

6. USER CONSIDERATIONS

6.1. INTRODUCTION

The methodology in this document has been earlier described as screening level in terms of theoretical sophistication, but site specific in its application. Chapter 2 described concepts of exposure and assigned values to exposure parameters which define, for purposes of demonstration, a central and a high end exposure pattern. Chapters 3 and 4 described algorithms for the fate, transport, and transfer of dioxin-like compounds, and also assigned parameter values for purposes of demonstration. The methodology was demonstrated in Chapter 5, using exposure and fate and transport parameters which had been laid out in earlier chapters. Those who wish to use the methodology for further analysis of incremental exposures to sources of dioxin-like compounds are now in a position to use the same algorithms, perhaps many of the same parameter values. The purpose of this chapter is to provide guidance on some key issues for potential users.

Section 6.2 discusses the use of the parameter values selected for the demonstration scenarios in Chapter 5 for other applications. Section 6.3 is a sensitivity analysis exercise on the parameters required for algorithms estimating exposure media concentrations. Section 6.4 addresses the issue of mass balance with regard to the source strength terms of the four source categories.

6.2. CATEGORIZATION OF METHODOLOGY PARAMETERS

Table 6-1 lists all the parameters, including names, definitions, and units, that are required for the methodologies of this assessment except the exposure parameters. Exposure parameters are given in Table 2-1 of Chapter 2. Table 6-1 also gives four additional pieces of information for each parameter listed. Three are numerical values which were used in the sensitivity analysis exercises that are described in Section 6.3. below. The parameter values labeled "selected" were the ones used in the demonstration of the methodologies in Chapter 5. Section 6.3. below justifies the high and low values of parameters selected for sensitivity analysis. Other users of this methodology may wish to view these high and low values as reasonable high and low possible values for their applications; note however that the chemical specific parameters are those only for 2,3,7,8-TCDD. The fourth piece of information is a qualitative judgement on the part of the authors of this document as to the appropriateness of using the "selected" parameter values for other assessments. This judgement is categorized in three ways:

1) **First Order Defaults, or FOD:** As defaults, these parameters are independent of site specific characteristics and can be used for any assessment. Also, as first order defaults, it is felt that the values selected for the demonstration scenarios carry a sufficient weight of evidence from current literature such that these values are recommended for other assessments. Several of the chemical specific parameters, such as the Henry's Constant, H, and the organic carbon partition coefficient, Koc, fall into this category. The qualifier above, "current literature", indicates that new information could lead to changes in these values.

2) **Second Order Defaults, or SOD:** Like the above category, these parameters are judged to be independent of site specific characteristics. However, unlike the above category, the current scientific weight of evidence is judged insufficient to describe values selected for demonstration purposes as first order defaults. SOD parameters of principal note are the bioconcentration parameters specific to the chemicals, such the Biota Sediment Accumulation Factor, or BSAF. This parameter translates the ratio of a bottom sediment concentration to a fish tissue concentration. The science is evolving for this parameter, including thought on the extent to which BSAFs generated for one species at one site can be generalized to other sites and/or species, the differences in BSAF between column and bottom feeders, the differences between past and ongoing contamination, and so on. Users should carefully review the justification for the SOD values selected for the demonstration scenarios before using the same values.

3) **Site Specific, or SS:** These parameters should or can be assigned values based on site-specific information. The information provided on their assignment for the demonstration scenarios, and for selection of high and low values for sensitivity analysis testing, is useful for determining alternate values for a specific site. A key class of SS parameters included in Table 6-1 above are the source strength terms - the soil concentrations, effluent discharge rates, and stack emission rates. There are likely to be site-specific applications of this methodology for which detailed information is unavailable. Often the midrange values selected for the demonstration scenarios are suitable for site specific applications when data is unavailable. An example of this category of parameters would be the soil characteristics, such as the porosity, bulk density, and so on.

The exposure parameters have not been categorized as have the contaminant fate and transport/transfer parameters. Assignment of these values are critical as LADD estimates are linearly related to parameter assignments - doubling exposure duration assumptions double LADDs, and so on. All exposure parameters were developed based on information and recommendations in EPA's *Exposure Factors Handbook* (EPA,1989;1997) and *Dermal Exposure Assessment: Principals and Applications* (EPA, 1992). Some of the exposure parameters of

Table 2-1, Chapter 2, are appropriately described as FOD. These include: lifetime, body weights, water ingestion rates, inhalation rates, and an exposure duration for a childhood pattern of soil ingestion. All of the other exposure parameters are better described as either SOD or SS. Attaining site-specific information is recommended for them. However, this is often difficult for site specific assessments and impractical if the procedures in this assessment are used in general assessments. In the absence of site specific information, the following parameters can be considered SOD: adult exposure durations of 9 years for central scenarios (whether they be modeled after "residential" settings or not) and 30 years for high end scenarios (whether "farming" be the model for high end exposures or not), childhood soil ingestion rates, the fruit/vegetable food ingestion rates, the fraction of fruit/vegetable consumption that comes from a home garden, the food preparation factors that were developed for home produced meats, and the fractions of time spent at home (which are applied to inhalation and water ingestion pathways). The remaining exposure parameters pertain to the exposure pathways evaluated as most critical to dioxin exposures. For this reason, users should either pursue site specific information or carefully justify parameter selections in the absence of site specific information. These include the rate of beef, milk, and fish ingestion and the fraction of these food products which are produced at home and hence impacted by the source. Fish ingestion rates for the demonstration of methodologies in this assessment were 8 g/day as the central assumption and 25 g/day for the high end assumption. These were the mean values for the central and upper end ingestion rates from several fish consumption studies characterized as "recreational" fishing studies in EPA (1997). These rates are both more than a national average estimate of fish consumption that was published in an water quality criteria document for 2,3,7,8-TCDD, 6.5 g/day (EPA, 1984). The setting for the demonstration scenarios was a rural setting which contained farm and non-farm residences, and which contained a major water body for recreational fishing purposes. The other parameters are the ingestion rates and contact fractions for beef, milk, chicken, and egg ingestion. The ingestion rates for these food products were developed in EPA (1997) from the 1987-88 National Food Consumption Survey (NFCS) conducted by USDA, and specifically, they were from the "household" portion of the NFCS. This portion of the survey included questions on consumption of home produced foods, which was why it was felt to be appropriate for the demonstration scenarios of this assessment. The contact fractions assigned for the high end scenarios were also developed from information in the household survey of the NFCS.

In addition to the above qualifications, the parameters of this methodology have been categorized in terms of their role in the methodology. The following is a brief description of three principal categories.

Category 1. Human behavior exposure parameters

These are the contact rates, contact fractions, exposure durations, lifetime and body weights used in the following equation for lifetime average daily dose:

$$\text{Lifetime Average Daily Dose (LADD)} = \frac{(\text{exposure media concentration} \times \text{contact rate} \times \text{contact fraction} \times \text{exposure duration})}{(\text{body weight} \times \text{lifetime})} \quad (6-1)$$

Category 2. Fate, transport, and transfer parameters

These parameters are all the parameters required to estimate exposure media concentrations, except those specifically associated with a contaminant - chemical-specific parameters are included in Category 3 below. All fate, transport, and transfer parameters are listed, defined, and further subcategorized in Table 6-1. Not included in the discussions in Section 6.3 are perhaps the most important terms in this category, and these are critical source strength terms: the concentrations of dioxin-like compounds for the soil contamination scenario, and the release quantities of dioxin-like compounds into the air for the stack emission source category and into the surface water for the effluent discharge source category. A general comment that can be made for fate and transport parameters is that values for the demonstration scenarios were selected to be midrange and plausible, and that this document provides information on selecting alternate values for site-specific applications. Most of the parameters in this category fall under the SS qualification. Subcategories within the fate and transport category include:

- Contaminated and exposure site characteristics: These are areas, soil properties, and depths of tillage (which are depths to which residues transported by erosion or deposition are mixed in conditions of tillage such as agriculture or gardening, and no tillage). Like the soil concentration term, the area of contamination is a site-specific parameter. Soil properties were assigned to be midrange and typical of agricultural soils. Depths of mixing for tilled and untilled circumstances are not known with certainty, and these two parameters were characterized as SOD.

- Soil and sediment delivery parameters: These include parameters associated the erosion of contaminated soil from a site of contamination to a nearby site of exposure and/or to a

nearby surface water body. All but one of the parameters in this subcategory are physical, site-specific parameters which should be evaluated for site specific applications. The one parameter not of this description is the enrichment ratio, which describes the enrichment of eroded soil with dioxin-like compounds, and was assigned a rating of SOD. Geometric parameters include watershed drainage area, water body volumes, and distances. Physical parameters include soil loss estimates, organic carbon contents, water body suspended solids, and background watershed contaminant concentrations.

- Volatilization and dust suspension parameters: These parameters are associated with suspension, dispersion, and transport of contaminants from contaminated soils. One parameter included in this category is the exposure duration, which appears to be misplaced. In fact, the exposure duration is used to determine the average vapor phase air concentration - this is further discussed in Section 6.3 below. Parameters in this category are site-specific and should be evaluated for specific methodology applications.

- Bioconcentration and biotransfer parameters: These include parameters describing the biota and the media surrounding the biota which influence the transfer of dioxin-like compounds from the media to the biota. Some of these parameters are site-specific, although obtaining values may be difficult. Included here are annual rainfall, fish lipid contents, a fresh to dry vegetable weight conversion factor, and yields and intercept fractions for vegetation categories. Others are theoretical; values for these were determined from the literature and can be used for other assessments if better information is unavailable. Included here are atmospheric deposition velocities of particles, washout of wind-suspended particles from the atmospheric, the retention of wet particle depositions on vegetation, empirical correction factors for vapor-phase air-to-plant transfers and soil-to-plant transfers, and the bioavailability of soil as compared to vegetation as a vehicle of transfer of dioxin-like compounds to terrestrial animals. These were given a rating of SOD. A third group describes exposure of the terrestrial animals to dioxin-like compounds through their diet. These include fractions of animal diet which are soil, pasture grass, and feed, and the extent to which these three are impacted by the source of contaminant. Sensitivity analysis below was conducted on beef parameters only, not on the dairy cow, chicken, or egg parameters. It is expected that, in general, the trends should be the same for all the terrestrial animals. The analysis below shows how beef concentrations are impacted by changes in assumptions of how cattle are exposed to dioxin-like compounds through their diet. Since terrestrial animal exposures are most critical for human exposure, the animal exposure assumptions made for demonstrating the methodologies of this assessment should be carefully considered before using them for other assessments.

- Effluent discharge source category: These are three physical parameters that can be determined on a site-specific basis, and include flow rates of the effluent and receiving water body, organic carbon contents of suspended solids in the effluent and the receiving water body, and suspended solids content of the effluent and the receiving water body.

- Stack emission source category: In fact, most of the parameters required to evaluate the impact of stack emissions to a nearby site of exposure have been included in other categories. Sensitivity analysis only focuses on parameters and issues unique to this category. One set of input values are contaminant wet and dry deposition rates. Three depositions are required: one for the site of exposure, one to represent depositions on watershed soils which drain into the water body, and one to represent direct deposition onto the water body. These were all generated using the ISCST3 model, as described in Chapter 3. Two other key inputs generated by the ISCST3 model are the ambient air vapor phase and particle phase concentrations of contaminant at the site of exposure. All such quantities are a function of that model's algorithms and parameter input requirements, particularly the release rate from the stack. Information on the ISCST3 model and its application is given in Chapter 3 and not discussed further in this chapter. Users can determine air concentrations and contaminant deposition rates in other ways, and use those in the methodologies to determine impacts and exposures. The no-till depth of mixing at the site of exposure, d_{not} , is required for the contaminated soil source algorithm as well. It's selected value for the stack emission source category was 2 cm, similar to the 2 cm used in the soil contamination source demonstration. The only other unique parameters not included in other subcategories are the average watershed mixing depth (used for determining watershed soil concentrations, which are then used to determine impacts to water bodies) and the fraction of particles depositing on water bodies which remain in suspension. These are both theoretical values and can be used in other assessments lacking better information.

Category 3. Chemical properties of dioxin-like compounds

The thirteen chemical-specific parameters required for the algorithms of this assessment fall under two categories, FOD and SOD. As such, they are all independent of the specifics of the site. The parameters deemed FOD are chemical fate and transport parameters, some of which are common and often determined in laboratory conditions. These include the Henry's Constant, the organic carbon partition coefficient, and the molecular diffusivity in air. The selected values for these parameters are, in the authors' opinion, the best values derivable from current data. A second set of chemical specific parameters are associated with bioconcentration/biotransfer algorithms. Some of them are determined from field data (data on dioxin-like compounds or

other compounds), and others are determined by experimentation and with that experimentation, development of empirical relationships between a critical transfer factor and the chemical's octanol water partition coefficient. The authors cannot be definitive in a judgement that values given to these parameters be considered default, hence the SOD rating. For these compounds, field/experimental data is conflicting or there simply is a lack of appropriate data. Parameters included in this category are a soil to below ground vegetation transfer factor, two air-to-plant factors: the air-to-leaf vapor phase transfer coefficient and the plant washoff rate constant, two water body to fish parameters: the biota to sediment accumulation factor and the related biota to suspended solids accumulation factor, and the bioconcentration factors for beef, milk, chicken, and eggs. The sorbed fraction was given a "SOD/SS" rating because its assignment is a function of chemical properties as well as an assumption regarding particle density in the airshed. This assessment assumed, "background plus local sources" as the appropriate descriptor for particle density in the airshed. This particle density selection is the site-specific aspect to this parameter assignment. Therefore, for other applications where this airshed particle density is appropriate, users may consider the values for the particle density to be, SOD.

6.3. SENSITIVITY ANALYSIS

Sensitivity analysis was undertaken in order to evaluate the impact of model results with changes in model parameters. The following sections describe the limitations, methodology and parameter selections, and results.

6.3.1. Limitations of the Sensitivity Analysis Exercises

The exercises were not comprehensive and/or definitive. Following are some key limiters:

! The ISCST3 model was not evaluated in this section. Chapter 3 describes the ISCST3 model. No sensitivity analysis runs were performed on ISCST3 model output for this chapter. This section does evaluate the impact of different deposition rates and modeled ambient air concentrations on exposure sites soils, surface water, and biota. Chapter 7 describes a model validation exercise on the ISCST3 model, and this exercise includes an evaluation of the impacts of selecting different meteorological data and different source strength terms (i.e., different stack emission rates of dioxins).

! Sensitivity to changes in exposure parameters was not evaluated. The basic equation for evaluating lifetime average daily dose was given above as Equation (6-1).

Chapter 2 described all terms in this equation except the exposure media concentration, which was the focus of Chapter 4. Because LADD estimates are a linear function of all exposure parameters, sensitivity analysis was not performed on LADD exposure estimates. The focus of this section instead is on the fate, transport, and bioconcentration/biotransfer algorithms used to estimate the exposure media concentration term in Equation (6-1).

! The analysis was not exhaustive in its coverage. Principal algorithms in the fate, transport, and transfer of dioxin-like compounds were evaluated, and all parameters required for algorithms were tested at least once. However, not all possible tests were conducted. Before noting those, following is a list of algorithms which were tested:

- Volatilization/suspension and transport/dispersion of vapor/particle phase airborne residues from a site of contamination to a site of exposure (using algorithms for the soil contamination source category);
- Transport via erosion of contaminants at a site of soil contamination to a nearby site of exposure to impact exposure site soils (soil contamination source category);
- Transport via erosion of contaminants at a site of soil contamination to a nearby surface water body, to impact bottom sediments, water, and fish (soil contamination source category);
- Transfers of contaminants from soils to below ground vegetables and from air to above ground vegetation (soil contamination source category);
- Transfers of contaminants from soils to vegetation to beef (soil contamination source category) and from air to vegetation to beef (stack emission source category);
- Direct discharges of dioxin-like compounds into surface water bodies, and the effect of surface water and effluent parameters on fish and water concentration estimation (effluent discharge source category); and
- Particle depositions and ambient air concentrations, which result from stack emissions, onto exposure site soils, watershed soils, surface water bodies, and biota (stack emission source category);

The exercise was purposefully limited since several possible exercises would have been duplicative. For example, impacts to terrestrial animal products was limited to an evaluation of the algorithm estimating beef concentrations. Similar trends are expected for the milk, chicken, and egg bioconcentration algorithms. For all the animal pathways, including fish ingestion, the impact to changes in the lipid, or fat, contents was not evaluated in this exercise. All the bioconcentration algorithms estimate the concentration of the dioxin-like compound in fat tissue. The fraction of fat parameters are all required simply to translate a fat concentration to a whole product concentration for purposes of exposure estimation. Therefore, changes to the assumption

of fat contents will translate to a linear change in the estimation of the whole animal product concentration.

A related limitation has to do with the cascading effect of certain parameters. For example, a key contaminant parameter is the organic partition coefficient, Koc, which impacts (among other concentrations) vapor phase air concentrations. Air concentrations are used to estimate above ground vegetation concentrations, including those of grass and cattle feed. Beef concentrations are a function of concentrations in grass and cattle feed. The impact of Koc is evaluated in the context of the soil contamination source category. What is not done in the sensitivity analysis below for this important model parameter (and others as well) is to evaluate the impact of changes in Koc to beef concentrations. What is done, however, is as follows. The sensitivity of air concentration predictions to changes in the partition coefficient are evaluated. Then, the sensitivity to grass and cattle feed concentrations to plus and minus one order of magnitude differences in estimated vapor phase air concentrations are evaluated. In this way, any possible parameter change(s) which influences air concentrations within a plus/minus order of magnitude range is evaluated for grass and feed concentrations. Finally, beef concentration estimations are evaluated within a similar plus/minus order of magnitude change for grass and feed concentrations. With some examination, therefore, the effect of cascading impacts can be determined.

The impact of changing soil concentrations (in the soil contamination source category) to estimates of exposure media concentrations (air, water, biota) is linear and direct in all cases - i.e., increasing soil concentrations by a factor of five increases all impacted exposure media by the same factor of five. For this reason, soil concentrations are not displayed in the sensitivity graphs displayed in the next section, with one exception. This was in the estimation of beef concentrations from soil contamination. Beef concentrations are a function of concentrations in the dry matter diet of the cattle, including soil, grass, and cattle feed. Therefore, if soil concentrations were to change and concentrations on the other intakes were to not change, than beef concentrations would not be a linear and direct function of soil concentrations. However, and in the context of this sensitivity analysis, when changing only soil concentrations, vegetative concentrations are linearly and directly impacted by the same order of magnitude change. Therefore, beef and milk concentrations turn out to be linearly related to soil concentrations.

A final limitation to note is that this exercise does not evaluate the multiple effects of changing more than one independent parameter simultaneously. Other numerical methods, particularly Monte Carlo, can be used to evaluate the impact of simultaneous changes to model

parameters. Applications of this technique to dioxin exposure assessments are discussed in Chapter 8 of this volume.

There are instances where parameters were evaluated as dependent and changes were made simultaneously. One example is in three parameters which are related to the size of a watershed (also termed the "effective drainage area" since such an area might be smaller than a surrounding river system watershed), and which are important in determining the impact of a bounded area of soil contamination to a nearby surface water body. These three include the watershed size, the watershed sediment delivery ratio (which decreases as watershed size increases), and the surface water body volume (which increases as watershed size increases, assuming sources of water - surface runoff, interflow, and groundwater recharge - remain the same on a per unit area basis). To test the impact of watershed size to surface water and sediment concentrations, all three parameters were changed simultaneously in modeling a small and a large watershed. One set of parameters which might not be independent, but which were treated as such in the sensitivity testing, are the chemical specific parameters. For example, a higher organic carbon partition coefficient might be associated with a lower Henry's Constant - tighter binding to soils means less of a tendency to volatilize. Empirical relationships between such chemical specific parameters have not been established, and since there is uncertainty in precise values selected for the dioxin-like compounds, chemical specific parameters were treated as independent parameters.

! Only a high and a low value for model parameters were tested; no discussions of likelihood for parameter values or distributions of parameter values are included. Certainly the identification of all model parameters and the justification for assignment of high and low values will be helpful to others using the methodology. Assignment of parameter values for purposes of demonstrating the methodologies in Chapter 5 should be carefully considered when users apply this methodology for specific purposes or specific sites.

6.3.2. Methodology Description and Parameter Assignments

Only two of the six example scenarios of Chapter 5 served as "baselines" in the sensitivity analysis exercises. The single scenario for the soil contamination source category, Scenario 3 in Chapter 5, served as the basis for testing on these algorithms: 1) transport of vapor and particulate phase airborne contaminants from a site of contamination to a nearby site of exposure, 2) transport of soils via erosion to nearby sites of exposure and to surface water bodies to impact bottom sediments, fish, and water, 3) impacts of soil concentrations and other parameters to below ground vegetation, and air concentrations and other parameters to above ground

vegetation, and 4) impacts of soil, grass, and feed concentrations, and other parameters, to beef concentrations. The source strength for this scenario, in summary, was a 40,000 m² (4 ha, 10 ac) area of soil concentrations of 1 µg/kg (ppb) within a watershed of size 4,000 ha (40,000,000 m²; 10,000 ac; 15.5 mi²) with soils otherwise at 0.0 ppb. Most of the sensitivity analyses focused on predictions that were to occur at the exposure site, which was a farm located 150 meters away. The high end example scenario for the stack emission source category, example scenario #5, served as the basis for the testing the impact of particle depositions and ambient air concentrations on soils and biota. The ambient air concentrations and deposition rates at the site of exposure 500 meters from the stack served as the baseline source strength terms. The single scenario for the effluent discharge source category, example scenario #6, was used to evaluate the impact of parameters required for that source category on fish and water concentrations. The source strength in that case was a discharge of 0.0315 mg/hr into a surface water body with a harmonic mean flow rate of 4.7x10⁸ L/hr. Assignment of that baseline discharge was based on data from the 104 pulp and paper mill study, and then considering reductions in discharges which have occurred in these pulp and paper mills since the 104 mill study in 1988.

The baseline chemical for all these sensitivity runs was 2,3,7,8-TCDD; i.e., all the chemical specific parameters were those assigned to this example compound. The high and low values for parameter testings were determined starting with the 2,3,7,8-TCDD assignments. Care was not taken to encompass a range of possible values for all dioxin-like compounds. However, the ranges that were tested are mostly inclusive of the dioxin-like compounds. What will be noted and discussed below is that mostly the model response to chemical-specific parameters is linear or nearly linear, so that model responses to values outside the ranges tested can be evaluated easily.

All the initial parameter values required for all four source categories, and the values selected for high and low sensitivity analysis were listed above in Table 6-1. Following are brief discussions on the selection of these high and low values. Longer discussions on all parameter values can be found in Chapter 4, which included justifications for all parameter values selected for the demonstration of the methodologies in Chapter 5. Often, ranges of possible values were discussed in Chapter 4; those ranges were the basis of high and low parameter values selected below. Discussions in Chapter 4 are not repeated here, but are referenced below. The summaries below are organized in the same order as the parameter listings in Table 6-1.

! Contaminated and exposure site characteristics: These are the area and distance parameters, and the soil characteristic parameters of the site of contamination and the site of exposure. The "site of contamination" refers to the bounded area of high soil concentration for the soil contamination source category. The "site of exposure" for these sensitivity runs is the small farm which was the basis for the definition of the "high end" example scenarios demonstrated in Chapter 5. The area of the site of exposure, **AES**, and site of contamination, **ASC**, are both 40,000 m² in the demonstration scenarios, which is equal to 4 ha or 10 ac. Low and high values tested were 4,000 m² (0.4 ha, 1 ac) and 400,000 m² (40 ha, 100 ac). The soil description parameters include soil porosity, **ESLP**, particle bulk density, **Psoil**, soil bulk density, **Bsoil**, and the organic carbon fraction, **OCsl**. The assignment of high/low values to these parameters were developed from Brady (1984) and cover a reasonable range of agricultural field soils. The no-till and tillage depths, **d_{not}** and **d_t**, refer to the depth to which eroded soil or depositing particulates mix at the site of exposure. The no-till depth was set at 2 cm and was varied between 1 and 10 cm, and the tilled depth was varied between 10 and 30 cm. The no-till concentrations were used to estimate soil concentrations for soil related exposures: soil ingestion and soil dermal contact, and also for the beef and milk bioconcentration algorithm. The tilled concentrations were used only to estimate the concentration in below ground vegetation.

! Soil and Sediment Delivery Parameters: Contaminated soil erodes from a site of contamination, a 4 ha site in the demonstration scenarios, to a nearby site of exposure and also to a nearby river. The distance to the site of exposure from a site of contamination, **DL_e**, was set at 150 meters for the example scenarios, and varied between 50 and 1000 meters in this exercise. The same initial distance of 150 meters was the distance to the nearby river, **DL_w**, and it was also varied between 50 and 1000 meters. The unit amount of soil eroding off the site of contamination, **SL_s**, was initialized at 21520 kg/ha-yr, equal to 9.6 Eng. ton/ac-yr (abbreviated t/ac-yr hereafter). Assumptions inherent in this estimate include: midcontinent range of annual rainfall erosivity (which is also the middle of the range of rainfall intensities of the US), midrange agricultural soil erosivity, a gentle 2% slope, no man-made erosion protection (ditches, etc.), and bare soil conditions. A doubling of this amount to 42,000 kg/ha-yr (19 t/ac-yr) was used as a high erosion estimate off the site of contamination. This could reflect any number of different assumptions, such as more erosive soil, more erosive rainfall, steeper slopes, and so on. A low estimate of one-tenth the default value, at 2100 kg/ha-yr (1 t/ac-yr), could reflect all the same assumptions except a dense cover of grass or weeds, which changes the bare soil

assumption leading to a "C" (cropping management factor) of 1.0 to a C of 0.1. The erosion amount of 2152 kg/ha-yr was the initial amount assumed for a second unit erosion term needed in this assessment, a unit erosion typical of land area between the contaminated and the exposure site, SL_{ec} . The critical assumption in this initialization was that all conditions for this land area were similar to the contaminated site, except that the ground was densely covered with grass or weeds. The value of SL_{ec} was reduced to 0 kg/ha-yr for the low value, which is unrealistically low but might give a sense of how the algorithm would perform if mixing with soil between the contaminated and exposure site were not considered. The high value was 21,000 kg/ha-yr, which is similar to the initial assumption for the contaminated site, could reflect similar erosion conditions between the contaminated site and the exposure site. The third unit soil loss parameter required is one which reflects average erosion conditions within the watershed draining into the water body, SL_w . This was initialized at 6455 kg/ha-yr (2.88 t/ac-yr) which reflects similar erosion conditions as the contaminated site (soil erosivity, rainfall intensity, average slopes, lack of support practices) except some erosion protection due to vegetation - C equal to 0.3 instead of 1.0. It was reduced to 2100 kg/ha-yr, which might translate to C equal to 0.1, and increased to 21,000, which was equal to the initial higher erosion from the contaminated site. The range of the enrichment ratio, ER, was noted at between 1 and 5 for its application in agricultural runoff field data and model simulations, and was given an initial value of 3 in this application. High and low values tested were 5 and 1. An average watershed concentration of contaminant was set at 0 for the soil contamination demonstration scenarios, where the soil concentration of 2,3,7,8-TCDD (and the other example compounds) was set at 1 ppb. This was selected so that the impact to surface water bodies could be demonstrated as an incremental impact. A concentration of 2,3,7,8-TCDD of 1 ppt was chosen to represent "background" conditions. This value is near the 0.3 ppt that was measured in the background setting near Columbus, Ohio, and used in the demonstration of the background scenarios. The value was used to evaluate the impact of a bounded site at 1 ppb when a background concentration of 1 ppt is also assumed to exist. Four parameters reflect watershed size. These include the effective drainage area, A_w , the watershed sediment delivery ratio, SD_w , the volume of the receiving water body, VOL_w , and the surface area of the water body, $AREA_w$. These are related and should therefore be changed in tandem. The initial watershed size of 100,000 ha (385 mi²) was reduced to 10,000 ha (39 m²) and increased to 1,000,000 ha (3850 mi²). Since the water body volume was estimated using a in/yr runoff times an area, it was concurrently reduced 1 order of magnitude for the small watershed test and increased one order of magnitude for the large watershed. The surface area of the water body was also increased or reduced by an order of

magnitude with the concurrent change in water body volume. The values of SD_w were estimated using Figure 4-4 (Chapter 4), which shows watershed delivery ratios as a function of watershed area. The remaining three parameters further described the water body, and were the total suspended solids, **TSS**, and the organic carbon contents of suspended and bottom sediments, OC_{ssed} and OC_{sed} . The initial value of TSS of 10 mg/L is typical of a moving water body (stream, river) supportive of fish and other aquatic life. It was reduced to 2 mg/L, which is typical of a stationary water body (pond, lake, reservoir) and increased to 50 mg/L, which begins to be high for a water body expected to be supportive of fish. The organic carbon contents were initialized at 0.05 for OC_{ssed} and 0.03 for OC_{sed} . The premise was that they were related - that sediments in suspension were lighter and likely to be higher in organic carbon content than bottom sediments. They were also changed in tandem to 0.02 (OC_{ssed}) and 0.01 (OC_{sed}) for a low organic carbon sensitivity test and 0.10 and 0.05 for a high organic carbon test.

! Volatilization and Dust Suspension Parameters: Distances and areas are pertinent to estimating vapor-phase and particulate-phase air concentrations, and these have been discussed above in the first two categories. One parameter included for sensitivity testing in this category is the exposure duration, **ED**. It is included in these exercises because the estimation of average volatilization flux over a period of time is a function of that period of time. The derivation of the flux model assumed contamination originates at the soil surface at time zero, and over time, originates from deeper within the soil profile. Therefore, the flux decreases over time (because residues have to migrate from deeper in the profile), and the average flux over a period of time will decrease as that period of time increases. This is further discussed in Chapter 4, Section 4.3.3., and in the original citation for the volatilization flux algorithm, Hwang, et al. (1986). The exposure duration assumed in the high end scenarios was 30 years, this was changed to 1 and 70 years in sensitivity tests. A range of average windspeeds, U_m , around the U.S. was noted at 2.8 and 6.3 m/sec, and these two values were used around the selected value of 4.0 m/sec. The frequency with which wind blows from a site of contamination to a site of exposure, **FREQ**, was set at 0.15, which is appropriate if one assumes that wind blows in all directions roughly equally. It was changed to 0.05 and 0.50, which might translate to an assumption of a prevailing wind direction, either away from or towards a site of exposure. The remaining parameters, fraction of vegetative cover, **V**, threshold wind speed, U_t , and model specific function, **F(x)**, all refer to the wind erosion algorithm which suspends contaminated particulates into the air. Sensitivity tests were applied to this trio for the on-site and the off-site source categories. **V** for the off-site scenario was initialized at zero, implying bare ground cover; it was increased to 0.9 reflecting

dense ground cover in the single sensitivity test here. It was set at 0.5 for the on-site small farm demonstration scenario, reflecting some bare ground conditions (in the agricultural fields, e.g.) as well as some dense vegetation (in other grassed areas of the farm property). It was decreased to 0 and increased to 0.9. The parameters U_t and $F(x)$ reflect intrinsic erodibility of the soil and were varied together. Values were selected to reflect a high and low wind erodibility soil, following guidance in EPA (1985), the primary reference for the wind erosion algorithm.

! Bioconcentration and Biotransfer Parameters: Several parameters are required for the vegetation concentration algorithm, most of which were associated with the algorithm for dry plus wet deposition of particulates in the soil contamination source category. One parameter not associated with fate and transport was the dry to fresh weight conversion factor, **FDW**. The algorithm calculates vegetative matter concentrations on a dry weight basis, which is appropriate for the role of vegetation in the beef/milk bioconcentration algorithm. However, ingestion rates of fruits and vegetables are on a fresh weight basis, so dry weight concentrations have to be converted to a fresh weight basis. The initial value of 0.15 assumes that fruits and vegetables are 85% liquid. The high and low values tested for this parameter were 0.30 (70% liquid) and 0.05 (95% liquid). Four parameters are described as empirical correction factors for the air-to-leaf algorithm adopted for vapor phase transfers to vegetation (three of the parameters), and for the soil-water-to-root algorithm adopted for below ground vegetation. There is one each for the four principal vegetation considered: below ground vegetables/fruits - VG_{bg} , above ground vegetables/fruits - VG_{vg} , grass - VG_{gr} , and feed - $VG_{ctfd/chfd}$ (cattle and chicken feed, respectively). The concept for assignment of values to these parameters was the same, and briefly is as follows. The principal biotransfer factors, vapor phase air-to-leaf and soil-water-to-root, were developed for relatively thin vegetation, grass leaves for air-to-leaf transfers and barley roots for soil-water-to-root transfers. Concurrently, there is evidence that the strongly hydrophobic/lipophilic dioxin-like compounds are found only in outer portions of vegetation and not inner portions of bulky vegetation; there is very little translocation of dioxin-like compounds into and within vegetation. Therefore, the full vegetation concentrations of bulky vegetation are expected to be much lower than the concentrations that would be found in their thin outer layers. For above ground bulky fruits/vegetables, two considerations were included in the final assignment of 0.01 to VG_{vg} : 1) a surface area to volume ratio based on this tendency not to translocate into inner portions of the vegetation, and 2) additional reductions in whole fruit/vegetable concentrations that would occur due to washing or peeling. For bulky below ground vegetation, a final value of 0.25 was selected based on: 1) again, this tendency not to translocate into inner portions of below ground

vegetation, and 2) experimental evidence on carrots and potatoes that did indicate more within plant translocations than have been measured for above ground vegetation. The above ground VG_{ag} was reduced to 0.001 and increased to 0.10 in sensitivity testing, and the below ground VG_{bg} was reduced to 0.01 and increased to 1.00. The VG_{gr} was set at 1.00 since the air-to-leaf vapor transfer factors were developed from data on grass, so no correction is warranted. Although there is no justification to change VG_{gr} , a lower value of 0.50 was chosen simply for illustration. The VG_{ctfd} was set at 0.50, recognizing that some cattle feed is unprotected and thin vegetation such as the leaves in silage, while others are protected grains such as corn grain. That value was changed to 0.25 and 0.75 in sensitivity testing. There is one required parameter for the dry deposition algorithm, and this is the particle deposition velocity by gravity settling, V_p , in m/yr. The initial value of 3.2×10^5 m/yr, from a velocity assumption of 1 cm/sec, was given by Seinfeld (1986) as the gravitational settling velocity for 10 μ m particles. This is the appropriate size to consider since the wind erosion algorithm was developed only for inhalable size particulates, those less than 10 μ m (EPA, 1985). This was reduced to 0.5 cm/sec and 2 cm/sec (transformed to m/yr) for sensitivity testing. Three of the vegetation bioconcentration parameters are associated with the particulate wet deposition algorithm. These are the atmospheric washout ratio, W_p , the retention of particles on vegetation, R_w , and the annual rainfall amount, R . The definition, derivation, and ranges for these values are described in Chapter 4, Section 4.3.4.2, and are not repeated here (the ranges are given in Table 6.1). The remaining bioconcentration parameters are the yield and crop intercept values for the three above ground vegetation: vegetables/fruits (Y_{veg} , INT_{veg}), grass (Y_{gr} , INT_{gr}), and cattle feed (Y_{ctfd} , INT_{ctfd}). Again, discussions of chosen, and high and low, values for these quantities are given in Chapter 4, Section 4, and displayed in Table 6.1. It is noted that these two terms are correlated - high yields are correlated with high interception amounts. In sensitivity testing, therefore, these parameters were changed in tandem.

The remaining bioconcentration/biotransfer parameters are for the terrestrial animal bioconcentration algorithms, for beef, milk, chicken, and eggs. For the sake of brevity, only the beef bioconcentration algorithm will be evaluated. The trends found in the testing of this algorithm are expected to be duplicated for the other terrestrial animal products. One of the parameters relates the bioavailability of soil relative to the bioavailability of vegetation, where bioavailability refers to the efficiency of transfer of a contaminant attached to a vehicle. Fries and Paustenbach (1990) developed the bioconcentration factor, BCF, from studies where cattle were given contaminated feed. The studies of McLachlan, et al. (1990), from which BCFs for dioxin congeners were derived and used for this assessment, also used standard cattle feeds. This

feed is assumed to be analogous to the vegetation in cattle diet; therefore, the experimental BCFs can be directly applied to vegetation in cattle diets. However, Fries and Paustenbach also hypothesized that soil is less bioavailable than feed, based on some rat feeding studies, and therefore the BCF developed from feed cannot directly be used on a soil concentration - it should be reduced. Information in Fries and Paustenbach led to an assignment of 0.65 for the soil bioavailability factor, B_s . This was reduced to 0.30 and increased to 0.90 in sensitivity testing. Three parameters describe the proportion of the dry matter in the diet of beef cattle that is soil, **BCSDF**, grass, **BCGDF**, and feed, **BCFDF**. The sum of these three terms, by definition, equals 1.00. Beef cattle are principally pastured (where incidental soil ingestion occurs), with supplemental feeds including hay, silages, and grain, particularly in cooler climates where they are housed during the winter. Values of 0.04 for BCSDF, 0.48 for BCGDF, and 0.48 for BCFDF were used in the demonstration scenarios. A final set of two parameters describes the proportion of these dietary intakes that are contaminated. One is defined as the fraction of grazing land that is contaminated, **BCGRA** for beef cattle. The initial assumption of 1.00 for this parameter meant that all the grass as well as all the soil in which the cattle grazed was contaminated (since soil was assumed to be ingested during grazing). The last one similarly is defined as the proportion of feed that is contaminated, **BCFOD** for beef cattle. It were also set at 1.00, perhaps indicating that feed was grown on-site. Rather than change these diet fraction assumptions and extent of contamination assumptions individually or in tandem (if necessary), what is done instead is to model four different scenarios relating to cattle exposures. These four scenarios and the parameter changes made are:

1) High and low soil ingestion

No changes to BCGRA or BCFOD; diet assumptions changed to reflect high and low soil ingestion patterns

Low: BCSDF = 0.01
BCGDF = 0.50
BCFDF = 0.49

High: BCSDF = 0.15
BCGDF = 0.43
BCFDF = 0.42

2) Low exposure conditions

Grazing is under lush conditions, so soil ingestion and diet pattern is modeled as "low" soil ingestion above; also, most feed is purchased externally and uncontaminated; BCFOD reduced from 1.00 to 0.25

BCSDF = 0.01
BCGDF = 0.50
BCFDF = 0.49
BCFOD = 0.25

3) Low extent of contamination

Diet assumptions are unchanged from initial assumptions; only it is assumed that 25% instead of 100% of dry matter in cattle diet is contaminated

BCGRA = 0.25

BCFOD = 0.25

4) High/low lifetime pasturing

Tests for beef cattle only assuming heavy lifetime pasturing, 90% grass, and light lifetime pasturing, 08% grass

Low: BCSDF = 0.02

BCGDF = 0.08

BCFDF = 0.90

High: BCSDF = 0.08

BCGDF = 0.90

BCFDF = 0.02

! Effluent Discharge Source Category: Section 4.6, Chapter 4, discusses briefly how data from the 104-mill pulp and paper mill study (EPA, 1990) were used to develop initial parameters required for this source category in its demonstration in Chapter 5. The use of the 104-mill data in a model evaluation exercise is expanded upon in Chapter 7, Section 7.3.6. The data is also used here to assign high and low values for four of the seven required parameters for this source category. Two have to do with flow rates: Q_e which is the effluent flow rate, and Q_u which is the receiving water flow rate. The range of Q_e is from 10^5 to 10^7 L/hr, which are the low and high surrounding the 4.1×10^6 rate used in the demonstration scenario in Chapter 5. The range of Q_u is 10^7 to 10^9 L/hr (excluding the top ten receiving water bodies, which were in the 10^{10} L/hr range and for which model did not appear to perform adequately), and these were the low and high around the 4.7×10^9 L/hr rate used in Chapter 5. Two parameters describe the suspended solids content of the effluent, TSS_e , and the suspended solids content of the receiving water body, TSS_u . TSS_e ranged from 10 to 250 mg/L in the 104-mill study, so this was the range around the 70 mg/L used as the initial value. Data from STORET used to develop TSS_u led to an average of 9.5 mg/L and a range of less than 1 to 50 mg/L; a range of 2 (a reasonable value for a stationary water body such as a pond or lake) to 50 mg/L was tested. One required parameter was, of course, the rate of contaminant discharge, LD , in units of mg/hr. The assumed value was 0.0315 mg/hr, and this decreased and increased an order of magnitude for low and high testing. The remaining two parameters are the organic carbon contents of effluent solids, OC_e , and upstream river suspended solids, OC_u . A range based on data was not available for these parameters. OC_e was assigned a value of 0.36 based on the fact that solids in effluent discharges are primarily biosolids, and this value was one cited for surface water algae; values of 0.15 and 0.50 were tested. The value of 0.05 for OC_u was the value assumed for demonstration of other

source categories, where the parameter was called OC_{ssed} . The same range of 0.02 to 0.10 for OC_{ssed} was used for OC_u .

! Stack Emission Source Category: The parameters in this category listed in Table 6-1 are the only ones which are unique to this source category. As seen, there are only a very few unique parameters. Most of these are associated with surface water impact, and one series of tests evaluated the impact of parameter changes to surface water concentrations and fish concentrations. These include the contaminant deposition rates, $RDEP_{wat}$ and $RDEP_{sw}$, which are depositions onto the watershed draining into the surface water body and the surface water body itself (units are $\mu\text{g}/\text{m}^2\text{-yr}$). The initial values for these were those modeled to occur 5000 meters from the stack. This assignment for the stack emission demonstration scenarios, #4 and #5 in Chapter 5, assumes that the stack is located reasonably distant from the impacted water body. These deposition rates are specific to 2,3,7,8-TCDD. Rates of 2,3,7,8-TCDD deposition at 200 meters and at 10,000 meters were used as high and low values, respectively. It should be noted that depositions are higher at 200 meters and lower at 10,000 meters as compared to 5,000 meters, but air concentrations are lower at 200 meters as compared to 5,000 meters. This trend occurs because wet deposition is highest nearest the stack. Total depositions are driven by these high wet deposition totals; hence total depositions at 200 meters exceed those at 5,000 meters. However, dispersion modeling shows that ambient air concentrations of contaminants in the vapor phase (given the wind data and all other parameters and assumptions in using the ISCST3 model for the demonstration scenarios) are highest 500-1000 meters from the stack. For sensitivity testing, differences in model performance as a function of distance from the stack will be evaluated. $RDEP_p$ is the deposition of particles themselves and was supplied in order to maintain a mass balance of solid materials entering the water body. The default value of $0.03 \text{ g}/\text{m}^2\text{-yr}$ was taken from Goeden and Smith (1989) for a study on the impacts of a resource recovery facility on a lake. They estimated a total deposition of particles to the lake from all sources was $74.4 \text{ g}/\text{m}^2\text{-yr}$. Assuming the stack is unlikely to contribute all sources of particles to a water body, a high value was chosen as $3 \text{ g}/\text{m}^2\text{-yr}$, and a low value was given as 0.003. The fraction of depositing particles remaining in suspension, f_{sd} , was initialized as 1.00 (meaning that all directly depositing particles remain in suspension) based on an argument that the small particles emitted from the stack and transported directly to the surface water body would settle to surface water bottoms much more slowly than other solids entering water bodies. A low value of 0.00 was tested (meaning that all solids directly depositing within a year settle quickly to become bottom sediments). The average watershed mixing zone depth, d_{wmx} , was initialized at 0.10 m

(10 cm) which is midway between the 2 cm assumed for non-tilled conditions and 20 cm assumed for tilled conditions. This assumption might translate to a rural watershed comprised equally of farmed and unfarmed land. It was reduced to 1 cm and increased to 20 cm in sensitivity testing. A second series of tests evaluated biota impacts at the site of exposure, vegetables/fruits and beef/milk. Parameter inputs for these tests include the ambient air concentration and depositions at the site of exposure, C_{va} and $RDEP_e$, and the no-till depth of mixing, d_{not} . The no-till depth of mixing was increased from 2 to 5 cm. Concentrations and depositions of 2,3,7,8-TCDD at 200 and 10,000 meters were tested. The baseline quantities at 5,000 meters were varied to reflect different vapor/particle partitioning assumptions. Currently, the assumption is that 2,3,7,8-TCDD emissions are 51% in the vapor phase and 49% in the particle phase. Linear adjustments to the emissions in vapor and in particle form can be made to stack emissions. Concentrations and depositions at specific locations are then adjusted in the same linear manner to reflect different vapor/particle partitioning assumptions. Two assumptions tested include 10% vapor/90% particle and 90% vapor/10% particle.

! Contaminant Physical and Chemical Properties: The initial values for testing of this category of parameters were the ones used for 2,3,7,8-TCDD. Generally, the high and low values tested are those which may represent a range for this contaminant only, not all dioxin-like compounds. However, several of the ranges also encompass values that could be pertinent to other compounds. It should be remembered that this is simply a model performance exercise and nothing else. Also, it could be argued that some of the parameters should be changed in tandem - that there may be a relationship between soil/water adsorption, as modeled by Koc, and bioconcentration. Such relationships were not explored in these exercises. Notes on the parameters are as follows:

1. **Henry's Constant, H** - The value of 3.29×10^{-5} atm-m³/mole was used for 2,3,7,8-TCDD. Except for a heptachloro-PCB, Henry's Constants for the dioxin-like compounds ranged from 10^{-6} to 10^{-4} . Because of this, the initial value was reduced and then increased an order of magnitude for this test.

2. **Molecular Diffusivity in Air, D_a** - This parameter is needed for the volatilization flux algorithm. Because no values were available for the dioxin-like compounds, values were estimated based on the ratios of molecular between a dioxin-like compound of interest and a compound for which a D_a was available - in this case, diphenyl. The range of values tested are 0.005 cm²/s as a low and 0.10 cm²/s around the initial value of 0.047 cm²/sec.

3. **Organic Carbon Partition Coefficient, K_{oc}:** The K_{oc} is perhaps the single most influential parameter governing the fate and transport of the dioxins from contaminated soils in this assessment, impacting surface water concentrations, vapor phase air concentrations, and directly or indirectly, all biomass concentrations (fish, vegetation, beef/milk). The literature for 2,3,7,8-TCDD shows a range of K_{oc} under 10⁶ (from Schroy, et al., 1985) to over 2x10⁷ L/kg (Jackson, et al., 1986). The value selected for 2,3,7,8-TCDD was 3.98*10⁶, based on an examination of available literature on the subject. The values tested were one order of magnitude less (4*10⁵) and one order of magnitude more (4*10⁷) than the value initially assumed for 2,3,7,8-TCDD.

4. **Air-to-Leaf Vapor Phase Transfer Factor, B_{vpa}:** The initial value for 2,3,7,8-TCDD was developed in a calibration exercise using field data which included air concentrations and grass concentrations which corresponded to these air concentrations. Details of this calibration are provided in Chapter 4, and will not be repeated here. Plus or minus an order of magnitude will be tested as a high and low value for B_{vpa}.

5. **Particle-Phase Fraction, ϕ :** This fraction was used in the stack emission source category for determining the portion of emitted contaminant that was and remained in the particle phase from stack to exposure site. Details on the measured and theoretical partitioning is given in Chapter 3 of this Volume. As discussed there, measured partitioning of 2,3,7,8-TCDD in ambient air showed a very small amount in the particle phase, 13%. However, speculation was that the monitoring method itself could lead to an underestimate in the particle phase, and for that reason, a theoretical approach was used to partition the dioxin. This led to a ϕ of 0.49 for 2,3,7,8-TCDD. The stack emission demonstration will be used to evaluate the impact of assuming 0.20 or 0.80 for 2,3,7,8-TCDD ϕ .

6. **Root Bioconcentration Factor, RCF:** The initial value for 2,3,7,8-TCDD was estimated as a function of octanol water partition coefficient, K_{ow}. Assuming a log K_{ow} of 6.8, RCF was solved as 5,200. Different assumptions for log K_{ow} were used to estimate high and low values of RCF for this exercise. Examining literature K_{ow} for the dioxin-like compounds, no log K_{ow} are less than 6.0 (the lowest at 6.2) and only one value estimated to exceed log K_{ow} equal 8.5. A high and low RCF were estimated, therefore, using log K_{ow} of 6 and 8.5. This led to tested values of RCF of 1,260 and 106,000.

7. **Beef/milk Bioconcentration Factor, BCF:** Unlike the RCF (but like the BSAF and BSSAF as noted blow), there are no empirical formulas developed for BCF as a function of more common parameters such as K_{ow}. The literature summary and interpretation of 2,3,7,8-TCDD cattle feeding studies by Fries and Paustenbach (1990) led them to assign a value of 5.0 for

2,3,7,8-TCDD. The study by McLachlan, et al. (1990) allowed for generation of BCF values for 16 of the 17 dioxin and furan congeners of dioxin toxicity equivalency, and the results from that study are used for this assessment. Fries, et al. (1999) presented another set of field-derived BCFs for 14 of the 17 dioxin-like dioxins and furans, and the BCF he calculated for 2,3,7,8-TCDD was 7.1. The 2,3,7,8-TCDD BCF used in this assessment was 5.76, which is close to the value of 5.0 promoted by Fries and Paustenbach (1990). Their summary, included in Table 4-5 in Chapter 4, showed BCF less than 1.0 for higher chlorinated dioxin-like compounds. For sensitivity testing, values of 1.0 and 10.0 were used as low and high values for BCF.

8. Biota Sediment and Biota Suspended Solids Accumulation Factors, BSAF and BSSAF: EPA (1993; 1995) summarizes several water column based and sediment (both suspended and bottom) based empirical parameters used to estimate fish concentrations given a water or sediment concentration. Two of these are the BSAF and BSSAF, which are used in this assessment. Although no data exists to determine values of the suspended solids factor, BSSAF, EPA (1993) suggests that BSAF values could be used. The range of BSAF values for 2,3,7,8-TCDD discussed in EPA (1993; 1995) is 0.03 to 0.30, and this was the low and high values selected for both BSAF and BSSAF. The literature summary on BSAF included in Chapter 4 of this assessment does include studies which imply higher BSAF for 2,3,7,8-TCDD. One study, which focused on bottom feeders (carp, catfish, etc.), found a BSAF for 2,3,7,8-TCDD (CDEP, 1992) of 0.76, whereas the range of 0.03 to 0.30 focused on column feeders. A high value of 2.94 (Kjeller, et al., 1990) was found in a lake in Sweden speculated to be impacted by an active pulp and paper mill. This high value appears to be an outlier not found in other field data sets.

9. First-order Plant Weathering Factor, kw: This is used to simulate the weathering of contaminated particulates which have settled on plant matter via dry and wet deposition. Several modeling efforts have used the same kw as used in this effort; that kw is 18.01 yr^{-1} , which corresponds to a half-life of 14 days. Values of 51 (half-life of 5 days) and 8.4 (half-life of 60 days) yr^{-1} were used to test the impact of this parameter.

10. Dissipation Rate Constant for Eroding or Depositing Contaminants, k: Evidence for soil degradation of the dioxin-like compounds indicates that residues even millimeters below the soil surface degrade at a very slow rate, if at all (see Chapter 2, Volume 2 of this assessment). This was the basis for not considering degradation of soil sources of dioxin-like compounds in this assessment. However, when residues migrate to impact only a thin layer of soil at a distant site, the processes of volatilization or photolysis (the one degradation process which appears to transform dioxin-like compounds in the environment) are likely to impact delivered residues. A rate constant of 0.0277 yr^{-1} , which corresponds to a 25-year half-life, was

used in two instances for this methodology - for erosion of off-site soils onto exposure site soils, and for deposition of stack emissions onto exposure site soils. This value was changed to 0.277 yr^{-1} (half-life of 2.5 years) and 0.00277 yr^{-1} (half-life of 250 years) in sensitivity testing.

6.3.3. Results

The results of the sensitivity analysis are principally described in a series of high/low bar graphs. The Y-axis is on a log scale and shows changes in media concentration estimation when the high and low parameter substitutions are made. The Y=1 line is the value of the media concentration with all baseline parameter selections; the precise value of that media concentration is noted on each graph. Other y-axis values are arrived at as the ratio of the pertinent media concentration estimated with the altered parameter over the baseline concentration; a y-axis value of 0.1, for example, means that the concentration with the parameter substitution was one-tenth the concentration under baseline conditions. Also noted on each graph is the pertinent source strength term - for air concentration sensitivities, soil concentrations are noted, and so on. The parameters tested are named on the x-axis, and these names correspond to the names in Table 6.1. The definition and baseline value of these key parameters are noted below each graph. The high and low values tested are appropriately placed either above (when the concentration increases with the parameter change) or below the bar graphs. These parameters are the only ones which impact the tested media concentration. Of course, the soil concentration also impacts the media concentration, but as noted in the previous section, soil concentrations have a direct and linear impact in all cases, and so are not displayed on the figures. Observations from each figure now follow.

6.3.3.1. *Estimation of Vapor-Phase and Particle-phase Air Concentrations Distant from a Site of Soil Contamination*

Results for this test are shown in Figures 6-1 and 6-2. For the test of the vapor-phase algorithm, Figure 6-1, no single change resulted in estimations over an order of magnitude different from that made with baseline parameters. The model is insensitive to porosity and particle bulk density parameters, E_{slp} and P_{soil} . The results are also reasonably insensitive to ranges for organic carbon content of soil, OC_{st} , and windspeed, U_m . For all other parameters, there appears to be roughly an order of magnitude spread over the range of parameters tested. Increasing the exposure duration to 70 years would decrease air concentration predictions by about 35% and decreasing the duration to 1 year would roughly double concentrations. As discussed earlier in Section 6.2, the volatilization algorithm assumes that contamination begins at

the soil surface at time zero, and residues available for volatilization originate from deeper in the profile over time. The result of this assumption is that the flux decreases as time increases. This is the only algorithm of this assessment where an assumption of a decreasing source strength over time is made.

Results from the test of the particle phase flux and dispersion algorithm are shown in Figure 6-2. The y-axis in this test spans two orders of magnitude since changes in the parameters describing the inherent wind erodibility of the soil, U_t and $F(x)$, results in over an order of magnitude higher and lower than concentration estimations as compared to estimations using the selected values of U_t and $F(x)$. The assumption of bare soil conditions at the site of contamination led to a value of 0.0 for V , the vegetative cover parameter. If the contaminated site had a reasonably dense vegetative cover leading to a V of 0.9, air concentrations at the nearby site of exposure would be about an order of magnitude less. The impact of area (ASC), distance (DL_c), and frequency (FREQ) on exposure site concentrations mirror those for vapor-phase air concentrations. That is because these three are used in the same far-field dispersion algorithm. Another parameter used for the far-field dispersion algorithm is windspeed, U_m . However, interestingly, the impact of that parameter is reversed between the vapor and particulate phase algorithms. For the particulate phase, the windspeed has more of an impact in increasing wind erosion and hence the reservoir of airborne contaminant - increasing windspeed increases air concentrations. For the vapor phase, windspeed does not play a role in estimating volatilization flux, but only a role in the far-field dispersion model. In that role, increasing wind speed increases dispersion and decreases concentrations.

Noteworthy for the particle phase algorithm is that estimated concentrations are independent of any chemical-specific parameters; wind erosion suspending the particles is only a function of climate, ground cover, and soil erodibility. Also noteworthy is that the baseline air concentration of contaminants on particles is over an order of magnitude lower than the baseline air concentration of contaminants in the vapor phase. Besides having implications for particle phase and vapor phase inhalation exposures, this difference also has implications for impacts to vegetation concentrations and subsequently to beef and milk concentrations.

The results shown in Figure 6-1 and 6-2 are specific to algorithms estimating emissions from soil, volatilization and wind erosion, and dispersion of those emissions to calculate an air concentration at a distant site. Chapter 4 also described an algorithm to estimate “near-field” dispersions, which can be used to estimate air concentrations above a site of soil contamination. Brief tests were conducted to evaluate the difference in impacts when the near field dispersion model is used instead of the far field dispersion model. One observation was that all parameters

associated with flux calculations had identical impacts to near-field air concentrations as compared to far-field concentrations. Included in this group were: for the volatilization algorithm - the exposure duration, ED, the organic carbon content, OC_{sl} , soil porosity, E_{slp} , particle bulk density, P_{soil} , and the three chemical-specific parameters, Henry's Constant, H, organic carbon partition coefficient, Koc, and molecular diffusivity, D_a , and for the wind erosion algorithm - fraction of vegetative cover, V, average windspeeds, U_m , and the parameters associated with the erodibility of the soil, U_t and F(x). The impact of area is different for concentrations calculated with the near-field algorithm compared to the far-field algorithm. This is because the area term, ASC, has a different role for the near field as compared to the far field algorithms. For the far field algorithm, ASC in effect impacts the source strength, with an order of magnitude increase in ASC increasing exposure site air concentrations by a little over 2 times (>200%). For the near field dispersion, ASC impacts the dispersion algorithm, and the same order of magnitude increase in area only increases concentrations by around 30%.

6.3.3.2. Estimation of Soil Erosion Impacts to Nearby Sites of Exposure

Results from this test are shown in Figure 6-3. This model shows little sensitivity to two parameters, the bulk density of soil at the site of exposure, B_{soil} , and the amount of "clean" soil (that which is between the contaminated and exposure site) which erodes onto the exposure site, SL_{ec} , along with the contaminated soil. These will not be discussed further. In contrast to SL_{ec} , the model has a direct linear impact with the amount of soil eroding from the contaminated site, SL_s . Decreasing that amount by a factor of 10 decreases exposure site soil concentrations by the same amount, and doubling contaminated site erosion also doubles exposure site soil concentrations.

The model appears to show insensitivity to the distance between the exposure and contaminated site, DL_e . However, this result should be viewed cautiously. The sediment delivery ratio equation was developed to estimate sediment loads from construction sites to nearby surface water bodies, and from distances up to 250 m. Its application to distances beyond that are questionable, and applications from one land area to another land area rather than from one land area to surface water, should also be questioned. At the model baseline distance of 150 m, the SD_s (sediment delivery ratio) is 0.26. At 1000 m, it is 0.17, which is a marginal dropoff for what appears to be a significant increase in distance. The distance becomes increasingly important when there are obstructions between the contaminated and the exposure site such as ditches, roads, and so on. When using this methodology, one should consider not relying on the sediment delivery ratio equation for: 1) transport of soils beyond 250 meters, 2) when the

exposure site is upgradient from the site of contamination (in its development for construction sites, the assumption that a water body is downgradient soil concentration at the exposure site only doubled; it did not increase by an order of magnitude. It is unreasonable to assume that all the eroded soil would crowd into the smaller exposure site. When the contaminated site decreased an order of magnitude to 4,000 m², the exposure site soil concentration likewise decreased by an order of magnitude. In this case, like the case when the contaminated and exposure site were of the same size, all the contaminated soil eroding in the direction of the exposure site mixes into exposure site soil, so the resulting average soil concentration at the exposure site is linearly related to the concentration at the contaminated site. A similar trend is noted with changes in the exposure site area term..

The impact to changes in depth of tillage is nearly, but not quite, linear. Decreasing the no till depth of mixing, d_{not} , from 0.02 m to 0.01 m increased soil concentrations by a factor of 1.4 roughly, while increasing d_{not} to 0.10 decreased concentrations by 70%. A similar, nearly linear, impact is noted with the changes tested for tillage depth, d_t . For figure clarity, these results were left off Figure 6-3, but decreasing the depth from an initial 0.20 m to 0.10 m increased concentrations by just under a factor 2, and decreasing it to 0.30 m decreased concentrations by just under 33%.

The impact of changing the dissipation rate is not linear. Decreasing the rate by an order of magnitude, which is equal to increasing the half-life from 25 to 250 years, only about doubles the predicted soil concentrations, while increasing the dissipation rate by an order of magnitude, or reducing the half-life to 2.5 years, reduces the soil concentration by a factor of 5.

It is interesting that some of the tested model parameter changes, including manipulation of the areas of contamination and exposure sites, and the dissipation rate, result in increasing the exposure site soil concentration to nearly the same concentration as the contaminated site. This is a somewhat counterintuitive result; it seems unlikely that an off-site location would have concentrations close to the contaminated site. If, in fact, the model has a tendency to overpredict exposure site concentrations, there are several reasons why this might occur: 1) overestimation of the sediment delivery ratio, which was discussed above, 2) a shallow mixing depth for untilled situations, 3) a low dissipation rate (which translates to a long half-life), 4) high estimates of erosion from the contaminated site, and/or 5) use of a steady state solution.

Regarding this latter point, a steady state solution means that if erosion continues indefinitely and the contaminated site soil concentrations do not lessen during this time, than the exposure site soil concentrations reaches the level predicted by the model. This could lead to a significant overestimation if the soil contamination was relatively recent. For example, if the

erosion from a contaminated site to an exposure site has been occurring for 25 years, it can easily be shown that the full solution to the soil concentration, Equation (4-16) in Chapter 4, will result in a soil concentration that is 72% of the concentration estimated using the steady state simplification, Equation (4-17) in Chapter 4. At 50 years, the modeled soil concentration will be 92% of the steady state solution. These calculations assumed the half-life of 25 years. Therefore, if the soil contamination occurred within 20 years or so, assessors may wish to model a lower and perhaps more accurate soil concentration by using the full solution rather than the steady state solution to estimate exposure site soil concentrations and impacts.

6.3.3.3. Estimation of Soil Erosion Impacts to Nearby Surface Water Bodies

Results from this test are shown in Figure 6-4. One immediate point to make about this bar graph is that the results displayed are essentially identical for water, bottom sediment, and fish concentrations, with the exception of two trends which will be described below. Also, since bottom and suspended sediment concentrations are assumed to be linearly related by the equation: $C_{ssed} = (OC_{ssed}/OC_{sed}) * C_{sed}$, where C_{ssed} and C_{sed} are suspended and bottom sediment concentrations, respectively, and OC_{ssed} and OC_{sed} are suspended and bottom organic carbon fractions, than the relationships in Figure 6-4 apply to suspended sediment concentrations as well.

One of the exceptions has to do with trends regarding partitioning of dioxins between sediments and water. The parameters involved in this algorithm are the organic carbon content parameters, OC_{ssed} and OC_{sed} , and the organic carbon partition coefficient, K_{oc} . First, the direction of the change is not the same. The sorption, and hence concentration, of dioxin-like compounds onto sediments can be increased by increasing the organic carbon content of the sediments or increasing the K_{oc} . However, doing either decreases the concentration in water. For the "low organics" test, water concentration increases by a factor of 2.7 rather than slightly decreases as in Figure 6-4, which for this case, displays only the impact to bottom sediments. For the "high organics" test, water concentrations decrease to 0.60 of what they were in baseline conditions. The high K_{oc} decreases water concentrations to 0.1, and the low K_{oc} increases water concentrations 7 times. Both these trends are distinctly different than the sediment trends; they were left out of the graph in order not to crowd the graph (or require another one be drafted), and also because water concentrations in the sub-ppq range are of minimal concern for exposure. The other exception has to do with the impact of changes to the organic carbon content of bottom and suspended sediments in the calculation of fish concentrations. Fish tissue concentrations for three of the four source categories of this assessment are a direct function of bottom sediment

concentrations; the one source category where this is not true is the effluent discharge source category, where fish tissue concentrations are a function of suspended sediment concentrations. As laid out in Chapter 4, whole fish tissue concentrations are estimated as: $(C_{sed}/OC_{sed}) * BSAF * f(\text{lipid})$, when fish tissue concentrations are a function of bottom sediment concentrations, and for the effluent source category, fish tissue concentrations are estimated as: $(C_{ssed}/OC_{ssed}) * BSSAF * f(\text{lipid})$. It is seen from Figure 6-4 that the concentration on bottom sediments, C_{sed} , is impacted by the value assigned to OC_{sed} . However, the impact to C_{sed} with changes to OC_{sed} is marginal and in the same direction. For example, reducing OC_{sed} from its baseline of 0.03 to 0.01, reduces C_{sed} by a small amount. The impact to fish tissue from changes in OC_{sed} is more pronounced and essentially in an inverse linear manner, as shown by the formulation above.

Other than these two exceptions, a principal message from Figure 6-4 is that all surface water impacts are identically impacted by surface soil and erosion parameters. The comments in the above section concerning the distance between the contaminated soil and the target site, which in the above section was the exposure site, but for here it is the surface water body, also pertains to this algorithm. Specifically, it was noted that the sediment delivery ratio equation seemed relatively insensitive to changes in distance. In Figure 6-4, this also seems to be the case, as little change in predicted water impacts occurs between the tested values of 50 and 1000 meters. However, if clear impediments such as roads or ditches are between the site and the target area as the distance increases, than it is quite possible that the sediment delivery ratio equation is not appropriate to use when predicting the delivery of contaminated soil to the water body. On the other hand, if a site is near a surface water body, it seems that the origins of the sediment delivery ratio equation - developed from data on construction sites near surface water bodies - are more appropriate.

The key source strength terms tested, the area of contamination, ASC, and the soil loss rate from the site of contamination, SL_s , both have a direct linear impact on the both sediment and surface water concentrations. The other soil loss term, the erosion rate for the watershed, SL_w , also has a direct linear impact. Somewhat less critical in this algorithm is the size of the watershed. The reduction of watershed size by about an order of magnitude increased water concentrations by about a factor of 2, and an increase in size by an order of magnitude reduced impacts by about 70%.

The algorithm seemed fairly insensitive to the remaining five parameters tested. The average watershed concentration, initialized at 0.0 in order to just show the incremental impact from the contaminated site, was increased to 1 ppt. This approximates a background concentration of 2,3,7,8-TCDD and was an order of magnitude lower than the contaminated site

concentration of 1 ppb. It is seen in Figure 6-4 that background soils have a marginal impact on a water body which is impacted from a site of elevated soil concentrations located near the water body. The impact of the organic carbon partition coefficient, K_{oc} , on bottom sediments appears small despite the fact that the K_{oc} range spans two orders of magnitude. This is an indication that it is so high for the dioxin-like compounds, that (at least in the algorithm of this assessment), its assignment is not critical for sediment concentration estimations. The same lack of impact appears to be the case for the organic carbon content of water body sediments, and the level of suspended solids in the water column. The range of enrichment ratios tested, 1 to 5, represents the appropriate high and low value this parameter would take, based on literature studies of this phenomena. As will be discussed in Chapter 7, a site in Connecticut had sediment concentrations in background settings about 2.8 times higher than surface soil concentrations. In this tested range, only a small impact to surface water is noted.

6.3.3.4. Vapor-Phase Transfers and Particle-Phase Depositions to Above Ground Vegetation

Concentrations in above ground vegetation are a function of vapor-phase transfers and particle phase depositions. Vapor and particle reservoirs originate from contaminated soils as volatilization and wind erosion, respectively. Atmospheric dispersion and deposition modeling delivers concentrations and depositions, respectively, from a stack to a site of exposure. The principal difference in the soil and stack emission source categories is in the relative proportions of the contaminant which are in the vapor and particle phases. As discussed below, more contaminant is delivered via particle depositions for the stack emission source category as compared to the soil contamination source category.

Vapor transfers and particle depositions for the soil contamination source category are evaluated in Figures 6-5 and 6-6. The same general trends shown in these figures also occurs in the stack emission source category. Three types of vegetation are modeled for this assessment, including vegetables/fruit, grass, and animal feeds. The latter two are for the terrestrial animal bioconcentration algorithms, the first for human exposure via consumption of unprotected fruits or vegetables.

For vapor-phase impacts shown in Figure 6-5, it would appear that changes to total vegetation concentrations are critically a function of parameters specific to the vapor transfer algorithm. There is between one and two orders of magnitude range of plant concentrations predicted over the range of the vapor phase transfer coefficient, B_{vpa} , tested. This parameter is uncertain as well as very influential in this methodology. There is about a one order of magnitude range for the vegetable/fruit category and a two order of magnitude range for the grass

and feed categories. The reason there is a difference in the influence of B_{vpa} in the vegetative categories has to do with the use of a second and also influential and uncertain parameter, the VG parameter. This parameter was introduced to model the difference between the leaves of the experiment for which B_{vpa} was developed and the bulky vegetation to which the B_{vpa} is applied, the VG parameters (VG_{veg} , VG_{gr} , and VG_{fod}). The need for such a correction factor is justified given the evidence that dioxin-like compounds do not translocate into vegetation. The grass leaf concentrations in the experiments for which B_{vpa} was derived are likely to be analogous only to the outer layer concentrations in bulky vegetation, not the whole plant (or whole fruit/vegetable) concentrations. This empirical parameter was set to 0.01 for bulky fruits/vegetables, but was set at 1.00 for grass, under the assumption that grass is similar to leaves, and 0.50 for cattle fodder, which is assumed to contain some bulky (grains) and leafy (hay) vegetation. Relatively speaking, therefore, the impact of grass concentrations to vapor phase concentrations are 100 times higher than the impact of vegetable/fruit concentrations to vapor phase concentrations because of this VG parameter. There is a linear impact for grass and feed to changes in VG - halving VG for grass halves the grass concentration, for example. The impact of changes to VG is less for vegetables/fruits, again because its influence is minimized due to its low initial value of 0.01.

A dry weight to fresh weight conversion factor, FDW, is required for estimating above ground concentrations of vegetable/fruits. This is because the algorithms estimate above ground vegetative concentrations on a dry weight basis, and the concentrations need to be diluted since fruit and vegetable consumption are given in this assessment on a fresh weight basis. The impact to concentrations is direct and linear, and since the range of likely FDW is small, the impact is small as well. This parameter is also required for the particle deposition algorithm, but is left out of Figure 6-6 for clarity. In fact, FDW is applied once vapor phase and particulate phase contributions to vegetable/fruit concentrations are already summed; in other words, it is not tied to either the vapor or particle phase algorithms.

The impact of all the particle phase parameters to overall plant concentrations is less than that of vapor transfers, as seen in a comparison between Figures 6-5 and 6-6. For the parameters including rainfall amount (R), washout factor (W_p), denseness of vegetation (as modeled by yield, Y, and intercept fraction, INT), velocity of particle deposition (V_p), and plant weather dissipation rate, kw, results in Figure 6-6 are for vegetable/fruits and not grass or fodder. Vegetables/fruits are more impacted by particle depositions than grass/fodder, and as seen, there is less than half an order of magnitude impact from the range of values for these parameters tested. As noted above, the impact of depositions on vegetable/fruit concentrations occurs because the correction factor for vegetables, VG_{veg} , is equal to 0.01, which minimizes the vapor-

phase contributions to vegetable concentrations in comparison to the contributions of the vapor phase concentrations for grass and fodder concentrations, which have correction factors of 1.00 (for grass) and 0.50 (for fodder).

This trend is quantified in Table 6-2. Model results on the proportion of above ground plant concentrations that are due to air-to-leaf transfer and particulate deposition were examined for the soil contamination and stack emission source categories for 2,3,7,8-TCDD, and results are summarized in Table 6-2. Results show that vapor phase transfers tend to dominate vegetative concentrations, although particle phase concentrations are important for bulky fruits and vegetables. Results also show that the relative impact of vapors and particles is a function of distance for the stack emission source category. For the central stack emission Scenario, #4, where the site of exposure is 5000 meters from the stack, vapor transfers generally have more of an impact to vegetation as compared to the high end Scenario, #5, where the site of exposure is 500 meters away.

It is possible that the impact of particle depositions is being underestimated, for at least four reasons:

- The wind erosion algorithm estimating air-borne contaminant concentrations for the soil contamination source category only estimates concentrations of PM-10, or inhalable size particulates, those 10 μm size diameter and less, while the ISCST3 model considers all size particulates emitted from stacks. Larger size air-borne particulates, while not inhalable, would deposit onto vegetation.
- For the demonstration of the soil contamination source category which involves soil contamination distant from the site of exposure, only the off-site locations provide the source of air-borne particulates. Meanwhile, algorithms are in place estimating exposure site contamination, albeit to thin surface levels. Certainly, the reservoir of air-borne particulates depositing onto vegetation would also include contributions from where the vegetation is located and the surrounding land, not only from the area of soil contamination.
- For the stack emission source category, resuspension of deposited particles and deposition onto plants is not considered. This omission is similar to the omission noted in the bullet above.
- The modeling does not consider the splash effect of rainfall, which would deposit soil onto the lower parts of plants. This would make the most impact for grass and for vegetables near the ground surface such as lettuce.

- For the soil contamination source category, an additional factor is on the way the model does not reapportion volatilized residues onto airborne particles. As was discussed in Chapter 5, the 2,3,7,8-TCDD vapor phase dominates the total air concentration and is about 95% of the total concentration. Residues which volatilize from the soil are assumed to remain in the vapor phase. In contrast, the 2,3,7,8-TCDD vapor phase is 51% of total air concentrations in the stack emission source category, because this is the fraction developed from the equilibrium vapor/particle partitioning algorithm. If dioxins were reapportioned after volatilizing, the vapor/particle partitioning for the soil contamination source category would shift over to the particle phase and the particle phase impacts to vegetation would be increased.

The precise impact of these factors might be investigated more fully in a later assessment with additional models. Tests were run for this sensitivity analysis by increasing the amount of particulate phase contaminants depositing onto vegetation by an order of magnitude to the soil contamination demonstration scenario, without changing the vapor phase contributions. The vapor phase/particulate phase contributions to above ground fruits and vegetables, originally 56%/44% (from Table 6-2), changed to 11%/89% with an order of magnitude increase in particulate phase contributions. Vegetable concentrations increased by a factor of 6. The impact was less for grass and fodder, with concentrations increasing by a factor of 1.7.

The impact of partitioning of airborne dioxins between a vapor and a particle phase was more fully investigated using results from the high end demonstration of the stack emission source, Scenario 5. The results from this analysis are shown in Figure 6-7. For this test, the partitioning of 2,3,7,8-TCDD was altered from the originally assigned values of 51% vapor/ 49% particle. The vegetation examined include above and below ground vegetable concentrations, and above ground grass and cattle feed.

The obvious trend to note from this figure is that the impact of this repartitioning is the opposite for vegetables/fruits, both above and below ground, as compared to grass and cattle feed. For above ground vegetation, this is the result of the use of the empirical correction factor, VG. As discussed above, assignment of the value of 0.01 for vegetable/fruit VG minimizes the impact of vapors on above ground vegetables/fruits. Therefore, when particle phase depositions are increased, as in the right-hand side of Figure 6-7, vegetable/fruit concentrations increase, and likewise, decreases in particle phase depositions decrease the concentrations. The reason that the trend is the same for below ground vegetables is that changes in particle depositions lead to concurrent changes in soil concentrations. Since the leafy vegetation of grass and cattle feed are

dominated by vapor phase transfers, reductions and increases in the vapor phase concentration lead to reductions and increases in the concentrations of these vegetation. Even at the lower vapor fraction, 20% in the right-hand side of Figure 6-7, vapor impacts still dominate the predicted concentrations for these vegetation.

6.3.3.5. *Estimation of Below Ground Vegetable Concentrations*

One important factor to note up front about below ground vegetable concentrations as compared to above ground vegetable concentrations (no underground fruits are assumed in this assessment) is that below ground vegetable concentrations of 2,3,7,8-TCDD are about four orders of magnitude higher than above ground vegetable concentrations for the soil contamination demonstration scenario. For the stack emission scenario, above and below ground concentrations of 2,3,7,8-TCDD are comparable. Also, the below ground vegetable ingestion rate of 1.16 g/kg-day is quite comparable to the above ground vegetable ingestion rate of 1.52 g/kg-day. Given the difference in concentration estimations in the soil contamination demonstration, below ground vegetables explain over 99% of the total exposure via ingestion of impacted vegetables in that demonstration. Again, they are about half the total vegetable exposure for the stack emission source category. Sensitivity of underground vegetable concentrations to parameter changes for the soil contamination source category becomes important from this perspective.

The reason for this dichotomy in performance between the soil contamination and stack emission source categories has been examined in other parts of this document, including the examination of vegetable results in Chapter 5, and the soil-to-air model testing in Chapter 7. To review these discussions, it was found that when soil is assumed to be source for air concentrations, as in the soil contamination source category, then a ratio of air to soil concentrations will be very low compared to an air to soil concentration ratio when the air is assumed to be source for soil concentrations, as in the stack emission source category. This air to soil ratio does not have any important meaning except in the context of this discussion. Two possible explanations were offered for this trend: 1) the models predicting volatilization and dispersion were underpredicting air concentrations, and/or 2) the soil to air models are not underpredicting air concentrations - the tendency for dioxins to escape soil (i.e., the fugacity of dioxins in soil to air transfers) is very low compared to the tendency for dioxins to move towards soil.

This question now is whether this dichotomy in performance is reasonable. A model exercise in Chapter 7 evaluated the air-to-soil algorithm and the soil-to-air algorithm using air

and soil data from the same rural site. It was shown that the air to soil model very reasonably was able to duplicate the soil concentrations, but that the predictions of air concentrations above the soil were much lower than observed, by about an order of magnitude. Again, this could be due to the fact that the models may be underpredicting air concentrations above them. Also, it could be due to the fact that air concentrations measured in the rural setting are due to long range transport from distant sources and not the soil concentrations. Given that the model appeared to perform well in air-to-soil modeling, it is expected that the observation that above, and below ground vegetable concentrations in the stack emission are comparable, is supportable. The same confidence cannot immediately be placed on the difference in modeling between above and below ground vegetables for the soil contamination source category.

In any case, the impacts of parameter changes for the algorithm predicting concentrations in underground vegetables are shown in Figure 6-8. These results were generated by the soil contamination source category, although analogous results would result for the stack emission, source category. All results are essentially linear, which is not surprising since below ground vegetable concentrations are a linear function of all the parameters tested: $C_{veg} = (C_{soil} * RCF * VG_{bg}) / (Koc * OC_{sl})$. The two orders of magnitude range for the root concentration factor, RCF, translates to a two order of magnitude range of concentration estimation. The same is true for the empirical correction factor applied to below ground vegetables, VG_{bg} , and the organic carbon partition coefficient, Koc. A smaller impact is noted for the organic carbon fraction of soil, OC_{sl} . Koc and OC_{sl} are required for this algorithm because vegetable concentrations are a function of soluble phase concentrations, not soil concentrations. Increasing Koc and/or increasing OC_{sl} results in decreasing the water concentrations, explaining why the high values for these parameters reduce vegetable concentrations. The smallest range in Figure 6-8 is the depth of tillage parameter, which directly influences the soil concentration, C_{soil} . Reducing the depth of tillage by 2 increases the soil concentration by about this same amount, as seen in Figure 6-8.

One final note is that the dry to fresh weight ratio, FDW, is not on this figure, while it does appear on Figure 6-7. This is because the RCF was developed on a fresh weight basis already, so no conversion to a fresh weight is required.

6.3.3.6. *Beef Fat Concentration Estimation in the Soil Contamination and Stack Emission Source Categories*

The impacts of parameter changes to beef fat concentration estimation for the soil contamination and stack emission source categories are shown in Figures 6-9 and 6-10. These sensitivity runs were both run on 2,3,7,8-TCDD, the only dioxin congener demonstrated for the

soil source category in Chapter 5, but 1 of the 17 dioxin-like congeners evaluated in the demonstration of the stack emission source in Chapter 5.

The overriding difference in the way the two source categories predict beef fat concentrations is that, in the soil contamination source category, the soil-to-cattle pathway dominates the prediction of beef fat concentration, whereas in the stack emission source category, the air-to-plant-to-cattle dominates. In Figure 6-9 showing results for the soil contamination source, there is essentially a linear relationship between changes in soil concentration and the beef impact, whereas in Figure 6-10 showing the stack emission relationships, a nearly linear impact is noted instead for changes in the grass and fodder concentrations. This overall trend is principally due to trends that have previously been discussed - that is, when soil is the source of contamination, the impact to air and above ground vegetation is proportionally smaller as compared to when air is the source of contamination.

This trend is further elucidated in the impact of two other soil related tests - one on the soil bioavailability factor, B_s , and one on the proportion of soil ingested in the cattle diet. In both cases, changes to these parameters have a significant impact in the soil source category but a minor impact in the stack emission category. Actually, the importance of soil exposure in the soil source category and the importance of vegetation in the stack emission category influences most of the other results on Figures 6-9 and 6-10. In the "low" exposure conditions, the reduction in soil intake from 4% of the diet to 1% of the diet influenced the results for the soil source category, but the influence was minor for the stack emission category because intake of contaminated grass was essentially unchanged and the "lower" exposure was mainly reflected in a reduction of intake of contaminated cattle feed. In the "extent of pasturing" test, the increase in soil intake from 4% to 8% resulted in a significant impact for the "high" condition in the soil source category, but less of an impact in the stack emission category, because again the vegetative intakes were not significantly changed for this test.

In addition to the sensitivity analysis shown in Figures 6-10 and 6-11, this trend can be described simply by displaying the following results from the demonstration of the soil source and stack emission source categories from Chapter 5:

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Description	Percent impact due to ingestion of:		
	Soil	Grass	Feed
Soil contamination, beef	98	< 1	> 1
Soil contamination, milk	97	< 1	> 2
Stack emission, beef	11	61	28
Stack emission, milk	7	14	79

As seen here, soil only accounts for 11 and 7% of beef and milk concentration impacts from stack emissions in the example scenario, but overwhelms the soil source category.

The only parameter which was equally influential for both categories, was the bioconcentration factor, BCF. To estimate beef fat concentrations, the concentrations in the soil and vegetation of the cattle diet are multiplied by this factor, so logically, its influence is separate from the modeling of concentrations in soil or vegetation. Also, the response to changes in this parameter are linear.

As seen in the above results, the relative impacts of soil and vegetation to milk fat is similar to that of beef fat in the two source categories. The baseline scenario for a dairy cow's exposure has a significantly greater amount in cattle feed, 90%, as compared to the beef cattle, 45%. That is why the percent of impact for milk is more driven by feed than grass as compared to beef in the stack omission source.

The free range chicken scenario is driven by soil in both the stack emission and the soil contamination scenario. The following results display this trend:

Description	Percent impact due to ingestion of:		
	Soil	Grass	Feed
Soil contamination, chicken and eggs	> 99.9	< 0.1	0
Stack emission, chicken and eggs	79	21	0

The reason for this trend is that the free range chicken exposure scenario has the chicken diet comprised of 10% soil, 5% incidental leafy vegetation while scavenging, and 85% residue free chicken feed. The justification for assuming that 85% of the chicken diet was residue free came

from Stephens, et al. (1995), who did not detect dioxins in the analysis of a standard chicken feed. They also developed the chicken/egg bioconcentration factors used in this assessment and assumed a 10% soil percent in the diet of the free range chicken. Further detail on the use of the Stephens, et al. (1995) data can be found in Chapter 4. In any case, it is expected that the chicken and egg models will respond to parameter changes in the same manner as the beef fat sensitivities as displayed in Figure 6-9, showing sensitivities in the soil contamination source category, rather than Figure 6-10, which shows the stack emission source sensitivities.

6.3.3.7. *Impact of Distance from the Stack Emission Source on Concentrations in Soil, Vegetables, and Beef Fat*

For this test, the high end scenario for the stack emission demonstration, Scenario 5, was used as the baseline. The exposure site was located 500 meters from the stack in the downwind direction. Two other locations, 200 and 5000 meters, were, evaluated, and predictions for soil, below and above ground vegetables, and beef fat were examined. The results of this examination are shown in Figure 6-11.

In the high end stack emission demonstration scenario, the farm was assumed to be 500 meters from the stack. Nearer to the stack at 200 meters, ambient air concentrations and dry deposition amounts were lower, but wet deposition was at its maximum. One effect of this was that vegetable concentrations increased. Below ground vegetables increased by about a factor of about 4, due to the same increase in soil concentration as a result of much higher wet deposition. Above ground vegetation increased by about 50%. As was described earlier, particle depositions dominated above ground vegetable/fruit concentrations. Therefore, an increase in overall particle depositions due to an increase in wet depositions led to increased above ground vegetable/fruit concentrations. However, the trend was not the same for beef fat. As discussed in earlier sections, vapor contributions dominated grass and feed concentrations for the stack emission source category. Therefore, a drop in ambient air vapor phase concentrations at 200 meters as compared to 500 meters dominated the result, and the net impact was to reduce beef fat concentrations. From Figure 6-11, it is seen that beef fat concentrations were reduced by about 30% when using ISCST3 output from 200 m instead of 500 m. Further from the stack at 5000 meters, all biota concentrations were lower. Vapor phase air concentrations were roughly halved as compared to what they were at 500 m, and dry and wet deposition were lower by 60 and 80% respectively compared to levels at 500 m. This led to substantial reductions in vegetable concentrations. Beef fat concentrations were also lower at 5000 meters as compared to 200 m

and the baseline distance of 500 m. Overall, beef fat concentrations were about 70% less at 5000 meters as compared to 500 m.

Trends for milk fat concentration are not exactly the same, but very similar to those of beef fat. Trends for chicken and egg are similar to that of soil and below ground vegetables, because these tissues are modeled primarily as a function of the free-range chicken exposure to soil - this was discussed in the previous section to this one.

6.3.3.8. *Water and Fish Concentrations Resulting from Effluent Discharges*

The impacts of parameter changes for algorithms estimating water and fish concentrations are shown in Figure 6-12. First, it should be noted that fish and water impacts are included in the same graph because the impacts to both concentrations are exactly the same with the noted changes in parameters, with one exception. This exception is the partition coefficient, K_{oc} . Increases in K_{oc} result in higher suspended sediment concentrations, which lead to higher fish tissue concentration estimations, but lower water concentration estimations. Increasing K_{oc} by an order of magnitude actually decreases water concentrations to 14% of its baseline value, or 0.14 on the y-axis of Figure 6-12. Decreasing K_{oc} by an order of magnitude increases water concentrations by a factor of 2.4. Roughly, the location of the high and low K_{oc} points on Figure 6-12 should be reversed for water concentration impacts. Also, the biota to suspended solids accumulation factor, BSSAF, and the fish lipid content, f_{lipid} , are specific to fish tissue estimations.

Clearly, both concentrations are mostly impacted by the loading rate - the impact is linear and direct. Of all the parameters describing the effluent stream and the receiving water body, only the two order of magnitude change in receiving water body flow rate seems to have about an order of magnitude range of predictions. The effluent flow rate is ultimately low in comparison to the receiving water body, so its impact is limited. The range of organic carbon contents of the effluent and of the suspended solids in the receiving water are reasonably assigned and appear to have a small impact.

Higher suspended solids content in the receiving water body can result in lower fish and water concentrations. This might be termed a "solids dilution effect". Few studies are available in the literature which support this result, but two studies were found which are consistent with a solids dilution effect. One "simulated field experiment" conducted by Isensee and Jones (1975) maintained a constant water concentration of 239 ppb, but reported a decrease in 2,3,7,8-TCDD concentrations in both mosquito fish (2200 ppb to 90 ppb) and catfish (720 to 90 ppb) as the amount of sediment increased from 20 to 440 g. Sherman (1992), in a review of this and other

simulated field experiments and laboratory flow through experiments, points out that a bioconcentration factor for these simulated field experiments would decrease as the sediment increases. He speculates that, in comparing water flow through experiments with field simulated data, the bioconcentration factors tend to be less in field simulated experiments because 2,3,7,8-TCDD may sorb to sediments and be less bioavailable. A second study supporting a solids dilution effect was conducted by Larsson, et al. (1992). They studied uptake of PCBs and p,p'-DDE in 341 northern pike in 61 lakes in southern Scandinavia. They found that the levels of these persistent pollutants in the fish decreased as productivity increased. Productivity was measured by total phosphorus, chlorophyll a, and lake water transparency, which was mainly influenced by phytoplankton biomass. Their hypothesis was that the levels decreased because humus adsorbs persistent pollutants, rendering them less available for uptake in fish.

The two order of magnitude range in Koc translates to about a one order of magnitude range in estimated fish and water concentration estimations. Fish tissue concentrations are linearly and directly related to the BSSAF and f_{lipid} . About an order of magnitude of concentration estimation is noted with about the same order of magnitude in likely values.

6.3.3.9. Water and Fish Concentrations Resulting from Stack Emissions

Results of sensitivity analysis of algorithms estimating surface water and fish concentrations resulting from stack emissions are shown in Figure 6-13. First, it is noted that the impact to both these media is the same with impacts to all parameters. The impact with changes in the deposition of particles onto the water body, $RDEP_p$, and with the fraction of deposited particles remaining in suspension, f_{sd} , is negligible. The assigned values to these parameters for the demonstration are, therefore, sufficient for any purpose. It is importantly noted the ISCST3 model or other atmospheric transport models do not need to estimate the concentration of contaminants on emitted particles - all that is required are mass emissions of contaminants (in g/sec units) and the delineation of size fractions of particles emitted. The ISCST3 model does not require a particle emission rate. An assumption of a greater deposition of particles directly into surface waters might translate back to an assumption of particle emissions. The $RDEP_p$ is only required to maintain a mass balance of solids entering the surface water body, and as it turns out, particles entering surface waters by this route are only a miniscule part of the total solids entering the body. There are no impacts to water or fish concentration estimations with reasonable values for this parameter. The same appears true for f_{sd} , which determines the extent to which directly depositing contaminants remain in suspension. The assigned value of 1.00 (meaning that all directly depositing contaminants remain in suspension), based on the argument

that particles emitted from stack are likely to be lighter than eroding soil particles, appears sufficient for general purposes.

Water body impacts are essentially linearly related to the average watershed depth of mixing. The value assigned for the demonstration scenario was 0.1 m, which is midway between the value assumed for non-tilled conditions, 0.02 m, and tilled conditions, 0.20. The value of 0.10 m suggests that half the watershed is tilled. The linear relationship underscores the importance of this uncertain parameter, and also suggests that erosion drives water body impacts rather than direct deposition. This trend is also apparent for the tests on depositions to the watershed, the RDEP_{wat} input, versus depositions directly onto the surface of the water body, the RDEP_{sw} input. The impact to changes in RDEP_{wat} are roughly linear - an increase in watershed depositions (but not depositions directly onto the water body) by about a factor of 13 leads to an increase in the water body impacts by a factor of 11. There was less but still a noteworthy change when depositions directly onto the water body increased or decreased - a 13-fold increase led to a 2.5 fold increase in water body impacts.

Changing the size of the watershed did not have much of an impact to water body impacts. In changing the size, the four parameters as noted on Figure 6-13 were changed simultaneously. Intuitively, increasing the size of watershed should increase water body impacts, since more land impacted by depositions would be draining into the water body. However, two factors counter this intuition: 1) the water body volume also changes concurrently, tending to dilute any additional soil inputs, and 2) soil inputs are not proportionally increased because the sediment delivery ratio decreases as the size of the watershed increases - from 0.06 in the baseline setting to 0.01 in the test for the large watershed. In fact, water body impacts dropped slightly for the large watershed and increased only very slightly for the smaller watershed. This increase was due also to the change in the sediment delivery ratio, which increased from 0.06 to 0.25.

6.3.4. Key Trends from the Sensitivity Analysis Testing

These are as follows:

- 1) Source terms are the most critical for exposure media impacts.** Source terms include soil concentrations, stack emissions, and effluent discharges. In nearly all cases, the impact to exposure media is linear with changes to source terms. Proximity to the source term can be important as well, as demonstrated with differences in distance from the stack emission source.
- 2) Chemical-specific parameters, particularly the bioconcentration/biotransfer parameters, are the second most critical model inputs.** Some of these have lesser impacts,

such as the organic carbon partition coefficient, K_{oc} , for surface water impacts. Generally, at least an order of magnitude in range in possible media concentrations is noted with the range of chemical-specific parameter ranges tested. The impact of changes to bioconcentration/biotransfer parameters is mostly linear. This is because these transfer factors estimate media concentrations as a linear transfer from one media to another - fish lipid concentrations are a linear function of the concentration of contaminants in sediments. These transfer parameters are also identified as uncertain parameters. Tested ranges sometimes spanned over an order of magnitude for 2,3,7,8-TCDD.

3) All other parameters had less of an impact as compared to source strength and chemical specific parameters; nearly all impacts were within an order of magnitude for the range of tested values. Part of the reason for this trend is that there is a reasonably narrow range for many of the parameters in this range - soil properties, wind speeds, vegetation yields, and others. It is important, nonetheless, to carefully consider all the model parameters. While impacts were generally within an order of magnitude of the values selected for the demonstration scenarios, there was often an order of magnitude or more difference between plausible high and low values for individual parameters.

4) A principle trend of note concerns the air to soil algorithm for the stack emission source category compared to the soil to air algorithm of the soil source category. Several tests in this chapter demonstrated the difference in model performance when soil is the source of contamination compared to when air is the source of contamination. The relationship between air and soil concentrations is distinctly different for the soil contamination source category as compared to the stack emission source category. It is found that the "air/soil" concentration ratio is much smaller in the soil source category as compared to that same ratio in the stack emission source category. This air to soil ratio does not have any important meaning except in the context of this discussion. An air-to-soil model validation exercise in Chapter 7 showed that the deposition modeling appeared to very reasonably predict soil concentrations. This exercise relied on concurrent measurements of air concentrations and soil concentrations in an actual rural background setting. The air concentrations became the independent variable used to model soil concentrations. The reasonable validation was the result of predicted soil concentrations matching observed soil concentrations. However, when the same exercise was turned around - i.e., the observed soil concentration was used to predict air concentration, it was found that the predicted air concentration was much lower than the observed air concentration. Two possible explanations were offered for this trend: 1) the models predicting volatilization and dispersion were underpredicting air concentrations, and/or 2) the soil to air models are not underpredicting

air concentrations - air concentrations over a soil are perhaps more a function of atmospheric transport from distant sources than volatilization or wind erosion from soils. In any case, this dichotomy in air/soil model performance had several cascading impacts as were found in this chapter as well as Chapter 5 demonstrating the methodologies. Results include, for example: 1) soil concentrations drive terrestrial animal food concentrations for the soil source category, since vegetation concentrations are so low as not to be a large influence in comparison to soil. On the other hand, the vegetation concentrations drive the terrestrial animal food concentrations in the stack emission source category - the air-to-plant pathway is most important here, and 2) below ground vegetable concentrations are four orders of magnitude higher than above ground vegetables for the soil contamination source category while they are roughly comparable for the stack emission source category.

6.4. MASS BALANCE CONSIDERATIONS

As has been discussed in this document more than once is the characterization of this methodology as a screening level methodology. Steady state, equilibrium partitioning, and assumptions of nondegradation of source strengths are key assumptions which lead to this qualification. Stacks are assumed to emit a constant amount of contaminant over a duration of exposure for the stack emission source category. Effluent discharges are assumed to continue unabated over a duration of exposure. These are both reasonable assumptions for evaluating the long-term impacts of these sources where no change in practices occur. Any violation of mass balance principals will, therefore, not be examined for these sources. The same assumption of unabated and constant releases might be questioned, however, for the soil contamination source category. Soil concentrations are assumed to remain constant, despite mechanisms which would dissipate concentrations over time. Volatilization and transport off-site, and wind erosion and transport off-site, are two mechanisms which dissipate residues into the air and deplete the source strength. Soil erosion off the site to a nearby exposure site and to nearby water bodies also is a mechanism of release. A key dissipation mechanism is soil degradation. There is evidence that photolysis is a mechanism of degradation of dioxin-like compounds, as discussed in Chapter 2 of Volume 11 of this assessment. However, this would only apply to those residues directly on the soil surface and, as such, it may be reasonable to make an assumption of nondegradation if a concurrent assumption is that residues exist below the soil surface. In any case, releases for a bounded area of soil contamination including volatilization, wind erosion, and soil erosion, which are estimated for purposes of estimating off-site impacts, are not also used to

estimate dissipation of the reservoir of contaminant in the soil. Said another way, the amount lost via these pathways is not a function of a soil reservoir which decreases over time.

The purpose of this section is to examine this assumption for the case of a bounded area of high soil concentration. The demonstration of the soil contamination source category will be the focus of discussions below. First, an estimate of the "reservoir" of 2,3,7,8-TCDD that is implied with the default parameters will be made. Then, an estimate of the rate at which this reservoir dissipates using the solution algorithms for dissipation: volatilization and wind erosion flux from soils, and soil erosion, will be made. Other routes of dissipation that will be examined are the soil ingestion by cattle and children, the loss via dermal contact, and the removal via harvest of below ground vegetation. These will be shown to be minuscule in comparison to air and soil erosion. The loss of soluble residues via surface runoff or leaching will be evaluated. Surface water bodies and above ground vegetation are sinks for dioxin-like compounds and therefore are not mechanisms of soil dissipation. If it can be shown, for example, that it takes several hundred years to dissipate a given reservoir, then it may be fair to conclude that exposures assuming non-dissipation over a 20 or even a 70 year exposure period are not significant overestimates. On the other hand, complete dissipation within a time period less than or even near to the period of exposure would mean that exposures and risks are being overestimated.

As will be shown, the rates of reservoir dissipation are very important considerations for soil contamination. Users of this methodology should consider dissipation of available residues and the discussions below when determining the duration of exposure for site-specific assessments. A recommended rule of thumb for users of this methodology is to evaluate the time to dissipation using the methodology below, and if it is less than or even near the assumed period of exposure (2 years to dissipate versus 20 years of assumed exposure, e.g.), then it may be appropriate to assign a duration of exposure equal or less than the calculated time to residue dissipation.

One of the key parameters in determining how rapidly residues will dissipate is one which is not required for this methodology. This is the depth of contamination. This depth, plus the initial concentration and the areal extent of contamination, describe the full extent of the source strength. The exercises below have assumed a shallow depth of 0.15 meters, or 6 inches, in soil. The impact of this assumption is demonstrated below. Also, the exercises below are specific to 2,3,7,8-TCDD.

The demonstration of the off-site soil contamination source category. were as follows:
 40,000 m² soil contaminated with an initial concentration of 1 ug/kg (ppb). It is assumed that the contamination extends to 0.15 meters (6 inches).

Step 1. Estimate the amount bound to soil:

		40,000 m ² * 10,000 cm ² /m ² * 15 cm =
		6 x 10 ⁹ cm ³
(soil bulk density)	x	1.5 gm/cm ³
(unitless 2,3,7,8-TCDD soil con., g/g)	x	(1/10 ⁹)
= grams 2,3,7,8-TCDD in soil		9 gms

Note: at a soil concentration of 1 µg/kg, there will also be some 2,3,7,8-TCDD in soil pore water. This amount is insignificant in comparison to the amount bound to soil, and will be neglected.

Step 2. Now estimate the amounts lost by various routes of dissipation

- Volatilization -Volatilization flux is a function of exposure duration, with less average flux calculated over longer durations - this is, in fact, the only model algorithm which accounts for reservoir depletion over time. The durations of exposure for the high end scenarios was 20 years. The release rate via volatilization is given as the term FLUX and is shown in Equation (4-22) in Chapter 4. Plugging in baseline parameter values for 2,3,7,8-TCDD and a duration of 20 years results in a calculated flux of 1.06x10⁻¹⁸ g/cm²-sec. Over a year and over the 40,000 m² contaminated area, this translates to an annual dissipation rate of 0.013 g/yr of 2,3,7,8-TCDD.

- Wind erosion: Unlike the volatilization algorithm, the flux due to wind erosion is not dependent on the duration of exposure. The wind erosion algorithm is described in Section 4.3.3 in Chapter 4. Plugging in baseline parameter values results in a flux of 2,3,7,8-TCDD of 5.74x10⁻²⁰ g/cm²-sec, or an annual flux over the 40,000 m² contaminated area of 0.0007 g/yr.

- Soil erosion: The annual erosion rate off the contaminated site was 21515 kg/hayr. This rate was assumed to erode towards the exposure site as well as towards the impacted surface water body. However, it would not be appropriate to double that quantity since it is used in two

different algorithms - the exposure site could be in the direction of the water body, for example. Or, if applied to a specific site, one could ascertain that the exposure site is upgradient from the contaminated site, and so on. In any case, 21515 kg/ha-yr can be translated to a cm/yr of soil erosion as follows:

$$\begin{array}{rcl}
 \text{volume per 1-cm hectare slice} & = & 10,000 \text{ m}^2/\text{ha} * 10,000 \text{ cm}^2/\text{m}^2 * 1 \text{ cm} = \\
 & & 1 \times 10^8 \text{ cm}^3 \\
 \text{soil bulk density} & \text{X} & 0.015 \text{ kg/cm}^3 \\
 \text{kilograms per 1 -cm hectare slice} & = & 150,000 \text{ kg/cm-hectare}
 \end{array}$$

Therefore, 21515 kg/ha-yr translates to a loss of soil equal to 0.14 cm/yr. Given that 9 g 2,3,7,8-TCDD are estimated to occur in 15 cm, the annual loss of 2,3,7,8-TCDD is 0.084 g/yr.

- Runoff and Leaching: Transport via water is not considered in this methodology since the dioxin-like compounds are so tightly sorbed that these are expected to be negligible. An estimate of loss via water will nonetheless be made for this exercise. Surface water body volume was estimated assuming a runoff rate of 15 in/yr, which was defined as all surface water contributions (surface runoff, interflow, and ground water recharge). This is a reasonable estimate for water-borne losses for this exercise. The annual amount of 2,3,7,8-TCDD lost in this water can be estimated using the soil partition coefficient, K_{d_s} , relationship, which is C_s/C_w . K_{d_s} is equal to 39,800 for 2,3,7,8-TCDD (organic carbon partition coefficient, K_{oc} of 3.98×10^6 * soil organic carbon, OC_{sl} of 0.01), so the concentration in water, C_w , given a soil concentration, C_s , of 1 $\mu\text{g}/\text{kg}$, is $2.5 \times 10^{-5} \mu\text{g}/\text{L}$, or $2.5 \times 10^{-11} \text{ g}/\text{L}$. Translated to a 40,000 m^2 area, 15 in/yr equals $1.524 \times 10^7 \text{ L}$, so the total annual loss in water equals 0.00038 g/yr 2,3,7,8-TCDD.

Except for soil degradation, these are the dissipation routes that would be considered for a site of soil contamination that is not used for any purpose - residence, agriculture, and so on. For the sake of completeness, other routes that will be looked at now include soil ingestion, soil dermal contact, and harvesting of underground vegetation.

- Soil Ingestion: Soil ingestion by children in the high end scenario is 600 mg/day, or 0.22 kg/yr. Soil ingestion by cattle will also be considered. First, an assumption of how many cattle would be feeding on a 40,000 m^2 area should be made. A daily cattle dry matter ingestion rate is 19 kg/day. For beef cattle that are assumed to principally graze, for 90% of their dry matter intake, the daily ingestion of grass would be 17.1 kg/day, and their daily intake of soil

while grazing, 8% of total dry matter intake, is 1.52 kg/day. With this daily ingestion of grass, their annual need for grass would be 6200+ kg/yr. The yield of grass assumed for other purposes in this assessment was 0.15 kg/m²-yr dry weight, or 6000 kg/40,000 m²-yr. Therefore, it appears that one grazing cow requires the 40,000 m² to himself (as a rough approximation). The annual intake of soil by this cow equals 555 kg/yr, which as expected, is much higher than child soil ingestion. The annual removal of 2,3,7,8-TCDD by cattle soil ingestion is 555 µg/yr, or 0.0006 g/yr.

- Dermal Contact: The dissipation of 2,3,7,8-TCDD residues via dermal contact is estimated as, $EV*CA*CR*C_s$, where EV = event frequency in terms of number of dermal contact events per year, which equals 365 in the high end scenario, CA = contact area, which ranges from 1000-10,000 cm², CR = contact rate, which ranges from 0.005-0.1 mg/cm²-event, and C_s = 2,3,7,8-TCDD concentration, which is 1 µg/kg, or in more convenient units, 10⁻¹² g/mg. Using the higher values, the annual loss via dermal contact is negligible at 3.7x10⁻⁷ g/yr.

- Underground Vegetation Harvests: The yield of vegetables required for other algorithms of this assessment, is 7.8 kg/m² fresh weight. The vegetable concentration/soil concentration ratio for tilled soils is about 0.033 (from results of the demonstration scenario). Therefore, for a 1 µg/kg soil concentration, the fresh weight vegetable concentration would be 0.033 µg/kg fresh weight. Therefore, the removal per m² is 0.26 µg/m², and the removal over 40,000 m² in g/yr is 0.01 g/yr if all the 40,000 m² were devoted to underground vegetables.

This exercise has shown that the principal mechanism of removal is soil erosion at 0.084 g/yr 2,3,7,8-TCDD, with volatilization explaining 0.013 g/yr removal. The sum of these two routes is 0.097 g/yr, and the sum of all the other routes examined briefly above is 0.01 g/yr, leading to a round total estimate of 0.11 g/yr. With an initial reservoir of 9 gr, it would take 82 years to dissipate the available reservoir, not including degradation and assuming that surface concentrations remain constant. The limited field data that is available on the loss of dioxins from surface soils suggested anywhere from 10 to 100 years for surface and subsurface residues. These losses would include degradation and transport. This assessment assumes a 25-year half-life for residues arriving at exposure sites from distant sources of contamination such as soils or stack emissions. As a rough estimate, half of the 9 gram reservoir would be dissipated at 25 years; 4.5 grams loss per 25 years translates to 0.18 g/yr lost. The algorithms of this assessment already lead to 0.11 g/yr lost, and therefore the observation that it would take about 80 years to

dissipate the reservoir appears sound. In other words, this simple exercise suggests that transport from a site, rather than degradation, could dominate the dissipation rates of 10 to 100 years that have been observed in the field.

This was not a definitive exercise, by any means, but it does lend some confidence that a principal of mass balance may not have been violated for the soil source categories, and for the assumption of 30 years exposure duration. As this section began, the algorithms of this assessment are characterized as screening level methodologies. Users of this methodology should be cognizant, nonetheless, of the possibility of depleting a reservoir of soil contamination prior to an assumed duration of exposure.

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Table 6-1. Parameters used to estimate exposure media concentrations for this assessment.

Parameter Name and Definition	Low ¹	Selected ¹	High ¹	Rating ²
1. Contaminated and Exposure Site Characteristics				
A. Site of Exposure				
AES Area of exposure site, m ²	4,000	40,000	400,000	SS
E _{slp} Soil porosity, unitless	0.35	0.50	0.60	SS
P _{soil} Particle bulk density, g/cm ³	2.55	2.65	2.75	FOD
B _{soil} Soil bulk density, g/cm ³	1.20	1.50	2.00	SS
OC _{sl} Soil organic carbon fraction	0.005	0.01	0.05	SS
d _t Depth of tillage, m	0.10	0.20	0.30	SOD
d _{not} No-till depth, m	0.01	0.02	0.10	SOD
B. Contaminated Site for Soil Contamination Source Demonstration				
C _s Soil concentration of 2,3,7,8-TCDD, µg/kg (ppb)	0.01	1.00	100.0	SS
ASC Area of contamination, ha	4,000	40,000	400,000	SS
E _{slp} Soil porosity, unitless	0.35	0.50	0.60	SS
P _{soil} Particle bulk density, g/cm ³	2.55	2.65	2.75	FOD
OC _{sl} Soil organic carbon fraction	0.001	0.01	0.05	SS

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Table 6-1. (cont'd)

Parameter Name and Definition		Low	Selected	High	Rating
2. Soil and Sediment Delivery Parameters					
SL _s	Contaminated site soil loss, kg/ha-yr	2,100	21,520	42,000	SS
SL _{ec}	Soil loss between cont. and exposure site, kg/ha-yr	0	2,150	21,000	SS
SL _w	Watershed soil loss, kg/ha-yr	2,100	6,455	21,500	SS
ER	Enrichment ratio	1	3.0	5.0	SOD
C _w	Watershed 2,3,7,8-TCDD concentration for contaminated soil source demonstration, pg/g (ppt)	0	0	1.00	SS
OC _{ssed}	Suspended sediment organic carbon fraction	0.02	0.05	0.10	SS
OC _{sed}	Bottom sediment organic carbon fraction	0.01	0.03	0.05	SS
A _w	Watershed drainage area, ha	10,000	100,000	1,000,000	SS
SD _w	Watershed sediment delivery ratio, unitless	0.25	0.06	0.01	SS
TSS	Total suspended sediment, mg/L	2	10	70	SS
DL _e	Distance from contaminated to exposure site, m	50	150	1,000	SS
DL _w	Distance from contaminated site to water body, m	50	150	1,000	SS
V _{wat}	Volume of water body, L/yr	5*10 ¹⁰	4.8*10 ¹¹	5*10 ¹²	SS
AREA _w	Surface area of water body, m ²	4*10 ⁵	4*10 ⁶	4*10 ⁷	SS

(continued on next page)

Table 6-1. (cont'd)

Parameter Name and Definition			Low	Selected	High	Rating
3. Volatilization and Dust Suspension Parameters						
ED	Exposure duration, yrs		1	30	70	SS
V	Fraction of vegetative cover at contaminated site		0	0	0.9	SS
U_m	Average windspeed, m/sec		2.8	4.0	6.3	SS
U_t	Threshold wind speed, m/sec		2.5	8.25	11.3	SS
F(x)	Model-specific parameter, unitless		0.87	0.50	0.05	SS
FREQ	Frequency wind blows to site, unitless		0.05	0.15	0.50	SS
4. Bioconcentration and Biotransfer Parameters						
Fish:	f_{lipid}	Fish lipid fraction	---	0.07	---	SS
Vegetation,	FDW	Dry to fresh weight conversion	0.05	0.15	0.30	SS
Particle	V_p	Particle deposition velocity, m/yr	$1.5 \cdot 10^5$	$3.2 \cdot 10^5$	$7.0 \cdot 10^5$	SOD
Impacts:	R	Annual rainfall, m/yr	0.30	1.00	2.00	SS
	W_p	Washout factor, unitless	2,000	50,000	1,000,000	SOD

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Table 6-1 (cont'd)

Parameter Name and Definition		Low	Selected	High	Rating
R_w	Fraction of wet deposition retained	0	0.30	1.00	SOD
Y_{gr}	Grass yield, kg/m ² dry	0.15	0.15	0.35	SS
INT_{gr}	Grass interception fraction	0.13	0.35	0.64	SS
Y_{ctfd}	Cattle feed yield, kg/m ² dry	0.25	0.63	1.30	SS
INT_{ctfd}	Cattle field interception fraction	0.20	0.62	0.93	SS
Y_{chfd}	Chicken feed yield, kg/m ² dry	---	0.63	---	SS
INT_{chfd}	Chicken feed interception fraction	---	0.62	---	SS
Y_{veg}	Above ground veg. yield, kg/m ² fresh	2.7	7.8	8.6	SS
INT_{veg}	Vegetable interception fraction	0.18	0.48	0.72	SS
Y_{ftr}	Fruit yield, kg/m ² fresh	---	7.8	---	SS
INT_{ftr}	Fruit interception fraction	---	0.48	---	SS
Vegetation,	VG_{vg} Vegetable/fruit correction factor	0.001	0.01	0.10	SOD
Vapor	VG_{gr} Grass correction factor	0.50	1.00	1.00	SOD
Impacts:	VG_{ctfd} Cattle feed correction factor	0.25	0.50	0.75	SOD
	VG_{chfd} Chicken feed correction factor	---	0.00	---	SOD

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Table 6-1. (cont'd)

Parameter Name and Definition			Low	Selected	High	Rating
Below Gr. Veg:	VG_{bg}	Below ground veg. correction factor	0.01	0.25	1.00	SOD
Beef:	BCSDF	Beef cattle soil diet fraction	0.01	0.04	0.15	SOD
	BCGDF	Beef cattle grass diet fraction	0.02	0.48	0.90	SOD
	BCFDF	Beef cattle feed diet fraction	0.02	0.48	0.90	SOD
	BCGRA	Beef cattle fraction of cont. grazing land	0.25	1.00	1.00	SOD
	BCFOD	Beef cattle fraction of cont. feed	0.25	1.00	1.00	SOD
	b_{fat}	Beef fat fraction	---	0.19	---	SS
Dairy:	DCSDF	Dairy cow soil diet fraction	---	0.02	---	SOD
	DCGDF	Dairy cow grass diet fraction	---	0.08	---	SOD
	DCFDF	Dairy cow feed diet fraction	---	0.90	---	SOD
	DCGRA	Dairy cow fraction of cont. grazing land	---	1.00	---	SOD
	DCFOD	Dairy cow fraction of cont. feed	---	1.00	---	SOD
	d_{fat}	Dairy fat fraction	---	0.035	---	SS
Chicken/Egg:	CSDF	Chicken soil diet fraction	---	0.10	---	SOD
	CGDF	Chicken grass diet fraction	---	0.00	---	SOD

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Table 6-1. (cont'd)

Parameter Name and Definition		Low	Selected	High	Rating
CFDF	Chicken feed diet fraction	---	0.90	---	SS
CGRA	Chicken fraction of cont. grazing land	---	1.00	---	SS
CFOD	Chicken fraction of cont. feed	---	1.00	---	SS
All animals:	B_s Bioavailability of dioxin in soil relative to vegetative feeds	0.30	0.65	0.90	SOD
5. Effluent Discharge Source Category					
LD	Loading to surface water body, mg/hr	0.00315	0.0315	0.315	SS
Q_e	Effluent flow rate, L/hr	$1*10^5$	$4.1*10^6$	$1*10^7$	SS
Q_u	Upstream receiving water flow, L/hr	$1*10^7$	$4.7*10^8$	$1*10^9$	SS
OC_e	Effluent organic carbon content, fraction	0.15	0.36	0.50	SS
OC_u	Upstream organic carbon content, fraction	0.02	0.05	0.10	SS
TSS_e	Effluent total suspended solids, mg/L	10	70	250	SS
TSS_u	Upstream total suspended solids, mg/L	2.0	9.5	50	SS

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Table 6-1. (cont'd)

Parameter Name and Definition	Low	Selected	High	Rating
6. Stack Emission Source Category				
RDEP _e Wet+dry deposition at high end exposure site, $\mu\text{g}/\text{m}^2\text{-yr}$	$1.82 \cdot 10^{-6}$	$1.13 \cdot 10^{-6}$	$1.43 \cdot 10^{-7}$	SS
RDEP _{wat} Wet+dry deposition onto watershed, $\mu\text{g}/\text{m}^2\text{-yr}$	$1.82 \cdot 10^{-6}$	$1.43 \cdot 10^{-7}$	$5.20 \cdot 10^{-8}$	SS
RDEP _{sw} Wet+dry deposition onto surface water, $\mu\text{g}/\text{m}^2\text{-yr}$	$1.82 \cdot 10^{-6}$	$1.43 \cdot 10^{-7}$	$5.20 \cdot 10^{-8}$	SS
C _{va} Vapor phase concentration at high end exp. site, $\mu\text{g}/\text{m}^3$	$4.34 \cdot 10^{-13}$	$6.99 \cdot 10^{-12}$	$2.49 \cdot 10^{-12}$	SS
RDEP _p Deposition of particles onto water body, $\text{g}/\text{m}^2\text{-yr}$	0.003	0.03	3.00	FOD
d _{wmx} Average mixing depth of deposition over watershed, m	0.01	0.10	0.20	SOD
f _{sd} Fraction of particles depositing onto water body from the atmosphere which remain in suspension	0	1.00	1.00	FOD
7. 2,3,7,8-TCDD Physical, Chemical, and Bioconcentration/Biotransfer Parameters				
H Henry's Constant, $\text{atm}\cdot\text{m}^3/\text{mole}$	$3.29 \cdot 10^{-6}$	$3.29 \cdot 10^{-5}$	$3.29 \cdot 10^{-4}$	FOD
D _a Molecular diffusivity in air, cm^2/s	0.005	0.047	0.10	FOD
Koc Organic carbon partition coefficient, L/kg	$4 \cdot 10^5$	$3.98 \cdot 10^6$	$4 \cdot 10^7$	FOD
ϕ Fraction of airborne reservoir sorbed	0.80	0.49	0.20	SOD/SS

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Table 6-1. (cont'd)

Parameter Name and Definition		Low	Selected	High	Rating
B _{vpa}	Air-to-leaf vapor phase transfer factor, unitless	6.55*10 ³	6.55*10 ⁴	6.55*10 ⁵	SOD
BCF	Beef/milk fat bioconcentration factor, unitless	1.00	5.76	10.00	SOD
CCF	Chicken fat bioconcentration factor, unitless	---	8.80	---	SOD
ECF	Egg fat bioconcentration factor, unitless	---	7.80	---	SOD
BSAF	Biota sediment accumulation factor, unitless	0.03	0.09	0.30	SOD/SS
BSSAF	Biota suspended sediment accumulation factor, unitless	0.03	0.09	0.30	SOD/SS
k	Soil dissipation rate for eroding/depositing dioxins, yr ⁻¹	0.0028	0.0277	0.28	SOD
kw	Plant weathering rate constant, yr ⁻¹	51.0	18.1	8.4	SOD
RCF	Root bioconcentration factor, unitless	1,600	5,200	100,000	SOD

Notes:

¹ “Selected” is the value chosen for the demonstration scenarios. The “Low” and “High” values were selected for the sensitivity analysis.

² “Ratings” are qualitative judgements pertaining to the use of the selected values for use in other assessments - see text for more detail.

³ “----” means that low and high values were not selected because these parameters were not tested in the sensitivity analysis exercises.

Trends with these parameters were demonstrated with related parameters.

Table 6-2. Contribution of above ground vegetation concentrations of 2,3,7,8-TCDD from air-to-leaf transfers and particulate depositions.¹

Description ²	Air-to-leaf vapor transfers	Particle depositions
Scenario 3: Soil contamination		
vegetables/fruit	56	44
grass	96	4
feed	97	3
Scenario 4: Stack emissions, central		
vegetables/fruit	35	65
grass	91	9
feed	92	8
Scenario 5: Stack emissions, high		
vegetables/fruit	20	80
grass	82	18
feed	87	13

¹ Results are in percent of total contribution.

² Scenario 3 demonstrated the soil contamination source category, where soil at a contaminated site 150meters away was initialized at 1 µg/kg (ppb) 2,3,7,8-TCDD; Scenarios 4 and 5 demonstrated the stack emission source category - in Scenario 4, the exposure site was 5000 meters from the emitting stack, and in Scenario 5, the exposure site was 500 meters from the stack.

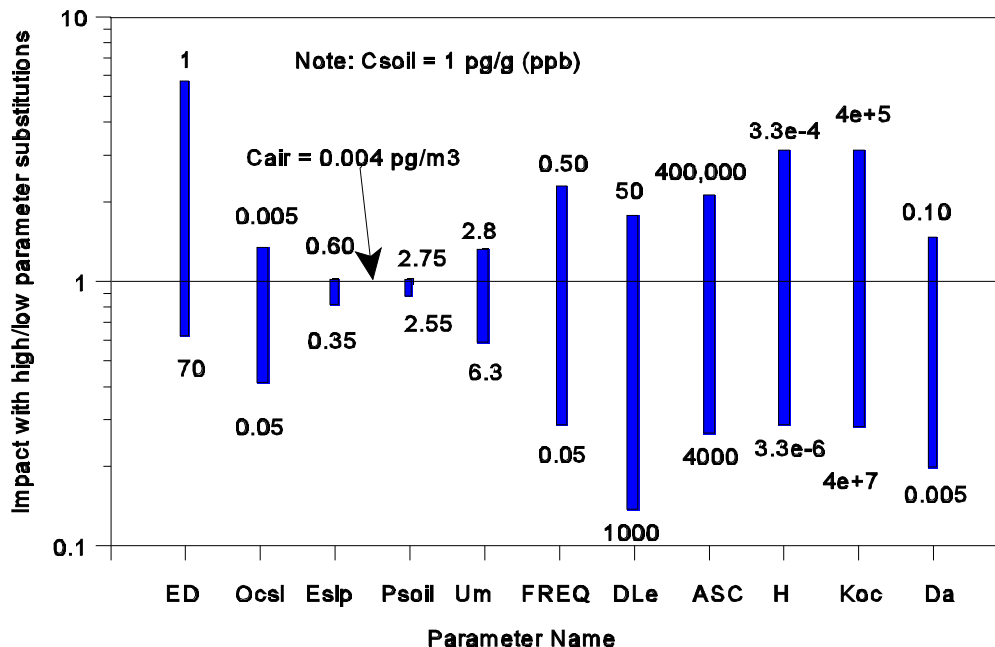


Figure 6-1. Results of sensitivity analysis of algorithms estimating exposure site vapor phase air concentrations resulting from a distant contaminated soil site.

Parameter Name	Definition	Selected
C_{soil}	soil concentration at contaminated area, ng/g (ppb)	1.00
C_{air}	air concentration at exposure site, pg/m ³	0.004
ED	exposure duration, yrs	30
OC_{sl}	soil organic carbon fraction	0.01
E_{slp}	soil porosity, unitless	0.50
P_{soil}	particle bulk den, g/cm ³	2.65
U_m	average windspeed, m/sec	4.0
FREQ	frequency wind blows to site, unitless	0.15
DL_e	distance to exposure site, m	150
ASC	area of off-site contamination, m ²	40,000
H	Henry's Constant, atm-m ³ /mole	3.29×10^{-5}
Koc	organic carbon partition coefficient, L/kg	3.98×10^6
D_a	molecular diffusivity in air, cm ² /s	0.047

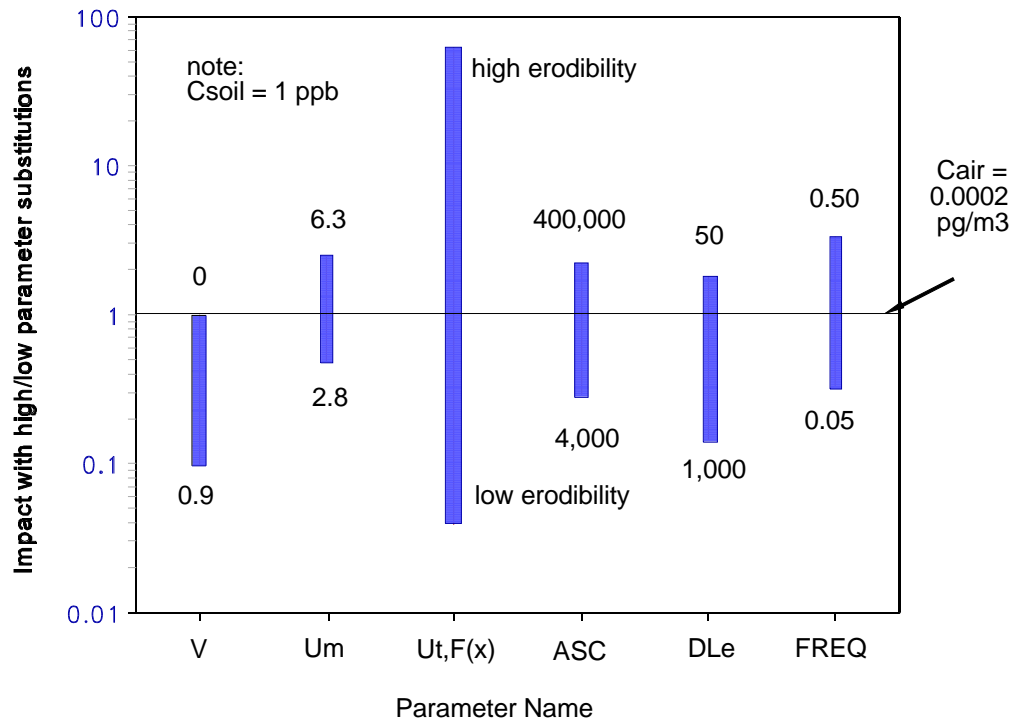


Figure 6-2. Results of sensitivity analysis of algorithms estimating exposure site particle phase air concentrations resulting from a distant contaminated soil site.

Parameter Name	Definition	Selected
C_{soil}	contaminated site soil concentration, ng/g (ppb)	1.00
C_{air}	exposure site air concentration, pg/m ³	0.0002
V	fraction of vegetative cover, unitless	0.0
U_m	average windspeed, m/sec	4.0
U_t	threshold wind speed, m/sec	8.25
F(x)	model-specific parameter	0.50
ASC	area of soil contamination, m ²	40,000
DL_e	distance to exposure site, m	150
FREQ	frequency wind blows to exposure site, unitless	0.15

