

Appendix K Equations For Estimating Concentrations of PB-HAP Compounds in Food and Drinking Water

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1.0 Introduction

This Appendix describes equations used by some multimedia models to estimate media concentrations for the recommended exposure scenarios presented in Part III. Most risk assessments will use a multimedia fate and transport model to perform these calculations; the particular equations used in a given model may differ slightly from those presented here, which are taken largely from EPA's 1998 *Peer Review Draft Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities, Volume I*.⁽¹⁾ The equations, and descriptions of the associated parameters, are presented here simply as a general reference, and are not intended to imply a recommendation over other equations, methods, or values for describing these processes. EPA's 1998 *Risk Assessment Protocol for Hazardous Waste Combustion Facilities* provides a more detailed discussion of the origin and development of each of these equations and many of their specific parameters. It should be noted that reference made throughout this chapter to "particle phase" is generic and made without distinction between particle and particle-bound. The remainder of this chapter is divided into seven sections:

- Section 2 describes the estimating media concentration equations for soils contaminated by PB-HAP compounds.
- Section 3 describes the estimating media concentration equations used to determine PB-HAP compound concentrations in produce.
- Sections 4 through 6 describe equations used to determine PB-HAP compound concentrations in animal products (such as milk, beef, pork, poultry, and eggs) resulting from animal ingestion of contaminated feed and soil.
- Section 7 describes equations used to determine PB-HAP compound concentrations in fish through bioaccumulation (or, for some compounds, bioconcentration) from the water column, dissolved water concentration, or bed sediment – depending on the PB-HAP compound.
- Section 8 describes equations for estimating the concentrations of doxins in breast milk.

2.0 Calculation of PB-HAP Compound Concentrations in Soil

PB-HAP compound concentrations in soil are calculated by summing the vapor phase and particle phase deposition of PB-HAP compounds to the soil. Wet and dry deposition of particles and vapors are considered, with dry deposition of vapors calculated from the vapor air concentration and the dry deposition velocity. The calculation of soil concentration incorporates a term that accounts for loss of PB-HAP compounds by several mechanisms, including leaching, erosion, runoff, degradation (biotic and abiotic), and volatilization. These loss mechanisms all lower the soil concentration associated with the deposition rate.

Soil concentrations may require many years to reach steady state. As a result, the equations used to calculate the average soil concentration over the period of deposition were derived by integrating the instantaneous soil concentration equation over the period of deposition. For carcinogenic PB-HAP compounds, EPA (1998)⁽¹⁾ recommends using two variations of the equation (average soil concentration over exposure duration). One form should be used if the exposure duration is greater than or equal to the operating lifetime of the emission source(s), and the other should be used if the exposure duration is less than the operating lifetime of the emission source(s).

For noncarcinogenic PB-HAP compounds, EPA (1998)⁽¹⁾ recommends using the second form of the carcinogenic equation to calculate the highest annual average PB-HAP compound soil concentration occurring during the exposure duration. These equations are described in more detail in Section 2.1.

Soil conditions such as pH, structure, organic matter content, and moisture content affect the distribution and mobility of PB-HAP compounds. Loss of PB-HAP compounds from the soil is modeled by using rates that depend on the physical and chemical characteristics of the soil. These variables and their use are described in the following subsections, along with the recommended equations.

2.1 Calculating Cumulative Soil Concentration (C_s)

EPA (1998)⁽¹⁾ recommends the use of Equations 1A, 1B, and 1C to calculate the cumulative soil concentration (C_s).

Carcinogens:

For $T_2 \leq tD$

$$C_s = \frac{D_s}{k_s \cdot (tD - T_1)} \cdot \left[\left(tD + \frac{\exp(-k_s \cdot tD)}{k_s} \right) - \left(T_1 + \frac{\exp(-k_s \cdot T_1)}{k_s} \right) \right] \quad (\text{Equation 1A})$$

For $T_1 < tD < T_2$

$$C_s = \frac{\left(\frac{D_s \cdot tD - C_{s,tD}}{k_s} \right) + \left(\frac{C_{s,tD}}{k_s} \right) \cdot \left(1 - \exp[-k_s \cdot (T_2 - tD)] \right)}{(T_2 - T_1)} \quad (\text{Equation 1B})$$

Noncarcinogens:

$$C_{s,tD} = \frac{D_s \cdot [1 - \exp(-k_s \cdot tD)]}{k_s} \quad (\text{Equation 1C})$$

where

- C_s = Average soil concentration over exposure duration (mg PB-HAP compound/kg soil)
- D_s = Deposition term (mg PB-HAP compound/kg soil/yr)
- T_1 = Time period at the beginning of emissions (yr)
- k_s = PB-HAP compound soil loss constant due to all processes (yr^{-1})
- tD = Time period over which deposition occurs (time period of emissions) (yr)
- $C_{s,tD}$ = Soil concentration at time tD (mg/kg)
- T_2 = Length of exposure duration (yr)

EPA (1998)⁽¹⁾ recommends Equation 1C when an exposure duration that is less than or equal to the operating lifetime of the emission source(s) ($T_2 \leq tD$); when an exposure duration greater than the operating lifetime of the emissions source(s) ($T_1 < tD < T_2$), Equation 1B is recommended. For noncarcinogenic PB-HAP compounds, Equation 1C is recommended.

The PB-HAP compound soil concentration averaged over the exposure duration, represented by C_s , can be used for carcinogenic compounds, where risk is averaged over the lifetime of an individual. Because the hazard quotient associated with noncarcinogenic PB-HAP compounds is based on a threshold dose rather than a lifetime exposure, the highest annual average PB-HAP compound soil concentration occurring during the exposure duration period is recommended to be used for noncarcinogenic PB-HAP compounds. The highest annual average PB-HAP compound soil concentration, $C_{s,tD}$, will typically occur at the end of the operating life of the emission source(s).

EPA (1998)⁽¹⁾ recommends using the highest 1-year annual average soil concentration, determined by using Equation 1C, to evaluate risk from noncarcinogenic PB-HAP compounds.

2.2 Calculating the PB-HAP compound Soil Loss Constant (ks)

Organic and inorganic PB-HAP compounds may be lost from the soil by several processes that may or may not occur simultaneously. The rate at which a PB-HAP compound is lost from the soil is known as the soil loss constant (ks). The constant ks is determined by using the soil's physical, chemical, and biological characteristics to consider the loss resulting from leaching, runoff, erosion, biotic and abiotic degradation, and volatilization. EPA (1998)⁽¹⁾ recommends that Equation 2 be used to calculate the PB-HAP compound soil loss constant (ks).

$$ks = ksg + kse + ksr + ksl + ksv \quad (\text{Equation 2})$$

where

- ks = PB-HAP compound soil loss constant due to all processes (yr^{-1})
- ksg = PB-HAP compound loss constant due to biotic and abiotic degradation (yr^{-1})
- kse = PB-HAP compound loss constant due to soil erosion (yr^{-1})
- ksr = PB-HAP compound loss constant due to surface runoff (yr^{-1})
- ksl = PB-HAP compound loss constant due to leaching (yr^{-1})
- ksv = PB-HAP compound loss constant due to volatilization (yr^{-1})

As highlighted in Section 2.1, the use of Equation 2 in Equations 1A and 1B assumes that PB-HAP compound loss can be defined by using first-order reaction kinetics. First-order reaction rates depend on the concentration of one reactant.⁽²⁾ The loss of a PB-HAP compound by a first-order process depends only on the concentration of the PB-HAP compound in the soil, and a constant fraction of the PB-HAP compound is removed from the soil over time. Those processes that apparently exhibit first-order reaction kinetics without implying a mechanistic dependence on a first-order loss rate are termed “apparent first-order” loss rates.⁽³⁾ The assumption that PB-HAP compound loss follows first-order reaction kinetics may be an oversimplification because – at various concentrations or under various environmental conditions – the loss rates from soil systems will resemble different kinetic expressions. However, at low concentrations, a

first-order loss constant may be adequate to describe the loss of the PB-HAP compound from soil (EPA 1990)⁽⁴⁾.

PB-HAP compound loss in soil can also follow zero or second-order reaction kinetics. Zero-order reaction kinetics are independent of reactant concentrations (Bohn, McNeal, and O'Connor 1985).⁽²⁾ Zero-order loss rates describe processes in which the reactants are present at very high concentrations. Under zero-order kinetics, a constant amount of a PB-HAP compound is lost from the soil over time, independent of its concentration. Processes that follow second-order reaction kinetics depend on the concentrations of two reactants or the concentration of one reactant squared (Bohn, McNeal, and O'Connor 1985)⁽²⁾. The loss constant of a PB-HAP compound following a second-order process can be contingent on its own concentration, or on both its concentration and the concentration of another reactant, such as an enzyme or catalyst.

Because PB-HAP compound loss from soil depends on many complex factors, it may be difficult to model the overall rate of loss. In addition, because the physical phenomena that cause PB-HAP compound loss can occur simultaneously, the use of Equation 2 may also overestimate loss rates for each process (Valentine 1986).⁽⁵⁾ When possible, the common occurrence of all loss processes should be taken into account. Combined rates of soil loss by these processes can be derived experimentally; values for some PB-HAP compounds are presented in EPA (1986).⁽⁶⁾

Sections 2.2.1 through 2.2.5 discuss issues associated with the calculation of the *ksl*, *kse*, *ksr*, *ksg*, and *ksv* variables.

2.2.1 PB-HAP compound Loss Constant Due to Biotic and Abiotic Degradation (*ksg*)

Soil losses resulting from biotic and abiotic degradation (*ksg*) are determined empirically from field studies and should be addressed in the literature (EPA 1990).⁽⁴⁾ Lyman et al. (1982)⁽⁷⁾ states that degradation rates can be assumed to follow first order kinetics in a homogenous medium. Therefore, the half-life of a compound can be related to the degradation rate constant. Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil media. Therefore, if the half-life of a compound (for all of the mechanisms of transformation) is known, the degradation rate can be calculated. However, literature sources do not provide sufficient data for all such mechanisms, especially for soil. EPA (1994a)⁽⁸⁾ recommends that *ksg* values for all PB-HAP compounds other than polycyclic organic matter (specifically 2,3,7,8-TCDD) should be set equal to zero. EPA (1998)⁽¹⁾ presents EPA recommended values for this compound-specific variable.

The rate of biological degradation in soils depends on the concentration and activity of the microbial populations in the soil, the soil conditions, and the PB-HAP compound concentration (Jury and Valentine 1986).⁽⁹⁾ First-order loss rates often fail to account for the high variability of these variables in a single soil system. However, the use of simple rate expressions may be appropriate at low chemical concentrations (e.g., nanogram per kilogram soil) at which a first-order dependence on chemical concentration may be reasonable. The rate of biological degradation is PB-HAP compound-specific, depending on the complexity of the PB-HAP compound and the usefulness of the PB-HAP compound to the microorganisms. Some substrates, rather than being used by the organisms as a nutrient or energy source, are simply degraded with other similar PB-HAP compounds, which can be further utilized. Environmental and PB-HAP compound-specific factors that may limit the biodegradation of PB-HAP compounds in the soil environment (Valentine and Schnoor 1986)⁽¹⁰⁾ include (1) availability of

the PB-HAP compound, (2) nutrient limitations, (3) toxicity of the PB-HAP compound, and (4) inactivation or nonexistence of enzymes capable of degrading the PB-HAP compound.

Chemical degradation of organic compounds can be a significant mechanism for removal of PB-HAP compounds in soil (EPA 1990).⁽⁴⁾ Hydrolysis and oxidation-reduction reactions are the primary chemical transformation processes occurring in the upper layers of soils (Valentine 1986).⁽⁵⁾ General rate expressions describing the transformation of some PB-HAP compounds by all non-biological processes are available, and these expressions are helpful when division into component reactions is not possible.

Hydrolysis in aqueous systems is characterized by three processes: acid-catalyzed, base-catalyzed, and neutral reactions. The overall rate of hydrolysis is the sum of the first-order rates of these processes (Valentine 1986).⁽⁵⁾ In soil systems, sorption of the PB-HAP compound can increase, decrease, or not affect the rate of hydrolysis, as numerous studies cited in Valentine (1986)⁽⁵⁾ have shown. The total rate of hydrolysis in soil can be predicted by adding the rates in the soil and water phases, which are assumed to be first-order reactions at a fixed pH (Valentine 1986).⁽⁵⁾ Methods for estimating these hydrolysis constants are described by Lyman et al. (1982).⁽⁷⁾

Organic and inorganic compounds also undergo oxidation-reduction (redox) reactions in the soil (Valentine 1986).⁽⁵⁾ Organic redox reactions involve the exchange of oxygen and hydrogen atoms by the reacting molecules. Inorganic redox reactions may involve the exchange of atoms or electrons by the reactants. In soil systems where the identities of oxidant and reductant species are not specified, a first-order rate constant can be obtained for describing loss by redox reactions (Valentine 1986).⁽⁵⁾ Redox reactions involving metals may promote losses from surface soils by making metals more mobile (e.g., leaching to subsurface soils).

2.2.2 PB-HAP compound Loss Constant Due to Soil Erosion (*kse*)

EPA (1998)⁽¹⁾ recommends that the constant for the loss of soil resulting from erosion (*kse*) is recommended to be set equal to zero in most cases. If soil erosion is a significant issue in the assessment area, EPA (1993b)⁽¹¹⁾ recommends the use of Equation 3 to calculate the constant for soil loss resulting from erosion (*kse*).

$$kse = \frac{0.1 \cdot X_e \cdot SD \cdot ER}{BD \cdot Z_s} \cdot \frac{Kd_s \cdot BD}{\theta_{sw} + (Kd_s \cdot BD)} \quad (\text{Equation 3})$$

where

- kse* = PB-HAP compound soil loss constant due to soil erosion
- 0.1 = Units conversion factor (1,000 g/kg/10,000 cm²-m²)
- X_e* = Unit soil loss (kg/m²-yr)
- SD* = Sediment delivery ratio (unitless)
- ER* = Soil enrichment ratio (unitless)
- Kd_s* = Soil-water partition coefficient (mL water/g soil)
- BD* = Soil bulk density (g soil/cm³ soil)
- Z_s* = Soil mixing zone depth (cm)
- θ_{sw}* = Soil volumetric water content (mL water/cm³ soil)

Unit soil loss (X_s) is calculated by using the Universal Soil Loss Equation (USLE) (See Section 7.2). Soil bulk density (BD) is described in Section 2.4.2. Soil volumetric water content (θ_{sw}) is described in Section 2.5.4.

For additional information on addressing kse , EPA (1998)⁽¹⁾ recommends consulting the methodologies described in EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Pathways of Exposure to Combustor Emissions* (EPA 1998)⁽¹²⁾.

2.2.3 PB-HAP compound Loss Constant Due to Runoff (ksr)

EPA (1998)⁽¹⁾ recommends that Equation 4 be used to calculate the constant for the loss of soil resulting from surface runoff (ksr).

$$ksr = \frac{RO}{\theta_{sw} \cdot Z_s} \cdot \left(\frac{1}{1 + (Kd_s \cdot BD / \theta_{sw})} \right) \quad \text{(Equation 4)}$$

where

- ksr = PB-HAP compound loss constant due to runoff (yr^{-1})
- RO = Average annual surface runoff from pervious areas (cm/yr)
- θ_{sw} = Soil volumetric water content (mL water/cm³ soil)
- Z_s = Soil mixing zone depth (cm)
- Kd_s = Soil-water partition coefficient (mL water/g soil)
- BD = Soil bulk density (g soil/cm³ soil)

Soil bulk density (BD) is described in Section 2.5.2. Soil volumetric water content (θ_{sw}) is described in Section 2.5.4.

2.2.4 PB-HAP compound Loss Constant Due to Leaching (ksl)

Losses of soil PB-HAP compounds due to leaching (ksl) depend on the amount of water available to generate leachate and soil properties such as bulk density, soil moisture, soil porosity, and soil sorption properties. EPA (1998)⁽¹⁾ recommends that Equation 5 be used to calculate the PB-HAP compound loss constant due to leaching (ksl) to account for runoff.

$$ksl = \frac{P + I - RO + E_v}{\theta_{sw} \cdot Z_s \cdot [1.0 + (BD \cdot Kd_s / \theta_{sw})]} \quad \text{(Equation 5)}$$

where

- ksl = PB-HAP compound loss constant due to leaching (yr^{-1})
- P = Average annual precipitation (cm/yr)
- I = Average annual irrigation (cm/yr)
- RO = Average annual surface runoff from pervious areas (cm/yr)
- E_v = Average annual evapotranspiration (cm/yr)
- θ_{sw} = Soil volumetric water content (mL water/cm³ soil)

- Z_s = Soil mixing zone depth (cm)
 Kd_s = Soil-water partition coefficient (cm³ water/g soil)
 BD = Soil bulk density (g soil/cm³ soil)

The average annual volume of water ($P + I - RO - E_v$) available to generate leachate is the mass balance of all water inputs and outputs from the area under consideration. These variables are described in Section 2.5.3. Soil bulk density (BD) is described in Section 2.5.2. Soil volumetric water content (θ_{sw}) is described in Section 2.5.4.

2.2.5 PB-HAP compound Loss Constant Due to Volatilization (k_{sv})

Semi-volatile and volatile PB-HAP compounds emitted in high concentrations may become adsorbed to soil particles and exhibit volatilization losses from soil. The loss of a PB-HAP compound from the soil by volatilization depends on the rate of movement of the PB-HAP compound to the soil surface, the chemical vapor concentration at the soil surface, and the rate at which vapor is carried away by the atmosphere (Jury 1986).⁽¹³⁾

EPA (1998)⁽¹⁾ recommends that in cases where high concentrations of volatile organic compounds are expected to be present in the soil that Equation 6A be used to calculate the constant for the loss of soil resulting from volatilization (k_{sv}).

$$k_{sv} = \left(\frac{3.1536 \times 10^7 \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \right) \cdot \left(\frac{D_a}{Z_s} \right) \cdot \left[1 - \left(\frac{BD}{\rho_{soil}} \right) - \theta_{sw} \right] \quad \text{(Equation 6A)}$$

where

- k_{sv} = PB-HAP compound loss constant due to volatilization (yr⁻¹)
 3.1536×10^7 = Units conversion factor (s/yr)
 H = Henry's Law constant (atm-m³/mol)
 Z_s = Soil mixing zone depth (cm)
 Kd_s = Soil-water partition coefficient (mL/g)
 R = Universal gas constant (atm-m³/mol-K)
 T_a = Ambient air temperature (K) = 298.1 K
 BD = Soil bulk density (g soil/cm³ soil) = 1.5 g/cm³
 D_a = Diffusivity of PB-HAP compound in air (cm²/s)
 θ_{sw} = Soil volumetric water content (mL/cm³ soil) = 0.2 mL/cm³
 ρ_{soil} = Solids particle density (g/cm³) = 2.7 g/cm³

The gas-phase mass transfer coefficient, K_t , based on general soil properties, can also be written as follows (Hillel 1980; Miller and Gardiner 1998)⁽¹⁴⁾:

$$K_t = \frac{D_a \cdot \theta_v}{Z_s} \quad \text{(Equation 6B)}$$

where

- K_t = Gas phase mass transfer coefficient (cm/s)
 Z_s = Soil mixing zone depth (cm)
 D_a = Diffusivity of PB-HAP compound in air (cm²/s)
 θ_v = Soil void fraction (cm³/cm³)

The soil void fraction (θ_v) is the volumetric fraction of a soil that does not contain solids or water and can be expressed as:

$$\theta_v = 1 - \left(\frac{BD}{\rho_{soil}} \right) - \theta_{sw} \quad (\text{Equation 6C})$$

where

- θ_v = Soil void fraction (cm³/cm³)
 θ_{sw} = Soil volumetric water content (mL water/cm³ soil) = 0.2 mL/cm³
 BD = Soil bulk density (g/cm³) = 1.5 g/cm³
 ρ_{soil} = Solids particle density (g/cm³) = 2.7 g/cm³

The expression containing bulk density (BD) divided by solids particle density (ρ_{soil}) gives the volume of soil occupied by pore space or voids (Miller and Gardiner 1998).⁽¹⁴⁾ Soil bulk density is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil (Hillel 1980)⁽¹⁴⁾; a range of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979).⁽¹⁵⁾ A default soil bulk density value of 1.5 g/cm³ is recommended based on a mean value for loam soil from Carsel et al. (1988).⁽¹⁶⁾ Blake and Hartge (1996)⁽¹⁷⁾ and Hillel (1980)⁽¹⁴⁾ both suggests that the mean density of solid particles is about 2.7 gm/cm³. The soil water content depends on both the available water and the soil structure of a particular soil. Values for θ_{sw} range from 0.03 to 0.40 mL/cm³ depending on soil type (Hoffman and Baes 1979).⁽¹⁵⁾ The lower values are typical of sandy soils, which cannot retain much water; the higher values are typical of soils such as clay or loam soils which can retain water. A mid-point default value of 0.2 mL water/cm³ soil is recommended as a default in the absence of site-specific information. However, since the soil water content of soil is unique for each soil type, site-specific information is highly recommended.

2.3 Calculating the Deposition Term (D_s)

EPA (1998)⁽¹⁾ recommends that Equation 7 be used to calculate the deposition term (D_s).

$$D_s = \left[\frac{100 \cdot Q}{Z_s \cdot BD} \right] \cdot \left[F_v \cdot (Dydv + Dywv) + (Dydp + Dywp) \cdot (1 - F_v) \right] \quad (\text{Equation 7})$$

where

- D_s = Deposition term (mg PB-HAP compound/kg soil/yr)
 100 = Units conversion factor (mg-m²/kg-cm²)
 Q = PB-HAP compound emission rate (g/s)
 Z_s = Soil mixing zone depth (cm)

- BD = Soil bulk density (g soil/cm³ soil)
 F_v = Fraction of PB-HAP compound air concentration in vapor phase (unitless)
 $Dydv$ = Unitized yearly average dry deposition from vapor phase (s/m²-yr)
 $Dyww$ = Unitized yearly average wet deposition from vapor phase (s/m²-yr)
 $Dydp$ = Unitized yearly average dry deposition from particle phase (s/m²-yr)
 $Dywp$ = Unitized yearly average wet deposition from particle phase (s/m²-yr)

2.4 Universal Soil Loss Equation (USLE)

EPA (1998)⁽¹⁾ recommends that the universal soil loss equation (USLE) be used to calculate the unit soil loss (X_e). This equation is further described in Section 7.2.

2.5 Site-Specific Parameters for Calculating Cumulative Soil Concentration

Calculating average soil concentration over the exposure duration (C_s) requires the use of site-specific parameters including the following:

- Soil mixing zone depth (Z_s)
- Soil bulk density (BD)
- Available water ($P + I - RO - E_v$)
- Soil volumetric water content (q_{sw})

Determination of values for these parameters is further described in the following subsections.

2.5.1 Soil Mixing Zone Depth (Z_s)

When exposures to PB-HAP compounds in soils are modeled, the depth of contaminated soils is important in calculating the appropriate soil concentration. PB-HAP compounds deposited onto soil surfaces may be moved into lower soil profiles by tilling, whether manually in a garden or mechanically in a large field.

EPA (1998)⁽¹⁾ recommends the following values for the soil mixing zone depth (Z_s):

- 2 cm for untilled soils; and
- 20 cm for tilled soils.

The assumption made to determine the value of Z_s may affect the outcome of the risk assessment, because soil concentrations that are based on soil depth are used to calculate exposure via several pathways: (1) ingestion of plants contaminated by root uptake; (2) direct ingestion of soil by humans, cattle, swine, or chicken; and (3) surface runoff into water bodies.

2.5.2 Soil Dry Bulk Density (BD)

Soil dry bulk density (BD) is the ratio of the mass of soil to its total volume. EPA (1998)⁽¹⁾ recommends the value of 1.50 g/cm³ for the soil dry bulk density (BD). EPA (1994c)⁽¹⁸⁾ recommended that wet soil bulk density be determined by weighing a thin-walled, tube soil sample (e.g., a Shelby tube) of known volume and subtracting the tube weight (ASTM Method

D2937).⁽¹⁹⁾ Moisture content can then be calculated (ASTM Method 2216)⁽²⁰⁾ to convert wet soil bulk density to dry soil bulk density.

2.5.3 Available Water ($P + I - RO - E_v$)

The average annual volume of water available ($P + I - RO - E_v$) for generating leachate is the mass balance of all water inputs and outputs from the area under consideration. A wide range of values for these site-specific parameters may apply in the various EPA regions.

The average annual precipitation (P), irrigation (I), runoff (RO), and evapotranspiration (E_v) rates and other climatological data may be obtained from either data recorded on site or from the Station Climatic Summary for a nearby airport.

Meteorological variables such as the evapotranspiration rate (E_v) and the runoff rate (RO) may also be found in resources such as Geraghty, Miller, van der Leeden, and Troise (1973).⁽²¹⁾ Surface runoff may also be estimated by using the Curve Number Equation developed by the U.S. Soil Conservation Service (EPA 1990).⁽⁴⁾ EPA (1985)⁽²²⁾ cited isopleths of mean annual cropland runoff corresponding to various curve numbers developed by Stewart, Woolhiser, Wischmeier, Caro, and Frere (1975).⁽²³⁾ Curve numbers are assigned to an area on the basis of soil type, land use or cover, and the hydrologic conditions of the soil (EPA 1990).⁽⁴⁾

Using these different references, however, introduces uncertainties and limitations. For example, Geraghty, Miller, van der Leeden, and Troise (1973)⁽²¹⁾ presented isopleths for annual surface water contributions that include interflow and ground water recharge. As noted in EPA (1994a)⁽⁸⁾, these values are recommended to be adjusted downward to reflect surface runoff only. EPA (1994a)⁽⁸⁾ recommended that these values be reduced by 50 percent.

2.5.4 Soil Volumetric Water Content (θ_{sw})

The soil volumetric water content (θ_{sw}) depends on the available water and the soil structure. A wide range of values for these variables may apply in the various EPA regions. EPA (1998)⁽¹⁾ recommends a value for θ_{sw} of 0.2 ml/cm³.

3.0 Calculation of PB-HAP Compound Concentrations in Produce

Indirect exposure resulting from ingestion of produce depends on the total concentration of PB-HAP compounds in the leafy, fruit, and tuber portions of the plant. Because of general differences in contamination mechanisms, consideration of indirect exposure separates produce into two broad categories: aboveground produce and belowground produce. In addition, aboveground produce can be further subdivided into exposed and protected aboveground produce for consideration of contamination as a result of indirect exposure.

Aboveground Produce

Aboveground exposed produce is assumed to be contaminated by three possible mechanisms:

- **Direct deposition of particles**—wet and dry deposition of particle phase PB-HAP compounds on the leaves and fruits of plants (Section 3.1).

- **Vapor transfer**—uptake of vapor phase PB-HAP compounds by plants through their foliage (Section 3.2).
- **Root uptake**—root uptake of PB-HAP compounds available from the soil and their transfer to the aboveground portions of the plant (Section 3.3).

The total PB-HAP compound concentration in aboveground exposed produce is calculated as a sum of contamination occurring through all three of these mechanisms. However, edible portions of aboveground protected produce, such as peas, corn, and melons, are covered by a protective covering; hence, they are protected from contamination through deposition and vapor transfer. Therefore, root uptake of PB-HAP compounds is the primary mechanism through which aboveground protected produce becomes contaminated (Section 3.3).

Belowground Produce

For belowground produce, contamination is assumed to occur only through one mechanism – root uptake of PB-HAP compounds available from soil (Section 3.3). Contamination of belowground produce via direct deposition of particles and vapor transfer are not considered because the root or tuber is protected from contact with contaminants in the vapor phase.

3.1 Aboveground Produce Concentration Due to Direct Deposition (*Pd*)

EPA (1998)⁽¹⁾ recommends the use of Equation 8 to calculate PB-HAP compound concentration in exposed and aboveground produce due to direct deposition.

$$Pd = \frac{1,000 \cdot Q \cdot (1 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1 - \exp(-kp \cdot T_p)]}{Yp \cdot kp} \quad \text{(Equation 8)}$$

where

- Pd* = Plant (aboveground produce) concentration due to direct (wet and dry) deposition (mg PB-HAP compound/kg DW)
- 1,000 = Units conversion factor (mg/g)
- Q* = PB-HAP compound emission rate (g/s)
- F_v* = Fraction of PB-HAP compound air concentration in vapor phase (unitless)
- Dydp* = Unitized yearly average dry deposition from particle phase (s/m²-yr)
- Fw* = Fraction of PB-HAP compound wet deposition that adheres to plant surfaces (unitless)
- Dywp* = Unitized yearly wet deposition from particle phase (s/m²-yr)
- Rp* = Interception fraction of the edible portion of plant (unitless)
- kp* = Plant surface loss coefficient (yr⁻¹)
- T_p* = Length of plant exposure to deposition per harvest of the edible portion of the *i*th plant group (yr)
- Yp* = Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m²)

3.1.1 Interception Fraction of the Edible Portion of Plant (R_p)

EPA (1998)⁽¹⁾ recommends the use of the weighted average R_p value of 0.39 as a default R_p value because it represents the most current parameters including standing crop biomass and relative ingestion rates.

3.1.2 Plant Surface Loss Coefficient (kp)

EPA (1998)⁽¹⁾ recommends use of a plant surface loss coefficient (kp) value of 18. The primary uncertainty associated with this variable is that the calculation of kp does not consider chemical degradation processes. However, information regarding chemical degradation of contaminants on plant surfaces is limited. The inclusion of chemical degradation processes would result in decreased half-life values and thereby increase kp values. Note that effective plant concentration decreases as kp increases. Therefore, use of a kp value that does not consider chemical degradation processes is protective.

3.1.3 Length of Plant Exposure to Deposition per Harvest of Edible Portion of Plant (T_p)

This value represents the time required from when a plant first emerges until harvest. EPA (1998)⁽¹⁾ recommends using a T_p value of 0.164 year as the best available default value. The primary uncertainty associated with the use of this value is that it is based on the growing season for hay rather than aboveground produce. The average period between successive hay harvests (60 days) may not reflect the length of the growing season or the period between successive harvests for aboveground produce at specific sites. To the extent that information documenting the growing season or period between successive harvests for aboveground produce is available, this information may be used to estimate a site-specific T_p value. Calculated plant concentrations will be affected most if the site-specific value of T_p is significantly less than 60 days.

3.1.4 Standing Crop Biomass (Productivity) (Y_p)

EPA (1998)⁽¹⁾ recommends the use of the weighted average Y_p value of 2.24 as a default Y_p value based on this value representing the most complete and thorough information available. The primary uncertainty associated with this variable is that the harvest yield (Y_h) and area planted (A_h) may not reflect site-specific conditions. To the extent to which site-specific information is available, the magnitude of the uncertainty introduced by the default Y_p value can be estimated.

3.2 Aboveground Produce Concentration Due to Air-to-Plant Transfer (P_v)

The methodology used to estimate PB-HAP compound concentration in exposed and aboveground produce due to air-to-plant transfer (P_v) considers limitations of PB-HAP compounds concentrations to transfer from plant surfaces to the inner portions of the plant. These limitations result from mechanisms responsible for inhibiting the transfer of the lipophilic PB-HAP compound (e.g., the shape of the produce) and the removal of the PB-HAP compounds from the edible portion of the produce (e.g., washing, peeling, and cooking). EPA (1998)⁽¹⁾ recommends the use of Equation 9 to calculate aboveground produce concentration due to air-to-plant transfer (P_v).

$$P_v = Q \cdot F_v \cdot \frac{C_{yv} \cdot B_{v_{ag}} \cdot VG_{ag}}{\rho_a} \quad (\text{Equation 9})$$

where

- P_v = Concentration of PB-HAP compound in the plant resulting from air-to-plant transfer ($\mu\text{g PB-HAP compound/g DW}$)
- Q = PB-HAP compound emission rate (g/s)
- F_v = Fraction of PB-HAP compound air concentration in vapor phase (unitless)
- C_{yv} = Unitized yearly average air concentration from vapor phase ($\mu\text{g-s/g-m}^3$)
- $B_{v_{ag}}$ = PB-HAP compound air-to-plant biotransfer factor ($[\text{mg PB-HAP compound/g DW plant}]/[\text{mg PB-HAP compound/g air}]$) (unitless)
- VG_{ag} = Empirical correction factor for aboveground produce (unitless)
- ρ_a = Density of air (g/m^3)

As discussed below in Section 3.2.1, the parameter VG_{ag} is dependent on lipophilicity of the PB-HAP compound, and assigned a value of 0.01 for lipophilic PB-HAP compounds ($\log K_{ow}$ greater than 4) or a value of 1.0 for PB-HAP compounds with a $\log K_{ow}$ less than 4.

Empirical Correction Factor for Aboveground Produce (VG_{ag})

The parameter VG_{ag} has been incorporated into Equation 9 to address the potential overestimation for lipophilic PB-HAP compounds to be transferred to the inner portions of bulky produce, such as apples. Because of the protective outer skin, size, and shape of bulky produce, transfer of lipophilic PB-HAP compounds ($\log K_{ow}$ greater than 4) to the center of the produce is not as likely as for non-lipophilic PB-HAP compounds and, as a result, the inner portions will be less affected. EPA (1998)⁽¹⁾ recommends the following empirical VG_{ag} values for aboveground produce:

- 0.01 for lipophilic PB-HAP compounds ($\log K_{ow}$ greater than 4); and
- 1.0 for PB-HAP compounds with a $\log K_{ow}$ less than 4 (these PB-HAP compounds are assumed pass more easily through the skin of produce).

Uncertainty may be introduced by the assumption of VG_{ag} values for leafy vegetables (such as lettuce) and for legumes (such as snap beans). Underestimation may be introduced by assuming a VG_{ag} value of 0.01 for legumes and leafy vegetables because these species often have a higher ratio of surface area to mass than other bulkier fruits and fruiting vegetables, such as tomatoes.

3.3 Produce Concentration Due to Root Uptake (Pr)

Root uptake of contaminants from soil may also result in PB-HAP compound concentrations in aboveground exposed produce, aboveground protected produce, and belowground produce. EPA (1998)⁽¹⁾ recommends the use of Equations 10A and 10B to calculate PB-HAP compound concentration aboveground and belowground produce due to root uptake (Pr).

Exposed and protected aboveground produce:

$$Pr = Cs \cdot Br \quad (\text{Equation 10A})$$

Belowground produce:

$$Pr = \frac{Cs \cdot RCF \cdot VG_{rootveg}}{Kd_s \cdot 1 \text{ kg / L}} \quad (\text{Equation 10B})$$

where

- Pr = Concentration of PB-HAP compound in produce due to root uptake (mg/kg)
 Br = Plant-soil bioconcentration factor for produce (unitless)
 $VG_{rootveg}$ = Empirical correction factor for belowground produce (unitless)
 Kd_s = Soil-water partition coefficient (L/kg)
 Cs = Average soil concentration over exposure duration (mg PB-HAP compound/kg soil)
 RCF = Root concentration factor (unitless)

Equation 10A is appropriate for evaluation of exposed and protected aboveground produce; however, it may not be appropriate for soil-to-belowground plant transfers. For belowground produce, Equation 10B includes a root concentration factor (RCF) developed by Briggs et al. (1982).⁽²⁴⁾ RCF is the ratio of PB-HAP compound concentration in the edible root to the PB-HAP compound concentration in the soil water. Since Briggs et al. (1982)⁽²⁴⁾ conducted their experiments in a growth solution, the PB-HAP compound soil concentration (Cs) must be divided by the PB-HAP compound-specific soil-water partition coefficient (Kd_s) (EPA 1994b).⁽²⁵⁾

Similar to VG_{ag} and as discussed in Section 3.2.1, $VG_{rootveg}$ is based on the lipophilicity of the PB-HAP compound. EPA (1998)⁽¹⁾ recommends the following empirical values for $VG_{rootveg}$:

- 0.01 for lipophilic PB-HAP compounds ($\log K_{ow}$ greater than 4) based on root vegetables like carrots and potatoes; and
- 1.0 for PB-HAP compounds with a $\log K_{ow}$ less than 4.

4.0 Calculation of PB-HAP Compound Concentrations in Beef and Dairy Products

PB-HAP compound concentrations in beef tissue and milk products are estimated on the basis of the amount of PB-HAP compounds that cattle are assumed to consume through their diet. The cattle's diet is assumed to consist of forage (primarily pasture grass and hay); silage (forage that has been stored and fermented), and grain. Additional contamination may occur through the cattle's ingestion of soil. The total PB-HAP compound concentration in the feed items (e.g., forage, silage, and grain) is calculated as a sum of contamination occurring through the following mechanisms:

- **Direct deposition of particles**—wet and dry deposition of particle phase PB-HAP compounds onto forage and silage (Section 4.1).

- **Vapor transfer**—uptake of vapor phase PB-HAP compounds by forage and silage through foliage (Section 4.2).
- **Root uptake**—root uptake of PB-HAP compounds available from the soil and their transfer to the aboveground portions of forage, silage, and grain (Section 4.3).

Feed items consumed by animals can be classified as exposed and protected, depending on whether it has a protective outer covering. Because the outer covering on the protected feed acts as a barrier, it is assumed that there is negligible contamination of protected feed through deposition of particles and vapor transfer. In this analysis, grain is classified as protected feed. As a result, grain contamination is assumed to occur only through root uptake. Contamination of exposed feed items, including forage and silage, is assumed to occur through all three mechanisms.

The amount of grain, silage, forage, and soil consumed is assumed to vary between dairy and beef cattle. Sections 4.4 (beef) and 4.5 (dairy) describe methods for estimating consumption rates and subsequent PB-HAP compound concentrations in cattle. EPA (1998)⁽¹⁾ recommends that 100 percent of the plant materials eaten by cattle be assumed to have been grown on soil contaminated by emission sources. Therefore, 100 percent of the feed items consumed are assumed to be contaminated.

4.1 Forage and Silage Concentrations Due to Direct Deposition (*Pd*)

PB-HAP compound concentrations in forage and silage result from wet and dry deposition onto exposed plant surfaces; similar to aboveground produce (Section 3.1). Equation 8, described in Section 3.1, is recommended for calculation of PB-HAP compound concentrations resulting from direct deposition onto plant surfaces of leafy plants and exposed produce (*Pd*). Therefore, EPA (1998)⁽¹⁾ recommends that Equation 8 also be used in calculating forage and silage concentrations due to direct deposition.

4.1.1 Interception Fraction of the Edible Portion of Plant (*Rp*)

EPA (1998)⁽¹⁾ recommends use of the *Rp* value of 0.5 for forage and the *Rp* value of 0.46 for silage. Note that the empirical relationships used to develop the default values for silage may not accurately represent site-specific silage types. However, the range of empirical constants used to develop the default value for forage is fairly small, and therefore the use of the midpoint should not significantly affect the *Rp* value and the resulting estimate of plant PB-HAP compound concentration.

4.1.2 Plant Surface Loss Coefficient (*kp*)

Section 3.1.2 presents the recommended value for plant surface loss coefficient *kp* for aboveground produce. The *kp* factor is derived in exactly the same manner for cattle forage and silage, and the uncertainties of *kp* for cattle forage and silage are similar to its uncertainties for aboveground produce.

4.1.3 Length of Plant Exposure to Deposition per Harvest of the Edible Portion of Plant (T_p)

As discussed in Section 3.1.3, T_p is treated as a constant, based on the average period between successive hay harvests. This period represents the length of time that aboveground vegetation (in this case, hay) would be exposed to particle deposition before being harvested. EPA (1998)⁽¹⁾ recommends the following T_p values: 0.12 year for forage; and 0.16 year for silage. The primary uncertainties associated with T_p are similar to those for aboveground produce, and are discussed in Section 3.1.3.

4.1.4 Standing Crop Biomass (Productivity) (Y_p)

As discussed in Section 3.1.4, the best estimate of Y_p is productivity, requires consideration of dry harvest yield (Y_h) and area harvested (A_h). EPA (1998)⁽¹⁾ recommends that forage Y_p be calculated as a weighted average of the calculated pasture grass and hay Y_p values. Weightings are assumed to be 0.75 for forage and 0.25 for hay, based on the fraction of a year that cattle are assumed to be pastured and eating grass (9 months per year) or not pastured and fed hay (3 months per year). The resulting value of 0.24 kg DW/m² is recommended as the Y_p for forage. For silage, EPA (1998)⁽¹⁾ recommends that a production-weighted U.S. average Y_p of 0.8 kg DW/m² be assumed. The primary uncertainty associated with this variable is that the harvest yield (Y_h) and area planted (A_h) may not reflect site-specific conditions. To the extent that site-specific information is available, the magnitude of the uncertainty introduced by the default Y_p value can be estimated. In addition, the weightings assumed in this discussion for the amount of time that cattle are pastured (and foraging) or stabled (and being fed silage) should be adjusted to reflect site-specific conditions, as appropriate.

4.2 Forage and Silage Concentrations Due to Air-to-Plant Transfer (P_v)

PB-HAP compound concentration in aboveground produce resulting from air-to-plant transfer (P_v), is calculated by using Equation 9 (Section 3.2). P_v is calculated for cattle forage and silage similarly to the way that it is calculated for aboveground produce. A detailed discussion of P_v is provided in Section 3.2. Differences in VG_{ag} values for forage and silage, as compared to the values for aboveground produce described in Section 3.2.1, are presented below in Section 4.2.1.

Empirical Correction Factor for Forage and Silage (VG_{ag})

EPA (1998)⁽¹⁾ recommends the use of VG_{ag} values of 1.0 for forage and 0.5 for silage. As discussed, the primary uncertainty associated with this variable is the lack of specific information on the proportions of each vegetation type of which silage may consist, leading to the default assumption of 0.5.

4.3 Forage, Silage, and Grain Concentrations Due to Root Uptake (P_r)

PB-HAP compound concentration in aboveground and belowground produce resulting from root uptake is calculated by using Equations 10A and 10B (Section 3.3). P_r is also calculated for cattle forage, silage, and grain in exactly the same way that it is calculated for aboveground produce. A detailed discussion describing calculation of P_r is provided in Section 3.3.

4.4 Beef Concentration Resulting from Plant and Soil Ingestion (A_{beef})

EPA (1998)⁽¹⁾ recommends that PB-HAP compound concentration in beef tissue (A_{beef}) be calculated by using Equation 11. Equation 11 calculates the daily amount of a PB-HAP compound that is consumed by cattle through the ingestion of contaminated feed items (plant) and soil. The equation includes biotransfer and metabolism factors to transform the daily animal intake of a PB-HAP compound (mg/day) into an animal PB-HAP compound tissue concentration (mg PB-HAP compound/kg tissue).

$$A_{beef} = \left(\sum (F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{beef} \cdot MF \quad (\text{Equation 11})$$

where

- A_{beef} = Concentration of PB-HAP compound in beef (mg PB-HAP compound/kg FW tissue)
 F_i = Fraction of plant type i grown on contaminated soil and ingested by the animal (cattle) (unitless)
 Qp_i = Quantity of plant type i eaten by the animal (cattle) per day (kg DW plant/day)
 P_i = Concentration of PB-HAP compound in each plant type i eaten by the animal (cattle) (mg/kg DW)
 Qs = Quantity of soil eaten by the animal (cattle) each day (kg/day)
 Cs = Average soil concentration over exposure duration (mg PB-HAP compound/kg soil)
 Bs = Soil bioavailability factor (unitless)
 Ba_{beef} = PB-HAP compound biotransfer factor for beef (day/kg FW tissue)
 MF = Metabolism factor (unitless)

The parameters F_i , Qp_i , P_i , Qs , Cs , Bs , and MF are described in Sections 4.4.1 through 4.4.7, respectively.

4.4.1 Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Cattle)(F_i)

EPA (1998)⁽¹⁾ recommends that 100 percent of the plant materials eaten by cattle be assumed to have been grown on soil contaminated by the emission sources being evaluated and therefore recommends a default value of 1.0 for F_i .

4.4.2 Quantity of Plant Type i Eaten by the Animal (Cattle) Each Day (Qp_i)

EPA (1998)⁽¹⁾ recommends the following beef cattle ingestion rates of forage, silage, and grain. These values are based on the total daily intake rate of about 12 kg DW/day.

- Forage = 8.8 kg DW/day;
- Silage = 2.5 kg DW/day; and
- Grain = 0.47 kg DW/day.

The principal uncertainty associated with Qp_i is the variability between forage, silage, and grain ingestion rates for cattle.

4.4.3 Concentration of PB-HAP compound in Plant Type *i* Eaten by the Animal (Cattle) (P_i)

The total PB-HAP compound concentration in forage, silage, and grain are recommended to be calculated by using Equation 12. Values for P_d , P_v , and P_r can be derived for each type of feed by using Equations 8, 17, and 10, respectively.

$$P_i = \sum_i (P_d + P_v + P_r) \quad (\text{Equation 12})$$

where

P_i = Concentration of PB-HAP compound in each plant type *i* eaten by the animal (mg PB-HAP compound/kg DW)

P_d = Plant concentration due to direct deposition (mg PB-HAP compound/kg DW)

P_v = Plant concentration due to air-to-plant transfer (mg PB-HAP compound/kg DW)

P_r = Plant concentration due to root uptake (mg PB-HAP compound/kg DW)

4.4.4 Quantity of Soil Eaten by the Animal (Cattle) Per Day (Q_s)

Additional cattle contamination occurs through ingestion of soil. EPA (1998)⁽¹⁾ recommends a value of 0.5 kg/day for the quantity of soil ingested by the animal (cattle).

4.4.5 Average Soil Concentration Over Exposure Duration (C_s)

PB-HAP compound concentration in soil is recommended to be calculated as discussed in Section 2.1, by using Equations 1A, 1B, and 1C.

4.4.6 Soil Bioavailability Factor (B_s)

The efficiency of transfer from soil may differ from efficiency of transfer from plant material for some PB-HAP compounds. If the transfer efficiency is lower for soils, than this ratio would be less than 1.0. If it is equal or greater than that of vegetation, the B_s value would be equal to or greater than 1.0. Until more PB-HAP compound-specific data becomes available for this parameter, EPA (1998)⁽¹⁾ recommends a default value of 1 for B_s .

4.4.7 Metabolism Factor (MF)

The metabolism factor (MF) represents the estimated amount of PB-HAP compound that remains in fat and muscle. EPA (1998)⁽¹⁾ recommends a MF of 1.0 for all PB-HAP compounds.

Considering the recommended values for this variable, MF has no quantitative effect on A_{beef} . MF applies only to mammalian species, including beef cattle, dairy cattle, and pigs. It does not relate to metabolism in produce, chicken, or fish. In addition, since exposures evaluated in this chapter are intake driven, the use of a metabolism factor applies only to ingestion of beef, milk, and pork. In summary, use of a MF does not apply for direct exposures to soil or water, or to ingestion of produce, chicken, or fish.

4.5 PB-HAP compound Concentration In Milk Due to Plant and Soil Ingestion (A_{milk})

Equation 11 (Section 4.4) describes the calculation of PB-HAP compound concentrations in beef cattle (A_{beef}). Equation 11 can be modified to calculate PB-HAP compound milk concentrations (A_{milk}), as follows:

$$A_{milk} = \left(\sum (F_i \cdot Q_{pi} \cdot P_i) + Q_s \cdot C_s \cdot B_s \right) \cdot Ba_{milk} \cdot MF \quad (\text{Equation 13})$$

where

A_{milk}	=	Concentration of PB-HAP compound in milk (mg PB-HAP compound/kg milk)
F_i	=	Fraction of plant type i grown on contaminated soil and ingested by the animal (dairy cattle) (unitless)
Q_{pi}	=	Quantity of plant type i eaten by the animal (dairy cattle) each day (kg DW plant/day)
P_i	=	Concentration of PB-HAP compound in plant type i eaten by the animal (dairy cattle) (mg/kg DW)
Q_s	=	Quantity of soil eaten by the animal (dairy cattle) each day (kg soil/day)
C_s	=	Average soil concentration over exposure duration (mg PB-HAP compound/kg soil)
B_s	=	Soil bioavailability factor (unitless)
Ba_{milk}	=	PB-HAP compound biotransfer factor for milk (day/kg WW tissue)
MF	=	Metabolism factor (unitless)

EPA (1998)⁽¹⁾ recommends the use of Equation 13 to estimate dairy cattle milk PB-HAP compound concentration (A_{milk}). The discussion in Section 4.4 of the variables F_i , Q_{pi} , P_i , Q_s , C_s , and MF for beef cattle generally applies to the corresponding variables for dairy cattle. However, there are some differences in assumptions made for dairy cattle; these differences are summarized in the following subsections.

4.5.1 Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Dairy Cattle) (F_i)

The calculation of F_i for dairy cattle is identical to that for beef cattle (Section 4.4.1).

4.5.2 Quantity of Plant Type i Eaten by the Animal (Dairy Cattle) Per Day (Q_{pi})

As discussed in Section 4.4.2, the daily quantity of forage, silage, and grain feed consumed by cattle is estimated for each category of feed material. However, daily ingestion rates for dairy cattle are estimated differently than for beef cattle. The daily quantity of feed consumed by cattle is recommended to be estimated on a dry weight basis for each category of plant feed.

EPA (1998)⁽¹⁾ recommends a default total ingestion rate of 20 kg DW/day for dairy cattle, divided among forage, silage, and grain, as follows:

- Forage = 13.2 kg DW/day;
- Silage = 4.1 kg DW/day; and
- Grain = 3.0 kg DW/day

Uncertainties associated with the estimation of Q_{pi} include the estimation of forage, grain, and silage ingestion rates, which will vary from site to site. The assumption of uniform contamination of plant materials consumed by cattle also introduces uncertainty.

4.5.3 Concentration of PB-HAP compound in Plant Type i Eaten by the Animal (Dairy Cattle) (P_i)

The estimation of P_i for dairy cattle is identical to that for beef cattle (Section 4.4.3).

4.5.4 Quantity of Soil Eaten by the Animal (Dairy Cattle) Per Day (Q_s)

As discussed in Section 4.4.4, contamination of dairy cattle also results from the ingestion of soil. EPA (1998)⁽¹⁾ recommends a soil ingestion rate of 0.4 kg/day for dairy cattle. Uncertainties associated with Q_s include the lack of current empirical data to support soil ingestion rates for dairy cattle. The assumption of uniform contamination of soil ingested by cattle also adds uncertainty.

4.5.5 Average Soil Concentration Over Exposure Duration (C_s)

The calculation of C_s for dairy cattle is the same as for beef cattle (Section 4.4.5).

4.5.6 Soil Bioavailability Factor (B_s)

The calculation of B_s for dairy cattle is the same as for beef cattle (Section 4.4.6).

4.5.7 Metabolism Factor (MF)

The recommended values for MF are identical to those recommended for beef cattle (Section 4.4.7).

5.0 Calculation of PB-HAP Compound Concentrations in Pork

PB-HAP compound concentrations in pork tissue are estimated on the basis of the amount of PB-HAP compounds that swine are assumed to consume through their diet; assumed to consist of silage and grain. Additional PB-HAP compound contamination of pork tissue may occur through the ingestion of soil by swine.

5.1 Concentration of PB-HAP compound In Pork

Equation 11 (Section 4.4) describes the calculation of PB-HAP compound concentration in beef cattle (A_{beef}). Equation 11 can be modified to calculate PB-HAP compound concentrations in swine (A_{pork}), as follows:

$$A_{pork} = \left(\sum (F_i \cdot Q_{pi} \cdot P_i) + Q_s \cdot C_s \cdot B_s \right) \cdot Ba_{pork} \cdot MF \quad (\text{Equation 14})$$

where

A_{pork}	=	Concentration of PB-HAP compound in pork (mg PB-HAP compound/kg FW tissue)
F_i	=	Fraction of plant type i grown on contaminated soil and ingested by the animal (swine)(unitless)
Qp_i	=	Quantity of plant type i eaten by the animal (swine) each day (kg DW plant/day)
P_i	=	Concentration of PB-HAP compound in plant type i eaten by the animal (swine) (mg/kg DW)
Qs	=	Quantity of soil eaten by the animal (swine) (kg/day)
Cs	=	Average soil concentration over exposure duration (mg PB-HAP compound/kg soil)
Bs	=	Soil bioavailability factor (unitless)
Ba_{pork}	=	PB-HAP compound biotransfer factor for pork (day/kg FW tissue)
MF	=	Metabolism factor (unitless)

EPA (1998)⁽¹⁾ recommends that Equation 14 be used to calculate PB-HAP compound pork concentrations (A_{pork}). The discussion in Section 4.5 of the variables F_i , Qp_i , P_i , Qs , Cs and MF for beef cattle generally applies to the corresponding variables for pork. However, different assumptions are made for pork. These differences are summarized in the following subsections.

5.1.1 Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Swine) (F_i)

The calculation of F_i for pork is identical to that for beef cattle (Section 4.4.1).

5.1.2 Quantity of Plant Type i Eaten by the Animal (Swine) Each Day (Qp_i)

As discussed in Section 4.4.2, the daily quantity of forage, silage, and grain feed consumed by beef cattle is estimated for each category of feed material. However, daily ingestion rates for pork are estimated differently than for beef cattle. Because swine are not grazing animals, they are assumed not to eat forage, and EPA (1998)⁽¹⁾ recommends that the daily quantity of plant feeds (kilograms of DW) consumed by swine be estimated for each category of plant feed.

EPA (1990)⁽⁴⁾ and NC DEHNR (1997)⁽²⁶⁾ did not differentiate between subsistence and typical hog farmers as for cattle. EPA (1990)⁽⁴⁾ and NC DEHNR (1997)⁽²⁶⁾ recommended grain and silage ingestion rates for swine as 3.0 and 1.3 kg DW/day, respectively. NC DEHNR (1997)⁽²⁶⁾ references EPA (1990)⁽⁴⁾ as the source of these ingestion rates. EPA (1990)⁽⁴⁾ reported total dry matter ingestion rates for hogs and lactating sows as 3.4 and 5.2 kg DW/day, respectively. EPA (1990)⁽⁴⁾ cites Boone, Ng, and Palm (1981)⁽²⁷⁾ as the source of the ingestion rate for hogs, and NAS (1987)⁽²⁸⁾ as the source of the ingestion rate for a lactating sow. Boone, Ng, and Palm (1981)⁽²⁷⁾ reported a grain ingestion rate of 3.4 kg DW/day for a hog. NAS (1987)⁽²⁸⁾ reported an average ingestion rate of 5.2 kg DW/day for a lactating sow. EPA (1990)⁽⁴⁾ recommended using the average of these two rates (4.3 kg DW/day). EPA (1990)⁽⁴⁾ assumed that 70 percent of the swine diet is grain and 30 percent silage to obtain the grain ingestion rate of 3.0 kg DW/day and the silage ingestion rate of 1.3 kg DW/day. EPA (1990)⁽⁴⁾ cited EPA (1982)⁽²⁹⁾ as the source of the grain and silage dietary fractions. EPA (1995)⁽³⁰⁾ recommended an ingestion rate of 4.7 kg DW/day for a swine, referencing NAS (1987).⁽²⁸⁾ NAS (1987)⁽²⁸⁾ reported an average daily intake of 4.36 kg DW/day for a gilt (young sow) and a average daily intake of 5.17 kg DW/day for a sow, which averages out to 4.7 kg/DW/day. Assuming the 70 percent grain to 30 percent silage diet noted above, estimated ingestion rates of 3.3 kg DW/day (grain) and 1.4 kg DW/day (silage) are derived.

EPA (1998)⁽¹⁾ recommends the use of the following Qp_i values for pork:

- Grain = 3.3 kg DW/day; and
- Silage = 1.4 kg DW/day.

Uncertainties associated with this variable include the variability of actual grain and silage ingestion rates from site to site. Site-specific data can be used to mitigate this uncertainty. In addition, the assumption of uniform contamination of plant materials consumed by swine produces some uncertainty.

5.1.3 Concentration of PB-HAP compound in Plant Type i Eaten by the Animal (Swine) (P_i)

The calculation of P_i for pork is identical to that for beef cattle (Section 4.4.3).

5.1.4 Quantity of Soil Eaten by the Animal (Swine) Each Day (Q_s)

As discussed in Section 4.4.4, additional contamination of swine results from ingestion of soil. EPA (1998)⁽¹⁾ recommends the following soil ingestion rate for swine: 0.37 kg DW/day. Uncertainties associated with this variable include the lack of current empirical data to support soil ingestion rates for swine, and the assumption of uniform contamination of soil ingested by swine.

5.1.5 Average Soil Concentration Over Exposure Duration (C_s)

The calculation of C_s for pork is the same as for beef cattle (Section 4.4.5).

5.1.6 Soil Bioavailability Factor (B_s)

The calculation of B_s for pork is the same as for beef cattle (Section 4.4.6)

5.1.7 Metabolism Factor (MF)

The recommended values for MF are identical to those recommended for beef cattle (Section 4.4.7).

6.0 Calculation of PB-HAP Compound Concentrations in Chicken and Eggs

Estimates of the PB-HAP compound concentrations in chicken and eggs are based on the amount of PB-HAP compounds that chickens consume through ingestion of grain and soil. The uptake of PB-HAP compounds via inhalation and via ingestion of water is assumed to be insignificant relative to other pathways. Chickens are assumed to be housed in a typical manner that allows contact with soil; and therefore, are assumed to consume 10 percent of their diet as soil. The remainder of the diet (90 percent) is assumed to consist of grain. Grain ingested by chickens is assumed to have originated from the exposure scenario location; therefore, 100 percent of the grain consumed is assumed to be contaminated. The uptake of PB-HAP compounds via ingestion of contaminated insects and other organisms (e.g., worms, etc.), which may also

contribute to the ingestion of PB-HAP compounds, is not accounted for in the equations and may be a limitation depending on the site-specific conditions under which the chickens are raised.

The PB-HAP compound concentration in grain is estimated by using the algorithm for aboveground produce described in Section 3. Grain is considered to be a feed item that is protected from deposition of particles and vapor transfer. As a result, only contamination due to root uptake of PB-HAP compounds is considered in the calculation of PB-HAP compound concentration in grain.

6.1 Concentration of PB-HAP compound in Chicken and Eggs

EPA (1998)⁽¹⁾ recommends the use of Equation 15 to calculate PB-HAP compound concentrations in chicken and eggs. It is recommended that PB-HAP compound concentrations in chicken and eggs be determined separately.

$$A_{chicken} \text{ or } A_{egg} = \left(\sum [F_i \cdot Qp_i \cdot P_i] + Qs \cdot Cs \cdot Bs \right) \cdot \left(Ba_{egg} \text{ or } Ba_{chicken} \right) \quad (\text{Equation 15})$$

where

- $A_{chicken}$ = Concentration of PB-HAP compound in chicken (mg PB-HAP compound/kg FW tissue)
- A_{egg} = Concentration of PB-HAP compound in eggs (mg PB-HAP compound/kg FW tissue)
- F_i = Fraction of plant type i (grain) grown on contaminated soil and ingested by the animal (chicken)(unitless)
- Qp_i = Quantity of plant type i (grain) eaten by the animal (chicken) each day (kg DW plant/day)
- P_i = Concentration of PB-HAP compound in plant type i (grain) eaten by the animal (chicken) (mg/kg DW)
- Qs = Quantity of soil eaten by the animal (chicken) (kg/day)
- Cs = Average soil concentration over exposure duration (mg PB-HAP compound/kg soil)
- Bs = Soil bioavailability factor (unitless)
- $Ba_{chicken}$ = PB-HAP compound biotransfer factor for chicken (day/kg FW tissue)
- Ba_{egg} = PB-HAP compound biotransfer factor for eggs (day/kg FW tissue)

EPA (1998)⁽¹⁾ describes determination of compound specific parameters $Ba_{chicken}$ and Ba_{egg} . The remaining parameters are discussed in the following subsections.

6.1.1 Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Chicken)(F_i)

The calculation of F_i for chicken is identical to that for beef cattle (Section 4.4.1).

6.1.2 Quantity of Plant Type i Eaten by the Animal (Chicken) Each Day (Qp_i)

Because chickens are not grazing animals, they are assumed not to eat forage. Chickens are assumed not to consume any silage. The daily quantity of plant feeds (kilograms of DW)

consumed by chicken only should be estimated for grain feed. EPA (1998)⁽¹⁾ recommends the use of the following ingestion rate (Q_{p_i}): Grain = 0.2 kg DW/day. Uncertainties associated with this variable include the variability of actual grain ingestion rates from site to site. In addition, the assumption of uniform contamination of plant materials consumed by chicken produces some uncertainty.

6.1.3 Concentration of PB-HAP compound in Plant Type i Eaten by the Animal (Chicken) (P_i)

The total PB-HAP compound concentration is the PB-HAP compound concentration in grain and can be calculated by using Equation 16. Values for Pr can be derived by using Equation 10.

$$P_i = \sum_i (Pr) \quad \text{(Equation 16)}$$

where

P_i = Concentration of PB-HAP compound in each plant type i eaten by the animal (mg PB-HAP compound/kg DW)

Pr = Plant concentration due to root uptake (mg PB-HAP compound/kg DW)

6.1.4 Quantity of Soil Eaten by the Animal (Chicken) Each Day (Q_s)

PB-HAP compound concentration in chickens also results from intake of soil. As discussed earlier, chickens are assumed to consume 10 percent of their total diet as soil. EPA (1998)⁽¹⁾ recommends the following soil ingestion rate for chicken: 0.022 kg DW/day. Uncertainties associated with this variable include the lack of current empirical data to support soil ingestion rates for chicken, and the assumption of uniform contamination of soil ingested by chicken.

6.1.5 Average Soil Concentration Over Exposure Duration (C_s)

The calculation of C_s for chicken is the same as for beef cattle (Section 4.4.5).

6.1.6 Soil Bioavailability Factor (B_s)

The calculation of B_s for chicken is the same as for beef cattle (Section 4.4.6)

7.0 Calculation of PB-HAP Compound Concentrations in Drinking Water and Fish

PB-HAP compound concentrations in surface water are calculated for all water bodies selected for evaluation in the risk assessment; specifically, evaluation of the drinking water and/or fish ingestion exposure pathways. Mechanisms considered for determination of PB-HAP compound loading of the water column are:

- (1) Direct deposition,
- (2) Runoff from impervious surfaces within the watershed,
- (3) Runoff from pervious surfaces within the watershed,
- (4) Soil erosion over the total watershed,
- (5) Direct diffusion of vapor phase PB-HAP compounds into the surface water, and
- (6) Internal transformation of compounds chemically or biologically.

Other potential mechanisms may need consideration on a case-by-case basis (e.g., tidal influences), however, contributions from other potential mechanisms are assumed to be negligible in comparison with those being evaluated.

The USLE and a sediment delivery ratio are used to estimate the rate of soil erosion from the watershed. In the ISCST3 model, surface water concentration algorithms include a sediment mass balance, in which the amount of sediment assumed to be buried and lost from the water body is equal to the difference between the amount of soil introduced to the water body by erosion and the amount of suspended solids lost in downstream flow. As a result, the assumptions are made that sediments do not accumulate in the water body over time, and an equilibrium is maintained between the surficial layer of sediments and the water column. The total water column PB-HAP compound concentration is the sum of the PB-HAP compound concentration dissolved in water and the PB-HAP compound concentration associated with suspended solids. Partitioning between water and sediment varies with the PB-HAP compound. The total concentration of each PB-HAP compound is partitioned between the sediment and the water column. The assumptions for other multimedia models may differ.

To evaluate the PB-HAP compound loading to a water body from its associated watershed, it is recommended that the PB-HAP compound concentration in watershed soils be calculated. As described in Section 2, the equation for PB-HAP compound concentration in soil includes a loss term that considers the loss of contaminants from the soil after deposition. These loss mechanisms all lower the soil concentration associated with a specific deposition rate.

The ISCST3 model approach for modeling PB-HAP compound loading to a water body represents a simple steady-state model to solve for a water column in equilibrium with the upper sediment layer. This approach may be limited in addressing the dynamic exchange of contaminants between the water body and the sediments following changes in external loadings. While appropriate for calculating risk under long-term average conditions, the evaluation of complex water bodies or shorter term loading scenarios may be improved through the use of a dynamic modeling framework [e.g., Exposure Analysis Modeling System (EXAMS)]. Although typically more resource intensive, such analysis may offer the ability to refine modeling of contaminant loading to a water body. Additionally, the computations may better represent the exposure scenario being evaluated.

For example, EXAMS allows computations to be performed for each defined segment or compartment of a water body or stream. These compartments are considered physically homogeneous and are connected via advective and dispersive fluxes. Compartments can be defined as littoral, epilimnion, hypolimnion, or benthic. Such resolution also makes it possible to assign receptor locations specific to certain portions of a water body where evaluation of exposure is of greatest interest.

Some considerations regarding the selection and use of a dynamic modeling framework or simulation model to evaluate water bodies may include the following:

- Will a complex surface water modeling effort provide enhanced results over the use of the more simplistic steady-state equations;

- Are the resources needed to conduct, as well as review, a more complex modeling effort justified in comparison to the refinement to results provided;
- Has the model been used previously for regulatory purposes, and therefore, already has available documentation to support such uses;
- Can the model conduct steady-state and dynamic analysis; and
- Does the model require calibration with field data, and if so, are there sufficient quantity and quality of site-specific data available to support calibration.

7.1 Total PB-HAP compound Load to the Water Body (L_T)

EPA (1998)⁽¹⁾ recommends the use of Equation 17 to calculate the total PB-HAP compound load to a water body (L_T).

$$L_T = L_{DEP} + L_{dif} + L_{RI} + L_R + L_E + L_I \quad (\text{Equation 17})$$

where

- L_T = Total PB-HAP compound load to the water body (including deposition, runoff, and erosion) (g/yr)
- L_{DEP} = Total (wet and dry) particle phase and vapor phase PB-HAP compound direct deposition load to water body (g/yr)
- L_{dif} = Vapor phase PB-HAP compound diffusion load to water body (g/yr)
- L_{RI} = Runoff load from impervious surfaces (g/yr)
- L_R = Runoff load from pervious surfaces (g/yr)
- L_E = Soil erosion load (g/yr)
- L_I = Internal transfer (g/yr)

Due to the limited data and uncertainty associated with the chemical or biological internal transfer, L_I , of compounds into daughter products, EPA (1998)⁽¹⁾ recommends a default value for this variable of zero. However, if a permitting authority determines that site-specific conditions indicate calculation of internal transfer may need to be considered, EPA (1998)⁽¹⁾ recommends following the methodologies described in EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Pathways of Exposure to Combustor Emissions* (EPA 1998).⁽¹²⁾ Calculation of each of the remaining variables (L_{DEP} , L_{dif} , L_{RI} , L_R , and L_E) is discussed in the following subsections.

7.1.1 Total (Wet and Dry) Particle Phase and Vapor Phase PB-HAP compound Direct Deposition Load to Water Body (L_{DEP})

EPA (1998)⁽¹⁾ recommends Equation 18 to calculate the load to the water body from the direct deposition of wet and dry particles and vapors onto the surface of the water body (L_{DEP}).

$$L_{DEP} = Q \cdot \left[F_v \cdot Dytwv + (1 - F_v) \cdot Dytyp \right] \cdot A_w \quad (\text{Equation 18})$$

where

- L_{DEP} = Total (wet and dry) particle phase and vapor phase PB-HAP compound direct deposition load to water body (g/yr)
 Q = PB-HAP compound emission rate (g/s)
 F_v = Fraction of PB-HAP compound air concentration in vapor phase (unitless)
 D_{ytwv} = Unitized yearly (water body or watershed) average total (wet and dry) deposition from vapor phase (s/m²-yr)
 D_{ytwp} = Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase (s/m²-yr)
 A_w = Water body surface area (m²)

7.1.2 Vapor Phase PB-HAP compound Diffusion Load to Water Body (L_{dif})

EPA (1998)⁽¹⁾ recommends using Equation 19 to calculate the vapor phase PB-HAP compound diffusion load to the water body (L_{dif}).

$$L_{dif} = \frac{K_v \cdot Q \cdot F_v \cdot C_{yvw} \cdot A_w \cdot 1 \times 10^{-6}}{H \cdot R \cdot T_{wk}} \quad \text{(Equation 19)}$$

where

- L_{dif} = Vapor phase PB-HAP compound diffusion load to water body (g/yr)
 K_v = Overall PB-HAP compound transfer rate coefficient (m/yr)
 Q = PB-HAP compound emission rate (g/s)
 F_v = Fraction of PB-HAP compound air concentration in vapor phase (unitless)
 C_{yvw} = Unitized yearly (water body or watershed) average air concentration from vapor phase (µg-s/g-m³)
 A_w = Water body surface area (m²)
 10^{-6} = Units conversion factor (g/µg)
 H = Henry's Law constant (atm-m³/mol)
 R = Universal gas constant (atm-m³/mol-K)
 T_{wk} = Water body temperature (K)

The overall PB-HAP compound transfer rate coefficient (K_v) is calculated by using Equation 29 (see section 7.4.4). EPA (1998)⁽¹⁾ recommends a water body temperature (T_{wk}) of 298 K (or 25°C).

7.1.3 Runoff Load from Impervious Surfaces (L_{RI})

In some watershed soils, a fraction of the total (wet and dry) deposition in the watershed will be to impervious surfaces. This deposition may accumulate and be washed off during rain events. EPA (1998)⁽¹⁾ recommends the use of Equation 20 to calculate impervious runoff load to a water body (L_{RI}).

$$L_{RI} = Q \cdot [F_v \cdot Dytwv + (1.0 - F_v) \cdot Dytwp] \cdot A_I \quad (\text{Equation 20})$$

where

- L_{RI} = Runoff load from impervious surfaces (g/yr)
- Q = PB-HAP compound emission rate (g/s)
- F_v = Fraction of PB-HAP compound air concentration in vapor phase (unitless)
- $Dytwv$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from vapor phase (s/m²-yr)
- $Dytwp$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase (s/m²-yr)
- A_I = Impervious watershed area receiving PB-HAP compound deposition (m²)

Impervious watershed area receiving PB-HAP compound deposition (A_I) is the portion of the total effective watershed area that is impervious to rainfall (such as roofs, driveways, streets, and parking lots) and drains to the water body.

7.1.4 Runoff Load from Pervious Surfaces (L_R)

EPA (1998)⁽¹⁾ recommends the use of Equation 21 to calculate the runoff dissolved PB-HAP compound load to the water body from pervious soil surfaces in the watershed (L_R).

$$L_R = RO \cdot (A_L - A_I) \cdot \frac{Cs \cdot BD}{\theta_{sw} + Kd_s + BD} \cdot 0.01 \quad (\text{Equation 21})$$

where

- L_R = Runoff load from pervious surfaces (g/yr)
- RO = Average annual surface runoff from pervious areas (cm/yr)
- A_L = Total watershed area receiving PB-HAP compound deposition (m²)
- A_I = Impervious watershed area receiving PB-HAP compound deposition (m²)
- Cs = Average soil concentration over exposure duration (in watershed soils) (mg PB-HAP compound/kg soil)
- BD = Soil bulk density (g soil/cm³ soil)
- θ_{sw} = Soil volumetric water content (mL water/cm³ soil)
- Kd_s = Soil-water partition coefficient (cm³ water/g soil)
- 0.01 = Units conversion factor (kg-cm²/mg-m²)

The calculation of the PB-HAP compound concentration in watershed soils (Cs) are discussed in Section 2.1. Soil bulk density (BD) is described in Section 2.5.2. Soil water content (θ_{sw}) is described in Section 2.5.4.

7.1.5 Soil Erosion Load (L_E)

EPA (1998)⁽¹⁾ recommends the use of Equation 22 to calculate soil erosion load (L_E).

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s + BD} \cdot 0.001 \quad (\text{Equation 22})$$

where

- L_E = Soil erosion load (g/yr)
- X_e = Unit soil loss (kg/m²-yr)
- A_L = Total watershed area (evaluated) receiving PB-HAP compound deposition (m²)
- A_I = Impervious watershed area receiving PB-HAP compound deposition (m²)
- SD = Sediment delivery ratio (watershed) (unitless)
- ER = Soil enrichment ratio (unitless)
- Cs = Average soil concentration over exposure duration (in watershed soils) (mg PB-HAP compound/kg soil)
- BD = Soil bulk density (g soil/cm³ soil)
- θ_{sw} = Soil volumetric water content (mL water/cm³ soil)
- Kd_s = Soil-water partition coefficient (mL water/g soil)
- 0.001 = Units conversion factor (k-cm²/mg-m²)

Unit soil loss (X_e) is described in Section 7.2. Watershed sediment delivery ratio (SD) is calculated as described in Section 7.3. PB-HAP compound concentration in soils (Cs) is described in Section 2.1. Soil bulk density (BD) is described in Section 2.5.2. Soil water content (θ_{sw}) is described in Section 2.5.4.

7.2 Universal Soil Loss Equation - USLE

EPA (1998)⁽¹⁾ recommends that the universal soil loss equation (USLE), Equation 22A, be used to calculate the unit soil loss (X_e) specific to each watershed.

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047} \quad (\text{Equation 22A})$$

where

- X_e = Unit soil loss (kg/m²-yr)
- RF = USLE rainfall (or erosivity) factor (yr⁻¹)
- K = USLE erodibility factor (ton/acre)
- LS = USLE length-slope factor (unitless)
- C = USLE cover management factor (unitless)
- PF = USLE supporting practice factor (unitless)
- 907.18 = Units conversion factor (kg/ton)
- 4047 = Units conversion factor (m²/acre)

The USLE RF variable, which represents the influence of precipitation on erosion, is derived from data on the frequency and intensity of storms. This value is typically derived on a storm-by-storm basis, but average annual values have been compiled (U.S. Department of Agriculture 1982).⁽³¹⁾ Information on determining site-specific values for variables used in calculating X_e is provided in U.S. Department of Agriculture (U.S. Department of Agriculture 1997)⁽³²⁾ and EPA guidance (EPA 1985).⁽²²⁾

7.3 Sediment Delivery Ratio (SD)

EPA (1998)⁽¹⁾ recommends the use of Equation 23 to calculate sediment delivery ratio (SD).

$$SD = a \cdot (A_L)^{-b} \quad \text{(Equation 23)}$$

where

SD = Sediment delivery ratio (watershed) (unitless)

a = Empirical intercept coefficient (unitless)

b = Empirical slope coefficient (unitless)

A_L = Total watershed area (evaluated) receiving PB-HAP compound deposition (m^2)

A_L is the total watershed surface area evaluated that is affected by deposition and drains to the body of water (see Chapter 2). In assigning values to the watershed surface area affected by deposition, the following may be a consideration:

- Distance from the emission source;
- Location of the area affected by deposition fallout with respect to the point at which drinking water is extracted or fishing occurs; and
- The watershed hydrology.

7.4 Total Water Body PB-HAP compound Concentration (C_{wtot})

EPA (1998)⁽¹⁾ recommends the use of Equation 24 to calculate total water body PB-HAP compound concentration (C_{wtot}). The total water body concentration includes both the water column and the bed sediment.

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} \cdot k_{wt} \cdot A_W \cdot (d_{wc} + d_{bs})} \quad \text{(Equation 24)}$$

where

C_{wtot} = Total water body PB-HAP compound concentration (including water column and bed sediment) (g PB-HAP compound/ m^3 water body)

L_T = Total PB-HAP compound load to the water body (including deposition, runoff, and erosion) (g/yr)

Vf_x = Average volumetric flow rate through water body (m^3 /yr)

f_{wc} = Fraction of total water body PB-HAP compound concentration in the water column (unitless)

k_{wt} = Overall total water body PB-HAP compound dissipation rate constant (yr^{-1})

- A_W = Water body surface area (m²)
- d_{wc} = Depth of water column (m)
- d_{bs} = Depth of upper benthic sediment layer (m)

The total PB-HAP compound load to the water body (L_T) – including deposition, runoff, and erosion – is described in Section 7.1. The depth of the upper benthic layer (d_{bs}), which represents the portion of the bed that is in equilibrium with the water column, cannot be precisely specified; however, EPA (1998)⁽¹⁾ recommends a default value of 0.03. Issues related to the remaining parameters are summarized in the following subsections.

7.4.1 Fraction of Total Water Body PB-HAP compound Concentration in the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

EPA (1998)⁽¹⁾ recommends using Equation 25A to calculate fraction of total water body PB-HAP compound concentration in the water column (f_{wc}), and Equation 25B to calculate total water body contaminant concentration in benthic sediment (f_{bs}).

$$f_{wc} = \frac{(1 + kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z}{(1 + kd_{sw} \cdot TSS \cdot 10^{-6}) \cdot d_{wc} / d_z + (\theta_{bs} + Kd_{bs} \cdot C_{BS}) \cdot d_{bs} / d_z} \quad \text{(Equation 25A)}$$

$$f_{bs} = 1 - f_{wc} \quad \text{(Equation 25B)}$$

where

- f_{wc} = Fraction of total water body PB-HAP compound concentration in the water column (unitless)
- f_{bs} = Fraction of total water body PB-HAP compound concentration in benthic sediment (unitless)
- Kd_{sw} = Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
- TSS = Total suspended solids concentration (mg/L)
- 1×10^{-6} = Units conversion factor (kg/mg)
- d_z = Total water body depth (m)
- θ_{bs} = Bed sediment porosity (L_{water}/L_{sediment})
- Kd_{bs} = Bed sediment/sediment pore water partition coefficient (L water/kg bottom sediment)
- C_{BS} = Bed sediment concentration (g/cm³ [equivalent to kg/L])
- d_{wc} = Depth of water column (m)
- d_{bs} = Depth of upper benthic sediment layer (m)

The partition coefficient Kd_{sw} describes the partitioning of a contaminant between sorbing material, such as soil, surface water, suspended solids, and bed sediments. Due to variability in water body specific values, EPA (1998)⁽¹⁾ recommends the use of water body-specific measured total suspended solids (TSS) values representative of long-term average annual values for the water body of concern. Average annual values for TSS are generally expected to be in the range

of 2 to 300 mg/L; with additional information on anticipated *TSS* values available in the EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Pathways of Exposure to Combustor Emissions* (EPA 1998).⁽¹²⁾ If measured data are not available, or of unacceptable quality, a calculated *TSS* value can be obtained for non-flowing water bodies using Equation 25C.

$$TSS = \frac{X_e \cdot (A_L - A_I) \cdot SD \cdot 1 \times 10^3}{Vf_x + D_{ss} \cdot A_W} \quad \text{(Equation 25C)}$$

where

- TSS* = Total suspended solids concentration (mg/L)
- X_e* = Unit soil loss (kg/m²-yr)
- A_L* = Total watershed area (evaluated) receiving PB-HAP compound deposition (m²)
- A_I* = Impervious watershed area receiving PB-HAP compound deposition (m²)
- SD* = Sediment delivery ratio (watershed) (unitless)
- Vf_x* = Average volumetric flow rate through water body (value should be 0 for quiescent lakes or ponds) (m³/yr)
- D_{ss}* = Suspended solids deposition rate (a default value of 1,825 for quiescent lakes or ponds) (m/yr)
- A_W* = Water body surface area (m²)
- 1x10⁻³ = Units conversion factor (g/kg)

The default value of 1,825 m/yr provided for *D_{ss}* is characteristic of Stoke's settling velocity for an intermediate (fine to medium) silt.

Also, to evaluate the appropriateness of watershed-specific values used in calculating the unit soil loss (*X_e*), as described in Section 7.2, the water-body specific measured *TSS* value can be compared to the calculated *TSS* value obtained using Equation 25C. If the measured and calculated *TSS* values differ significantly, parameter values used in calculating *X_e* can be re-evaluated. This re-evaluation of *TSS* and *X_e* can also be conducted if the calculated *TSS* value is outside of the normal range expected for average annual measured values, as discussed above.

Bed sediment porosity (*θ_{bs}*) can be calculated from the bed sediment concentration by using Equation 26 (EPA 1993b)⁽¹¹⁾:

$$\theta_{bs} = 1 - \frac{C_{BS}}{\rho_s} \quad \text{(Equation 26)}$$

where

- θ_{bs}* = Bed sediment porosity (L_{water}/L_{sediment})
- ρ_s* = Bed sediment density (kg/L)
- C_{BS}* = Bed sediment concentration (kg/L)

EPA (1998)⁽¹⁾ recommends the default value of $0.6 \frac{L_{\text{water}}}{L_{\text{sediment}}}$ for bed sediment porosity (θ_{bs}). This assumes a bed sediment density (ρ_s) of 2.65 kg/L and a bed sediment concentration (C_{BS}) of 1.0 kg/L.

7.4.2 Overall Total Water Body PB-HAP compound Dissipation Rate Constant (k_{wt})

EPA (1998)⁽¹⁾ recommends the use of Equation 27 to calculate the overall dissipation rate of PB-HAP compounds in surface water, resulting from volatilization and benthic burial.

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b \quad (\text{Equation 27})$$

where

- k_{wt} = Overall total water body dissipation rate constant (yr^{-1})
- f_{wc} = Fraction of total water body PB-HAP compound concentration in the water column (unitless)
- k_v = Water column volatilization rate constant (yr^{-1})
- f_{bs} = Fraction of total water body PB-HAP compound concentration in benthic sediment (unitless)
- k_b = Benthic burial rate constant (yr^{-1})

The variables f_{wc} and f_{bs} are discussed in Section 7.4.1, and Equations 25A and 25B.

7.4.3 Water Column Volatilization Rate Constant (k_v)

EPA (1998)⁽¹⁾ recommends using Equation 28 to calculate water column volatilization rate constant.

$$k_v = \frac{K_v}{d_z \cdot (1 + kd_{sw} \cdot TSS \cdot 1 \times 10^{-6})} \quad (\text{Equation 28})$$

where

- k_v = Water column volatilization rate constant (yr^{-1})
- K_v = Overall PB-HAP compound transfer rate coefficient (m/yr)
- d_z = Total water body depth (m)
- Kd_{sw} = Suspended sediments/surface water partition coefficient (L water/kg suspended sediments)
- TSS = Total suspended solids concentration (mg/L)
- 1×10^{-6} = Units conversion factor (kg/mg)

Total water body depth (d_z), suspended sediment and surface water partition coefficient (Kd_{sw}), and total suspended solids concentration (TSS), are described in Section 7.4.1. The overall transfer rate coefficient (K_v) is described in Section 7.4.4.

7.4.4 Overall PB-HAP compound Transfer Rate Coefficient (K_v)

Volatile organic chemicals can move between the water column and the overlying air. The overall transfer rate K_v , or conductivity, is determined by a two-layer resistance model that assumes that two “stagnant films” are bounded on either side by well-mixed compartments. Concentration differences serve as the driving force for the water layer diffusion. Pressure differences drive the diffusion for the air layer. From balance considerations, the same mass must pass through both films; the two resistances thereby combine in series, so that the conductivity is the reciprocal of the total resistance.

EPA (1998)⁽¹⁾ recommends the use of Equation 29 to calculate the overall transfer rate coefficient (K_v).

$$K_v = \left(K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right)^{-1} \cdot \theta^{T_{wk}-293} \quad (\text{Equation 29})$$

where

- K_v = Overall PB-HAP compound transfer rate coefficient (m/yr)
- K_L = Liquid phase transfer coefficient (m/yr)
- K_G = Gas phase transfer coefficient (m/yr)
- H = Henry’s Law constant (atm-m³/mol)
- R = Universal gas constant (atm-m³/mol-K)
- T_{wk} = Water body temperature (K)
- θ = Temperature correction factor (unitless)

The value of the conductivity K_v depends on the intensity of turbulence in the water body and the overlying atmosphere. As Henry’s Law constant increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. Conversely, as Henry’s Law constant decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

The liquid and gas phase transfer coefficients, K_L and K_G , respectively, vary with the type of water body. The liquid phase transfer coefficient (K_L) is calculated by using Equations 30A and 30B (described in Section 7.4.5). The gas phase transfer coefficient (K_G) is calculated by using Equations 31A and 31B (described in Section 7.4.6).

Henry’s Law constants generally increase with increasing vapor pressure of a PB-HAP compound and generally decrease with increasing solubility of a PB-HAP compound. Henry’s Law constants are compound-specific and are presented in Appendix D. The universal ideal gas constant, R , is 8.205×10^{-5} atm-m³/mol-K, at 20°C. The temperature correction factor (θ), which is equal to 1.026, is used to adjust for the actual water temperature. Volatilization is assumed to occur much less readily in lakes and reservoirs than in moving water bodies.

7.4.5 Liquid Phase Transfer Coefficient (K_L)

EPA (1998)⁽¹⁾ recommends using Equations 30A and 30B to calculate liquid phase transfer coefficient. (K_L).

$$K_L = \sqrt{\frac{(1 \times 10^{-4}) \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7 \quad (\text{Equation 30A})$$

$$K_L = (C_d^{0.5} \cdot W) \cdot \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot \frac{\mu_w}{\rho_w \cdot D_w} \cdot 3.1536 \times 10^7 \quad (\text{Equation 30B})$$

where

K_L	=	Liquid phase transfer coefficient (m/yr)
D_w	=	Diffusivity of PB-HAP compound in water (cm ² /s)
u	=	Current velocity (m/s)
1×10^{-4}	=	Units conversion factor (m ² /cm ²)
d_z	=	Total water body depth (m)
C_d	=	Drag coefficient (unitless)
W	=	Average annual wind speed (m/s)
ρ_a	=	Density of air (g/cm ³)
ρ_w	=	Density of water (g/cm ³)
k	=	von Karman's constant (unitless)
λ_z	=	Dimensionless viscous sublayer thickness (unitless)
μ_w	=	Viscosity of water corresponding to water temperature (g/cm-s)
3.1536×10^7	=	Units conversion factor (s/yr)

For a flowing stream or river, the transfer coefficients are controlled by flow-induced turbulence. For these systems, the liquid phase transfer coefficient is calculated by using Equation 30A. For a stagnant system (quiescent lake or pond), the transfer coefficient is controlled by wind-induced turbulence, and the liquid phase transfer coefficient can be calculated by using Equation 30B. The total water body depth (d_z) for liquid phase transfer coefficients is discussed in Section 7.4.1. EPA (1998)⁽¹⁾ recommends the use of the following default values:

- A diffusivity of chemical in water ranging (D_w) from 1.0×10^{-5} to 8.5×10^{-2} cm²/s;
- A dimensionless viscous sublayer thickness (λ_z) of 4;
- A von Karman's constant (k) of 0.4;
- A drag coefficient (C_d) of 0.0011;
- An air density (ρ_a) of 0.0012 g/cm³ at standard conditions (temperature = 20°C or 293 K, pressure = 1 atm or 760 millimeters of mercury);
- A water density of (ρ_w) of 1 g/cm³; and
- A water viscosity (μ_w) of a 0.0169 g/cm-s corresponding to water temperature.

7.4.6 Gas Phase Transfer Coefficient (K_G)

EPA (1998)⁽¹⁾ recommends using Equations 31A and 31B to calculate gas phase transfer coefficient (K_G).

For flowing streams or rivers:

$$K_G = 36,500 \text{ m / yr} \quad (\text{Equation 31A})$$

For quiescent lakes or ponds:

$$K_G = \left(C_d^{0.5} \cdot W \right) \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_a}{\rho_a \cdot D_a} \right)^{-0.67} \cdot 3.1536 \times 10^7 \quad (\text{Equation 31B})$$

where

- K_G = Gas phase transfer coefficient (m/yr)
- C_d = Drag coefficient (unitless)
- W = Average annual wind speed (m/s)
- k = von Karman's constant (unitless)
- λ_z = Dimensionless viscous sublayer thickness (unitless)
- μ_a = Viscosity of air corresponding to air temperature (g/cm-s)
- ρ_a = Density of air corresponding to water temperature (g/cm³)
- D_a = Diffusivity of PB-HAP compound in air (cm²/s)
- 3.1536×10^7 = Units conversion factor (s/yr)

EPA (1998)⁽¹⁾ recommends 1.81×10^{-4} g/cm-s for the viscosity of air corresponding to air temperature.

7.4.7 Benthic Burial Rate Constant (k_b)

EPA (1998)⁽¹⁾ recommends using Equation 32 to calculate benthic burial rate (k_b).

$$k_b = \left(\frac{X_e \cdot A_L \cdot SD \cdot 1 \times 10^3 - Vf_x \cdot TSS}{A_W \cdot TSS} \right) \cdot \left(\frac{TSS \cdot 1 \times 10^{-6}}{C_{BS} \cdot d_{bs}} \right) \quad (\text{Equation 32})$$

where

- k_b = Benthic burial rate constant (yr⁻¹)
- X_e = Unit soil loss (kg/m²-yr)
- A_L = Total watershed area (evaluated) receiving deposition (m²)
- SD = Sediment delivery ratio (watershed) (unitless)
- Vf_x = Average volumetric flow rate through water body (m³/yr)
- TSS = Total suspended solids concentration (mg/L)
- A_W = Water body surface area (m²)

C_{BS} = Bed sediment concentration (g/cm³)
 d_{bs} = Depth of upper benthic sediment layer (m)
 1×10^{-6} = Units conversion factor (kg/mg)
 1×10^3 = Units conversion factor (g/kg)

The benthic burial rate constant (k_b), can also be expressed in terms of the rate of burial (Wb) (Equation 33):

$$Wb = k_b \cdot d_{bs} \quad \text{(Equation 33)}$$

where

Wb = Rate of burial (m/yr)
 k_b = Benthic burial rate constant (yr⁻¹)
 d_{bs} = Depth of upper benthic sediment layer (m)

EPA (1998)⁽¹⁾ recommends the following default value of 1.0 kg/L for bed sediment concentration (C_{BS}).

Section 7.2 discusses the unit soil loss (X_e). Section 7.3 discusses sediment delivery ratio (SD) and watershed area evaluated receiving PB-HAP compound deposition (A_L). Section 7.4 discusses the depth of the upper benthic sediment layer (d_{bs}). Average volumetric flow rate through the water body (Vf_x) and water body surface area (A_w) are discussed further in EPA (1998).⁽¹⁾ Section 7.4.1 discusses total suspended solids concentration (TSS).

The calculated value for k_b is expected to range from 0 to 1.0; with low k_b values expected for water bodies characteristic of no or limited sedimentation (rivers and fast flowing streams), and k_b values closer to 1.0 expected for water bodies characteristic of higher sedimentation (lakes). This range of values is based on the relation between the benthic burial rate and rate of burial expressed in Equation 33; with the depth of upper benthic sediment layer held constant. For k_b values calculated as a negative (water bodies with high average annual volumetric flow rates in comparison to watershed area evaluated), EPA (1998)⁽¹⁾ recommends assigning a k_b value of 0 for use in calculating the total water body PB-HAP compound concentration (C_{wtot}) in Equation 34 (see next section). If the calculated k_b value exceeds 1.0, re-evaluation of the parameter values used in calculating X_e is recommended to be conducted.

7.4.8 Total PB-HAP compound Concentration in Water Column (C_{wctot})

EPA (1998)⁽¹⁾ recommends using Equation 34 to calculate total PB-HAP compound concentration in water column (C_{wctot}).

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}} \quad (\text{Equation 34})$$

where

C_{wctot} = Total PB-HAP compound concentration in water column (mg PB-HAP compound/L water column)

f_{wc} = Fraction of total water body PB-HAP compound concentration in the water column (unitless)

C_{wtot} = Total water body PB-HAP compound concentration, including water column and bed sediment (mg PB-HAP compound/L water body)

d_{wc} = Depth of water column (m)

d_{bs} = Depth of upper benthic sediment layer (m)

Total water body PB-HAP compound concentration – including water column and bed sediment (C_{wtot}) and fraction of total water body PB-HAP compound concentration in the water column (f_{wc}) – can be calculated by using Equation 34 and Equation 35 (see next section). Depth of upper benthic sediment layer (d_{bs}) is discussed in Section 7.4.1.

7.4.9 Dissolved Phase Water Concentration (C_{dw})

EPA (1998)⁽¹⁾ recommends the use of Equation 35 to calculate the concentration of PB-HAP compound dissolved in the water column (C_{dw}).

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}} \quad (\text{Equation 35})$$

where

C_{dw} = Dissolved phase water concentration (mg PB-HAP compound/L water)

C_{wctot} = Total PB-HAP compound concentration in water column (mg PB-HAP compound/L water column)

Kd_{sw} = Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)

TSS = Total suspended solids concentration (mg/L)

1×10^{-6} = Units conversion factor (kg/mg)

The total PB-HAP compound concentration in water column (C_{wctot}) is calculated by using the Equation 34. Section 7.4.1 discusses the surface water partition coefficient (Kd_{sw}) and total suspended solids concentration (TSS).

7.4.10 PB-HAP compound Concentration Sorbed to Bed Sediment (C_{sb})

EPA (1998)⁽¹⁾ recommends the use of Equation 36 to calculate PB-HAP compound concentration sorbed to bed sediment (C_{sb}).

$$C_{sb} = f_{bs} \cdot C_{wtot} \cdot \left(\frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot C_{BS}} \right) \cdot \left(\frac{d_{wc} + d_{bs}}{d_{bs}} \right) \quad (\text{Equation 36})$$

where

- C_{sb} = PB-HAP compound concentration sorbed to bed sediment (mg PB-HAP compound/kg sediment)
- f_{bs} = Fraction of total water body PB-HAP compound concentration in benthic sediment (unitless)
- C_{wtot} = Total water body PB-HAP compound concentration, including water column and bed sediment (mg PB-HAP compound/L water body)
- Kd_{bs} = Bed sediment/sediment pore water partition coefficient (L PB-HAP compound/kg water body)
- θ_{bs} = Bed sediment porosity ($L_{\text{pore water}}/L_{\text{sediment}}$)
- C_{BS} = Bed sediment concentration (g/cm^3)
- d_{wc} = Depth of water column (m)
- d_{bs} = Depth of upper benthic sediment layer (m)

Bed sediment porosity (θ_{bs}) and bed sediment concentration (C_{BS}) are discussed in Section 7.4.1. Depth of water column (d_{wc}) and depth of upper benthic layer (d_{bs}) are discussed in Section 7.4.

7.5 Concentration of PB-HAP compound in Fish (C_{fish})

The PB-HAP compound concentration in fish is calculated using either a PB-HAP compound-specific bioconcentration factor (BCF), a PB-HAP compound-specific bioaccumulation factor (BAF), or a PB-HAP compound-specific biota-sediment accumulation factor ($BSAF$). For compounds with a $\log K_{ow}$ less than 4.0, $BCFs$ are used. Compounds with a $\log K_{ow}$ greater than 4.0 (except for extremely hydrophobic compounds such as polycyclic organic matter and PCBs), are assumed to have a high tendency to bioaccumulate, therefore, $BAFs$ are used. While extremely hydrophobic PB-HAP compounds are also assumed to have a high tendency to bioaccumulate, they are expected to be sorbed to the bed sediments more than associated with the water phase. Therefore, for polycyclic organic matter and PCBs, EPA (1998)⁽¹⁾ recommends using $BSAFs$ to calculate concentrations in fish.

BCF and BAF values are generally based on dissolved water concentrations. Therefore, when BCF or BAF values are used, the PB-HAP compound concentration in fish is calculated using dissolved water concentrations. $BSAF$ values are based on benthic sediment concentrations. Therefore, when $BSAF$ values are used, PB-HAP compound concentration in fish is calculated using benthic sediment concentrations. The equations used to calculate fish concentrations are described in the subsequent subsections.

7.5.1 Fish Concentration (C_{fish}) from Bioconcentration Factors Using Dissolved Phase Water Concentration

EPA (1998)⁽¹⁾ recommends the use of Equation 37 to calculate fish concentration from $BCFs$ using dissolved phase water concentration.

$$C_{fish} = C_{dw} \cdot BCF_{fish} \quad (\text{Equation 37})$$

where

C_{fish} = Concentration of PB-HAP compound in fish (mg PB-HAP compound/kg FW tissue)

C_{dw} = Dissolved phase water concentration (mg PB-HAP compound/L)

BCF_{fish} = Bioconcentration factor for PB-HAP compound in fish (L/kg)

The dissolved phase water concentration (C_{dw}) is calculated by using Equation 35.

7.5.2 Fish Concentration (C_{fish}) from Bioaccumulation Factors Using Dissolved Phase Water Concentration

EPA (1998)⁽¹⁾ recommends the use of Equation 38 to calculate fish concentration from $BAFs$ using dissolved phase water concentration.

$$C_{fish} = C_{dw} \cdot BAF_{fish} \quad (\text{Equation 38})$$

where

C_{fish} = Concentration of PB-HAP compound in fish (mg PB-HAP compound/kg FW tissue)

C_{dw} = Dissolved phase water concentration (mg PB-HAP compound/L)

BAF_{fish} = Bioaccumulation factor for PB-HAP compound in fish (L/kg FW tissue)

The dissolved phase water concentration (C_{dw}) is calculated by using Equation 35.

7.5.3 Fish Concentration (C_{fish}) from Biota-To-Sediment Accumulation Factors Using PB-HAP compound Sorbed to Bed Sediment

EPA (1998)⁽¹⁾ recommends the use of Equation 39 to calculate fish concentration from $BSAFs$ using PB-HAP compound sorbed to bed sediment for very hydrophobic compounds (polycyclic organic matter and PCBs).

$$C_{fish} = \frac{C_{sb} \cdot f_{lipid} \cdot BSAF}{OC_{sed}} \quad (\text{Equation 39})$$

where

C_{fish} = Concentration of PB-HAP compound in fish (mg PB-HAP compound/kg FW tissue)

- C_{sb} = Concentration of PB-HAP compound sorbed to bed sediment (mg PB-HAP compound/kg bed sediment)
 f_{lipid} = Fish lipid content (unitless)
 $BSAF$ = Biota-to-sediment accumulation factor (unitless)
 OC_{sed} = Fraction of organic carbon in bottom sediment (unitless)

The concentration of PB-HAP compound sorbed to bed sediment (C_{sb}) is calculated by using Equation 36. EPA recommended default values for the fish lipid content (f_{lipid}) and for the fraction of organic carbon in bottom sediment (OC_{sed}) are given in EPA (1998).⁽¹⁾

Values for the fraction of organic carbon in bottom sediment recommended by EPA (1993b)⁽¹¹⁾ range from 0.03 to 0.05 (OC_{sed}). These values are based on an assumption of a surface soil OC content of 0.01. This document states that the organic carbon content in bottom sediments is higher than the organic carbon content in soils because (1) erosion favors lighter-textured soils with higher organic carbon contents, and (2) bottom sediments are partially comprised of detritus materials.

The fish lipid content (f_{lipid}) value is site-specific and dependent on the type of fish. As stated in EPA (1998)⁽¹⁾, a default range of 0.03 to 0.07 is recommended specific to warm or cold water fish species. EPA (2000)⁽³³⁾ provides information supporting a value of 0.03 (3 percent lipid content of the edible portion). EPA (1993a)⁽³⁴⁾ recommended a default value of 0.04 for OC_{sed} , which is the midpoint of the specified range. EPA (1993b; 1993a)⁽¹¹⁾⁽³⁴⁾ recommended the use of 0.07, which was originally cited in Cook et al. (1991).⁽³⁵⁾

8.0 Concentrations of Dioxins in Breast Milk

EPA (1998)⁽¹⁾ recommends the use of Equation 40 to estimate the concentrations of dioxins in breast milk.

$$C_{milkfat} = \frac{m \cdot 1 \times 10^9 \cdot h \cdot f_1}{0.6932 \cdot f_2} \quad (\text{Equation 40})$$

where

- $C_{milkfat}$ = Concentration of dioxin in milk fat of breast milk for a specific exposure scenario (pg dioxin/kg milk fat)
 m = Average maternal intake of dioxin for each adult exposure scenario (mg dioxin/kg BW-day)
 1×10^9 = Units conversion factor (pg/mg)
 h = Half-life of dioxin in adults (days)
 f_1 = Fraction of ingested dioxin that is stored in fat (unitless)
 f_2 = Fraction of mother's weight that is fat (unitless)

The values of m , h , f_1 , and f_2 are site-specific and dependent on the specific species of dioxin present. EPA (1998)⁽¹⁾ recommends a default value of 2,555 days for h , a default value of 0.9 for f_1 , and a default value of 0.3 for f_2 . Additional references for the derivation of this equation and these default values are given in EPA (1998).⁽¹⁾

Uncertainties associated with this equation include:

- The most significant uncertainties are associated with the variable m . Because m is calculated as the sum of numerous potential intakes, estimates of m incorporate uncertainties associated with each exposure pathway. Therefore, m may be under- or over-estimated.
- This equation assumes that the concentration of dioxin in breast milk fat is the same as in maternal fat. To the extent that this is not the case, uncertainty is introduced.

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