with the Scioto (550 cfs). Average width = 50 m, and depth = 0.33 m. Current Velocity:  $14.1 \text{ m}^3/\text{s} \div 17 \text{ m}^2 = 0.83 \text{ m}^3/\text{m}^2\text{-s}$ .

• Combined Water Body:  $0.36 \text{ m}^3/\text{m}^2\text{-s}$ , where flow rate = 300 cfs =  $8.5 \text{ m}^3/\text{s}$ , based on the average of the stations along Alum Creek (104 cfs and 196 cfs) and Big Walnut Creek (217 cfs and 481 cfs) and the estimated flow at the intersection with the Scioto (500 cfs). Average width = 75 m, and depth = 0.31 m. Current Velocity:  $8.5 \text{ m}^3/\text{s} \div 23.3 \text{ m}^2 = 0.36 \text{ m}^3/\text{m}^2\text{-s}$ .

## Chemical-Independent Properties -- Documentation for OH WTE Dioxin Site

**Bulk Flow Rates.** The bulk flow rates between water bodies were determined using flow data at appropriate USGS gaging stations located near the junction of the water bodies.

- Olentangy River to Scioto River: 550 cfs =  $1.34\text{E}+06 \text{ m}^3/\text{day}$ , based on 450 cfs estimate at upstream station (Olentangy R NR Worthington OH) and assuming a 100 cfs increase in flow from station to junction with the Scioto River; 100 cfs increase was estimated using the increase in flow in the Scioto River when it merged with the Olentangy River.

- Combined Water Body to Scioto River: 500 cfs =  $1.22\text{E}+06 \text{ m}^3/\text{day}$ , based on estimates ranging from 468 to 496 cfs at station (Big Walnut C at Rees OH) just upstream from junction with the Scioto River and assuming a small increase in flow from the station to the junction.

**Runoff Rates.** The overall erosion rate for the Ohio site was estimated using a regional erosion rate (van der Leeden et al. 1990) and assuming that the rate was approximately uniform throughout the modeled site. Runoff and erosion fractions between parcels were estimated using the basic methods described in the TRIM.FaTE User's Guide (U.S. EPA 2003b). Watershed data and USGS 1:24,000 scale topographic maps were used for the site. A transparent overlay with parcel boundaries was created to place over the topographic map. Erosion and runoff fractions were determined using this parcel layout and identifying watershed boundaries and flow paths on the map.

**Flushing Rates.** Flush rates for water bodies that flow out of the modeled area were calculated by dividing the flow rate leaving the water body by the water body's volume. Flow rates were calculated using USGS data, and water body volumes are a product of area (based on GIS data) and depth (see following section on surface water properties).

- Scioto River: 564.1 flushes/yr, calculated by dividing the annual mean flow rate leaving the modeling region ( $1.88\text{E}+09 \text{ m}^3/\text{yr}$ ) by the volume of the water body ( $3.32\text{E}+06 \text{ m}^3$ ). The flow rate was estimated based on sum of the flows from an upstream station on the Scioto River of 1,432 cfs, from a downstream station representing the flow from the Combined Creek of 500 cfs, and an approximated flow of 170 cfs due to the runoff from the remaining portion of the river (i.e., downstream from where the Combined Creek merges into the Scioto River to the edge of the modeling region). The volume was calculated by multiplying the area of the water body ( $4.96\text{E}+06 \text{ m}^2$ ) by the depth (0.67 m).

# Chemical-Independent Properties -- Documentation for OH WTE Dioxin Site

## Surface Water Properties

Where possible, site-specific or regional values were used for water body parameters, such as algae properties, chloride and chlorophyll concentrations, depth, suspended sediment properties, pH, and water temperature. Site-specific properties for the Scioto and Olentangy Rivers were available from USGS monitoring stations in the river (USGS 2003a,b,c,d). Specific site data for the Ohio site were also available from the EPA's STORET database (U.S. EPA 2003a) and from Alum and Big Walnut Creeks (USGS 2003c,d). The time period of the data collection (number of years, period) were checked to verify representation of annual conditions. Data from the specific water body were used, if available. If data were not available, the next closest site was used, minding distance and location (e.g., north) from downtown Columbus. More general "default" values obtained from the literature were defined for the remaining required parameters where site-specific or regional measurements were not found. Details of assumptions for all calculated properties in the various water bodies are included below. See Appendix A for specific values and data sources for all surface water properties.

### Chloride Concentration.

- Scioto River: 42.1 mg/L, based on the average of 31 measurements from 1965-1996 at USGS station on Scioto River at Columbus, OH (near center of volume element).
- Olentangy River: 48.2 mg/L, based on the average of 39 measurements from 1964-1977 at USGS station on Olentangy River near Worthington, OH (near northern tip of volume element).
- Combined Water Body: 39.0 mg/L, based on the average of values from USGS station on Alum Creek (near center of volume element) and values from Big Walnut Creek (just north of volume element).

### Chlorophyll Concentration.

- Scioto and Olentangy Rivers: 1.48E-02 mg/L, based on the average of 20 Chl-A and 17 Chl-B measurements from 1988-1995 at USGS station on Olentangy River near I270 Bridge station.
- Combined Water Body: 1.83E-02 mg/L, based on the average of 19 Chl-A and 19 Chl-B measurements at Alum Creek-Columbus USGS station.

**Depth.** The mean depth of each of the surface water bodies was approximated using stream orders that were estimated based on watershed maps and USGS mean annual discharge data in cfs, using the information in Table 1 of Keup (1985).

• Scioto River: Based on mapping, the Scioto River appears to be either a 4th or 5th order stream. The annual average discharge of the Scioto River ranges from 815 cfs to 1,431 cfs, which falls between the calculated discharges in Table 1 of 5th (380 cfs) and 6th (1,800 cfs) order streams. Based on this and the stream order of the Olentangy River (see below, because the order of the Olentangy River influences the order of the Scioto River since they merge), the Scioto River was assumed to be a 5th order stream. Mean depth = 2.20 ft.

• Olentangy River: Based on mapping, the Olentangy River appears to be either a 3rd or 4th order stream. The annual average discharge of the Olentangy River ranges from 158 cfs to 450 cfs, which falls between the calculated discharges in Table 1 of 4th (73 cfs) and 5th (380 cfs) order streams. Therefore, the Olentangy River was assumed to be a 4th order stream. Mean depth = 1.10 ft.

## Chemical-Independent Properties -- Documentation for OH WTE Dioxin Site

- Alum Creek: Based on mapping, Alum Creek appears to be a 3rd order stream. The annual average discharge of Alum Creek ranges from 110 cfs to 177 cfs. These values fall between the calculated discharges in Table 1 of 4th (73 cfs) and 5th (380 cfs) order streams, but are closer to the values for 4th order streams. The calculated discharge of 3rd order streams (according to Table 1) is 15.6 cfs. Because the measured discharge is higher and the mapping process includes uncertainties, an average of the mean depth values for 3rd (0.58 feet) and 4th (1.10 feet) order streams was used. Mean depth =  $(0.58 + 1.10)/2 = 0.84$  ft.

- Big Walnut Creek: Based on mapping, Big Walnut Creek appears to be a 3rd order stream. The annual average discharge of Big Walnut Creek ranges from 114 cfs to 478 cfs, which is substantially higher than the calculated discharge for 3rd order streams in Table 1 (15.6 cfs). These discharge values fall between the calculated discharges in Table 1 of 4th (73 cfs) and 6th (1,800 cfs) order streams. Because it is fairly clear from the map that Big Walnut Creek is not a 5th or 6th order stream, but because the discharge data indicate that Big Walnut Creek is larger than a 3rd order stream, Big Walnut Creek was assumed to be a 4th order stream. Mean depth = 1.10 feet.

- Combined Water Body: Big Walnut Creek mean depth was weighted twice as much as Alum Creek mean depth because its flow contributed approximately twice as much to the overall flow for the combined water body. Mean depth =  $(0.84 + 2*1.10)/3 = 1.013$  feet.

### pH.

- Scioto River: 7.72, based on the average of 34 measurements from 1965-1996 at USGS station on Scioto River at Columbus, OH.

- Olentangy River: 7.87, based on the average of 40 measurements from 1964-1989 at USGS station on Olentangy River near Worthington, OH.

- Combined Water Body: 7.88, based on the average of values from USGS station on Alum Creek and values from Big Walnut Creek.

**Total Suspended Sediment Concentration.** Based on data available from around Columbus, OH, suspended sediment concentrations are very site-specific and variable, due to impact from several environmental variables (e.g., sediment type, flow volume, flow velocity, runoff volume, land-use around the area). When available, site-specific data were therefore used over regional data.

- Scioto River and Combined Water Body:  $2.63E-01$  kg[sediment]/m<sup>3</sup>[water column], based on the average of 49 measurements from 1969-1973 at USGS station on Alum Creek at Africa, OH. Data were not available for either the Scioto River or Big Walnut Creek. The station at Africa, OH was chosen because it is upstream of Columbus and probably would be less impacted by urban activities.

- Olentangy River:  $4.50E-02$  kg[sediment]/m<sup>3</sup>[water column], based on the average of 4 measurements from 1966 at USGS station on Olentangy River near Worthington, OH.

## **Chemical-Independent Properties -- Documentation for OH WTE Dioxin Site**

### **Water Temperatures.**

- Scioto River: 16.2 degrees C, based on average temp from 51 measurements from 1965-1996 at USGS station on Scioto River at Columbus, OH.
- Olentangy River: 16.8 degrees C, based on average temp from 48 measurements from 1965-1989 at USGS station on Olentangy River near Worthington, OH.
- Combined Waterbody: 13.9 degrees C, based on average of 54 measurements taken over 28 years at monitoring station on Big Walnut Creek and 33 measurements taken over 12 years at monitoring station on Alum Creek. Big Walnut Creek average temperature was weighted twice as much as Alum Creek average temperature because its flow contributed approximately twice as much to the overall flow for the combined water body.

## Terrestrial Vegetation Types -- Documentation for OH WTE Dioxin Test Case<sup>a</sup>

### Terrestrial Vegetation

Surface Soil Volume Element	Deciduous Forest	Grasses/Herbs	Agricultural	None
Source				X
NNW1		X		
WNW1		X		
WSW2		X		
SW1		X		
E1		X		
WNW2		X		
WSW3		X		
SW2		X		
SE2		X		
ESE2			X	
SE3		X		
ESE3		X		
NE2	X			
NNE2		X		
NNW2		X		
NW2		X		
NWFarm			X	
NNW3		X		
NW3		X		

<sup>a</sup> Assignments made based on review of land use maps.



**Chemical-Independent/Biotic -- Documentation for OH WTE Dioxin Test Case**  
**(same values used for all terrestrial vegetation compartments of a given type)**  
**Terrestrial Vegetation Compartment Types**

		Deciduous <sup>a</sup>		Grass/Herb <sup>a</sup>		Agricultural <sup>a</sup>	
Parameter Name	Units	Value Used	Reference	Value Used	Reference	Value Used	Reference
Leaf Compartment Type							
Allow exchange	1=yes, 0=no	seasonal <sup>b</sup>	See note b	seasonal <sup>b</sup>	See note b	seasonal <sup>b</sup>	See note b
Average leaf area index	m <sup>2</sup> [total leaf area]/m <sup>2</sup> [underlying soil area]	3.4	Harvard Forest, dom. red oak and red maple, CDIAC website	5	Mid-range of 4-6 for old fields, R.J. Luxmoore, ORNL	2	GLEAMS 1993, average for crops
Calculate wet dep interception fraction	1=yes, 0=no	0	Professional judgment	0	Professional judgment	0	Professional judgment
Correction exponent, octanol to lipid	unitless	0.76	Trapp 1995, from roots	0.76	Trapp 1995, from roots	0.76	Trapp 1995, from roots
Degree stomatal opening	unitless	1	Set to 1 for daytime based on professional judgment (stomatal diffusion is turned off at night using a different property, IsDay)	1	Set to 1 for daytime based on professional judgment (stomatal diffusion is turned off at night using a different property, IsDay)	1	Set to 1 for daytime based on professional judgment (stomatal diffusion is turned off at night using a different property, IsDay)
Density of wet leaf	kg[leaf wet wt]/m <sup>3</sup> [leaf]	820	Paterson et al. 1991	820	Paterson et al. 1991	820	Paterson et al. 1991
Leaf wetting factor	m	3.00E-04	Muller and Prohl 1993, 1E-04 to 6E-04 for different crops and elements	3.00E-04	Muller and Prohl 1993, 1E-04 to 6E-04 for different crops and elements	3.00E-04	Muller and Prohl 1993, 1E-04 to 6E-04 for different crops and elements
Length of leaf	m	0.1	Professional judgment	0.05	Professional judgment	0.05	Professional judgment
Lipid content	kg[lipid]/kg[leaf wet wt]	0.00224	Riederer 1995, European beech	0.00224	Riederer 1995, European beech	0.00224	Riederer 1995, European beech
Litter fall rate	1/day	seasonal <sup>c</sup>	See note c	seasonal <sup>c</sup>	See note c	seasonal <sup>c</sup>	See note c
Stomatal area, normalized for effective diffusion path length	1/m	200	Wilmer and Fricker 1996	200	Wilmer and Fricker 1996	200	Wilmer and Fricker 1996
Vegetation attenuation factor	m <sup>2</sup> /kg	2.9	Baes et al. 1984, grass/hay	2.9	Baes et al. 1984, grass/hay	2.9	Baes et al. 1984, grass/hay
Water content	unitless (kg[water]/kg[leaf wet wt])	0.8	Paterson et al. 1991	0.8	Paterson et al. 1991	0.8	Paterson et al. 1991
Wet dep interception fraction	unitless	0.2	Calculated based on 5 years of met data from the Maine test case, 1987-1991	0.2	Calculated based on 5 years of met data from the Maine test case, 1987-1991	0.2	Calculated based on 5 years of met data from the Maine test case, 1987-1991
Wet mass of leaf per unit area	kg[fresh leaf]/m <sup>2</sup> [area]	0.6	Calculated from leaf area index, leaf thickness (Simonich & Hites, 1994), density of wet foliage	0.6	Calculated from leaf area index and Leith 1975	0.4	Calculated from leaf area index and Leith 1975
Particle on Leaf Compartment Type							
Allow exchange	1=yes, 0=no	seasonal <sup>b</sup>	Professional judgment	seasonal <sup>b</sup>	Professional judgment	seasonal <sup>b</sup>	Professional judgment

**Chemical-Independent/Biotic -- Documentation for OH WTE Dioxin Test Case**  
**(same values used for all terrestrial vegetation compartments of a given type)**

**Terrestrial Vegetation Compartment Types**

Parameter Name	Units	Deciduous <sup>a</sup>		Grass/Herb <sup>a</sup>		Agricultural <sup>a</sup>	
		Value Used	Reference	Value Used	Reference	Value Used	Reference
Volume particle per area leaf	m <sup>3</sup> [leaf particles]/m <sup>2</sup> [leaf]	1.00E-09	Coe and Lindberg. 1987, based on particle density and size distribution for atmospheric particles measured on an adhesive surface	1.00E-09	Coe and Lindberg. 1987, based on particle density and size distribution for atmospheric particles measured on an adhesive surface	1.00E-09	Coe and Lindberg. 1987, based on particle density and size distribution for atmospheric particles measured on an adhesive surface
<b>Root Compartment Type - Nonwoody Vegetation Only<sup>d</sup></b>							
Allow exchange	1=yes, 0=no			seasonal <sup>b</sup>	Professional judgment	seasonal <sup>b</sup>	Professional judgment
Correction exponent, octanol to lipid	unitless			0.76	Trapp 1995	0.76	Trapp 1995
Lipid content of root	kg[lipid]/kg [root wet wt]			0.011	Calculated	0.011	Calculated
Water content of root	kg[water]/kg[root wet wt]			0.8	Professional judgment	0.8	Professional judgment
Wet density of root	kg[leaf wet wt]/m <sup>3</sup> [root]			820	soybean, Paterson et al. 1991	820	soybean, Paterson et al. 1991
Wet mass per area	kg[root wet wt]/m <sup>2</sup> [soil]			1.4	temperate grassland, Jackson et al. 1996	0.15	crops, Jackson et al. 1996
<b>Stem Compartment Type - Nonwoody Vegetation Only<sup>d</sup></b>							
Allow exchange	1=yes, 0=no			seasonal <sup>b</sup>	Professional judgment	seasonal <sup>b</sup>	Professional judgment
Correction exponent, octanol to lipid	unitless			0.76	from roots, Trapp 1995	0.76	Trapp 1995
Density of phloem fluid	kg[phloem]/m <sup>3</sup> [phloem]			1,000	Professional judgment	1,000	Professional judgment
Density of xylem fluid	kg[xylem]/m <sup>3</sup> [xylem]			900	Professional judgment	900	Professional judgment
Flow rate of transpired water per leaf area	m <sup>3</sup> [water]/m <sup>2</sup> [leaf]-day			0.0048	Crank et al. 1981	0.0048	Crank et al. 1981
Fraction of transpiration flow rate that is phloem rate	unitless			0.05	Paterson et al. 1991	0.05	Paterson et al. 1991
Lipid content of stem	kg[lipid]/kg [stem wet wt]			0.00224	Riederer 1995, leaves of European beech	0.00224	Riederer 1995, leaves of European beech
Water content of stem	kg[water]/kg[stem wet wt]			0.8	Paterson et al. 1991	0.8	Paterson et al. 1991
Wet density of stem	kg[stem wet wt]/m <sup>3</sup> [root]			830	Professional judgment	830	Professional judgment
Wet mass per area	kg[stem wet wt]/m <sup>2</sup> [soil]			0.24	Calculated from leaf and root biomass density, based on professional judgment	0.16	Calculated from leaf and root biomass density, based on professional judgment

<sup>a</sup>See attached table for assignment of vegetation types to surface soil volume elements.

<sup>b</sup>Begins April 15 (set to 1), ends November 5 (set to 0). Set to average days of last and first frost, based on meteorological data for Ohio site.

<sup>c</sup>Begins November 5, ends December 4; rate = 0.15/day during this time (value assumes first-order relationship and that 99 percent of leaves fall in 30 days). Rate is zero at all other times.

<sup>d</sup>Roots and stems are not modeled for deciduous forests in the current version of TRIM.FaTE.

## Chemical-Dependent/Independent of Compartment Type -- Documentation for the OH WTE Dioxin Test Case

Chemical	Diffusion coefficient in pure air		Diffusion coefficient in pure water		Henry's Law Constant	
	Value (m <sup>2</sup> /d)	Reference	Value (m <sup>2</sup> /d)	Reference	Value (Pa-m <sup>3</sup> /mol)	Reference
2,3,7,8-TCDD	1.06E-01	U.S. EPA 1999	5.68E-05	U.S. EPA 1999	3.33	Mackay et al. 1992 as cited in U.S. EPA 2000a
1,2,3,7,8-PeCDD	1.01E-01	U.S. EPA 1999	3.65E-05	U.S. EPA 1999	3.33	Mackay et al. 1992 as cited in U.S. EPA 2000a; value is for 2,3,7,8-TCDD
1,2,3,4,7,8-HxCDD	9.58E-02	U.S. EPA 1999	3.43E-05	U.S. EPA 1999	1.08	Mackay et al. 1992 as cited in U.S. EPA 2000
1,2,3,6,7,8-HxCDD	9.58E-02	U.S. EPA 1999	3.43E-05	U.S. EPA 1999	1.08	Mackay et al. 1992 as cited in U.S. EPA 2000a; value is for 1,2,3,4,7,8-HxCDD
1,2,3,7,8,9-HxCDD	9.58E-02	U.S. EPA 1999	3.43E-05	U.S. EPA 1999	1.08	Mackay et al. 1992 as cited in U.S. EPA 2000a; value is for 1,2,3,4,7,8-HxCDD
1,2,3,4,6,7,8-HpCDD	9.25E-02	U.S. EPA 1999	3.24E-05	U.S. EPA 1999	1.28	Mackay et al. 1992 as cited in U.S. EPA 2000a
1,2,3,4,6,7,8,9-OCDD	8.83E-02	U.S. EPA 1999	3.08E-06	U.S. EPA 1999	0.68	Mackay et al. 1992 as cited in U.S. EPA 2000a
2,3,7,8-TCDF	1.49E-01	U.S. EPA 1999	4.04E-05	U.S. EPA 1999	1.46	Mackay et al. 1992 as cited in U.S. EPA 2000a
1,2,3,7,8-PeCDF	1.42E-01	U.S. EPA 1999	3.76E-05	U.S. EPA 1999	0.50	Mackay et al. 1992 as cited in U.S. EPA 2000a; value is for 2,3,4,7,8-PeCDF
2,3,4,7,8-PeCDF	1.42E-01	U.S. EPA 1999	3.76E-05	U.S. EPA 1999	0.50	Mackay et al. 1992 as cited in U.S. EPA 2000a
1,2,3,4,7,8-HxCDF	1.35E-01	U.S. EPA 1999	3.53E-05	U.S. EPA 1999	1.45	Calculated by the VP/WS ratio technique as cited in U.S. EPA 2000a
1,2,3,6,7,8-HxCDF	1.35E-01	U.S. EPA 1999	3.53E-05	U.S. EPA 1999	0.74	Mackay et al. 1992 as cited in U.S. EPA 2000a
1,2,3,7,8,9-HxCDF	1.35E-01	U.S. EPA 1999	3.53E-05	U.S. EPA 1999	0.74	Mackay et al. 1992 as cited in U.S. EPA 2000a; value is for 1,2,3,6,7,8-HxCDF
2,3,4,6,7,8-HxCDF	1.35E-01	U.S. EPA 1999	3.53E-05	U.S. EPA 1999	0.74	Mackay et al. 1992 as cited in U.S. EPA 2000a; value is for 1,2,3,6,7,8-HxCDF
1,2,3,4,6,7,8-HpCDF	1.29E-01	U.S. EPA 1999	3.33E-05	U.S. EPA 1999	1.43	Mackay et al. 1992 as cited in U.S. EPA 2000a
1,2,3,4,7,8,9-HpCDF	1.29E-01	U.S. EPA 1999	3.33E-05	U.S. EPA 1999	1.43	Mackay et al. 1992 as cited in U.S. EPA 2000a; value is for 1,2,3,4,6,7,8-HpCDF
1,2,3,4,6,7,8,9-OCDF	1.23E-01	U.S. EPA 1999	3.15E-05	U.S. EPA 1999	0.19	Calculated by the VP/WS ratio technique as cited in U.S. EPA 2000a

## Chemical-Dependent/Independent of Compartment Type -- Documentation for the OH WTE Dioxin Test Case

Chemical	Octanol-water partition coefficient (K <sub>ow</sub> )		Melting Point		Molecular Weight	
	Value (unitless)	Reference	Value (Kelvin)	Reference	Value (g/mol)	Reference
2,3,7,8-TCDD	6.31E+06	Mackay et al. 1992 as cited in U.S. EPA 2000a	578	Mackay et al. 2000, U.S. EPA 2000b	322	Mackay et al. 2000, NLM 2002
1,2,3,7,8-PeCDD	4.37E+06	Sijm et al. 1989 as cited in U.S. EPA 2000a	513	U.S. EPA 2000b	356.4	ATSDR 1998
1,2,3,4,7,8-HxCDD	6.31E+07	Mackay et al. 1992 as cited in U.S. EPA 2000a	546	Mackay et al. 2000, U.S. EPA 2000b	391	Mackay et al. 2000
1,2,3,6,7,8-HxCDD	1.62E+08	U.S. EPA 2000b; calculated	558	U.S. EPA 2000b	390.84	NLM 2002
1,2,3,7,8,9-HxCDD	1.62E+08	U.S. EPA 2000b; calculated	517	NLM 2002	390.84	NLM 2002
1,2,3,4,6,7,8-HpCDD	1.00E+08	Mackay et al. 1992 as cited in U.S. EPA 2000a	538	Mackay et al. 2000, ATSDR 1998	425.2	Mackay et al. 2000
1,2,3,4,6,7,8,9-OCDD	1.58E+08	Mackay et al. 1992 as cited in U.S. EPA 2000a	603	Mackay et al. 2000, NLM 2002, U.S. EPA 2000b	460	Mackay et al. 2000
2,3,7,8-TCDF	1.26E+06	Mackay et al. 1992 as cited in U.S. EPA 2000a	500	Mackay et al. 2000	306	Mackay et al. 2000
1,2,3,7,8-PeCDF	6.17E+06	Sijm et al. 1989 as cited in U.S. EPA 2000a	499	ATSDR 1998	340.42	ATSDR 1998, Atkinson 1996 as cited in U.S. EPA 2000a, U.S. EPA 2000b
2,3,4,7,8-PeCDF	3.16E+06	Mackay et al. 1992 as cited in U.S. EPA 2000a	469.25	Mackay et al. 2000	340.42	Mackay et al. 2000, ATSDR 1998, Atkinson 1996 as cited in U.S. EPA 2000a, U.S. EPA 2000b
1,2,3,4,7,8-HxCDF	1.00E+07	Mackay et al. 1992 as cited in U.S. EPA 2000a	499	Mackay et al. 2000	374.87	Mackay et al. 2000, ATSDR 1998, Atkinson 1996 as cited in U.S. EPA 2000a, U.S. EPA 2000b
1,2,3,6,7,8-HxCDF	8.24E+07	U.S. EPA 2000b; calculated	506	ATSDR 1998	374.87	ATSDR 1998, Atkinson 1996 as cited in U.S. EPA 2000a, U.S. EPA 2000b
1,2,3,7,8,9-HxCDF	3.80E+07	U.S. EPA 2000b; calculated	508.95	U.S. EPA 2000b	374.87	ATSDR 1998, Atkinson 1996 as cited in U.S. EPA 2000a, U.S. EPA 2000b
2,3,4,6,7,8-HxCDF	8.31E+07	U.S. EPA 2000b; calculated	512.5	ATSDR 1998	374.87	ATSDR 1998, Atkinson 1996 as cited in U.S. EPA 2000a, U.S. EPA 2000b
1,2,3,4,6,7,8-HpCDF	2.51E+07	Mackay et al. 1992 as cited in U.S. EPA 2000a	236.5	Mackay et al. 2000	409.31	Mackay et al. 2000, ATSDR 1998, Atkinson 1996 as cited in U.S. EPA 2000a, U.S. EPA 2000b
1,2,3,4,7,8,9-HpCDF	7.94E+06	Mackay et al. 2000; calculated	222	Mackay et al. 2000	409.31	Mackay et al. 2000, ATSDR 1998, Atkinson 1996 as cited in U.S. EPA 2000a, U.S. EPA 2000b
1,2,3,4,6,7,8,9-OCDF	1.00E+08	Mackay et al. 1992 as cited in U.S. EPA 2000a	259	Mackay et al. 2000	443.76	Mackay et al. 2000, ATSDR 1998, U.S. EPA 2000b

**Chemical-Dependent/Abiotic -- Documentation for the OH WTE Dioxin Test Case**  
**(same values used for all abiotic compartments of a given type, except where noted)**

Property Type	Units	Value							Reference
		2,3,7,8-TCDD	1,2,3,7,8-PeCDD	1,2,3,4,7,8-HxCDD	1,2,3,6,7,8-HxCDD	1,2,3,7,8,9-HxCDD	1,2,3,4,6,7,8-HpCDD	1,2,3,4,6,7,8,9-OCDD	
Air Compartment									
Halflife <sup>a</sup>	day	12	18	42	28	28	64	162	Atkinson 1996 as cited in U.S. EPA 2000s; vapor phase reaction with hydroxyl radical
Groundwater									
Halflife	day	1008	1008	1008	1008	1008	1008	1008	Average value of the range presented in Mackay et al. 2000; based on estimated unacclimated aerobic biodegradation half-life, value is for 2,3,7,8-TCDD
Sediment									
Halfliife <sup>a</sup>	day	1095	1095	1095	1095	1095	1095	1095	Estimation based on Adriaens and Grbic-Galic 1992,1993 and Adriaens et al. 1995 as cited in U.S. EPA 2000a
Soil - Root Zone									
Halfliife <sup>a</sup>	day	3650	3650	3650	3650	3650	3650	3650	Mackay et al. 2000; the degradation rate was cited by multiple authors, value is for 2,3,7,8-TCDD
Soil - Surface									
Halflife <sup>a</sup>	day	3650	3650	3650	3650	3650	3650	3650	Mackay et al. 2000; the degradation rate was cited by multiple authors, value is for 2,3,7,8-TCDD
Soil - Vadose Zone									
Halflife <sup>a</sup>	day	1008	1008	1008	1008	1008	1008	1008	Average value of the range presented in Mackay et al. 2000; based on estimated unacclimated aerobic biodegradation half-life, value is for 2,3,7,8-TCDD
Surface water									
Halflife <sup>a</sup>	day	2.7	2.7	6.3	6.3	6.3	47	0.67	2,3,7,8-TCDD and 1,2,3,7,8-PeCDD: Podoll et al. 1986 as cited in U.S. EPA 2000a; sunlight, water: acetonitrile (1:1 v/v), value is for 2,3,7,8-TCDD; All HxCDD's: Choudry and Webster 1989 as cited in U.S. EPA 2000a; Hg lamp, water:acetonitrile (2:3 v/v) (value for 1,2,3,4,7,8-HxCDD); 1,2,3,4,6,7,8-HpCDD: Choudry and Webster 1989 as cited in U.S. EPA 2000a; Hg lamp, water:acetonitrile; 1,2,3,4,6,7,8,9-OCDD: Kim and O'Keefe 1998 as cited in U.S. EPA 2000; sunlight, water from 7 ponds/lakes.

<sup>a</sup>See "Discussion of Half-life value selection in TRIM.FaTE vs. Lorber et al. (2000)" following this table.

**Chemical-Dependent/Abiotic -- Documentation for the OH WTE Dioxin Test Case**  
**(same values used for all abiotic compartments of a given type, except where noted)**

Property Type	Units	Value										Reference
		2,3,7,8-TCDF	1,2,3,7,8-PeCDF	2,3,4,7,8-PeCDF	1,2,3,4,7,8-HxCDF	1,2,3,6,7,8-HxCDF	1,2,3,7,8,9-HxCDF	2,3,4,6,7,8-HxCDF	1,2,3,4,6,7,8-HpCDF	1,2,3,4,7,8,9-HpCDF	1,2,3,4,6,7,8,9-OCDF	
Air Compartment												
Halflife <sup>a</sup>	day	19	31	33	78	55	51	59	137	122	321	Atkinson 1996 as cited in U.S. EPA 2000a; vapor phase reaction with hydroxyl radical
Groundwater												
Halflife <sup>a</sup>	day	1008	1008	1008	1008	1008	1008	1008	1008	1008	1008	Average value of the range presented in Mackay et al. 2000; based on estimated unacclimated aerobic biodegradation half-life, value is for 2,3,7,8-TCDD
Sediment												
Halflife <sup>a</sup>	day	1095	1095	1095	1095	1095	1095	1095	1095	1095	1095	Estimation based on Adriaens and Grbic-Galic 1992,1993 and Adriaens et al. 1995 as cited in U.S. EPA 2000a
Soil - Root Zone												
Halflife <sup>a</sup>	day	3650	3650	3650	3650	3650	3650	3650	3650	3650	3650	Mackay et al. 2000; the degradation rate was cited by multiple authors, value is for 2,3,7,8-TCDD
Soil - Surface												
Halflife <sup>a</sup>	day	3650	3650	3650	3650	3650	3650	3650	3650	3650	3650	Mackay et al. 2000; the degradation rate was cited by multiple authors, value is for 2,3,7,8-TCDD
Soil - Vadose Zone												
Halflife <sup>a</sup>	day	1008	1008	1008	1008	1008	1008	1008	1008	1008	1008	Average value of the range presented in Mackay et al. 2000; based on estimated unacclimated aerobic biodegradation half-life, value is for 2,3,7,8-TCDD
Surface water												
Halflife <sup>a</sup>	day	0.18	0.19	0.19	0.58	0.58	0.58	0.58	0.58	0.58	0.58	2,3,7,8-TCDF: Kim and O'Keefe 1998 as cited in U.S. EPA 2000a; sunlight, water from 7 ponds/lakes; 1,2,3,7,8-PeCDF and 2,3,4,7,8-PeCDF: Friesen et al. 1993 as cited in U.S. EPA 2000a; sunlight, lake water (value for 2,3,4,7,8-PeCDF); All other furans: Kim and O'Keefe 1998 as cited in U.S. EPA 2000a; sunlight, water from 7 ponds/lakes (value is for OCDF).

<sup>a</sup>See "Discussion of Half-life value selection in TRIM.FaTE vs. Lorber et al. (2000)" following this table.

## Chemical-Dependent/Abiotic -- Documentation for the OH WTE Dioxin Test

### Discussion of Half-life value selection in TRIM.FaTE vs. Lorber et al. (2000)

The model results presented in the Lorber et al. (2000) report were calculated using a dioxin dissipation rate, which corresponds to a half-life of 25 years (the same value was used for all congeners). This rate included dioxin removal from the soil by both chemical degradation and physical processes (e.g., runoff and erosion). According to Lorber et al. (2000), 25 years was selected as a mid-range value between a half-life of ten years, which is often used for surface dioxin residues, and 100 years, which is speculated to be an upper range for subsurface dioxin residues. Also, a study was cited that reported a measured half-life of 20 years for physical and chemical removal processes of dioxins from soil.

TRIM.FaTE models chemical degradation and physical removal separately. The chemical degradation rate used by TRIM.FaTE for all congeners corresponds to a half-life of ten years. The ten-year degradation half-life for TRIM.FaTE was selected based on multiple studies cited in Mackay et al. (2000), most of which ranged from one to 12 years for soil or surface soil, although one study reported that half-lives could be as high as 100 years for subsurface soil. It is not always clear whether half-lives reported are degradation or dissipation half-lives. Because most of the dioxin mass remains in the surface soil (with a depth of 1 cm), ten years was selected as a half-life. Although ten years is near the top of the range given by Mackay et al. (excluding the subsurface soil value), the half-life when physical removal processes are taken into account is closer to the middle of the range.

The physical removal processes in TRIM.FaTE are not modeled with a single rate constant, but are modeled with multiple algorithms and parameters based on chemical properties and region-specific runoff and erosion parameters. To gauge the magnitude of the impact of these processes on the TRIM.FaTE effective dissipation half-life (i.e., chemical degradation plus physical removal processes), the dissipation half-life was calculated empirically from the decrease in soil concentration when there is no input from the source. The TRIM.FaTE effective dissipation half-life is different for each chemical because of different chemical properties, so half-lives for two representative chemicals, 2,3,7,8-TCDD and 1,2,3,4,6,7,8,9-OCDD, were calculated. The 2,3,7,8-TCDD dissipation half-life in the TRIM.FaTE surface soil is on average 6.5 years, and the 1,2,3,4,6,7,8,9-OCDD dissipation half-life is on average 9 years. The difference between the chemicals is due primarily to the higher volatilization rate of 2,3,7,8-TCDD. Therefore, due to the range of half-lives available in the literature, different assumptions for taking into account subsurface dissipation rates, and different methods used to account for physical removal processes, the dioxin dissipation half-life used by Lorber et al. is approximately three times longer than the effective dissipation half-life used in TRIM.FaTE.

**Chemical-Dependent/Biotic -- Documentation for the OH WTE Dioxin Test Case**  
**(same values used for all biotic compartments of a given type, except where noted)**

Compartment	Property	Units	Value							Reference
			2,3,7,8-TCDD	1,2,3,7,8-PeCDD	1,2,3,4,7,8-HxCDD	1,2,3,6,7,8-HxCDD	1,2,3,7,8,9-HxCDD	1,2,3,4,6,7,8-HpCDD	1,2,3,4,6,7,8,9-OCDD	
Terrestrial Vegetation										
Leaf - Agriculture - General in Agriculture - General	Halflife	day	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Leaf - Agriculture - General in Agriculture - General	TransferFactortoLeafParticle	1/day	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	Calculated as 1 percent of transfer factor to leaf; highly uncertain.
Leaf - Coniferous Forest in Coniferous Forest	Halflife	day	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Leaf - Coniferous Forest in Coniferous Forest	TransferFactortoLeafParticle	1/day	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	Calculated as 1 percent of transfer factor to leaf; highly uncertain.
Leaf - Deciduous Forest in Deciduous Forest	Halflife	day	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Leaf - Deciduous Forest in Deciduous Forest	TransferFactortoLeafParticle	1/day	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	Calculated as 1 percent of transfer factor to leaf; highly uncertain.
Leaf - Grasses/Herbs in Grasses/Herbs	Halflife	day	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Leaf - Grasses/Herbs in Grasses/Herbs	TransferFactortoLeafParticle	1/day	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	Calculated as 1 percent of transfer factor to leaf; highly uncertain.
Particle on Leaf - Agriculture - General in Agriculture - General	Halflife	day	4.4	4.4	4.4	4.4	4.4	4.4	4.4	McCrary and Maggard 1993; photodegradation sorbed to grass foliage in sunlight; assumed 10 hours of sunlight per day.
Particle on Leaf - Agriculture - General in Agriculture - General	TransferFactortoLeaf	1/day	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	Professional judgment based on U.S. EPA 2000a (an estimate for mercury) and Trapp 1995; highly uncertain.
Particle on Leaf - Coniferous Forest in Coniferous Forest	Halflife	day	4.4	4.4	4.4	4.4	4.4	4.4	4.4	McCrary and Maggard 1993; photodegradation sorbed to grass foliage in sunlight; assumed 10 hours of sunlight per day.
Particle on Leaf - Coniferous Forest in Coniferous Forest	TransferFactortoLeaf	1/day	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	Professional judgment based on U.S. EPA 2000a (an estimate for mercury) and Trapp 1995; highly uncertain.
Particle on Leaf - Deciduous Forest in Deciduous Forest	Halflife	day	4.4	4.4	4.4	4.4	4.4	4.4	4.4	McCrary and Maggard 1993; photodegradation sorbed to grass foliage in sunlight; assumed 10 hours of sunlight per day.
Particle on Leaf - Deciduous Forest in Deciduous Forest	TransferFactortoLeaf	1/day	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	Professional judgment based on U.S. EPA 2000a (an estimate for mercury) and Trapp 1995; highly uncertain.
Particle on Leaf - Grasses/Herbs in Grasses/Herbs	Halflife	day	4.4	4.4	4.4	4.4	4.4	4.4	4.4	McCrary and Maggard 1993; photodegradation sorbed to grass foliage in sunlight; assumed 10 hours of sunlight per day.
Particle on Leaf - Grasses/Herbs in Grasses/Herbs	TransferFactortoLeaf	1/day	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	Professional judgment based on U.S. EPA 2000a (an estimate for mercury) and Trapp 1995; highly uncertain.
Root - Agriculture - General in Agriculture - General	Halflife	day	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Root - Agriculture - General in Agriculture - General	RootSoilWaterInteraction_Alpha	unitless	0.95	0.95	0.95	0.95	0.95	0.95	0.95	Professional judgment
Root - Grasses/Herbs in Grasses/Herbs	Halflife	day	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Root - Grasses/Herbs in Grasses/Herbs	RootSoilWaterInteraction_Alpha	unitless	0.95	0.95	0.95	0.95	0.95	0.95	0.95	Professional judgment
Stem - Agriculture - General in Agriculture - General	Halflife	day	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Stem - Grasses/Herbs in Grasses/Herbs	Halflife	day	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.



**Chemical-Dependent/Biotic -- Documentation for the OH WTE Dioxin Test Case**  
**(same values used for all biotic compartments of a given type, except where noted)**

Compartment	Property	Units	Value										Reference
			2,3,7,8-TCDF	1,2,3,7,8-PeCDF	2,3,4,7,8-PeCDF	1,2,3,4,7,8-HxCDF	1,2,3,6,7,8-HxCDF	1,2,3,7,8,9-HxCDF	2,3,4,6,7,8-HxCDF	1,2,3,4,6,7,8-HpCDF	1,2,3,4,7,8,9-HpCDF	1,2,3,4,6,7,8,9-OCDF	
Terrestrial Vegetation													
Leaf - Agriculture - General in Agriculture - General	Half-life	day	70	70	70	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Leaf - Agriculture - General in Agriculture - General	TransferFactor to Leaf Particle	1/day	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	Calculated as 1 percent of transfer factor to leaf; highly uncertain.
Leaf - Coniferous Forest in Coniferous Forest	Half-life	day	70	70	70	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Leaf - Coniferous Forest in Coniferous Forest	TransferFactor to Leaf Particle	1/day	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	Calculated as 1 percent of transfer factor to leaf; highly uncertain.
Leaf - Deciduous Forest in Deciduous Forest	Half-life	day	70	70	70	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Leaf - Deciduous Forest in Deciduous Forest	TransferFactor to Leaf Particle	1/day	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	Calculated as 1 percent of transfer factor to leaf; highly uncertain.
Leaf - Grasses/Herbs in Grasses/Herbs	Half-life	day	70	70	70	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Leaf - Grasses/Herbs in Grasses/Herbs	TransferFactor to Leaf Particle	1/day	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	3.0E-03	Calculated as 1 percent of transfer factor to leaf; highly uncertain.
Leaf Particle - Agriculture - General in Agriculture - General	Half-life	day	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	McCrary and Maggard 1993; photodegradation of 2,3,7,8-TCDD sorbed to grass foliage in sunlight; assumed 10 hours of sunlight per day.
Leaf Particle - Agriculture - General in Agriculture - General	TransferFactor to Leaf	1/day	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	Professional judgment based on TCDD information in U.S. EPA 2000a (an estimate for mercury) and Trapp 1995; highly uncertain.
Leaf Particle - Coniferous Forest in Coniferous Forest	Half-life	day	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	McCrary and Maggard 1993; photodegradation of 2,3,7,8-TCDD sorbed to grass foliage in sunlight; assumed 10 hours of sunlight per day.
Leaf Particle - Coniferous Forest in Coniferous Forest	TransferFactor to Leaf	1/day	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	Professional judgment based on TCDD information in U.S. EPA 2000a (an estimate for mercury) and Trapp 1995; highly uncertain.
Leaf Particle - Deciduous Forest in Deciduous Forest	Half-life	day	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	McCrary and Maggard 1993; photodegradation of 2,3,7,8-TCDD sorbed to grass foliage in sunlight; assumed 10 hours of sunlight per day.
Leaf Particle - Deciduous Forest in Deciduous Forest	TransferFactor to Leaf	1/day	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	Professional judgment based on TCDD information in U.S. EPA 2000a (an estimate for mercury) and Trapp 1995; highly uncertain.
Leaf Particle - Grasses/Herbs in Grasses/Herbs	Half-life	day	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	4.4	McCrary and Maggard 1993; photodegradation of 2,3,7,8-TCDD sorbed to grass foliage in sunlight; assumed 10 hours of sunlight per day.
Leaf Particle - Grasses/Herbs in Grasses/Herbs	TransferFactor to Leaf	1/day	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	3.0E-01	Professional judgment based on TCDD information in U.S. EPA 2000a (an estimate for mercury) and Trapp 1995; highly uncertain.
Root - Agriculture - General in Agriculture - General	Half-life	day	70	70	70	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Root - Agriculture - General in Agriculture - General	RootSoilWater Interaction_Alpha	unitless	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	Professional judgment
Root - Grasses/Herbs in Grasses/Herbs	Half-life	day	70	70	70	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.
Root - Grasses/Herbs in Grasses/Herbs	RootSoilWater Interaction_Alpha	unitless	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	Professional judgment
Stem - Agriculture - General in Agriculture - General	Half-life	day	70	70	70	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.

**Chemical-Dependent/Biotic -- Documentation for the OH WTE Dioxin Test Case**  
**(same values used for all biotic compartments of a given type, except where noted)**

Compartment	Property	Units	2,3,7,8-TCDF	1,2,3,7,8-PeCDF	2,3,4,7,8-PeCDF	1,2,3,4,7,8-HxCDF	1,2,3,6,7,8-HxCDF	1,2,3,7,8,9-HxCDF	2,3,4,6,7,8-HxCDF	1,2,3,4,6,7,8-HpCDF	1,2,3,4,7,8,9-HpCDF	1,2,3,4,6,7,8,9-OCDF	Reference
Stem - Grasses/Herbs in Grasses/Herbs	Half-life	day	70	70	70	70	70	70	70	70	70	70	Arjmand and Sandermann 1985, as cited in Komoba, et al. 1995; soybean root cell culture metabolism test data for DDE.

## Meteorological and Other Settings --Documentation for the OH WTE Dioxin Test Case

Parameter Name	Units	Value Used	Reference
<b>Meteorological Inputs (all TRIM.FaTE scenario properties, except mixing height)<sup>a</sup></b>			
Air temperature	degrees K	varies hourly	From hourly local composite met data, 1989 and 1994
Horizontal wind speed	m/sec	varies hourly	From hourly local composite met data, 1989 and 1994
Wind direction	degrees clockwise from N (blowing from)	varies hourly	From hourly local composite met data, 1989 and 1994
Rainfall rate	m <sup>3</sup> [rain]/m <sup>2</sup> [surface area]-day	varies hourly	From hourly local composite met data, 1989 and 1994
Mixing height (used to set air VE property named "top")	m	varies hourly	From hourly local composite met data, 1989 and 1994 (used values for rural setting)
Day/night	1=day, 0=night	varies hourly	Based on sunrise/sunset data for source latitude and longitude
<b>Other Settings (all TRIM.FaTE scenario properties)</b>			
Start of simulation	date/time	1/1/1994 or 1/1/1989	Selected to match start of the air (1994) and soil (1989) simulations described in Lorber et al. 2000
End of simulation	date/time	1/1/1995 or 1/1/2001	Selected to match end of the air (1995) and soil (2001) simulations described in Lorber et al. 2000
Simulation time step	hr	1	Selected value
Output time step <sup>b</sup>	hr	1 or 730	Selected value of one hour for air simulation and 730 hours (approximatly one month) for the soil simulations.

<sup>a</sup>Input data used repeats in one-year cycle throughout modeling period for the 1989 met data.

<sup>b</sup>Output time step is set in TRIM.FaTE using the scenario property "simulationStepsPerOutputStep."

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## **Appendix C**

### **DOCUMENTATION OF FACILITY EMISSIONS FOR TRIM.FaTE INPUT PARAMETERS**

This appendix contains the following sets of tables, including calculations where appropriate, listing and describing the input parameters used in TRIM.FaTE for the Columbus, Ohio WTE Facility source emissions:

- summary of TRIM.FaTE source input parameters
- calculations for facility emissions for 1992 and 1994 stack test emissions

References are included at the end of the appendix.



## Source Data -- Documentation for Ohio Dioxin Application

Property	Units	Value
Stack Elevation	m	82.9
X-coordinate	m (UTM)	327174.5
Y-coordinate	m (UTM)	4418908.1

Chemical	Units	Emission Rate	
		1992 Stack Test	1994 Stack Test
1,2,3,4,6,7,8,9-OCDD	g/day	4.41E+00	6.53E+00
1,2,3,4,6,7,8,9-OCDF	g/day	1.79E+00	2.00E+00
1,2,3,4,6,7,8-HpCDD	g/day	4.00E+00	2.87E+00
1,2,3,4,6,7,8-HpCDF	g/day	7.40E+00	4.54E+00
1,2,3,4,7,8,9-HpCDF	g/day	3.02E+00	3.41E-01
1,2,3,4,7,8-HxCDD	g/day	6.04E-01	3.59E-01
1,2,3,4,7,8-HxCDF	g/day	2.46E+00	7.36E-01
1,2,3,6,7,8-HxCDD	g/day	7.96E-01	2.93E-01
1,2,3,6,7,8-HxCDF	g/day	2.61E+00	6.56E-01
1,2,3,7,8,9-HxCDD	g/day	7.46E-01	2.31E-01
1,2,3,7,8,9-HxCDF	g/day	5.03E-01	2.93E-02
1,2,3,7,8-PeCDD	g/day	7.18E-01	2.16E-01
1,2,3,7,8-PeCDF	g/day	1.58E+00	1.91E-01
2,3,4,6,7,8-HxCDF	g/day	2.96E+00	9.01E-01
2,3,4,7,8-PeCDF	g/day	1.63E+00	3.50E-01
2,3,7,8-TCDD	g/day	1.64E-01	1.38E-02
2,3,7,8-TCDF	g/day	5.99E-01	8.64E-02
<b>All 17 dioxin/furans</b>	g TEQ/day	2.69E+00	7.22E-01
<b>All 17 dioxin/furans</b>	g TEQ/sec	3.10E-05	8.35E-06

Percent reduction from 1992 to 1994 emissions (for TEQ) = 73

## Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility - Documentation for Ohio Dioxin Application

### Steps to convert data from 1992 stack tests to emissions data for TRIM.FaTE:

- 1) Compiled stack data using information Table 2 in the Ohio EPA report from Sept 1994
- 2) Converted data from grains per dry standard cubic foot (gr/DSCF) to grams per DSCF (g/DSCF)
- 3) Using flow rates (DSCF/min) from Ohio EPA (1994) report, converted data to grams per minute
- 4) Converted stack emissions to grams per second
- 5) Adjusted stack emissions for usage, based on the assumption that on average 4.22 boilers are used continuously (i.e., multiplied by 4.22)
- 6) Converted emissions to grams per day to be consistent with units in TRIM.FaTE
- 7) Converted emissions to toxicity equivalent (TEQ) emissions by multiplying by toxicity equivalency factors (TEFs) for comparison (from Ohio EPA 1994; same as Lorber et al. 2000)
- 8) Compared TEQ (in grams per year) to Lorber et al., 1996 and 2000 reports

### ***Conversion factors and other constants:***

<b>grams per grain</b>	6.48E-02
<b>sec/min</b>	60
<b>sec/day</b>	8.64E+04
<b>Number of boilers in use</b>	4.22

Flow Rate (DSCF/min)				
Run 1	Run 2	Run 3	Run 3-1	Run 3-2
1.17E+05	1.16E+05	1.15E+05	1.15E+05	1.05E+05

**Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility -  
Documentation for Ohio Dioxin Application**

	<b>STEP 1</b>				
	<b>Stack Emissions (gr/DSCF)</b>				
	<b>Run 1</b>	<b>Run 2</b>	<b>Run 3</b>	<b>Run 3-1</b>	<b>Run 3-2</b>
2,3,7,8 TCDD	2.65E-09	5.13E-09	4.84E-09	3.95E-09	1.50E-09
1,2,3,7,8 PeCDD	1.64E-08	2.20E-08	1.91E-08	2.03E-08	9.35E-10
1,2,3,4,7,8 HxCDD	1.52E-08	1.59E-08	1.20E-08	1.56E-08	8.29E-09
1,2,3,6,7,8 HxCDD	2.02E-08	2.08E-08	1.40E-08	2.27E-08	1.04E-08
1,2,3,7,8,9 HxCDD	1.77E-08	2.20E-08	1.53E-08	1.91E-08	8.29E-09
1,2,3,4,6,7,8 HpCDD	9.98E-08	1.08E-07	7.01E-08	1.17E-07	4.81E-08
OCDD	1.52E-07	1.10E-07	8.03E-08	8.86E-08	5.62E-08
2,3,7,8 TCDF	1.01E-08	1.59E-08	1.66E-08	1.56E-08	8.28E-09
1,2,3,7,8 PeCDF	2.65E-08	4.64E-08	4.46E-08	4.31E-08	1.39E-08
2,3,4,7,8 PeCDF	3.54E-08	4.27E-08	3.70E-08	4.31E-08	2.24E-08
1,2,3,4,7,8 HxCDF	5.69E-08	6.96E-08	5.61E-08	6.22E-08	2.67E-08
1,2,3,6,7,8 HxCDF	5.69E-08	7.82E-08	6.12E-08	6.70E-08	2.48E-08
1,2,3,7,8,9 HxCDF	1.25E-08	2.08E-08	1.12E-08	7.66E-09	3.21E-09
2,3,4,6,7,8 HxCDF	4.30E-08	1.83E-07	3.19E-08	4.43E-08	2.41E-08
1,2,3,4,6,7,8 HpCDF	2.02E-07	1.83E-07	1.53E-07	1.91E-07	8.82E-08
1,2,3,4,7,8,9 HpCDF	1.90E-08	2.69E-07	1.66E-08	1.91E-08	9.09E-09
OCDF	6.19E-08	5.62E-08	4.84E-08	6.10E-11	3.21E-08

	<b>STEP 2</b>				
	<b>Stack Emissions (g/DSCF)</b>				
	<b>Run 1</b>	<b>Run 2</b>	<b>Run 3</b>	<b>Run 3-1</b>	<b>Run 3-2</b>
2,3,7,8 TCDD	1.7E-10	3.3E-10	3.1E-10	2.6E-10	9.69E-11
1,2,3,7,8 PeCDD	1.1E-09	1.4E-09	1.2E-09	1.3E-09	6.06E-11
1,2,3,4,7,8 HxCDD	9.8E-10	1.0E-09	7.8E-10	1.0E-09	5.37E-10
1,2,3,6,7,8 HxCDD	1.3E-09	1.3E-09	9.1E-10	1.5E-09	6.75E-10
1,2,3,7,8,9 HxCDD	1.1E-09	1.4E-09	9.9E-10	1.2E-09	5.37E-10
1,2,3,4,6,7,8 HpCDD	6.5E-09	7.0E-09	4.5E-09	7.6E-09	3.12E-09
OCDD	9.8E-09	7.1E-09	5.2E-09	5.7E-09	3.64E-09
2,3,7,8 TCDF	6.6E-10	1.0E-09	1.1E-09	1.0E-09	5.37E-10
1,2,3,7,8 PeCDF	1.7E-09	3.0E-09	2.9E-09	2.8E-09	9.00E-10
2,3,4,7,8 PeCDF	2.3E-09	2.8E-09	2.4E-09	2.8E-09	1.45E-09
1,2,3,4,7,8 HxCDF	3.7E-09	4.5E-09	3.6E-09	4.0E-09	1.73E-09
1,2,3,6,7,8 HxCDF	3.7E-09	5.1E-09	4.0E-09	4.3E-09	1.61E-09
1,2,3,7,8,9 HxCDF	8.1E-10	1.3E-09	7.3E-10	5.0E-10	2.08E-10
2,3,4,6,7,8 HxCDF	2.8E-09	1.2E-08	2.1E-09	2.9E-09	1.56E-09
1,2,3,4,6,7,8 HpCDF	1.3E-08	1.2E-08	9.9E-09	1.2E-08	5.71E-09
1,2,3,4,7,8,9 HpCDF	1.2E-09	1.7E-08	1.1E-09	1.2E-09	5.89E-10
OCDF	4.0E-09	3.6E-09	3.1E-09	4.0E-12	2.08E-09

**Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility -  
Documentation for Ohio Dioxin Application**

STEP 3	Stack Emissions (g/min)				
	Run 1	Run 2	Run 3	Run 3-1	Run 3-2
2,3,7,8 TCDD	2.02E-05	3.84E-05	3.62E-05	2.95E-05	1.02E-05
1,2,3,7,8 PeCDD	1.25E-04	1.65E-04	1.43E-04	1.52E-04	6.39E-06
1,2,3,4,7,8 HxCDD	1.15E-04	1.19E-04	8.96E-05	1.16E-04	5.66E-05
1,2,3,6,7,8 HxCDD	1.54E-04	1.56E-04	1.05E-04	1.70E-04	7.12E-05
1,2,3,7,8,9 HxCDD	1.35E-04	1.65E-04	1.14E-04	1.43E-04	5.66E-05
1,2,3,4,6,7,8 HpCDD	7.60E-04	8.05E-04	5.25E-04	8.76E-04	3.29E-04
OCDD	1.15E-03	8.24E-04	6.01E-04	6.62E-04	3.84E-04
2,3,7,8 TCDF	7.70E-05	1.19E-04	1.24E-04	1.16E-04	5.66E-05
1,2,3,7,8 PeCDF	2.02E-04	3.48E-04	3.34E-04	3.22E-04	9.49E-05
2,3,4,7,8 PeCDF	2.69E-04	3.20E-04	2.77E-04	3.22E-04	1.53E-04
1,2,3,4,7,8 HxCDF	4.33E-04	5.21E-04	4.20E-04	4.65E-04	1.83E-04
1,2,3,6,7,8 HxCDF	4.33E-04	5.85E-04	4.58E-04	5.01E-04	1.70E-04
1,2,3,7,8,9 HxCDF	9.51E-05	1.56E-04	8.39E-05	5.72E-05	2.19E-05
2,3,4,6,7,8 HxCDF	3.27E-04	1.37E-03	2.38E-04	3.31E-04	1.64E-04
1,2,3,4,6,7,8 HpCDF	1.54E-03	1.37E-03	1.14E-03	1.43E-03	6.02E-04
1,2,3,4,7,8,9 HpCDF	1.44E-04	2.01E-03	1.24E-04	1.43E-04	6.21E-05
OCDF	4.71E-04	4.21E-04	3.62E-04	4.56E-07	2.19E-04

STEP 4	Stack Emissions (g/sec)				
	Run 1	Run 2	Run 3	Run 3-1	Run 3-2
3.36E-07	6.40E-07	6.04E-07	4.92E-07	1.70E-07	
2.08E-06	2.74E-06	2.38E-06	2.53E-06	1.06E-07	
1.92E-06	1.98E-06	1.49E-06	1.94E-06	9.43E-07	
2.56E-06	2.59E-06	1.75E-06	2.83E-06	1.19E-06	
2.24E-06	2.74E-06	1.91E-06	2.39E-06	9.43E-07	
1.27E-05	1.34E-05	8.74E-06	1.46E-05	5.48E-06	
1.92E-05	1.37E-05	1.00E-05	1.10E-05	6.39E-06	
1.28E-06	1.98E-06	2.07E-06	1.94E-06	9.43E-07	
3.37E-06	5.79E-06	5.56E-06	5.36E-06	1.58E-06	
4.49E-06	5.34E-06	4.61E-06	5.36E-06	2.55E-06	
7.21E-06	8.69E-06	6.99E-06	7.75E-06	3.04E-06	
7.21E-06	9.76E-06	7.63E-06	8.35E-06	2.83E-06	
1.59E-06	2.59E-06	1.40E-06	9.54E-07	3.65E-07	
5.45E-06	2.29E-05	3.97E-06	5.51E-06	2.74E-06	
2.56E-05	2.29E-05	1.91E-05	2.39E-05	1.00E-05	
2.40E-06	3.36E-05	2.07E-06	2.39E-06	1.03E-06	
7.85E-06	7.02E-06	6.04E-06	7.61E-09	3.65E-06	

**Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility -  
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	<b>STEP 5</b>				
	<b>Facility Emissions, Adjusted for Usage (g/sec)</b>				
	<b>Run 1</b>	<b>Run 2</b>	<b>Run 3</b>	<b>Run 3-1</b>	<b>Run 3-2</b>
2,3,7,8 TCDD	1.42E-06	2.70E-06	2.55E-06	2.07E-06	7.19E-07
1,2,3,7,8 PeCDD	8.79E-06	1.16E-05	1.01E-05	1.07E-05	4.49E-07
1,2,3,4,7,8 HxCDD	8.12E-06	8.37E-06	6.30E-06	8.18E-06	3.98E-06
1,2,3,6,7,8 HxCDD	1.08E-05	1.09E-05	7.38E-06	1.19E-05	5.01E-06
1,2,3,7,8,9 HxCDD	9.47E-06	1.16E-05	8.05E-06	1.01E-05	3.98E-06
1,2,3,4,6,7,8 HpCDD	5.34E-05	5.66E-05	3.69E-05	6.16E-05	2.31E-05
OCDD	8.12E-05	5.79E-05	4.23E-05	4.66E-05	2.70E-05
2,3,7,8 TCDF	5.41E-06	8.36E-06	8.72E-06	8.18E-06	3.98E-06
1,2,3,7,8 PeCDF	1.42E-05	2.44E-05	2.35E-05	2.26E-05	6.68E-06
2,3,4,7,8 PeCDF	1.89E-05	2.25E-05	1.95E-05	2.26E-05	1.08E-05
1,2,3,4,7,8 HxCDF	3.04E-05	3.67E-05	2.95E-05	3.27E-05	1.28E-05
1,2,3,6,7,8 HxCDF	3.04E-05	4.12E-05	3.22E-05	3.52E-05	1.19E-05
1,2,3,7,8,9 HxCDF	6.69E-06	1.09E-05	5.90E-06	4.03E-06	1.54E-06
2,3,4,6,7,8 HxCDF	2.30E-05	9.65E-05	1.68E-05	2.33E-05	1.16E-05
1,2,3,4,6,7,8 HpCDF	1.08E-04	9.65E-05	8.05E-05	1.01E-04	4.24E-05
1,2,3,4,7,8,9 HpCDF	1.01E-05	1.42E-04	8.72E-06	1.01E-05	4.37E-06
OCDF	3.31E-05	2.96E-05	2.55E-05	3.21E-08	1.54E-05

**Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility -  
Documentation for Ohio Dioxin Application**

	STEP 6						
	Facility Emissions, Adjusted for Usage (g/day)						
	Run 1	Run 2	Run 3	Run 3-1	Run 3-2	Average	% Total
2,3,7,8 TCDD	1.23E-01	2.33E-01	2.20E-01	1.79E-01	6.21E-02	1.64E-01	0.5%
1,2,3,7,8 PeCDD	7.59E-01	1.00E+00	8.69E-01	9.24E-01	3.88E-02	7.18E-01	2.0%
1,2,3,4,7,8 HxCDD	7.01E-01	7.23E-01	5.45E-01	7.07E-01	3.44E-01	6.04E-01	1.7%
1,2,3,6,7,8 HxCDD	9.35E-01	9.45E-01	6.37E-01	1.03E+00	4.33E-01	7.96E-01	2.2%
1,2,3,7,8,9 HxCDD	8.18E-01	1.00E+00	6.95E-01	8.70E-01	3.44E-01	7.46E-01	2.1%
1,2,3,4,6,7,8 HpCDD	4.62E+00	4.89E+00	3.19E+00	5.33E+00	2.00E+00	4.00E+00	11.1%
OCDD	7.02E+00	5.01E+00	3.65E+00	4.03E+00	2.33E+00	4.41E+00	12.2%
2,3,7,8 TCDF	4.68E-01	7.23E-01	7.53E-01	7.07E-01	3.44E-01	5.99E-01	1.7%
1,2,3,7,8 PeCDF	1.23E+00	2.11E+00	2.03E+00	1.96E+00	5.77E-01	1.58E+00	4.4%
2,3,4,7,8 PeCDF	1.64E+00	1.95E+00	1.68E+00	1.96E+00	9.31E-01	1.63E+00	4.5%
1,2,3,4,7,8 HxCDF	2.63E+00	3.17E+00	2.55E+00	2.83E+00	1.11E+00	2.46E+00	6.8%
1,2,3,6,7,8 HxCDF	2.63E+00	3.56E+00	2.78E+00	3.04E+00	1.03E+00	2.61E+00	7.2%
1,2,3,7,8,9 HxCDF	5.78E-01	9.45E-01	5.10E-01	3.48E-01	1.33E-01	5.03E-01	1.4%
2,3,4,6,7,8 HxCDF	1.99E+00	8.34E+00	1.45E+00	2.01E+00	9.98E-01	2.96E+00	8.2%
1,2,3,4,6,7,8 HpCDF	9.35E+00	8.34E+00	6.95E+00	8.70E+00	3.66E+00	7.40E+00	20.6%
1,2,3,4,7,8,9 HpCDF	8.76E-01	1.22E+01	7.53E-01	8.70E-01	3.77E-01	3.02E+00	8.4%
OCDF	2.86E+00	2.56E+00	2.20E+00	2.77E-03	1.33E+00	1.79E+00	5.0%

**Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility -  
Documentation for Ohio Dioxin Application**

STEP 7							Average
TEF Converted Emissions (g/day)							
	Run 1	Run 2	Run 3	Run 3-1	Run 3-2	TEF	
2,3,7,8 TCDD	1.23E-01	2.33E-01	2.20E-01	1.79E-01	6.21E-02	1	1.64E-01
1,2,3,7,8 PeCDD	3.80E-01	5.00E-01	4.35E-01	4.62E-01	1.94E-02	0.5	3.59E-01
1,2,3,4,7,8 HxCDD	7.01E-02	7.23E-02	5.45E-02	7.07E-02	3.44E-02	0.1	6.04E-02
1,2,3,6,7,8 HxCDD	9.35E-02	9.45E-02	6.37E-02	1.03E-01	4.33E-02	0.1	7.96E-02
1,2,3,7,8,9 HxCDD	8.18E-02	1.00E-01	6.95E-02	8.70E-02	3.44E-02	0.1	7.46E-02
1,2,3,4,6,7,8 HpCDD	4.62E-02	4.89E-02	3.19E-02	5.33E-02	2.00E-02	0.01	4.00E-02
1,2,3,4,6,7,8,9-OCDD	7.02E-03	5.01E-03	3.65E-03	4.03E-03	2.33E-03	0.001	4.41E-03
2,3,7,8 TCDF	4.68E-02	7.23E-02	7.53E-02	7.07E-02	3.44E-02	0.1	5.99E-02
1,2,3,7,8 PeCDF	6.14E-02	1.06E-01	1.01E-01	9.78E-02	2.88E-02	0.05	7.90E-02
2,3,4,7,8 PeCDF	8.18E-01	9.73E-01	8.40E-01	9.78E-01	4.66E-01	0.5	8.15E-01
1,2,3,4,7,8 HxCDF	2.63E-01	3.17E-01	2.55E-01	2.83E-01	1.11E-01	0.1	2.46E-01
1,2,3,6,7,8 HxCDF	2.63E-01	3.56E-01	2.78E-01	3.04E-01	1.03E-01	0.1	2.61E-01
1,2,3,7,8,9 HxCDF	5.78E-02	9.45E-02	5.10E-02	3.48E-02	1.33E-02	0.1	5.03E-02
2,3,4,6,7,8 HxCDF	1.99E-01	8.34E-01	1.45E-01	2.01E-01	9.98E-02	0.1	2.96E-01
1,2,3,4,6,7,8 HpCDF	9.35E-02	8.34E-02	6.95E-02	8.70E-02	3.66E-02	0.01	7.40E-02
1,2,3,4,7,8,9 HpCDF	8.76E-03	1.22E-01	7.53E-03	8.70E-03	3.77E-03	0.01	3.02E-02
1,2,3,4,6,7,8,9-OCDF	2.86E-03	2.56E-03	2.20E-03	2.77E-06	1.33E-03	0.001	1.79E-03
TEQ (g/day)	2.61E+00	4.01E+00	2.70E+00	3.02E+00	1.11E+00		2.69E+00
TEQ (g/yr)	9.54E+02	1.47E+03	9.87E+02	1.10E+03	4.07E+02		9.83E+02

<b>STEP 8) Verify emissions with previous reports</b>		
	<b>TEQ (g/s)</b>	<b>TEQ (g/yr)</b>
Ohio EPA, 1994 (from Step 7)	-	9.83E+02
TEQ emissions used in Lorber et al, 1996	3.10E-05	9.78E+02
TEQ emissions used in Lorber et al, 2000	-	9.84E+02

## Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility - Documentation for Ohio Dioxin Application

### Steps to convert data from 1994 stack tests to emissions data for TRIM.FaTE:

- 1) Compiled stack data using information tables in the Solid Waste Authority of Central Ohio report dated October 26, 1994 (to EPA Region 5)
- 2) Converted data from nanograms per dry standard cubic meters (ng/DSCM) to grams per DSCM (g/DSCM)
- 3) Using flow rates (DSCM/min) from Solid Waste Authority report, converted data to grams per minute (g/min)
- 4) Converted stack emissions to grams per second (g/s)
- 5) Adjusted stack emissions for usage, based on the assumption that on average 4.22 boilers are used continuously (i.e., multiplied by 4.22)
- 6) Converted emissions to grams per day to be consistent with units in TRIM.FaTE
- 7) Converted emissions to toxicity equivalent (TEQ) emissions by multiplying by toxicity equivalency factors (TEFs) for comparison (from Ohio EPA 1994; same as Lorber et al. 2000)
- 8) Compared TEQ (in grams per year) to Lorber et al., 1996 and 2000 reports

### **Conversion factors and other constants:**

<b>g/ng</b>	1.0E-09
<b>sec/min</b>	60
<b>sec/day</b>	8.64E+04
<b>Number of boilers in use</b>	4.22

<b>Flow Rate (DSCM/min)</b>		
<b>Run 1</b>	<b>Run 2</b>	<b>Run 3</b>
1977	1936	1962



**Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility -  
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Stack C for boiler 6	STEP 1 Stack Emissions (ng/DSCM)			STEP 2 Stack Emissions (g/DSCM)			STEP 3 Stack Emissions (g/min)		
	Run 1	Run 2	Run 3	Run 1	Run 2	Run 3	Run 1	Run 2	Run 3
2,3,7,8 TCDD	2.08	0.89	0.487	2.1E-09	8.9E-10	4.9E-10	4.11E-06	1.72E-06	9.55E-07
1,2,3,7,8 PeCDD	28.9	18.3	7.23	2.9E-08	1.8E-08	7.2E-09	5.71E-05	3.54E-05	1.42E-05
1,2,3,4,7,8 HxCDD	43.3	33.0	14.2	4.3E-08	3.3E-08	1.4E-08	8.56E-05	6.39E-05	2.79E-05
1,2,3,6,7,8 HxCDD	34.4	28.0	11.4	3.4E-08	2.8E-08	1.1E-08	6.80E-05	5.42E-05	2.24E-05
1,2,3,7,8,9 HxCDD	29.7	20.2	8.21	3.0E-08	2.0E-08	8.2E-09	5.87E-05	3.91E-05	1.61E-05
1,2,3,4,6,7,8 HpCDD	281	294	148	2.8E-07	2.9E-07	1.5E-07	5.56E-04	5.69E-04	2.90E-04
OCDD	572	642	434.0	5.7E-07	6.4E-07	4.3E-07	1.13E-03	1.24E-03	8.52E-04
2,3,7,8 TCDF	11.2	6.78	3.77	1.1E-08	6.8E-09	3.8E-09	2.21E-05	1.31E-05	7.40E-06
1,2,3,7,8 PeCDF	25.4	14.9	7.83	2.5E-08	1.5E-08	7.8E-09	5.02E-05	2.88E-05	1.54E-05
2,3,4,7,8 PeCDF	44.6	29.5	14.0	4.5E-08	3.0E-08	1.4E-08	8.82E-05	5.71E-05	2.75E-05
1,2,3,4,7,8 HxCDF	88.3	64.5	32.6	8.8E-08	6.5E-08	3.3E-08	1.75E-04	1.25E-04	6.40E-05
1,2,3,6,7,8 HxCDF	79.9	54.3	31.0	8.0E-08	5.4E-08	3.1E-08	1.58E-04	1.05E-04	6.08E-05
1,2,3,7,8,9 HxCDF	3.1	2.83	1.46	3.1E-09	2.8E-09	1.5E-09	6.13E-06	5.48E-06	2.86E-06
2,3,4,6,7,8 HxCDF	92.5	85.3	49.4	9.3E-08	8.5E-08	4.9E-08	1.83E-04	1.65E-04	9.69E-05
1,2,3,4,6,7,8 HpCDF	479	423	243	4.8E-07	4.2E-07	2.4E-07	9.47E-04	8.19E-04	4.77E-04
1,2,3,4,7,8,9 HpCDF	32.3	34.8	18.9	3.2E-08	3.5E-08	1.9E-08	6.39E-05	6.74E-05	3.71E-05
OCDF	172	202	130	1.7E-07	2.0E-07	1.3E-07	3.40E-04	3.91E-04	2.55E-04

**Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility -  
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	STEP 4 Stack Emissions (g/sec)			STEP 5 Facility Emissions, Adjusted for			STEP 6 Facility Emissions, Adjusted for Usage (g/day)				% Total
	Run 1	Run 2	Run 3	Run 1	Run 2	Run 3	Run 1	Run 2	Run 3	Average	
2,3,7,8 TCDD	6.85E-08	2.87E-08	1.59E-08	2.89E-07	1.21E-07	6.72E-08	2.50E-02	1.05E-02	5.81E-03	1.38E-02	0.1%
1,2,3,7,8 PeCDD	9.52E-07	5.90E-07	2.36E-07	4.02E-06	2.49E-06	9.98E-07	3.47E-01	2.15E-01	8.62E-02	2.16E-01	1.1%
1,2,3,4,7,8 HxCDD	1.43E-06	1.06E-06	4.64E-07	6.02E-06	4.49E-06	1.96E-06	5.20E-01	3.88E-01	1.69E-01	3.59E-01	1.8%
1,2,3,6,7,8 HxCDD	1.13E-06	9.03E-07	3.73E-07	4.78E-06	3.81E-06	1.57E-06	4.13E-01	3.29E-01	1.36E-01	2.93E-01	1.4%
1,2,3,7,8,9 HxCDD	9.79E-07	6.52E-07	2.68E-07	4.13E-06	2.75E-06	1.13E-06	3.57E-01	2.38E-01	9.79E-02	2.31E-01	1.1%
1,2,3,4,6,7,8 HpCDD	9.26E-06	9.49E-06	4.84E-06	3.91E-05	4.00E-05	2.04E-05	3.38E+00	3.46E+00	1.76E+00	2.87E+00	14.1%
OCDD	1.88E-05	2.07E-05	1.42E-05	7.95E-05	8.74E-05	5.99E-05	6.87E+00	7.55E+00	5.17E+00	6.53E+00	32.1%
2,3,7,8 TCDF	3.69E-07	2.19E-07	1.23E-07	1.56E-06	9.23E-07	5.20E-07	1.35E-01	7.98E-02	4.49E-02	8.64E-02	0.4%
1,2,3,7,8 PeCDF	8.37E-07	4.81E-07	2.56E-07	3.53E-06	2.03E-06	1.08E-06	3.05E-01	1.75E-01	9.34E-02	1.91E-01	0.9%
2,3,4,7,8 PeCDF	1.47E-06	9.52E-07	4.58E-07	6.20E-06	4.02E-06	1.93E-06	5.36E-01	3.47E-01	1.67E-01	3.50E-01	1.7%
1,2,3,4,7,8 HxCDF	2.91E-06	2.08E-06	1.07E-06	1.23E-05	8.78E-06	4.50E-06	1.06E+00	7.59E-01	3.89E-01	7.36E-01	3.6%
1,2,3,6,7,8 HxCDF	2.63E-06	1.75E-06	1.01E-06	1.11E-05	7.39E-06	4.28E-06	9.60E-01	6.39E-01	3.70E-01	6.56E-01	3.2%
1,2,3,7,8,9 HxCDF	1.02E-07	9.13E-08	4.77E-08	4.31E-07	3.85E-07	2.01E-07	3.72E-02	3.33E-02	1.74E-02	2.93E-02	0.1%
2,3,4,6,7,8 HxCDF	3.05E-06	2.75E-06	1.62E-06	1.29E-05	1.16E-05	6.82E-06	1.11E+00	1.00E+00	5.89E-01	9.01E-01	4.4%
1,2,3,4,6,7,8 HpCDF	1.58E-05	1.36E-05	7.95E-06	6.66E-05	5.76E-05	3.35E-05	5.75E+00	4.98E+00	2.90E+00	4.54E+00	22.3%
1,2,3,4,7,8,9 HpCDF	1.06E-06	1.12E-06	6.18E-07	4.49E-06	4.74E-06	2.61E-06	3.88E-01	4.09E-01	2.25E-01	3.41E-01	1.7%
OCDF	5.67E-06	6.52E-06	4.25E-06	2.39E-05	2.75E-05	1.79E-05	2.07E+00	2.38E+00	1.55E+00	2.00E+00	9.8%

**Calculations for Emissions of Dioxin-like Compounds at the Columbus WTE Facility -  
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STEP 7 TEF Converted Emissions (g/day)					Average
Run 1	Run 2	Run 3	TEF		
2,3,7,8 TCDD	2.50E-02	1.05E-02	5.81E-03	1	1.38E-02
1,2,3,7,8 PeCDD	1.74E-01	1.08E-01	4.31E-02	0.5	1.08E-01
1,2,3,4,7,8 HxCDD	5.20E-02	3.88E-02	1.69E-02	0.1	3.59E-02
1,2,3,6,7,8 HxCDD	4.13E-02	3.29E-02	1.36E-02	0.1	2.93E-02
1,2,3,7,8,9 HxCDD	3.57E-02	2.38E-02	9.79E-03	0.1	2.31E-02
1,2,3,4,6,7,8 HpCDD	3.38E-02	3.46E-02	1.76E-02	0.01	2.87E-02
1,2,3,4,6,7,8,9-OCDD	6.87E-03	7.55E-03	5.17E-03	0.001	6.53E-03
2,3,7,8 TCDF	1.35E-02	7.98E-03	4.49E-03	0.1	8.64E-03
1,2,3,7,8 PeCDF	1.53E-02	8.76E-03	4.67E-03	0.05	9.56E-03
2,3,4,7,8 PeCDF	2.68E-01	1.74E-01	8.35E-02	0.5	1.75E-01
1,2,3,4,7,8 HxCDF	1.06E-01	7.59E-02	3.89E-02	0.1	7.36E-02
1,2,3,6,7,8 HxCDF	9.60E-02	6.39E-02	3.70E-02	0.1	6.56E-02
1,2,3,7,8,9 HxCDF	3.72E-03	3.33E-03	1.74E-03	0.1	2.93E-03
2,3,4,6,7,8 HxCDF	1.11E-01	1.00E-01	5.89E-02	0.1	9.01E-02
1,2,3,4,6,7,8 HpCDF	5.75E-02	4.98E-02	2.90E-02	0.01	4.54E-02
1,2,3,4,7,8,9 HpCDF	3.88E-03	4.09E-03	2.25E-03	0.01	3.41E-03
1,2,3,4,6,7,8,9-OCDF	2.07E-03	2.38E-03	1.55E-03	0.001	2.00E-03
TEQ (g/day)	1.05E+00	7.46E-01	3.74E-01		7.22E-01
TEQ (g/yr)	3.82E+02	2.72E+02	1.36E+02		2.63E+02

<b>STEP 8) Verify emissions with previous reports</b>		
	<b>TEQ (g/s)</b>	<b>TEQ (g/yr)</b>
(from Step 7)	-	2.63E+02
emission used in Lorber et al, 1996 * 0.27	8.37E-06	2.64E+02
emission used in Lorber et al, 2000 * 0.27	-	2.67E+02

## Source Data -- Documentation for Ohio Dioxin Application

### References

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

Lorber, M.; Cleverly, D.; and J. Schaum. 1996. A screening-level risk assessment of the indirect impacts from the Columbus waste to energy facility in Columbus, Ohio. Proceedings of an International Specialty Conference, sponsored by the Air and Waste Management Association and the United States Environmental Protection Agency, held April 18-21, 1996 in Washington, D.C. Published in Solid Waste Management: Thermal Treatment & Waste-to-Energy Technologies, VIP - 53. pp. 262-278. Air & Waste Management Association, One Gateway Center, Third Floor, Pittsburgh, PA 15222.

Lorber, M.; Eschenroeder, A.; 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 (2000), pp. 3995-4010.

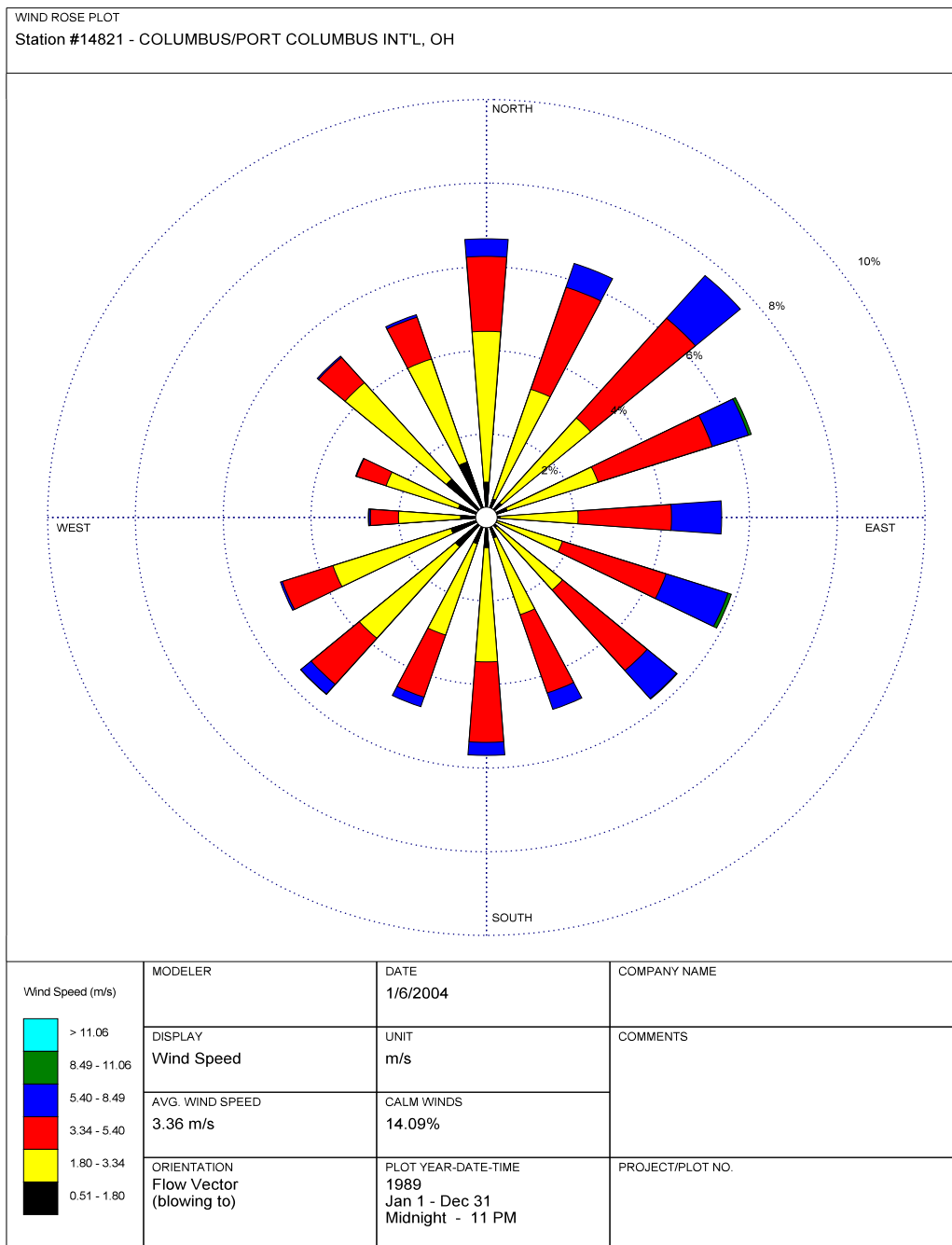
Ohio Environmental Protection Agency (OEPA) (1994) Risk assessment of potential health effects of dioxins and dibenzofurans emitted from the Columbus solid waste authority's reduction facility. The Ohio Environmental Protection Agency, Division of Air Pollution Control. February 28, 1994.

## **Appendix D. WIND ROSES**

This appendix contains the following wind roses using the appropriate meteorological data:

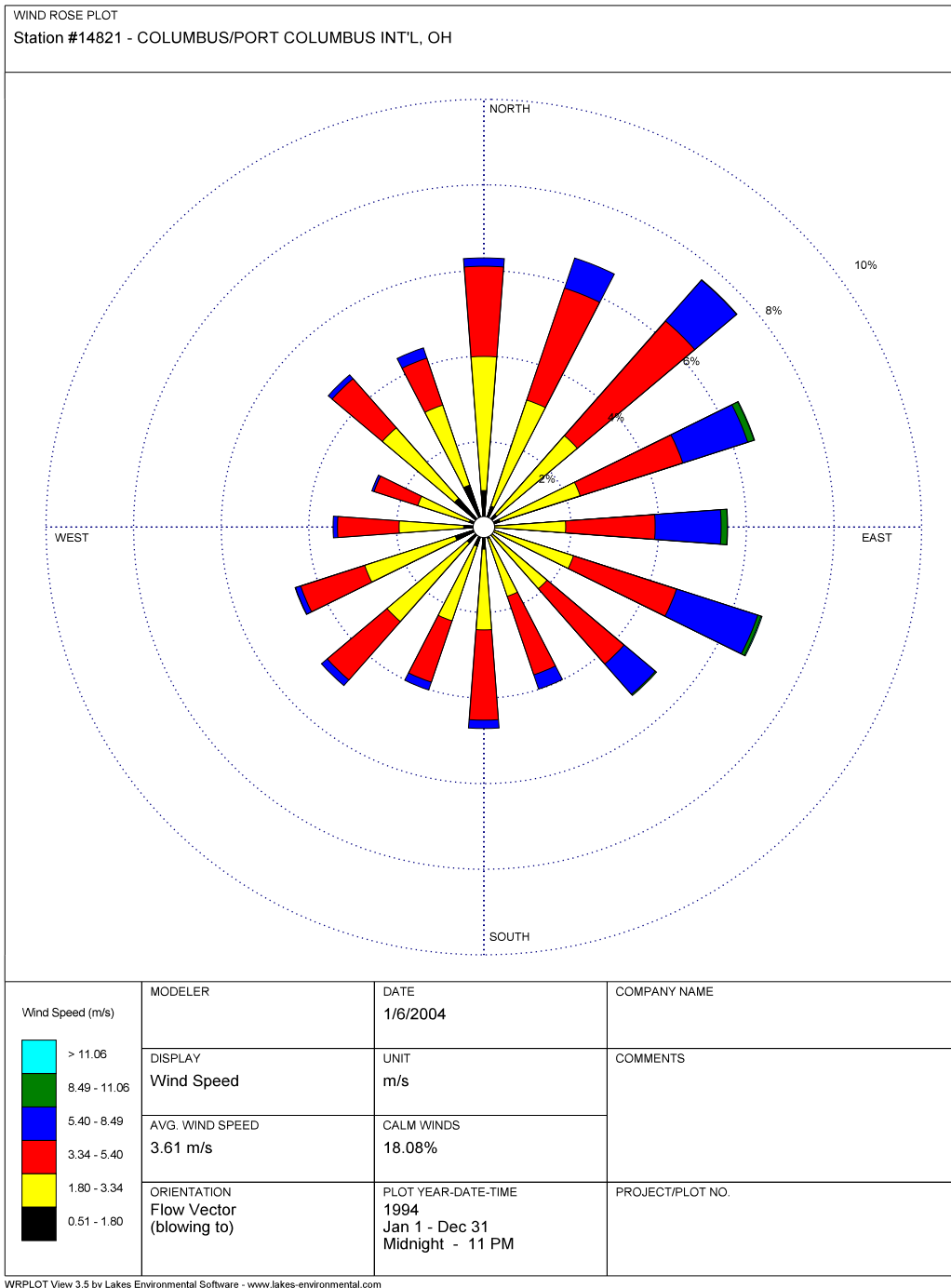
- Wind rose for Columbus, Ohio using local airport meteorological data from 1989;
- Wind rose for Columbus, Ohio using local airport meteorological data from 1994;
- Wind rose for Columbus, Ohio using local airport meteorological data from March 15 through 17, 1994.

## Wind Rose for Columbus, Ohio - 1989

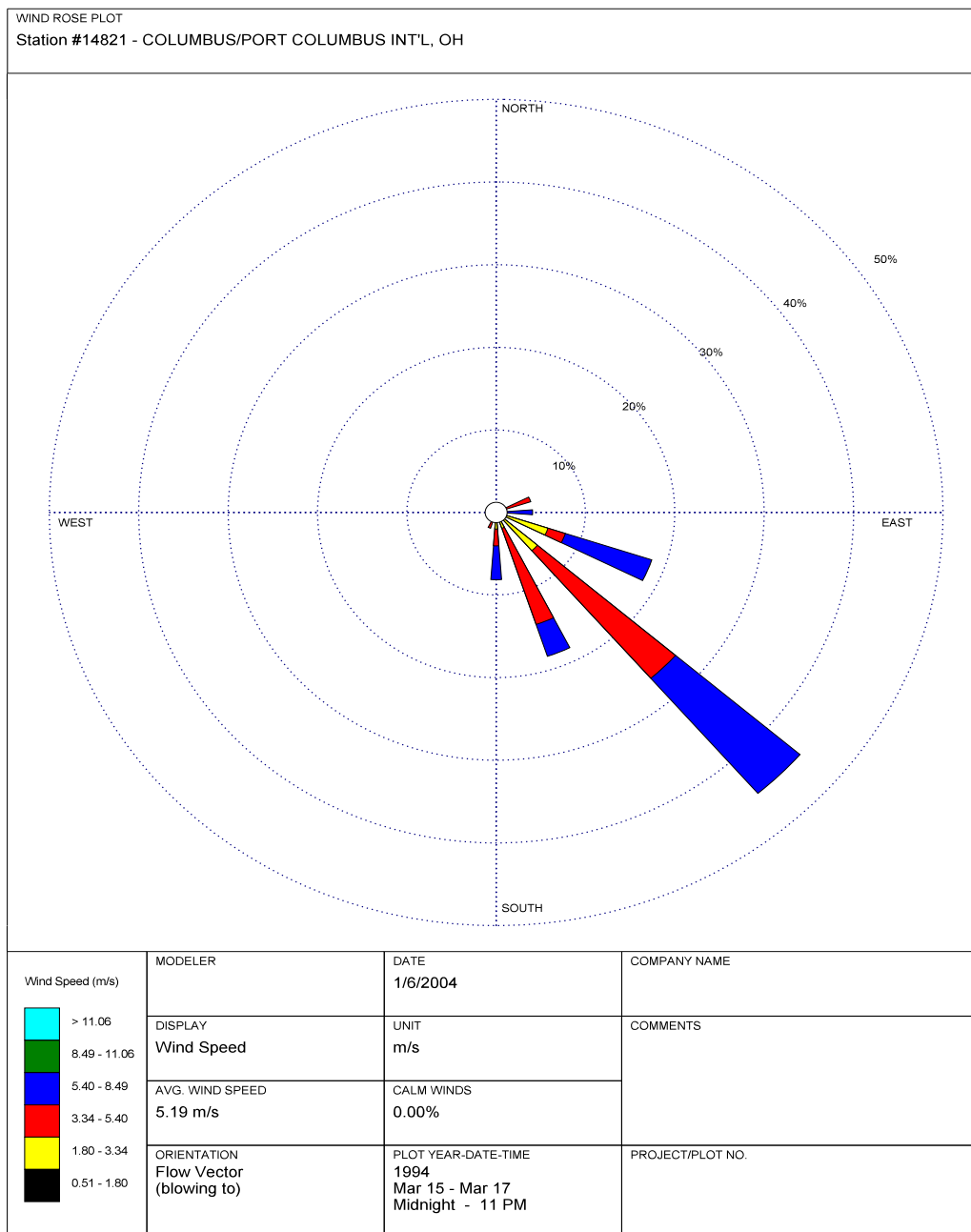


WRPLOT View 3.5 by Lakes Environmental Software - [www.lakes-environmental.com](http://www.lakes-environmental.com)

## Wind Rose for Columbus, Ohio - 1994



# **Wind Rose for Columbus, Ohio - March 15 through March 17, 1994**



WRPLOT View 3.5 by Lakes Environmental Software - www.lakes-environmental.com



## **Appendix E.**

### **DETAILED TRIM.FATE RESULTS BY CONGENER**

This appendix provides charts with congener specific TRIM.FaTE results for:

- The overall distribution of dioxin TEQ mass over time in compartments and sinks.
- The distribution of dioxin TEQ mass over time in abiotic compartments.

Figure E-1  
1,2,3,4,6,7,8-HpCDF Mass: Overall Distribution in Compartments and Sinks

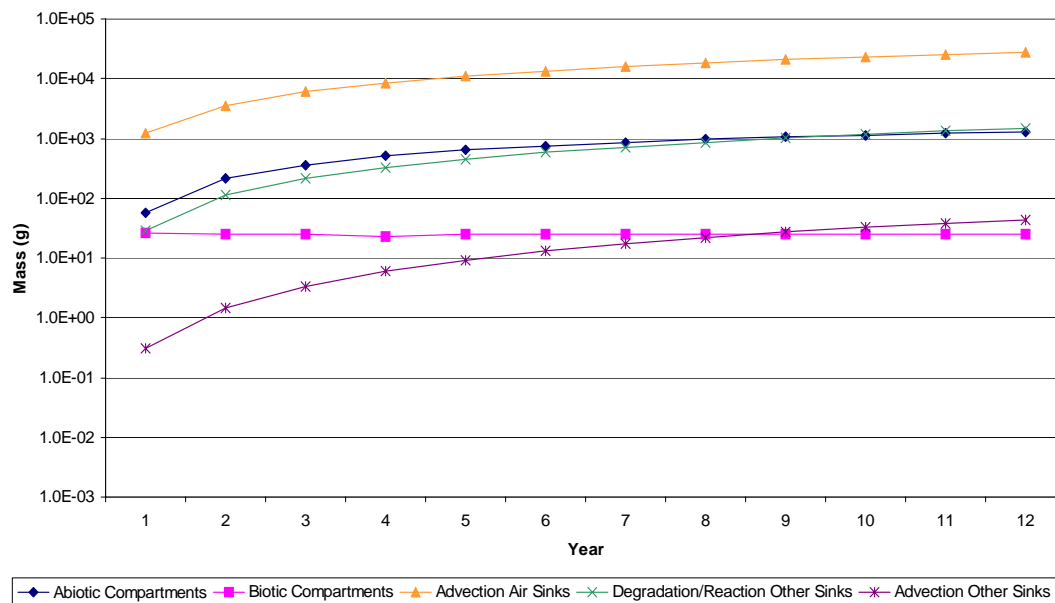


Figure E-2  
1,2,3,4,7,8-HxCDD Mass: Overall Distribution in Compartments and Sinks

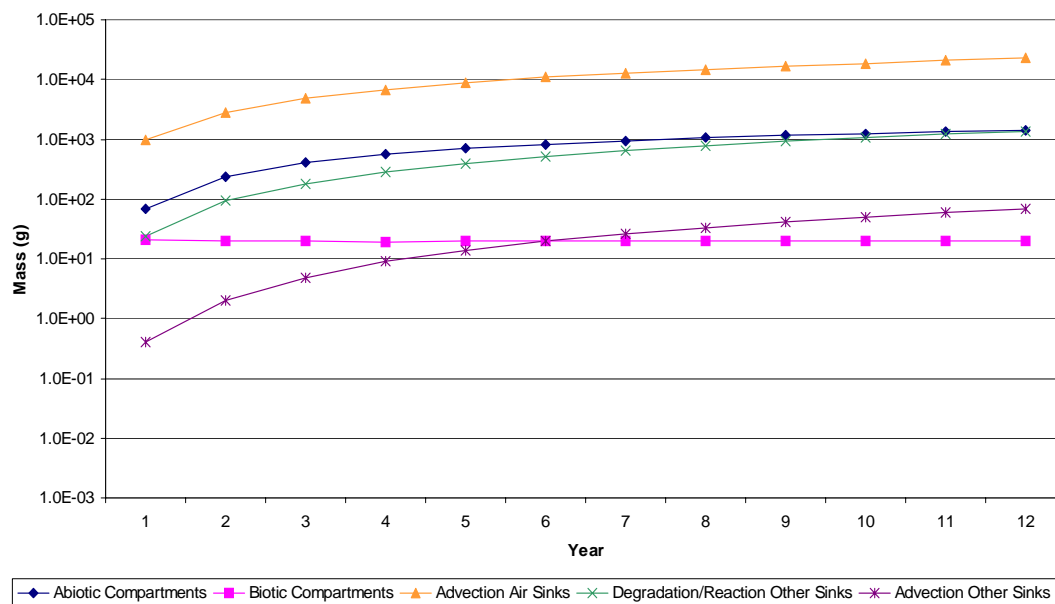


Figure E-3  
1,2,3,4,6,7,8,9-OCDD Mass: Overall Distribution in Compartments and Sinks

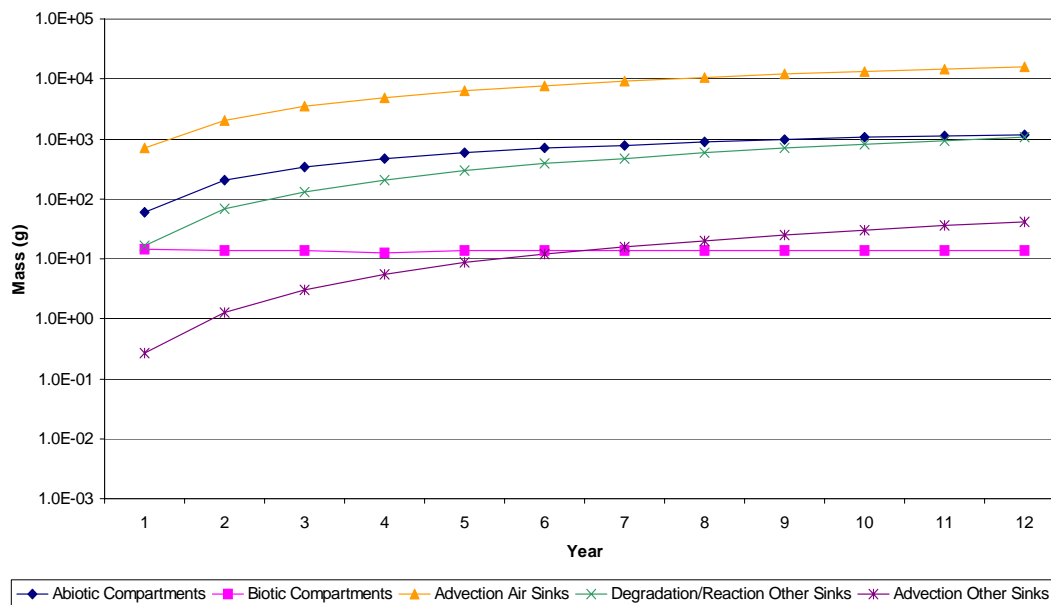


Figure E-4  
1,2,3,4,6,7,8-HpCDD Mass: Overall Distribution in Compartments and Sinks

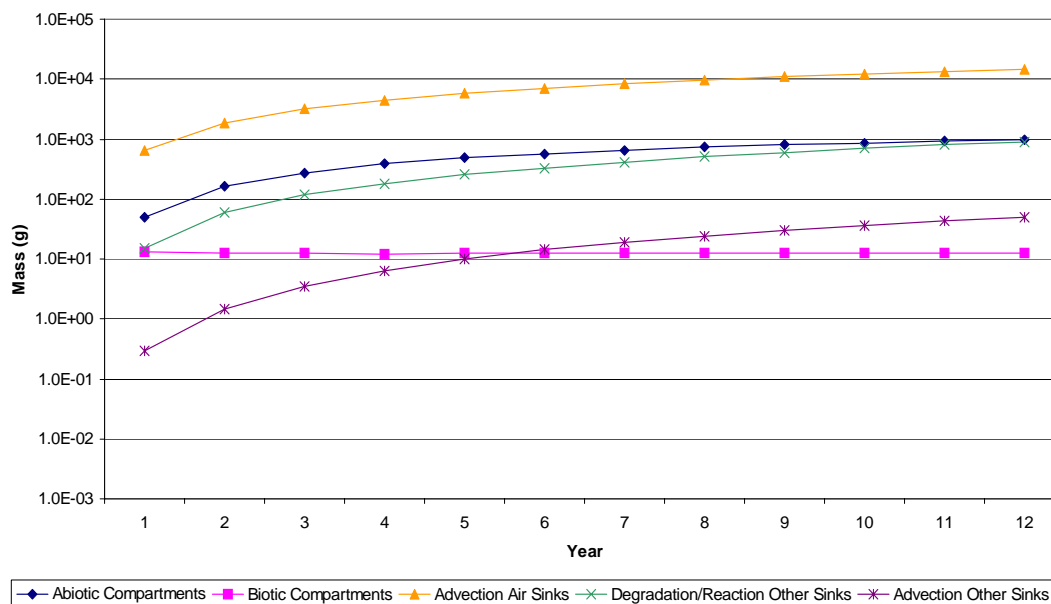


Figure E-5  
2,3,4,6,7,8-HxCDF Mass: Overall Distribution in Compartments and Sinks

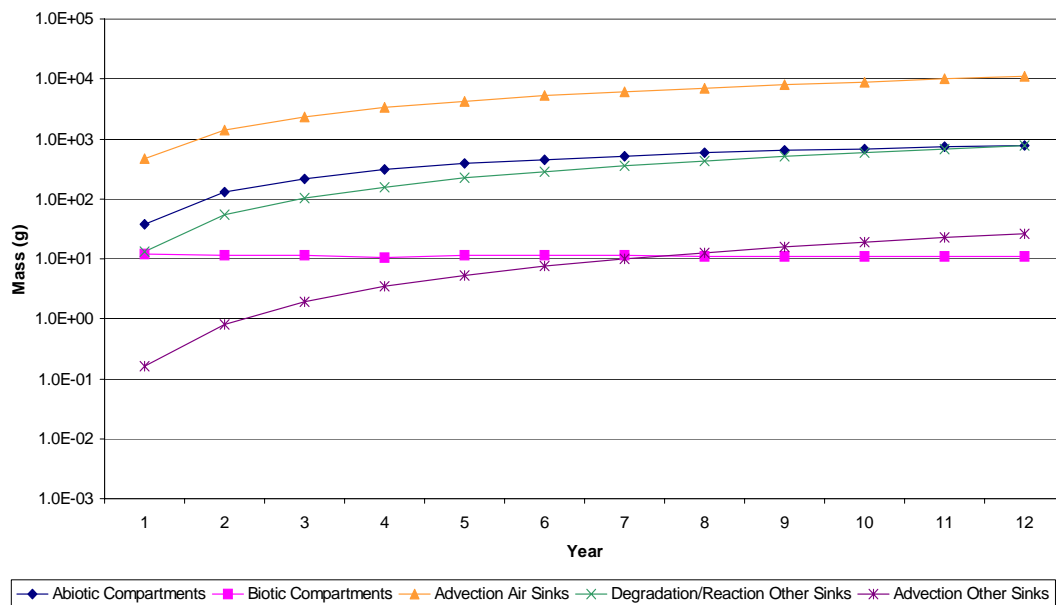


Figure E-6  
1,2,3,6,7,8-HxCDF Mass: Overall Distribution in Compartments and Sinks

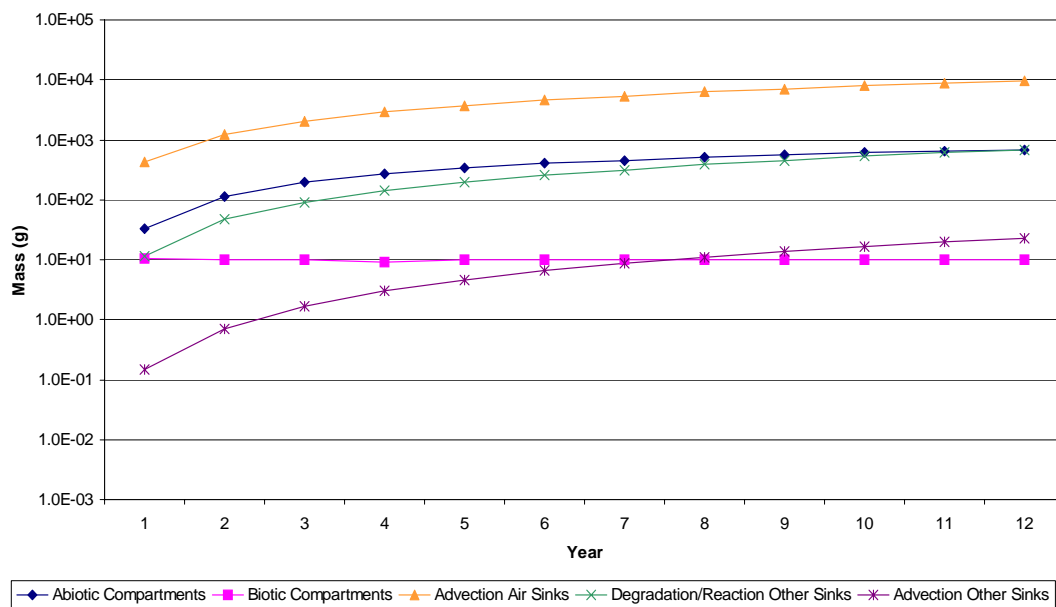


Figure E-7  
1,2,3,4,6,7,8,9-OCDF Mass: Overall Distribution in Compartments and Sinks

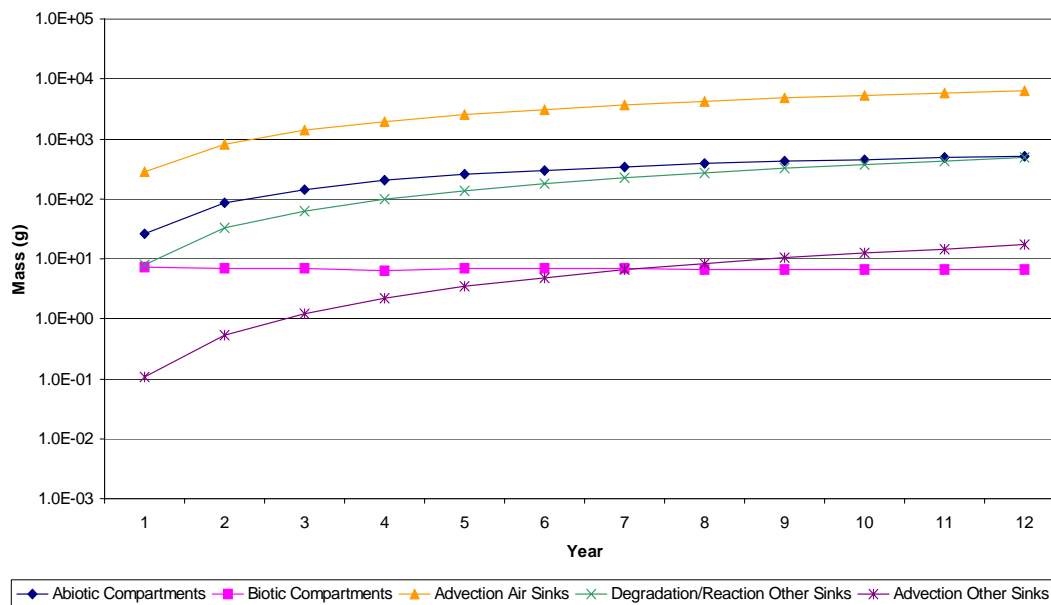


Figure E-8  
1,2,3,4,7,8,9-HpCDF Mass: Overall Distribution in Compartments and Sinks

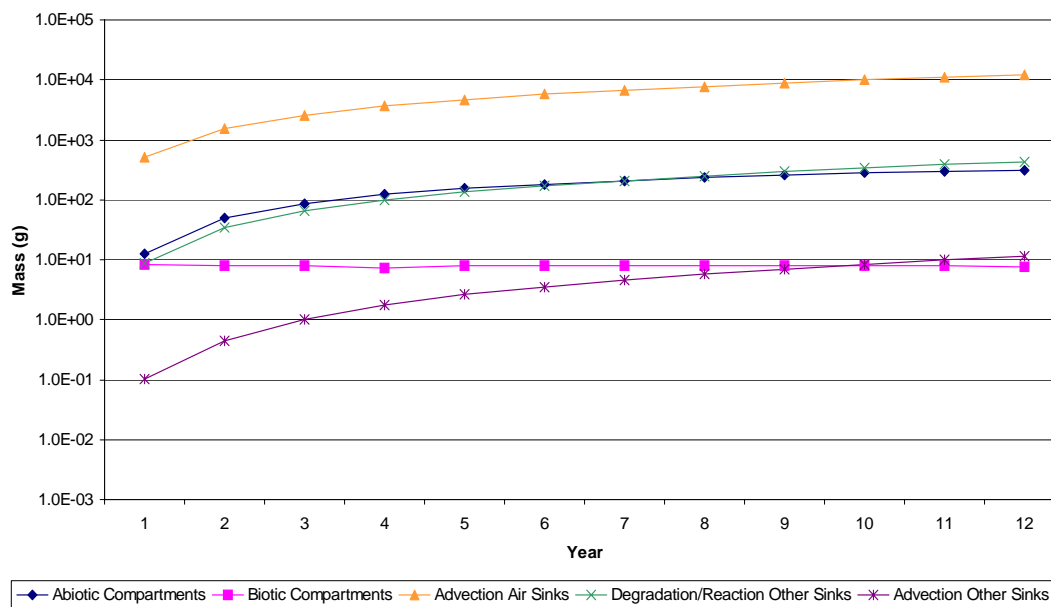


Figure E-9  
1,2,3,4,7,8-HxCDF Mass: Overall Distribution in Compartments and Sinks

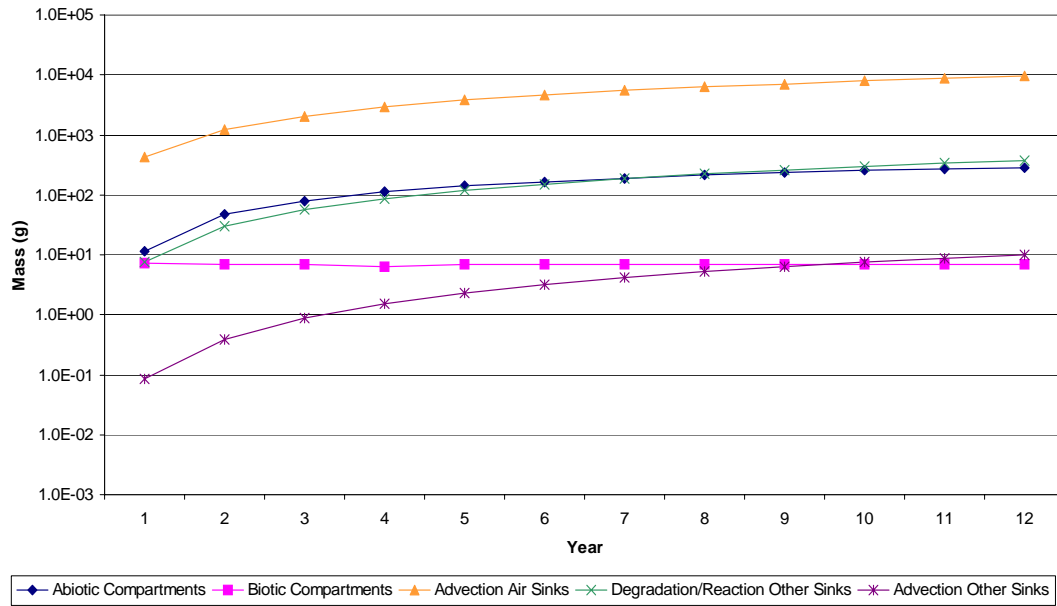


Figure E-10  
1,2,3,7,8-PeCDF Mass: Overall Distribution in Compartments and Sinks

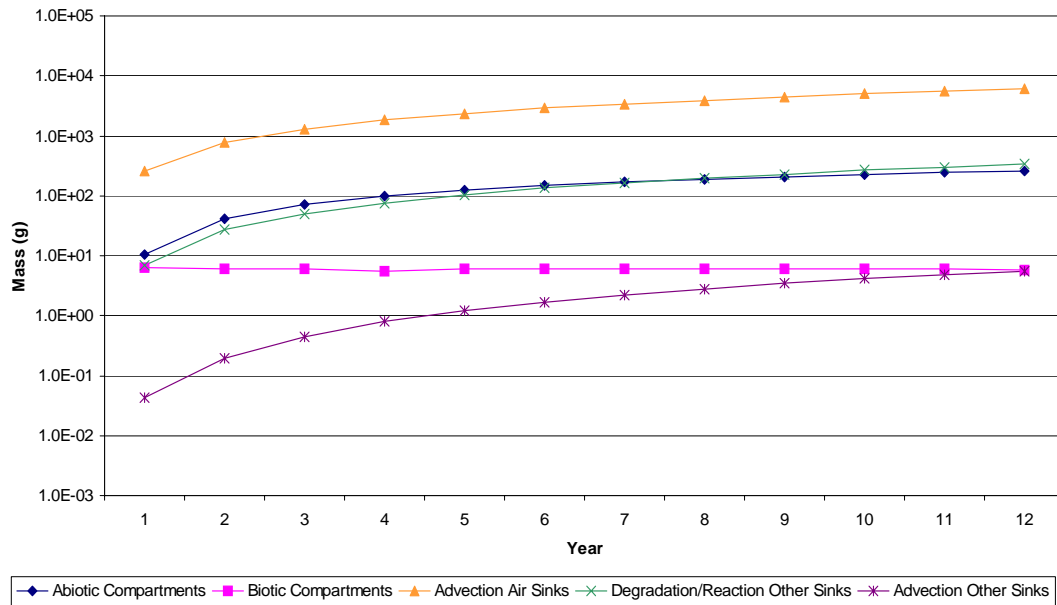


Figure E-11  
2,3,4,7,8-PeCDF Mass: Overall Distribution in Compartments and Sinks

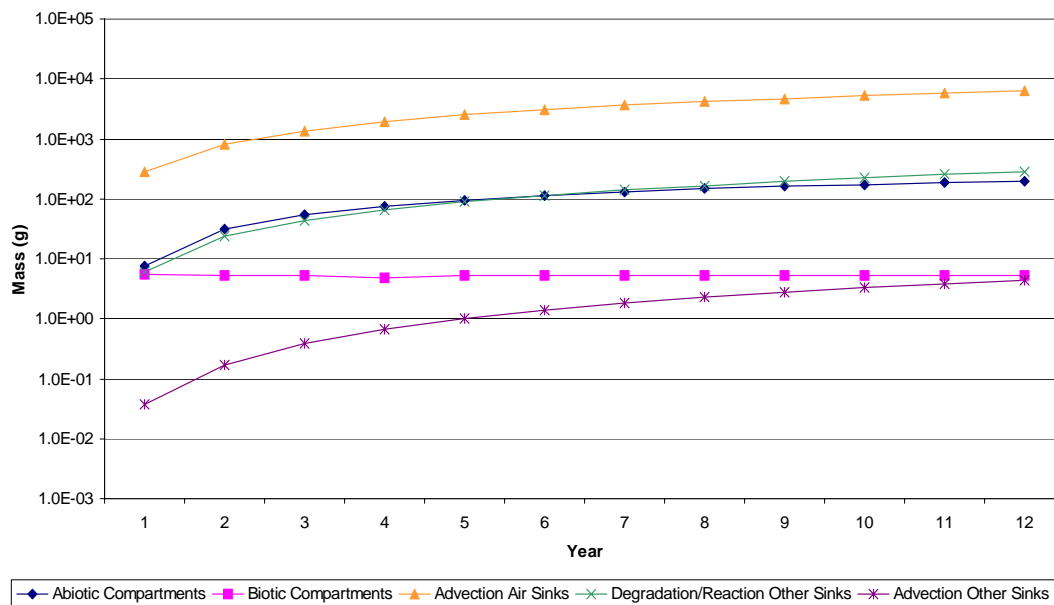


Figure E-12  
1,2,3,6,7,8-HxCDD Mass: Overall Distribution in Compartments and Sinks

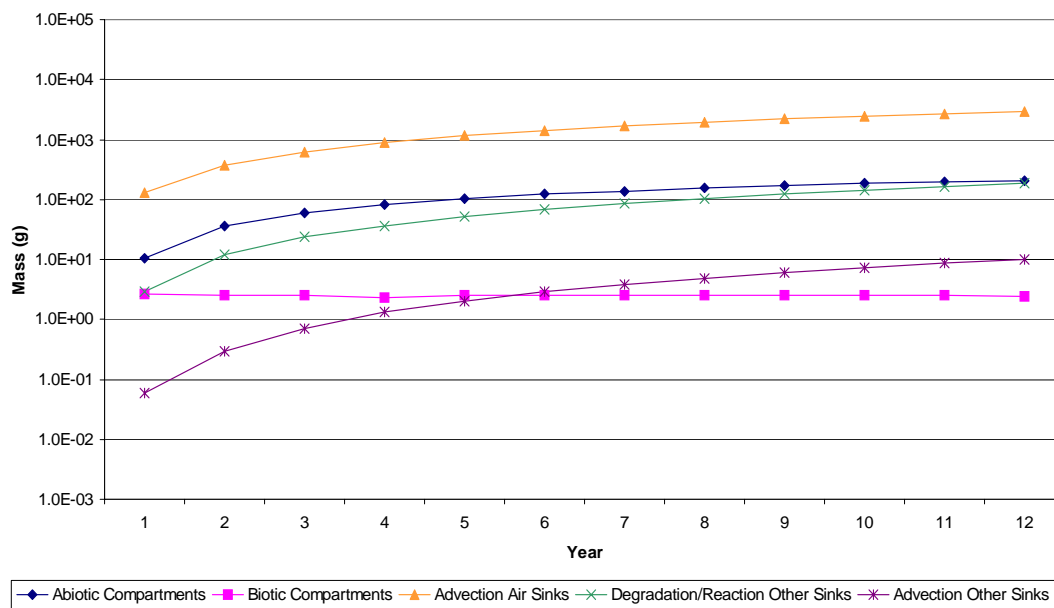


Figure E-13  
1,2,3,7,8,9-HxCDD Mass: Overall Distribution in Compartments and Sinks

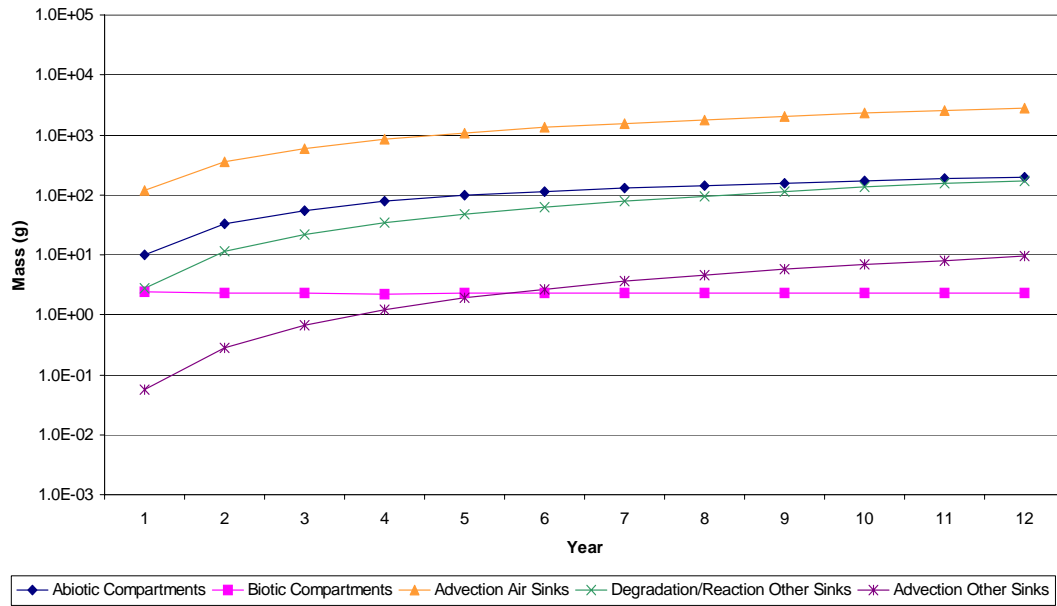


Figure E-14  
1,2,3,7,8,9-HxCDF Mass: Overall Distribution in Compartments and Sinks

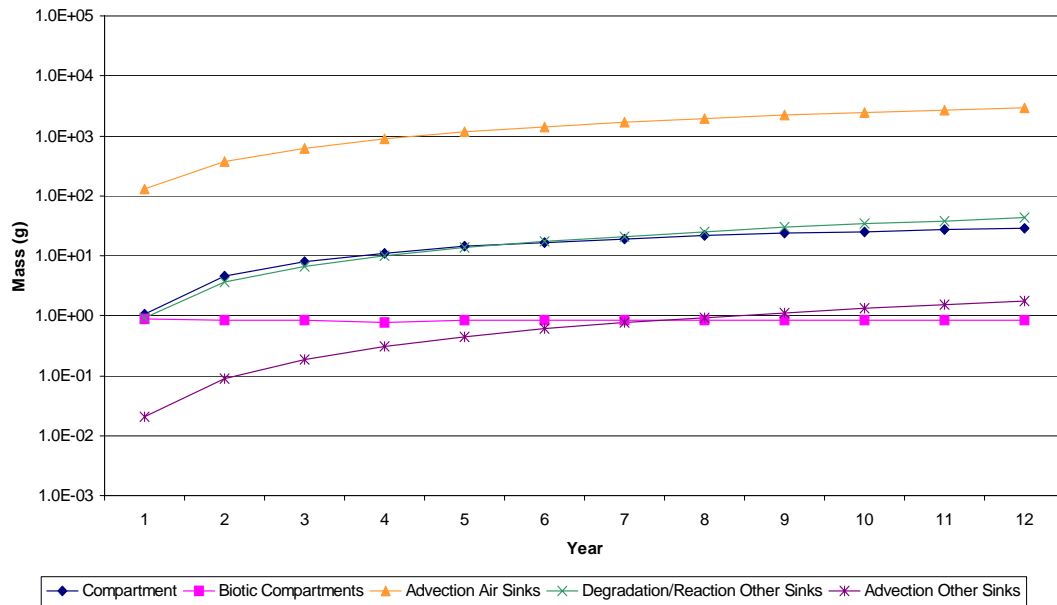




Figure E-15  
1,2,3,7,8-PeCDD Mass: Overall Distribution in Compartments and Sinks

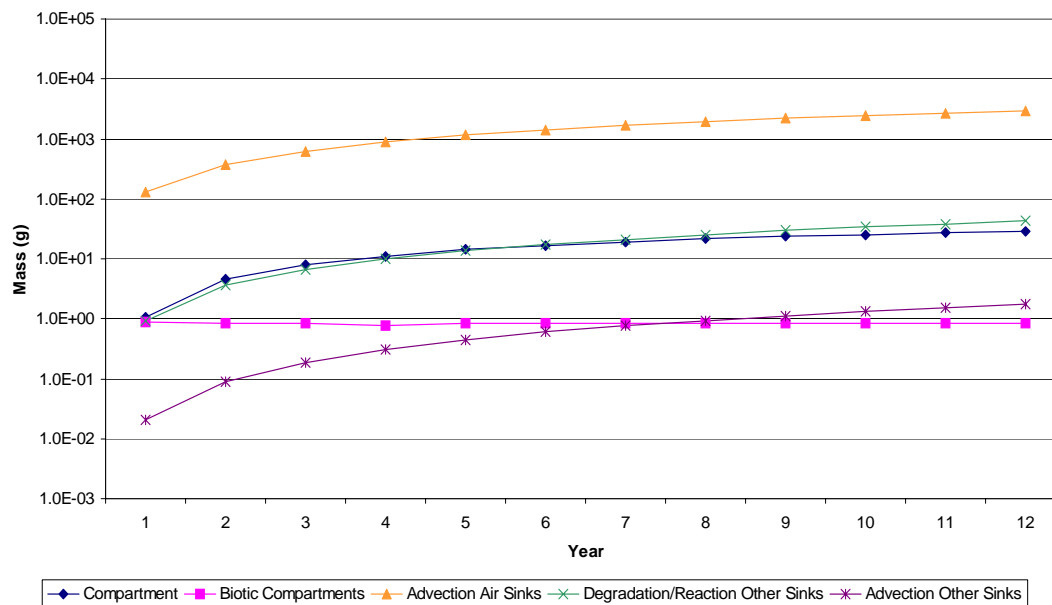


Figure E-16  
2,3,7,8-TCDF Mass: Overall Distribution in Compartments and Sinks

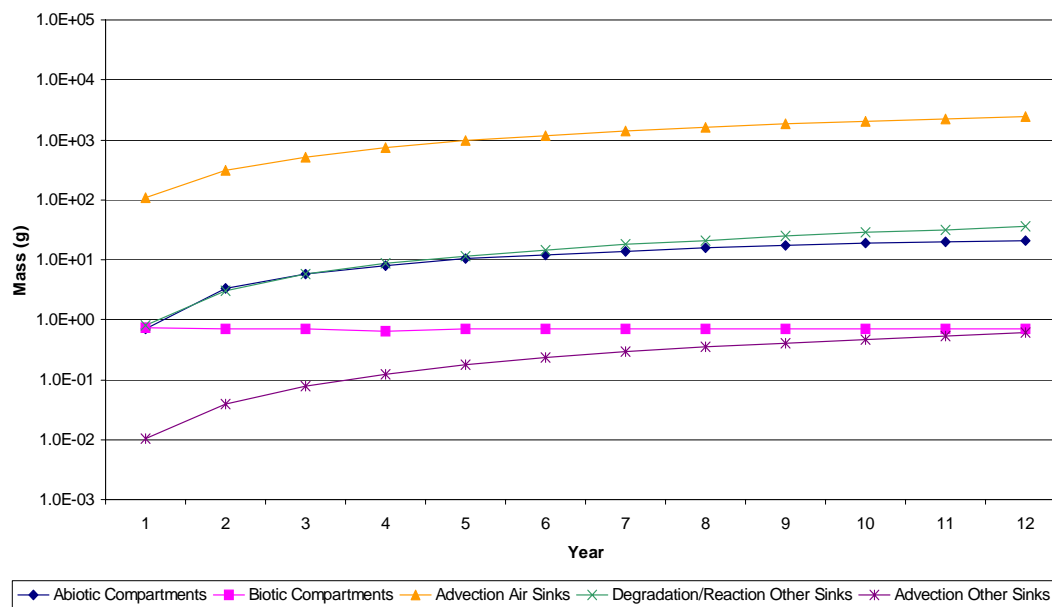


Figure E-17  
2,3,7,8-TCDD Mass: Overall Distribution in Compartments and Sinks

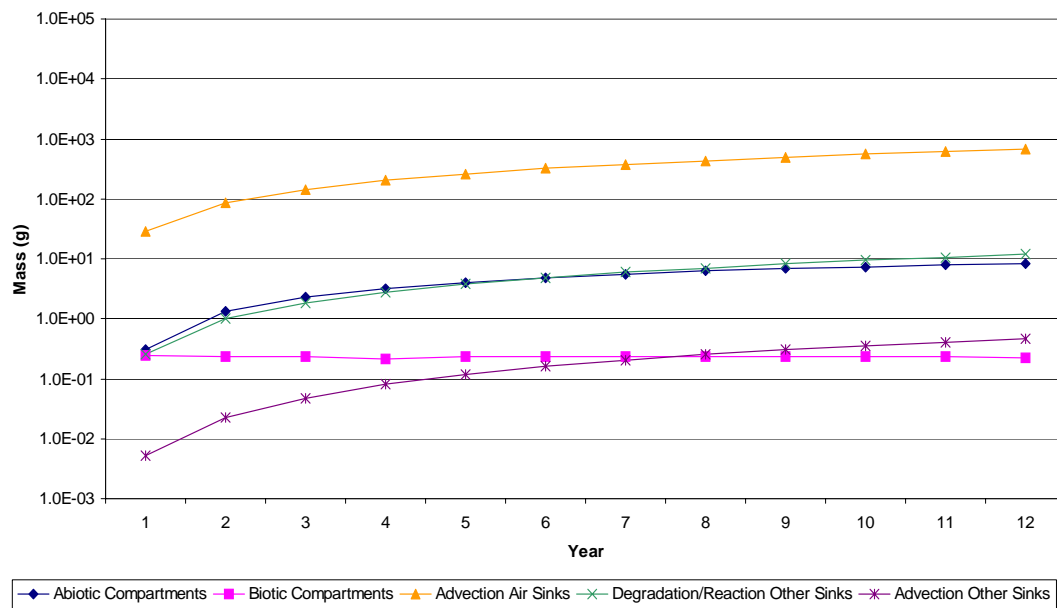


Figure E-18  
1,2,3,4,6,7,8-HpCDF Mass: Distribution in Abiotic Compartments

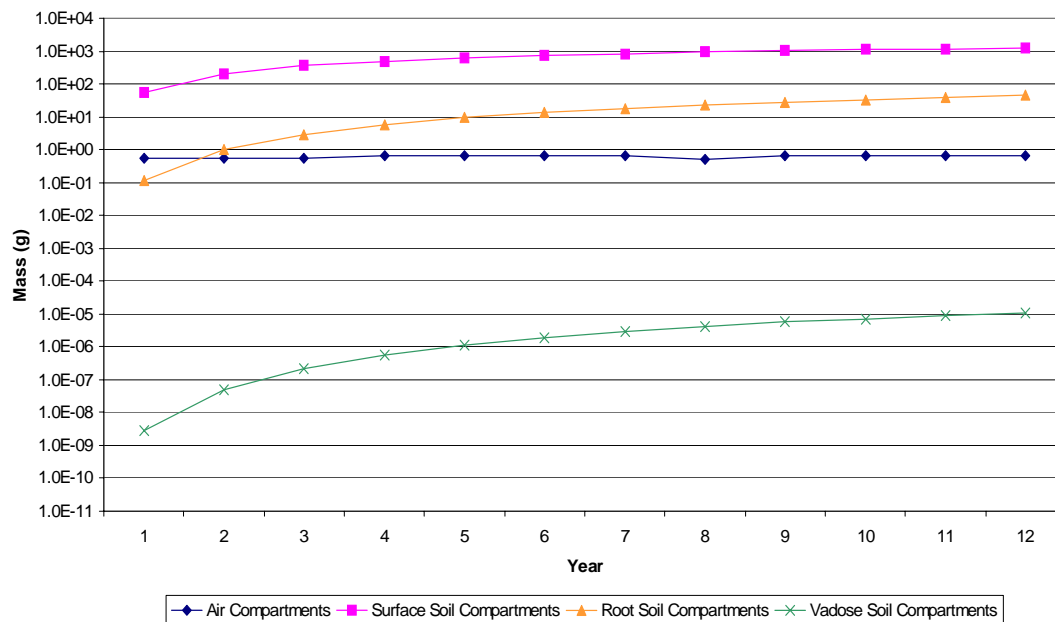


Figure E-19  
1,2,3,4,7,8-HxCDD Mass: Distribution in Abiotic Compartments

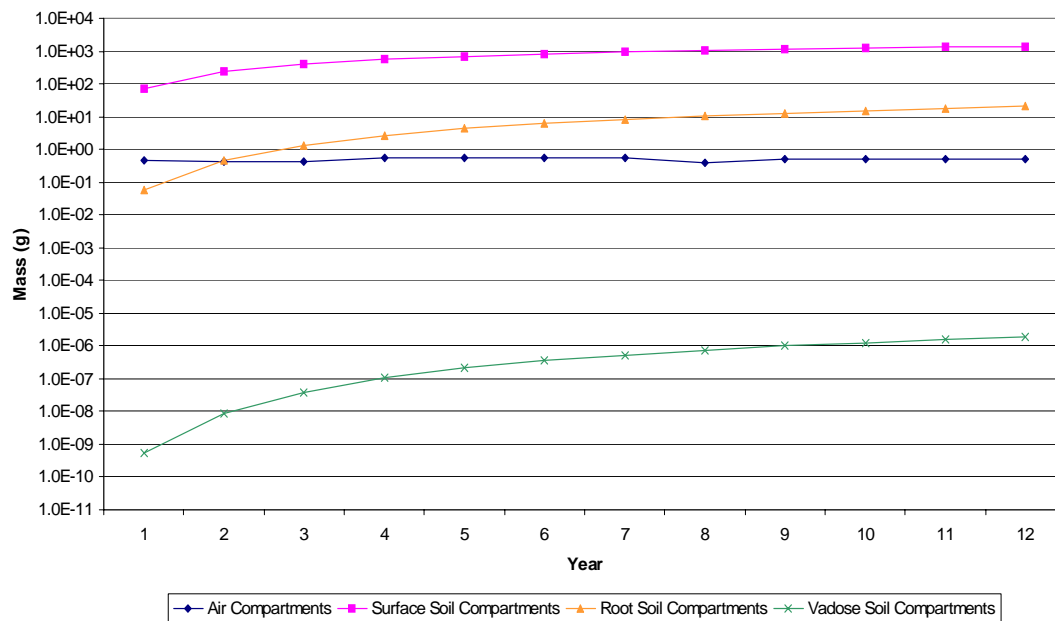


Figure E-20  
1,2,3,4,6,7,8,9-OCDD Mass: Distribution in Abiotic Compartments

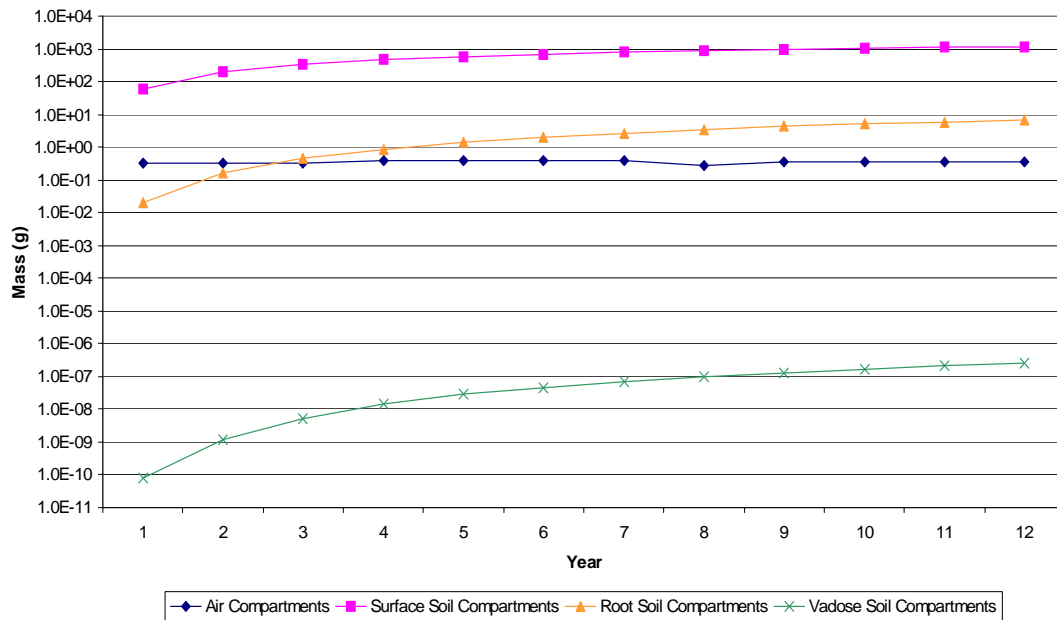


Figure E-21  
1,2,3,4,6,7,8-HpCDD Mass: Distribution in Abiotic Compartments

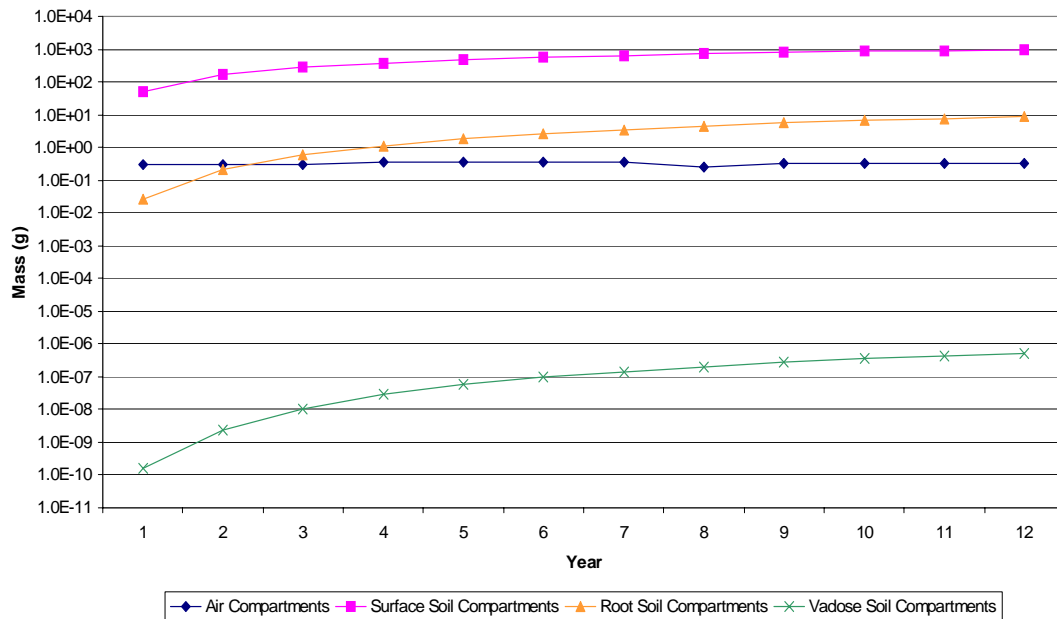


Figure E-22  
2,3,4,6,7,8-HxCDF Mass: Distribution in Abiotic Compartments

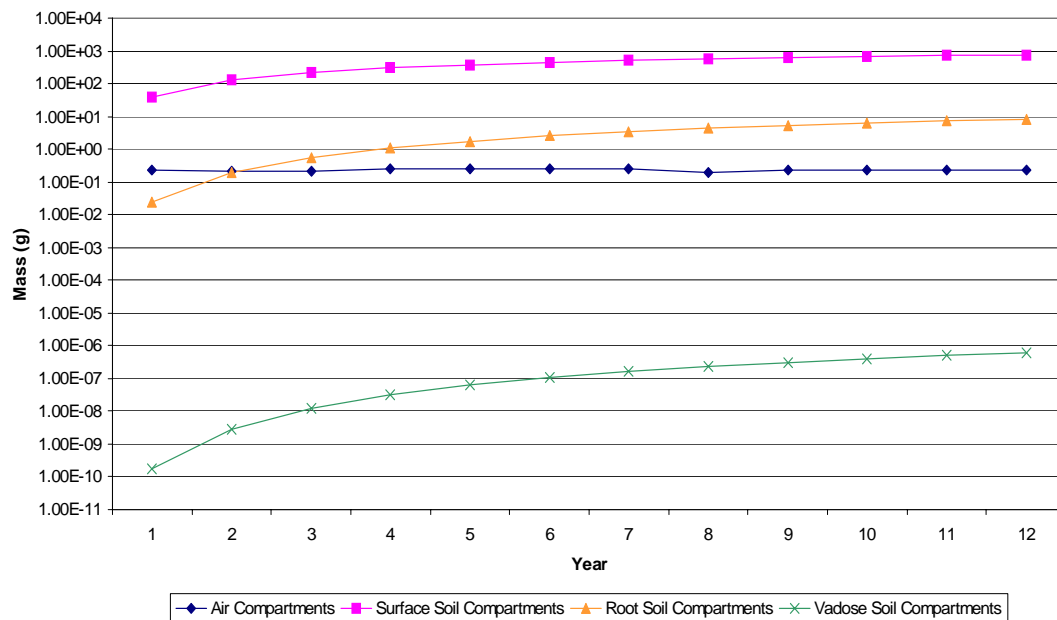


Figure E-23  
1,2,3,6,7,8-HxCDF Mass: Distribution in Abiotic Compartments

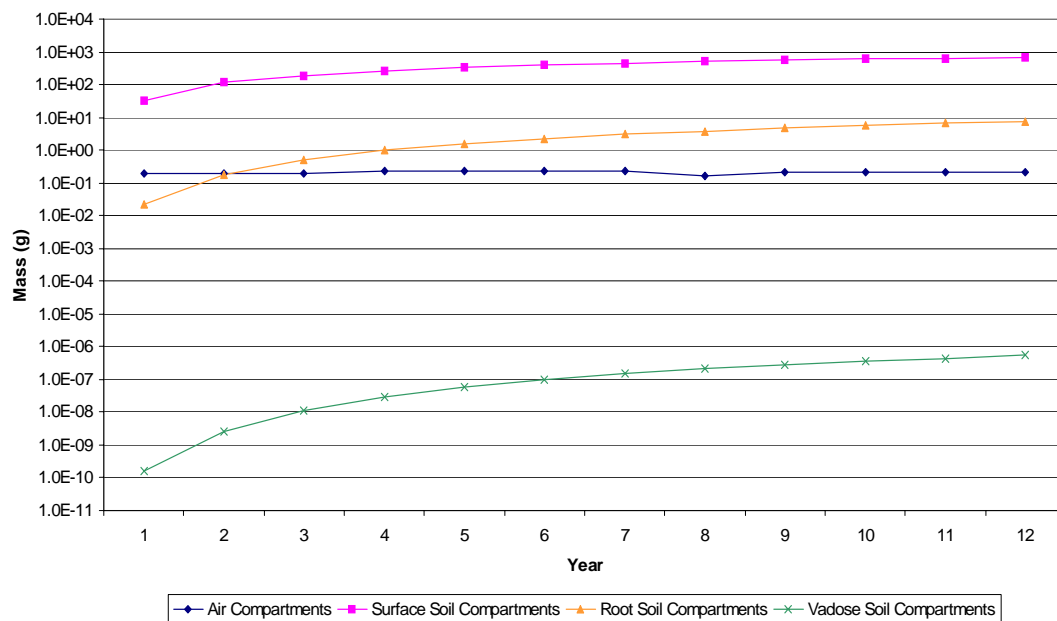


Figure E-24  
1,2,3,4,6,7,8,9-OCDF Mass: Distribution in Abiotic Compartments

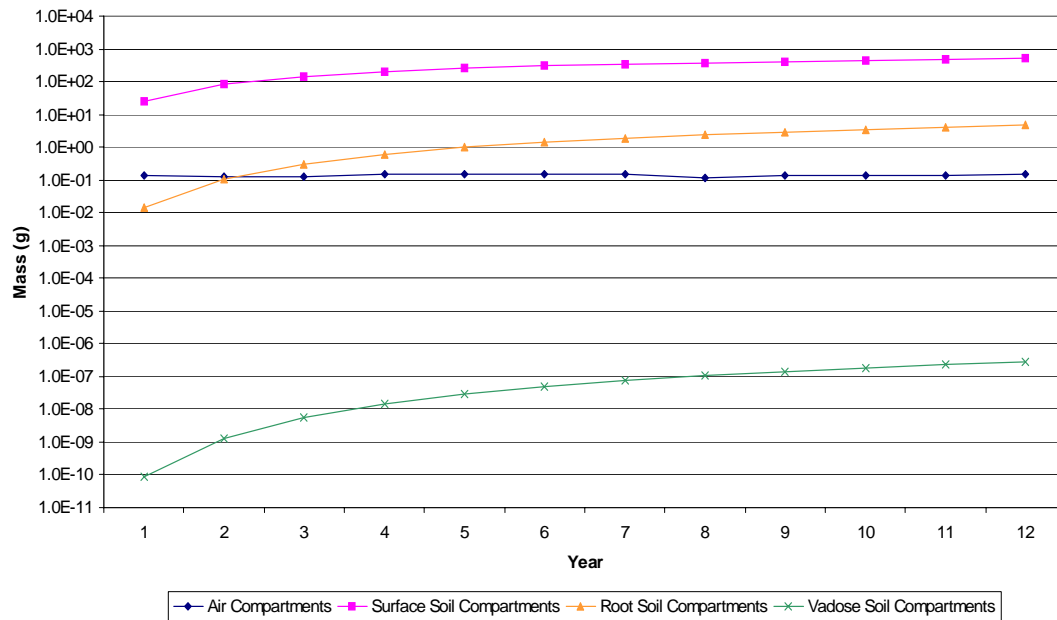


Figure E-25  
1,2,3,4,7,8,9-HpCDF Mass: Distribution in Abiotic Compartments

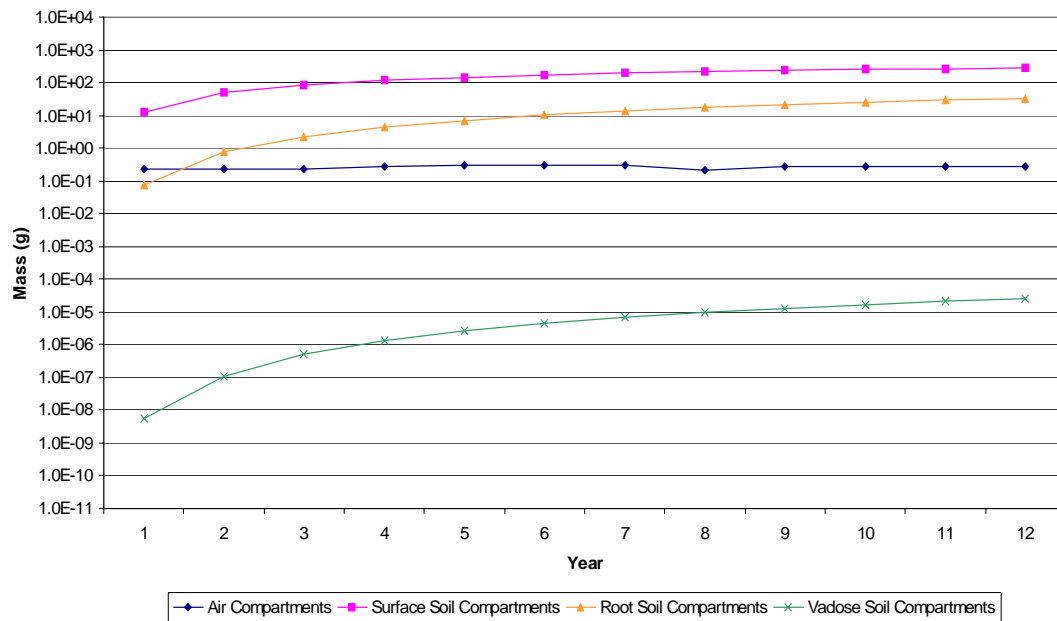


Figure E-26  
1,2,3,4,7,8-HxCDF Mass: Distribution in Abiotic Compartments

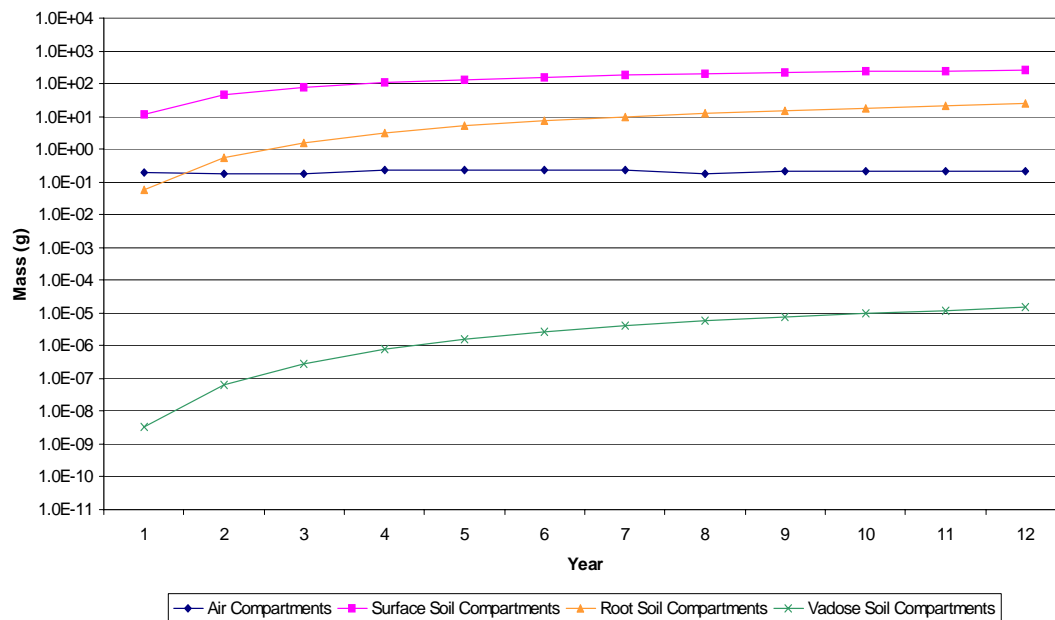


Figure E-27  
1,2,3,7,8-PeCDF Mass: Distribution in Abiotic Compartments

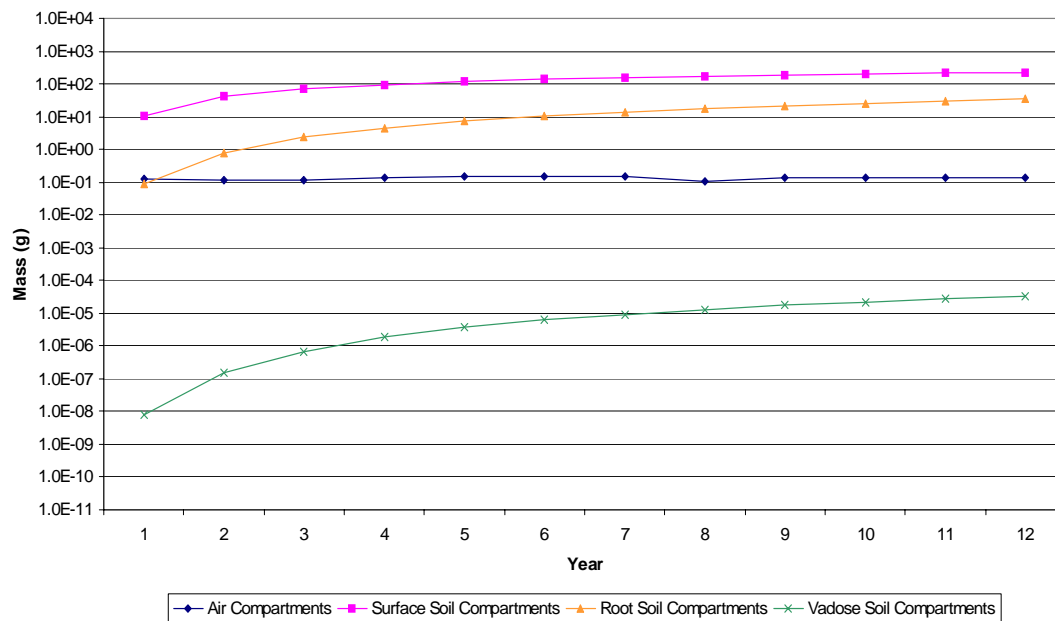


Figure E-28  
2,3,4,7,8-PeCDF Mass: Distribution in Abiotic Compartments

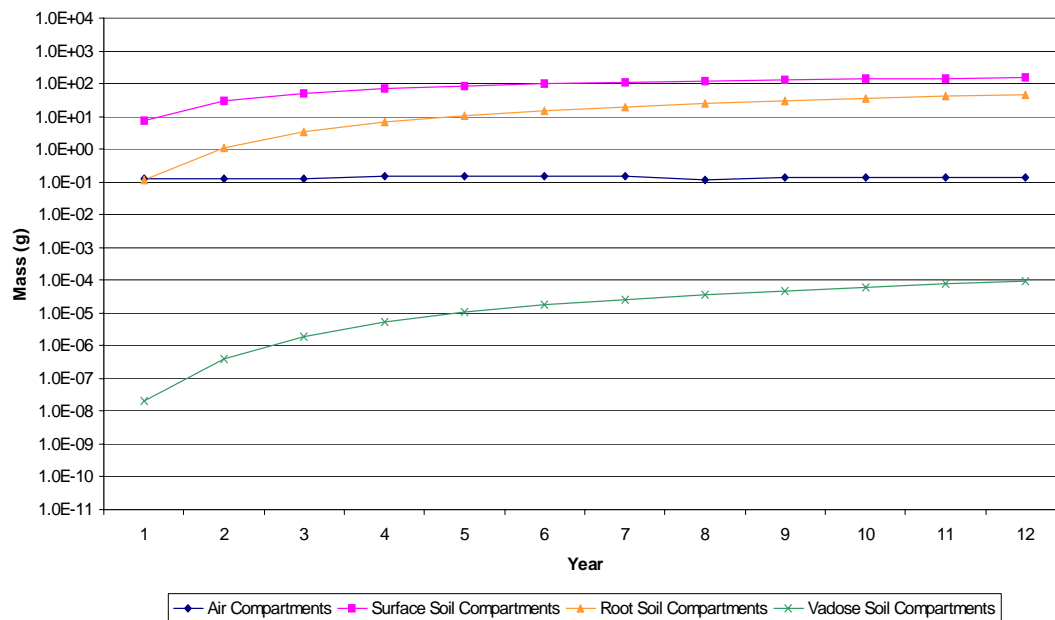


Figure E-29  
1,2,3,6,7,8-HxCDD Mass: Distribution in Abiotic Compartments

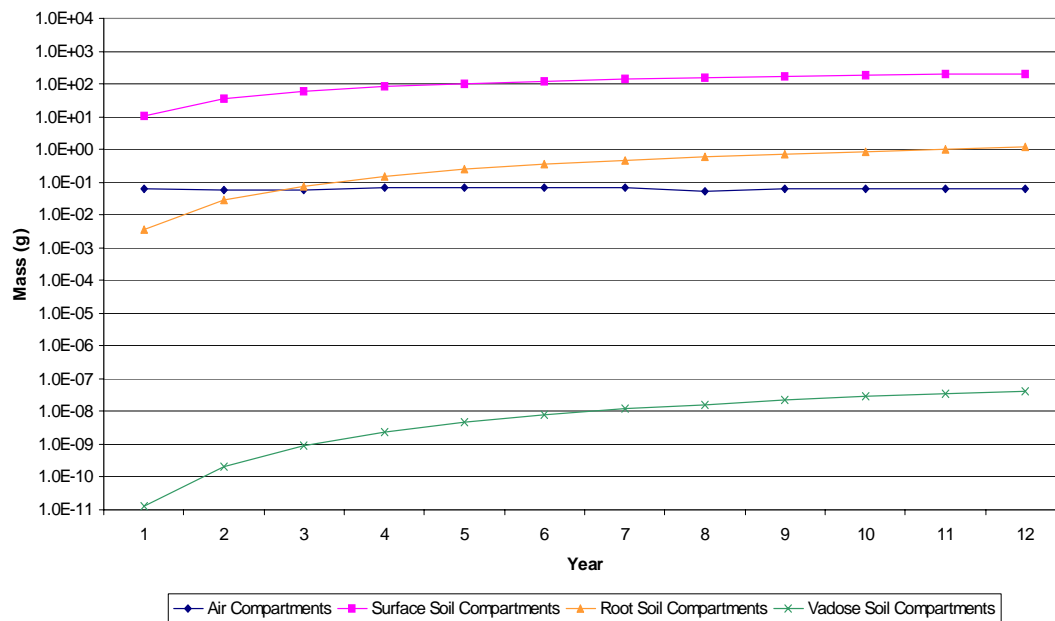




Figure E-30  
1,2,3,7,8,9-HxCDD Mass: Distribution in Abiotic Compartments

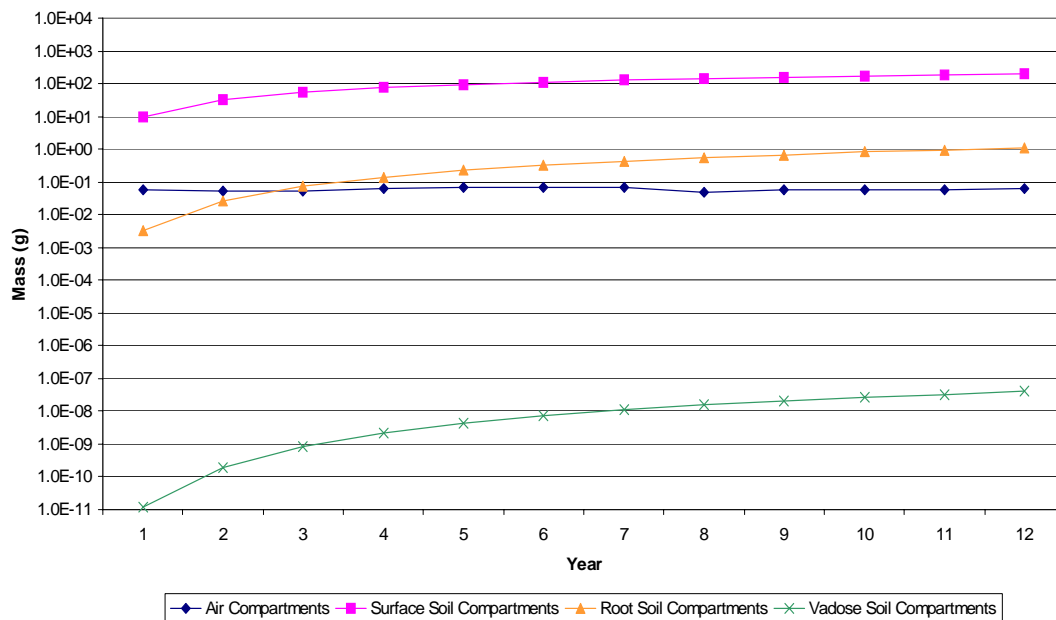


Figure E-31  
1,2,3,7,8,9-HxCDF Mass: Distribution in Abiotic Compartments

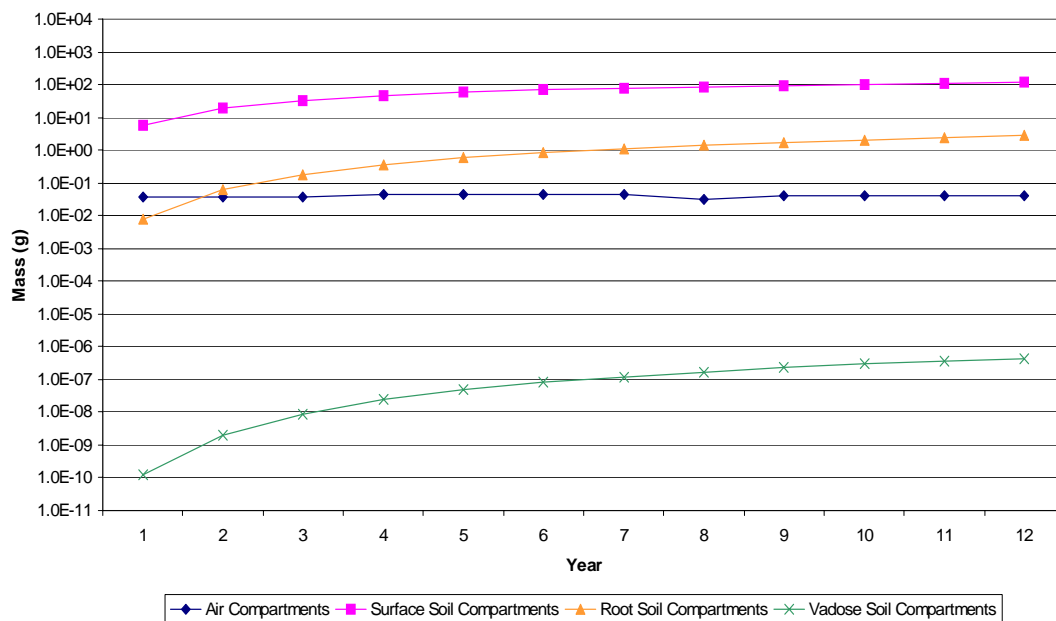


Figure E-32  
1,2,3,7,8-PeCDD Mass: Distribution in Abiotic Compartments

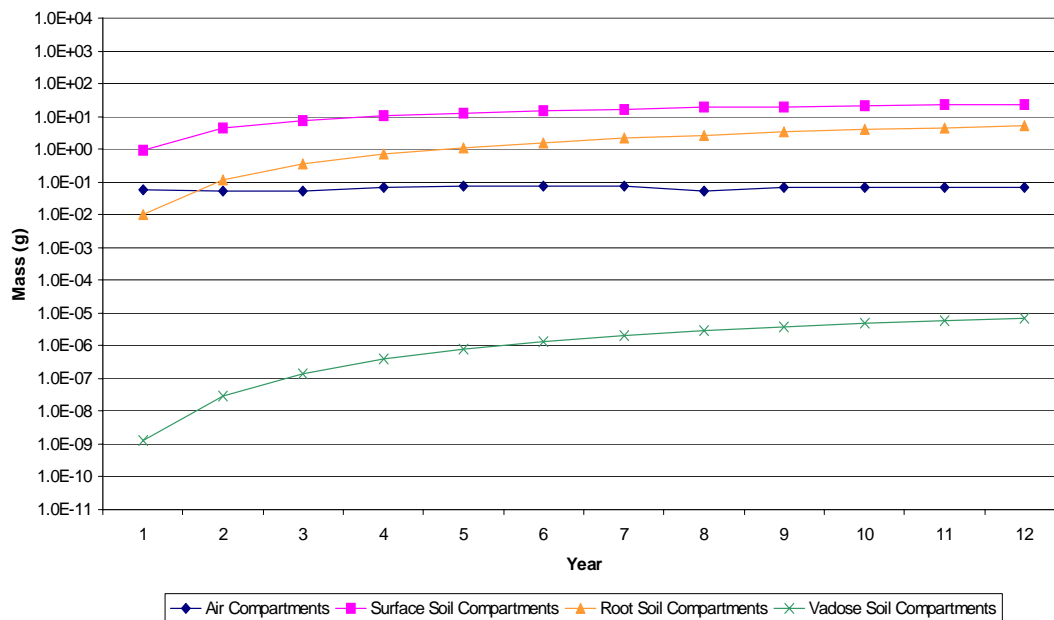


Figure E-33  
2,3,7,8-TCDF Mass: Distribution in Abiotic Compartments

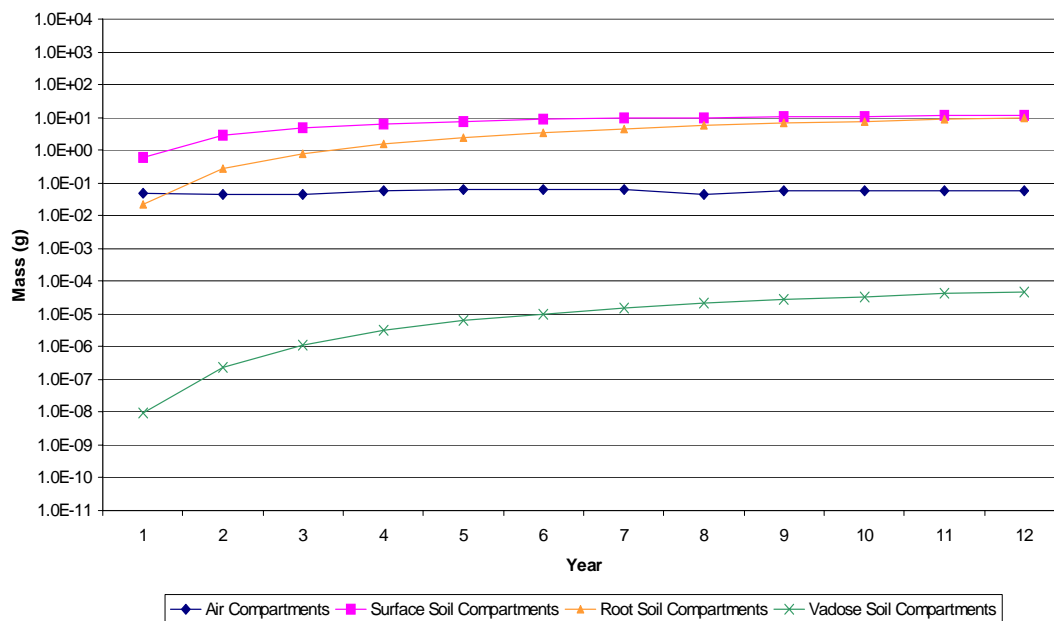
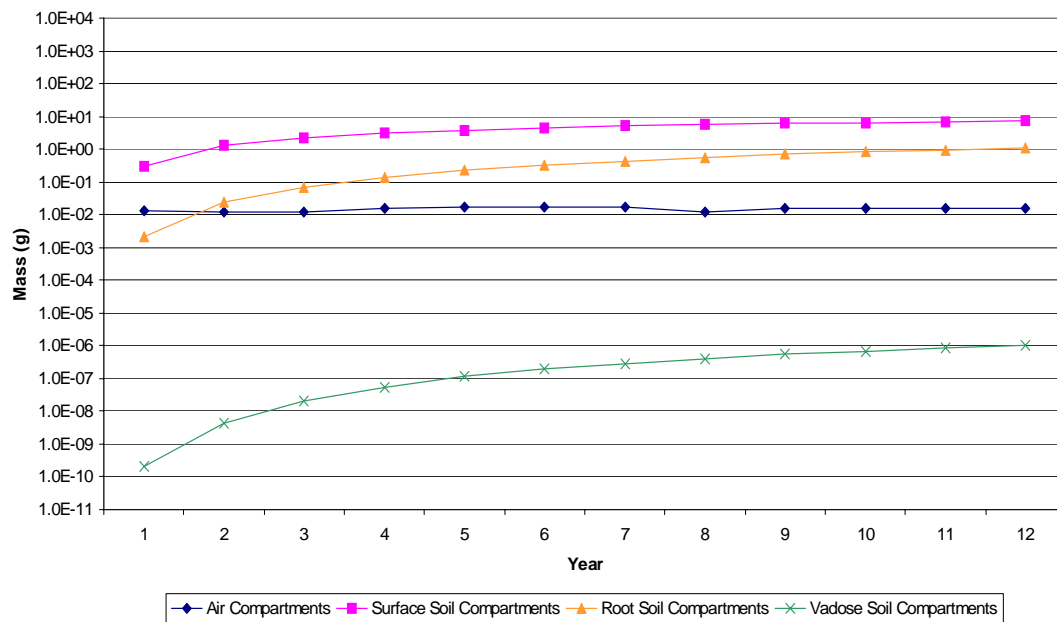


Figure E-34  
2,3,7,8-TCDD Mass: Distribution in Abiotic Compartments



## **Appendix F**

### **DOCUMENTATION OF TRIM.FaTE CONCENTRATION RESULTS - SPATIAL DISTRIBUTIONS**

This appendix contains the following sets of tables for the following TRIM.FaTE results:

- annual average air TEQ concentrations using 1994 stack test emissions and 1994 meteorological data;
- average 48-hour air individual congener and TEQ concentrations using 1994 stack test emissions and 1994 meteorological data;
- annual average (for year 12 of the simulation) surface soil, root zone soil, vadose zone soil groundwater, and surface water TEQ concentrations using 1992 stack test emissions and 1989 meteorological data.

**Total Dioxin TEQ Concentration:  
Air Compartments (1994 stack test emissions)**

<b>Air compartment</b>	<b>Annual Average TEQ Concentration (g/m3)</b>
Source	8.3E-12
NNW1	1.5E-12
NNE1	1.4E-12
SSW1	1.2E-12
WNW1	1.2E-12
SSE1	1.2E-12
WSW1	1.1E-12
ENE1	1.0E-12
ESE1	1.0E-12
NNW2	7.6E-13
NNE2	7.5E-13
SSW2	5.9E-13
WNW2	5.8E-13
SSE2	5.7E-13
WSW2	5.7E-13
ENE2	5.0E-13
ESE2	4.6E-13
NNE3	2.6E-13
NNW3	2.5E-13
SSE3	1.9E-13
SSW3	1.9E-13
WSW3	1.9E-13
WNW3	1.8E-13
ESE3	1.6E-13
ENE3	1.4E-13
NNW4	8.8E-14
NNE4	8.7E-14
WSW4	6.2E-14
SSW4	6.2E-14
WNW4	5.7E-14
SSE4	5.6E-14
ESE4	5.2E-14
ENE4	4.9E-14

**Individual Congeners and Total Dioxin TEQ Concentrations:  
Air Compartments (1994 stack test emissions)**

Air compartment	Average 48-hour Concentration (ug/m3)							
	1,2,3,4,6,7,8,9-OCDD	1,2,3,4,6,7,8,9-OCDF	1,2,3,4,6,7,8 HpCDD	1,2,3,4,6,7,8 HpCDF	1,2,3,4,7,8,9 HpCDF	1,2,3,4,7,8 HxCDD	1,2,3,4,7,8 HxCDF	1,2,3,6,7,8 HxCDD
Source	1.2E-05	3.6E-06	5.2E-06	8.3E-06	6.2E-07	6.5E-07	1.3E-06	5.3E-07
ESE1	5.1E-06	1.6E-06	2.2E-06	3.5E-06	2.7E-07	2.8E-07	5.7E-07	2.3E-07
SSE1	4.8E-06	1.5E-06	2.1E-06	3.4E-06	2.5E-07	2.7E-07	5.5E-07	2.2E-07
ESE2	3.0E-06	9.1E-07	1.3E-06	2.1E-06	1.6E-07	1.6E-07	3.4E-07	1.3E-07
SSE2	2.7E-06	8.4E-07	1.2E-06	1.9E-06	1.4E-07	1.5E-07	3.1E-07	1.2E-07
ENE1	2.7E-06	8.1E-07	1.2E-06	1.8E-06	1.4E-07	1.5E-07	3.0E-07	1.2E-07
SSW1	2.5E-06	7.6E-07	1.1E-06	1.7E-06	1.3E-07	1.4E-07	2.8E-07	1.1E-07
ENE2	1.1E-06	3.4E-07	4.9E-07	7.7E-07	5.8E-08	6.1E-08	1.3E-07	5.0E-08
ESE3	1.1E-06	3.4E-07	4.8E-07	7.7E-07	5.8E-08	6.0E-08	1.2E-07	4.9E-08
SSE3	9.9E-07	3.0E-07	4.3E-07	6.9E-07	5.2E-08	5.4E-08	1.1E-07	4.4E-08
SSW2	9.9E-07	3.0E-07	4.4E-07	6.9E-07	5.2E-08	5.4E-08	1.1E-07	4.4E-08
ESE4	4.2E-07	1.3E-07	1.8E-07	3.0E-07	2.2E-08	2.3E-08	4.8E-08	1.9E-08
SSE4	4.0E-07	1.2E-07	1.8E-07	2.8E-07	2.1E-08	2.2E-08	4.6E-08	1.8E-08
ENE3	3.0E-07	9.1E-08	1.3E-07	2.1E-07	1.6E-08	1.6E-08	3.4E-08	1.3E-08
SSW3	2.5E-07	7.7E-08	1.1E-07	1.7E-07	1.3E-08	1.4E-08	2.8E-08	1.1E-08
NNE1	1.7E-07	5.1E-08	7.4E-08	1.2E-07	8.8E-09	9.2E-09	1.9E-08	7.5E-09
ENE4	8.8E-08	2.7E-08	3.9E-08	6.2E-08	4.7E-09	4.9E-09	1.0E-08	4.0E-09
WSW1	8.9E-08	2.7E-08	3.9E-08	6.2E-08	4.7E-09	4.9E-09	1.0E-08	4.0E-09
NNW1	7.7E-08	2.4E-08	3.4E-08	5.4E-08	4.0E-09	4.3E-09	8.7E-09	3.5E-09
SSW4	7.4E-08	2.3E-08	3.3E-08	5.2E-08	3.9E-09	4.1E-09	8.5E-09	3.3E-09
NNE2	7.3E-08	2.2E-08	3.2E-08	5.1E-08	3.8E-09	4.0E-09	8.3E-09	3.3E-09
WNW1	4.3E-08	1.3E-08	1.9E-08	3.0E-08	2.2E-09	2.3E-09	4.8E-09	1.9E-09
WSW2	2.4E-08	7.2E-09	1.0E-08	1.6E-08	1.2E-09	1.3E-09	2.7E-09	1.1E-09
NNW2	2.1E-08	6.5E-09	9.3E-09	1.5E-08	1.1E-09	1.2E-09	2.4E-09	9.5E-10
NNE3	1.6E-08	4.9E-09	7.0E-09	1.1E-08	8.3E-10	8.7E-10	1.8E-09	7.1E-10
WNW2	7.2E-09	2.2E-09	3.2E-09	5.0E-09	3.8E-10	4.0E-10	8.1E-10	3.2E-10
WSW3	3.4E-09	1.0E-09	1.5E-09	2.4E-09	1.8E-10	1.9E-10	3.9E-10	1.5E-10
NNW3	3.1E-09	9.5E-10	1.4E-09	2.2E-09	1.6E-10	1.7E-10	3.5E-10	1.4E-10
NNE4	2.1E-09	6.3E-10	9.1E-10	1.4E-09	1.1E-10	1.1E-10	2.3E-10	9.2E-11
WNW3	7.3E-10	2.2E-10	3.2E-10	5.1E-10	3.8E-11	4.0E-11	8.3E-11	3.3E-11
NNW4	3.8E-10	1.2E-10	1.7E-10	2.7E-10	2.0E-11	2.1E-11	4.4E-11	1.7E-11
WSW4	3.6E-10	1.1E-10	1.6E-10	2.5E-10	1.9E-11	2.0E-11	4.1E-11	1.6E-11
WNW4	7.6E-11	2.3E-11	3.3E-11	5.3E-11	4.0E-12	4.2E-12	8.6E-12	3.4E-12

**Individual Congeners and Total Dioxin TEQ Concentrations:  
Air Compartments (1994 stack test emissions)**

Air compartment	Average 48-hour Concentration (ug/m3)									
	1,2,3,6,7,8 HxCDF	1,2,3,7,8,9 HxCDD	1,2,3,7,8,9 HxCDF	1,2,3,7,8 PeCDD	1,2,3,7,8 PeCDF	2,3,4,6,7,8 HxCDF	2,3,4,7,8 PeCDF	2,3,7,8 TCDD	2,3,7,8 TCDF	TEQ
Source	1.2E-06	4.2E-07	5.3E-08	3.9E-07	3.5E-07	1.6E-06	6.4E-07	2.5E-08	1.6E-07	1.3E-06
ESE1	5.1E-07	1.8E-07	2.3E-08	1.7E-07	1.5E-07	7.0E-07	2.7E-07	1.1E-08	6.7E-08	5.6E-07
SSE1	4.9E-07	1.7E-07	2.2E-08	1.6E-07	1.4E-07	6.7E-07	2.6E-07	1.0E-08	6.4E-08	5.4E-07
ESE2	3.0E-07	1.1E-07	1.3E-08	9.9E-08	8.7E-08	4.1E-07	1.6E-07	6.3E-09	3.9E-08	3.3E-07
SSE2	2.8E-07	9.7E-08	1.2E-08	9.1E-08	8.0E-08	3.8E-07	1.5E-07	5.8E-09	3.6E-08	3.0E-07
ENE1	2.7E-07	9.4E-08	1.2E-08	8.8E-08	7.8E-08	3.7E-07	1.4E-07	5.6E-09	3.5E-08	2.9E-07
SSW1	2.5E-07	8.8E-08	1.1E-08	8.2E-08	7.3E-08	3.4E-07	1.3E-07	5.3E-09	3.3E-08	2.8E-07
ENE2	1.1E-07	3.9E-08	5.0E-09	3.7E-08	3.3E-08	1.5E-07	6.0E-08	2.4E-09	1.5E-08	1.2E-07
ESE3	1.1E-07	3.9E-08	4.9E-09	3.7E-08	3.2E-08	1.5E-07	5.9E-08	2.3E-09	1.5E-08	1.2E-07
SSE3	9.9E-08	3.5E-08	4.4E-09	3.3E-08	2.9E-08	1.4E-07	5.3E-08	2.1E-09	1.3E-08	1.1E-07
SSW2	9.9E-08	3.5E-08	4.4E-09	3.3E-08	2.9E-08	1.4E-07	5.3E-08	2.1E-09	1.3E-08	1.1E-07
ESE4	4.2E-08	1.5E-08	1.9E-09	1.4E-08	1.2E-08	5.8E-08	2.3E-08	9.0E-10	5.7E-09	4.7E-08
SSE4	4.0E-08	1.4E-08	1.8E-09	1.4E-08	1.2E-08	5.5E-08	2.2E-08	8.6E-10	5.4E-09	4.5E-08
ENE3	3.0E-08	1.0E-08	1.3E-09	9.9E-09	8.7E-09	4.1E-08	1.6E-08	6.3E-10	3.9E-09	3.3E-08
SSW3	2.5E-08	8.9E-09	1.1E-09	8.3E-09	7.4E-09	3.5E-08	1.3E-08	5.3E-10	3.3E-09	2.8E-08
NNE1	1.7E-08	5.9E-09	7.5E-10	5.6E-09	4.9E-09	2.3E-08	9.0E-09	3.5E-10	2.2E-09	1.9E-08
ENE4	8.9E-09	3.1E-09	4.0E-10	3.0E-09	2.6E-09	1.2E-08	4.8E-09	1.9E-10	1.2E-09	9.9E-09
WSW1	8.9E-09	3.1E-09	4.0E-10	3.0E-09	2.6E-09	1.2E-08	4.8E-09	1.9E-10	1.2E-09	9.8E-09
NNW1	7.8E-09	2.7E-09	3.5E-10	2.6E-09	2.3E-09	1.1E-08	4.2E-09	1.6E-10	1.0E-09	8.6E-09
SSW4	7.5E-09	2.6E-09	3.3E-10	2.5E-09	2.2E-09	1.0E-08	4.0E-09	1.6E-10	1.0E-09	8.3E-09
NNE2	7.3E-09	2.6E-09	3.3E-10	2.4E-09	2.1E-09	1.0E-08	3.9E-09	1.6E-10	9.7E-10	8.1E-09
WNW1	4.3E-09	1.5E-09	1.9E-10	1.4E-09	1.2E-09	5.9E-09	2.3E-09	9.0E-11	5.7E-10	4.7E-09
WSW2	2.4E-09	8.4E-10	1.1E-10	7.8E-10	6.9E-10	3.3E-09	1.3E-09	5.0E-11	3.1E-10	2.6E-09
NNW2	2.1E-09	7.5E-10	9.5E-11	7.0E-10	6.2E-10	2.9E-09	1.1E-09	4.5E-11	2.8E-10	2.3E-09
NNE3	1.6E-09	5.6E-10	7.1E-11	5.3E-10	4.7E-10	2.2E-09	8.6E-10	3.4E-11	2.1E-10	1.8E-09
WNW2	7.2E-10	2.6E-10	3.2E-11	2.4E-10	2.1E-10	1.0E-09	3.9E-10	1.5E-11	9.6E-11	8.0E-10
WSW3	3.4E-10	1.2E-10	1.5E-11	1.1E-10	1.0E-10	4.7E-10	1.8E-10	7.2E-12	4.5E-11	3.8E-10
NNW3	3.1E-10	1.1E-10	1.4E-11	1.0E-10	9.2E-11	4.3E-10	1.7E-10	6.6E-12	4.2E-11	3.5E-10
NNE4	2.1E-10	7.3E-11	9.3E-12	6.9E-11	6.1E-11	2.8E-10	1.1E-10	4.4E-12	2.8E-11	2.3E-10
WNW3	7.4E-11	2.6E-11	3.3E-12	2.4E-11	2.2E-11	1.0E-10	3.9E-11	1.6E-12	9.8E-12	8.1E-11
NNW4	3.8E-11	1.4E-11	1.7E-12	1.3E-11	1.1E-11	5.3E-11	2.1E-11	8.2E-13	5.1E-12	4.3E-11
WSW4	3.6E-11	1.3E-11	1.6E-12	1.2E-11	1.1E-11	5.0E-11	2.0E-11	7.7E-13	4.8E-12	4.0E-11
WNW4	7.6E-12	2.7E-12	3.4E-13	2.5E-12	2.2E-12	1.0E-11	4.1E-12	1.6E-13	1.0E-12	8.4E-12

**Total Dioxin TEQ Concentration:**  
**Soil, Groundwater, Surface Water and Sediment Compartments (1992 stack test emissions)**

Compartment	Average Annual TEQ Concentration (Year 12)					
	Surface Soil	Root Zone Soil	Vadose Zone Soil	Groundwater	Surface Water	Sediment
	g/g dry weight	g/g dry weight	g/g dry weight	g/L	g/g dry weight	g/g dry weight
Source	1.6E-09	1.0E-12	7.3E-19	4.1E-25	N/A <sup>a</sup>	N/A <sup>a</sup>
W1	2.5E-10	2.2E-13	1.7E-19	9.9E-26		
N1	1.8E-10	1.5E-13	1.2E-19	6.7E-26		
SW1	1.4E-10	1.2E-13	9.4E-20	5.5E-26		
E1	1.1E-10	9.2E-14	7.1E-20	4.1E-26		
NWFarm	6.7E-11	4.8E-14	3.5E-20	2.0E-26		
NNW1	5.4E-11	4.7E-14	3.6E-20	2.1E-26		
WNNW1	5.1E-11	4.4E-14	3.4E-20	2.0E-26		
WSW1	5.0E-11	4.7E-14	3.7E-20	2.2E-26		
SW2	4.9E-11	4.3E-14	3.3E-20	2.0E-26		
E2	3.2E-11	2.7E-14	2.1E-20	1.3E-26		
NNW2	2.2E-11	1.9E-14	1.5E-20	8.6E-27		
NW2	2.0E-11	1.7E-14	1.4E-20	8.0E-27		
WSW3	1.9E-11	1.8E-14	1.4E-20	8.6E-27		
NNW3	1.9E-11	1.7E-14	1.3E-20	7.7E-27		
NNE2	1.8E-11	1.6E-14	1.3E-20	7.5E-27		
WSW2	1.7E-11	1.7E-14	1.4E-20	8.2E-27		
NW3	1.6E-11	1.4E-14	1.1E-20	6.8E-27		
WNNW3	1.6E-11	1.4E-14	1.1E-20	6.6E-27		
SW3	1.6E-11	1.4E-14	1.1E-20	6.5E-27		
SW4	1.5E-11	1.4E-14	1.1E-20	6.5E-27		
WNNW2	1.5E-11	1.4E-14	1.1E-20	6.5E-27		
SE2	1.2E-11	1.0E-14	8.0E-21	4.7E-27		
SE3	1.2E-11	1.1E-14	8.5E-21	5.0E-27		
ESE2	1.1E-11	8.0E-15	6.0E-21	3.4E-27		
NE2	1.1E-11	8.8E-15	6.8E-21	4.0E-27		
ESE3	1.0E-11	8.8E-15	6.9E-21	4.1E-27		

<sup>a</sup>Surface water and sediment results are not included because an incorrect value for the RatioOfConcnAlgaeToConcDissolvedInWater property was used. This property does not significantly impact any of the other abiotic results used in this report; however, it does impact the dissolved surface water concentrations and sediment concentrations, and thus, these values are not reported.



**Total Dioxin TEQ Concentration:  
Calculated Soil Compartments at a Depth of 7.5 cm (1994 stack test emissions)**

Compartment	Instantaneous TEQ Concentration (at Year 11.5)			
	Surface Soil	Root Zone Soil	Soil at 7.5 - minimum <sup>a</sup>	Soil at 7.5 - maximum <sup>b</sup>
	g/g dry weight	g/g dry weight	g/g dry weight	g/g dry weight
Source	2.8E-10	9.5E-14	3.7E-11	3.8E-11
W1	4.1E-11	1.9E-14	5.5E-12	5.7E-12
N1	3.0E-11	1.3E-14	4.0E-12	4.2E-12
SW1 <sup>c</sup>	2.2E-11	1.0E-14	3.0E-12	3.1E-12
E1 <sup>c</sup>	1.9E-11	8.0E-15	2.5E-12	2.6E-12
NWFarm <sup>c</sup>	1.1E-11	4.2E-15	1.5E-12	1.5E-12
NNW1 <sup>c</sup>	8.8E-12	4.0E-15	1.2E-12	1.2E-12
WNW1 <sup>c</sup>	8.3E-12	3.7E-15	1.1E-12	1.1E-12
WSW1 <sup>c</sup>	8.0E-12	3.9E-15	1.1E-12	1.1E-12
SW2 <sup>c</sup>	8.0E-12	3.6E-15	1.1E-12	1.1E-12
E2 <sup>c</sup>	5.3E-12	2.4E-15	7.1E-13	7.3E-13
NNW2 <sup>c</sup>	3.7E-12	1.6E-15	4.9E-13	5.0E-13
NW2 <sup>c</sup>	3.2E-12	1.5E-15	4.3E-13	4.5E-13
NNW3 <sup>c</sup>	3.1E-12	1.4E-15	4.1E-13	4.3E-13
WSW3 <sup>c</sup>	3.0E-12	1.5E-15	4.0E-13	4.2E-13
NNE2 <sup>c</sup>	2.9E-12	1.4E-15	3.9E-13	4.1E-13
WSW2 <sup>c</sup>	2.8E-12	1.4E-15	3.7E-13	3.8E-13
NW3 <sup>c</sup>	2.6E-12	1.2E-15	3.5E-13	3.7E-13
WNW3 <sup>c</sup>	2.6E-12	1.2E-15	3.5E-13	3.6E-13
SW3 <sup>c</sup>	2.6E-12	1.2E-15	3.4E-13	3.5E-13
SW4 <sup>c</sup>	2.5E-12	1.2E-15	3.3E-13	3.4E-13
WNW2 <sup>c</sup>	2.5E-12	1.2E-15	3.3E-13	3.4E-13
SE2 <sup>c</sup>	2.1E-12	8.9E-16	2.7E-13	2.8E-13
SE3 <sup>c</sup>	2.0E-12	9.2E-16	2.7E-13	2.8E-13
ESE2 <sup>c</sup>	1.8E-12	7.0E-16	2.4E-13	2.5E-13
NE2 <sup>c</sup>	1.7E-12	7.6E-16	2.3E-13	2.4E-13
ESE3 <sup>c</sup>	1.7E-12	7.6E-16	2.3E-13	2.3E-13

<sup>a</sup>Soil concentration calculated by dividing the surface soil concentration (i.e., total mass/volume) by 7.5

<sup>b</sup>Soil concentration calculated by dividing the total mass in the surface and root zone soil compartments by the volume to a depth of 7.5 cm

<sup>c</sup>Concentrations for this compartment are below the background concentration (4E-12 g/g) presented in Lorber et al. (2000)



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