Chapter 5
Estimating Media Concentrations

What's Covered in Chapter 5:

The purpose of this chapter is to describe the equations (and associated parameters) for estimating media concentration that we recommend using to evaluate the exposure scenarios presented in Chapter 4. In most cases, we include the origin and development of each of these equations, and describe the associated parameters. We also present the equations in Appendix B in a more condensed form (i.e. without derivation), and organize them according to exposure pathway. Discussions of ISCST3-modeled unitized air parameters are presented in Chapter 3. Appendix B also includes equations for modeling phase allocation and speciation of mercury concentrations. Appendix A-2 lists compound-specific parameters the equations need to estimate media concentrations, as well as our recommended hierarchies of sources. The HHRAP companion database provides recommended values for compound-specific parameters.

PLEASE NOTE: for the purposes of this guidance, "we" refers to the U.S. EPA OSW.

The HHRAP is written for the benefit of a varied audience, including risk assessors, regulators, risk managers, and community relations personnel. However, the "you" to which we speak in this chapter is the performer of a risk assessment: the person (or persons) who will actually put the recommended methods into practice.

Section 5.1 describes the equations that estimate air concentrations for evaluating direct inhalation of COPCs. Section 5.2 describes equations for estimating COPC concentrations in soils. Section 5.3

describes equations for estimating COPC concentrations in produce. Sections 5.4 through 5.6 describe equations for estimating COPC concentrations in animal products (such as milk, beef, pork, poultry, and eggs) resulting from animals ingesting contaminated feed and soil. Section 5.7 describes equations for estimating COPC concentrations in fish through bioaccumulation (or, for some compounds, bioconcentration) from the water column, dissolved water concentration, or bed sediment—depending on the COPC.

> ***Please Note***: references made throughout Chapter 5 to particle phase are generic and made without distinction between particle and particle-bound.

5.1 CALCULATING COPC CONCENTRATIONS IN AIR FOR DIRECT INHALATION

We recommend calculating COPC concentrations in air by summing the vapor phase and particle phase air concentrations of COPCs. To evaluate long-term or chronic exposure via direct inhalation, we generally recommend using unitized ***yearly*** air parameter values to calculate air concentrations, as specified in Appendix B, Table B-5-1. To evaluate short-term or acute exposure via direct inhalation, we recommend using unitized ***hourly*** air parameter values to calculate air concentrations, as specified in Appendix B, Table B-6-1.

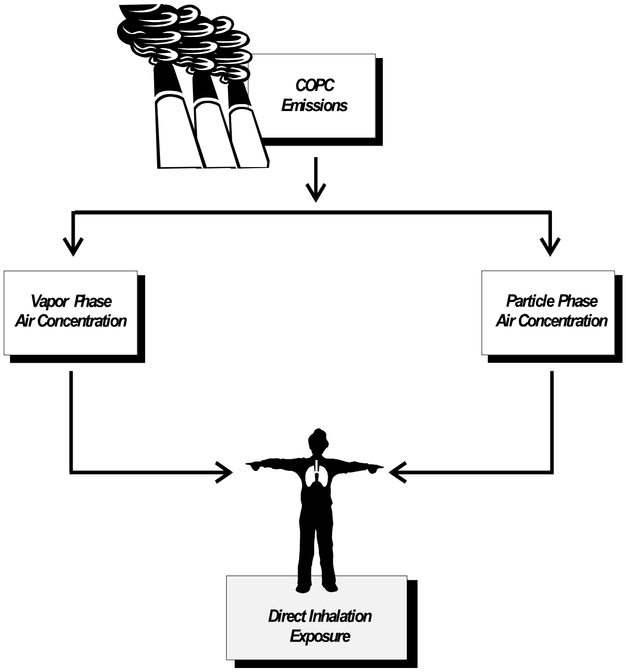
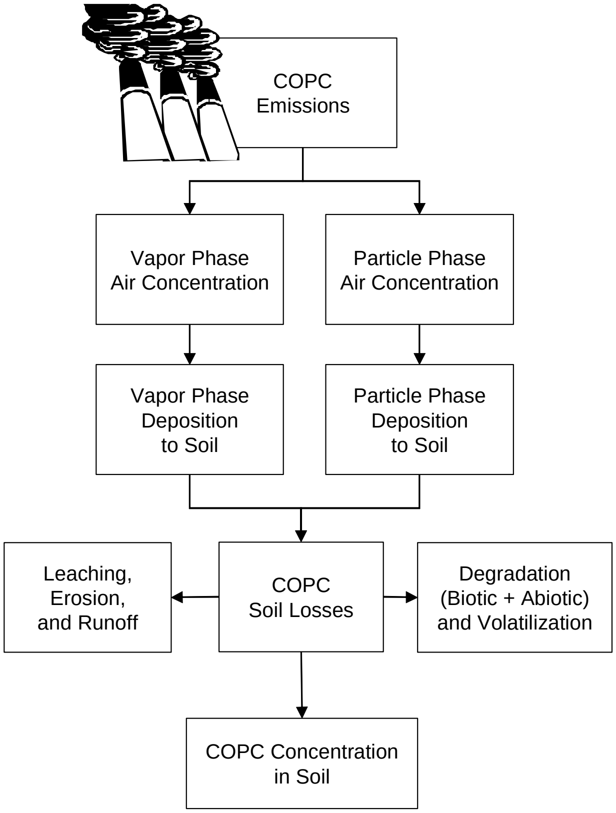


Figure 5-1 - COPC Concentration in Air for Direct Inhalation

5.2 CALCULATING COPC CONCENTRATIONS IN SOIL

We recommend estimating COPC concentrations in soil by summing the vapor phase and particle phase deposition of COPCs to the soil. We generally recommend considering wet and dry deposition of particles and vapors. Calculate dry deposition of vapors from the vapor air concentration and the dry deposition velocity. We consider it appropriate for soil concentration calculations to account for loss of COPCs 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. We present our recommended equations for calculating soil concentration and soil losses of COPCs in Appendix B, Tables B-1 for land use areas, and Tables B-4 for watersheds (see Section 5.7).

FIGURE 5-2 -
COPC CONCENTRATION IN SOIL



Soil concentrations might require many years to reach steady state. As a result, the equations we suggest 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 COPCs, we recommend using two variations of the equation (average soil concentration over exposure duration):

1. one variation if the exposure duration (*T2*) is ***greater than or equal to*** the operating lifetime of the emission source or time period of combustion, and
2. the other form if the exposure duration is ***less*** than the operating lifetime of the emission source or time period of combustion.

For noncarcinogenic COPCs, we recommend using the second form of the carcinogenic equation. This equation calculates the highest annual average COPC soil concentration occurring during the exposure duration. We describe these equations in more detail in Section 5.2.1.

Soil conditions—such as pH, structure, organic matter content, and moisture content—affect the distribution and mobility of COPCs. Modeling the loss of COPCs from soil uses rates specific to the physical and chemical characteristics of the soil. We describe these variables and their use in the following subsections, along with the recommended equations.

5.2.1 Calculating Cumulative Soil Concentration (*Cs*)

U.S. EPA (1990e) recommended using Equation 5-1—adapted from Travis, et al. (1983)—to calculate cumulative soil concentration:

$$Cs = \frac{100 \cdot (Dydp + Dywv) \cdot [1.0 - \exp\ (-ks \cdot tD)]}{Z_s \cdot BD \cdot ks} \qquad \text{Equation 5-1}$$

where

Cs = Average soil concentration over exposure duration (mg COPC/kg soil)
100 = Units conversion factor (mg-m^2/kg-cm^2)
$Dydp$ = Unitized yearly dry deposition from particle phase (s/m^2-yr)
$Dywv$ = Unitized yearly wet deposition from vapor phase (s/m^2-yr)
ks = COPC soil loss constant due to all processes (yr^{-1})
tD = Time period over which deposition occurs (time period of combustion) (yr)
Z_s = Soil mixing zone depth (cm)
BD = Soil bulk density (g soil/cm^3 soil)

U.S. EPA (1993f) stated that Equation 5-1 evaluated deposition of particle phase COPCs, but failed to consider vapor phase deposition or diffusion. To account for vapor phase diffusion, U.S. EPA (1998c) recommended using the following equation:

$$Cs = \frac{100 \cdot (Dydp + Dywv + L_{dif}) \cdot [1.0 - \exp\ (-ks \cdot tD)]}{Z_s \cdot BD \cdot ks} \qquad \text{Equation 5-1A}$$

where

Cs = Average soil concentration over exposure duration (mg COPC/kg soil)
100 = Units conversion factor (mg-m^2/kg-cm^2)
$Dydp$ = Unitized yearly dry deposition from particle phase (s/m^2-yr)
$Dywv$ = Unitized yearly wet deposition from vapor phase (s/m^2-yr)
L_{dif} = Dry vapor phase diffusion load to soil (g/m^2-yr)
ks = COPC soil loss constant due to all processes (yr^{-1})
tD = Time period over which deposition occurs (time period of combustion) (yr)

Z_s = Soil mixing zone depth (cm)
BD = Soil bulk density (g soil/cm^3 soil)

Other guidance (U.S. EPA 1994g) recommended the original Equation 5-1, but only for calculating *Cs* for 2,3,7,8-TCDD. U.S. EPA (1994g) also recommended setting the COPC soil loss constant (*ks*) equal to 0 for all other COPCs. For COPCs other than 2,3,7,8-TCDD, U.S. EPA (1994g) recommended Equation 5-1B—which eliminates the COPC soil loss constant:

$$Cs = 100 \cdot \frac{Dyd + Dyw}{Z_s \cdot BD} \cdot tD \qquad \text{Equation 5-1B}$$

where

Cs = Average soil concentration over exposure duration (mg COPC/kg soil)
100 = Units conversion factor (mg-m^2/kg-cm^2)
Dyd = Yearly dry deposition rate of pollutant (g/m^2-yr)
Dyw = Yearly wet deposition rate of pollutant (g/m^2-yr)
tD = Time period over which deposition occurs (time period of combustion) (yr)
Z_s = Soil mixing zone depth (cm)
BD = Soil bulk density (g soil/cm^3 soil)

More recent guidance documents—U.S. EPA (1994r) and NC DEHNR (1997)—recommended using two different equations (Equations 5-1C and 5-1D) with carcinogenic COPCs. Equation 5-1C was recommended for $T_2 \leq tD$ and Equation 5-1D was recommended for $T_1 < tD < T_2$. For noncarcinogenic COPCs, Equation 5-1E was recommended.

We recommend using Equations 5-1C, 5-1D, and 5-1E to calculate *Cs*. Appendix B, Table B-1-1 discusses further how to use these equations.

Recommended Equations for Calculating: Cumulative Soil Concentration (*Cs*)

Carcinogens:

For $T_2 \leq tD$

$$Cs = \frac{Ds}{ks \cdot (tD - T_1)} \cdot \left[\left(tD + \frac{\exp\ (-ks \cdot tD)}{ks} \right) - \left(T_1 + \frac{\exp(-ks \cdot T_1)}{ks} \right) \right] \quad \text{Equation 5-1C}$$

For $T_1 < tD < T_2$

$$Cs = \frac{\left(\frac{Ds \cdot tD - Cs_{tD}}{ks}\right) + \left(\frac{Cs_{tD}}{ks}\right) \cdot (1 - \exp\ [-ks \cdot (T_2 - tD)])}{(T_2 - T_1)} \quad \text{Equation 5-1D}$$

Noncarcinogens:

$$Cs_{tD} = \frac{Ds \cdot [1 - \exp(-ks \cdot tD)]}{ks} \quad \text{Equation 5-1E}$$

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where

Cs = Average soil concentration over exposure duration (mg COPC/kg soil)
Ds = Deposition term (mg COPC/kg soil/yr)
ks = COPC soil loss constant due to all processes (yr^{-1})
tD = Time period over which deposition occurs (time period of combustion) (yr)
T_1 = Time period at the beginning of combustion (yr)
Cs_{tD} = Soil concentration at time *tD* (mg/kg)
T_2 = Length of exposure duration (yr)

We discuss the deposition term further in this Section, as well as Section 5.2.3. Section 5.2.2 discusses the COPC-specific soil loss constant (*ks*). Chapter 2 discusses how the period of time at the beginning of combustion (T_1) relates to characterizing site conditions immediately preceding the study period. Chapter 2 also addresses the time period during which burning - and therefore deposition - occurs (*tD*), as it relates to setting emission rates. Chapter 3 addresses air dispersion modeling aspects of *tD*. Chapter 6 further discusses how the duration of exposure (T_2) relates to characterizing exposure.

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-1C when you model an exposure duration that is ***less than or equal to*** the operating lifetime of the emission source or hazardous waste combustor ($T_2 \leq tD$). We recommend using Equation 5-1D when you model an exposure duration ***greater than*** the operating lifetime of the hazardous waste combustor ($T_1 < tD < T_2$). For noncarcinogenic COPCs, we recommend Equation 5-1E.

We generally recommend using the COPC soil concentration averaged over the exposure duration (represented by *Cs*) for carcinogenic compounds. Carcinogenic risk is averaged over the lifetime of an individual. Because the hazard quotient associated with noncarcinogenic COPCs is based on a threshold dose rather than a lifetime exposure, we recommend using the highest annual average COPC soil concentration (Cs_{tD}) occurring during the exposure duration period for noncarcinogenic COPCs. Cs_{tD} typically occurs at the end of the operating life of the emission source or the time period of combustion.

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using the highest 1-year annual average soil concentration, determined using Equation 5-1E, to evaluate risk from noncarcinogenic COPCs (see Chapter 7).

5.2.2 Calculating the COPC Soil Loss Constant (*ks*)

Organic and inorganic COPCs can be lost from the soil by several processes that may or may not occur simultaneously. The rate at which a COPC is lost from the soil is known as the soil loss constant (*ks*). We recommend determining *ks* by using the soil's physical, chemical, and biological characteristics, to estimate the COPC-specific loss resulting from:

(1) leaching,
(2) runoff,
(3) erosion,
(4) biotic and abiotic degradation, and
(5) volatilization.

U.S. EPA (1990e) recommended Equation 5-2 to calculate *ks*:

$$ks = ksl + ksg + ksv \qquad \text{Equation 5-2}$$

where

ks = COPC soil loss constant due to all processes (yr^{-1})
ksl = COPC loss constant due to leaching (yr^{-1})
ksg = COPC loss constant due to biotic and abiotic degradation (yr^{-1})
ksv = COPC loss constant due to volatilization (yr^{-1})

We recommend using Equation 5-2A to calculate *ks*. We describe this equation further in Appendix B, Table B-1-2. Using Equation 5-2A is consistent with U.S. EPA (1994g), U.S. EPA (1994r), U.S. EPA (1998c) and NC DEHNR (1997).

Recommended Equation for Calculating: COPC Soil Loss Constant (*ks*)

$$ks = ksg + kse + ksr + ksl + ksv \qquad \text{Equation 5-2A}$$

where

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

Section 5.2.2.1 discusses loss due to biotic and abiotic degradation (*ksg*). Section 5.2.2.2 discusses loss due to erosion (*kse*). Section 5.2.2.3 discusses loss due to surface runoff (*ksr*). Section 5.2.2.4 discusses Loss due to leaching (*ksl*). Section 5.2.2.5 discusses loss due to volatilization (*ksv*).

As highlighted in Section 5.2.1, using Equation 5-2A in Equations 5-1C and 5-1D assumes that you can define COPC loss using first-order reaction kinetics. First-order reaction rates depend on the concentration of one reactant (Bohn et al. 1985). The loss of a COPC by a first-order process depends only on the concentration of the COPC in the soil, and a constant fraction of the COPC 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 (Sparks 1989). The assumption that COPC 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 COPC from soil (U.S. EPA 1998c).

COPC loss in soil can also follow zero or second-order reaction kinetics. Zero-order reaction kinetics are independent of reactant concentrations (Bohn et al. 1985). 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 COPC 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 et al. 1985). The loss constant of a COPC 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 COPC 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 COPC loss can occur simultaneously, using Equation 5-2A might also overestimate loss rates for each process (Valentine 1986). We recommend, when possible, taking into account the common occurrence of all loss processes. It's possible to derive combined rates of soil loss by these processes experimentally. U.S. EPA (1986c) presents values for some COPCs.

5.2.2.1 COPC 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 available in the literature (U.S. EPA 1998c). According to Lyman et al. (1982), it's reasonable to assume that degradation rates follow first order kinetics in a homogenous media. You're therefore able to relate the half-life of a compound 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, you can calculate the degradation rate. However, literature sources don't provide sufficient data for all such mechanisms, especially for soil. Earlier Agency guidance (U.S. EPA 1994g) recommended setting *ksg* for all COPCs other than 2,3,7,8-TCDD equal to zero. The HHRAP companion database presents our recommended values for this COPC-specific variable.

Recommended Values for:
COPC Loss Constant Due to Biotic and Abiotic Degradation (ksg)

COPC-Specific
(See the HHRAP companion database)

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

- availability of the COPC;
- nutrient limitations;
- toxicity of the COPC; and
- inactivation or nonexistence of enzymes capable of degrading the COPC.

Chemical degradation of organic compounds can be a significant mechanism for removing COPCs from soil (U.S. EPA 1998c). Hydrolysis and oxidation-reduction reactions are the primary chemical transformation processes occurring in the upper layers of soils (Valentine 1986). General rate expressions describing the transformation of some COPCs by all non-biological processes are available. These expressions are helpful when division into component reactions isn't 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). In soil systems, sorption of the COPC can increase, decrease, or not affect the rate of hydrolysis, as numerous studies cited in Valentine (1986) have shown. We recommend predicting the overall (i.e. total) rate of hydrolysis in soil by adding the rates in the soil and water phases. We recommend assuming that these rates are first-order reactions at a fixed pH (Valentine 1986). Lyman et al. (1982) describes methods for estimating these hydrolysis constants.

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

5.2.2.2 COPC Loss Constant Due to Soil Erosion (*kse*)

U.S. EPA (1998c) recommended using Equation 5-3 to calculate the constant for soil loss resulting from erosion (*kse*).

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

Equation 5-3

where

kse = COPC soil loss constant due to soil erosion
0.1 = Units conversion factor (1,000 g-kg/10,000 cm^2-m^2)
X_e = Unit soil loss (kg/m^2-yr)
SD = Sediment delivery ratio (unitless)
ER = Soil enrichment ratio (unitless)
BD = Soil bulk density (g soil/cm^3 soil)
Z_s = Soil mixing zone depth (cm)
Kd_s = Soil/water partition coefficient (ml water/g soil)
θ_{sw} = Soil volumetric water content (ml water/cm^3 soil) = 0.2 ml/cm^3

We recommend using the Universal Soil Loss Equation (USLE) to calculate unit soil loss (X_e)(See Section 5.7.2). We describe soil bulk density (BD) in Section 5.2.4.2. We describe Soil mixing depth (Z_s) in Section 5.2.4.1. We describe soil volumetric water content (θ_{sw}) in Section 5.2.4.4. We discuss site-specific variables associated with Equation 5-3 further in Appendix B.

U.S. EPA (1994g and 1994r) recommended setting all *kse* values equal to zero. U.S. EPA (1994r) recommended setting *kse* equal to zero because contaminated soil erodes both onto and off of the site.

As in U.S. EPA (1994g and 1994r), we recommend setting *kse* equal to zero.

Recommended Value for: **COPC Loss Constant Due to Erosion (*kse*)**
0

For additional information on addressing *kse*, we recommend consulting U.S. EPA (1998c). We also further describe using *kse* values in Appendix B, Table B-1-3.

5.2.2.3 COPC Loss Constant Due to Runoff (*ksr*)

Earlier U.S. EPA guidance (1994g) recommended setting all *ksr* values equal to zero.

As in U.S. EPA (1994r; 1998c) and NC DEHNR (1997), we recommend using Equation 5-4 to calculate *ksr*. We further discuss using Equation 5-4 in Appendix B, Table B-1-4.

Recommended Equation for Calculating:
COPC Loss Constant Due to Runoff (*ksr*)

$$ksr = \frac{RO}{\theta_{sw} \cdot Z_s} \cdot \left(\frac{1}{1 + (Kd_s \cdot BD / \theta_{sw})} \right) \qquad \text{Equation 5-4}$$

where

ksr = COPC 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/cm^3 soil) = 0.2 ml/cm^3
Z_s = Soil mixing zone depth (cm)
Kd_s = Soil/water partition coefficient (ml water/g soil)
BD = Soil bulk density (g soil/cm^3 soil) = 1.5 g/cm^3

The average annual surface runoff from pervious surfaces (RO) is a site-specific water loss term discussed in Section 5.2.4.3. Section 5.2.4.4 describes soil volumetric water content (θ_{sw}). Section 5.2.4.1 discusses the depth of soil mixing (Z_s). Appendix A-2 explains how we recommend calculating the COPC-specific soil/water partition coefficient (Kd_s). Section 5.2.4.2 describes soil bulk density (*BD*).

5.2.2.4 COPC Loss Constant Due to Leaching (*ksl*)

Losses of soil COPCs 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.

U.S. EPA (1990e) recommended using Equation 5-5 to calculate *ksl*.

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

where

ksl = COPC loss constant due to leaching (yr^{-1})
P = Average annual precipitation (cm/yr)
I = Average annual irrigation (cm/yr)
E_v = Average annual evapotranspiration (cm/yr)
θ_{sw} = Soil volumetric water content (ml water/cm^3 soil) = 0.2 ml/cm^3
Z_s = Soil mixing zone depth (cm)
Kd_s = Soil/water partition coefficient (ml water/g soil)
BD = Soil bulk density (g soil/cm^3 soil)

U.S. EPA (1993f) determined that Equation 5-5 does not properly account for surface runoff. U.S. EPA (1994g) recommended setting all *ksl* values to zero.

More recent guidance (U.S. EPA 1994r; 1998c; NC DEHNR 1997) have recommended using Equation 5-5A to calculate *ksl*. As with U.S. EPA (1994r), U.S. EPA (1998c), and NC DEHNR (1997), we recommend using Equation 5-5A to account for runoff while calculating *ksl*. We further discuss the use of this equation in Appendix B, Table B-1-5.

Recommended Equation for Calculating:
COPC Loss Constant Due to Leaching (*ksl*)

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

where

ksl = COPC 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/cm^3 soil) = 0.2 ml/cm^3
Z_s = Soil mixing zone depth (cm)
BD = Soil bulk density (g soil/cm^3 soil) = 1.5 g/cm^3
Kd_s = Soil/water partition coefficient (cm^3 water/g soil)

Appendix B describes how we suggest acquiring site-specific variables associated with Equation 5-5A. The average annual volume of water available to generate leachate is the mass balance of all water inputs and outputs from the area under consideration ($P + I - RO - E_v$). These variables are described in Section 5.2.4.3. Section 5.2.4.4 describes soil volumetric water content (θ_{sw}). Section 5.2.4.1 describes the soil mixing depth (Z_s). Section 5.2.4.2 soil bulk density (BD). Appendix A-2 describes how we recommend calculating the COPC-specific soil/water partition coefficient (Kd_s).

5.2.2.5 COPC Loss Constant Due to Volatilization (*ksv*)

Semi-volatile and volatile COPCs emitted in high concentrations may become adsorbed to soil particles and exhibit volatilization losses from soil. The loss of a COPC from the soil by volatilization depends on the rate of movement of the COPC 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).

U.S. EPA (1990e; 1993f; 1998c) recommended using Equation 5-6 to calculate *ksv*.

$$ksv = Ke \cdot Kt \qquad \text{Equation 5-6}$$

where

ksv = COPC loss constant due to volatilization (yr^{-1})
Ke = Equilibrium coefficient (s/cm-yr)
Kt = Gas phase mass transfer coefficient (cm/s)

U.S. EPA (1990e; 1993f; 1998c) don’t identify a reference for Equation 5-6. U.S. EPA (1993f) stated that Equation 5-6 had been independently verified as accurately representing volatilization loss, but that the equation for *Kt* (Equation 5-8) appeared to fit to data empirically. U.S. EPA (1993f) also stated that *ksv* is modeled as a means of limiting soil concentration. Because this mass flux never experiences rain out, or washout and subsequent re-deposit, soil COPC concentrations are underestimated for soluble volatile COPCs. U.S. EPA (1993f) further recommended that additional research be conducted to determine the magnitude of the uncertainty introduced for volatile COPCs. U.S. EPA (1998c) recommended not considering the volatilized residues of semi-volatile COPCs (such as dioxin). U.S. EPA (1994g) recommended setting all *ksv* values to zero.

U.S. EPA guidance (1994r) and NC DEHNR (1997) recommended using Equation 5-6A to calculate *ksv*. Equation 5-6A appears to incorporate equations that U.S. EPA (1990e) recommended for calculating *Ke* (equilibrium coefficient) and *Kt* (gas phase mass transfer coefficient).

$$ksv = \left(\frac{3.1536 \times 10^{7} \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \right) \cdot \left(0.482 \cdot W^{0.78} \cdot \left[\frac{\mu_a}{\rho_a \cdot D_a} \right]^{-0.67} \cdot \left[\sqrt{\frac{4 \cdot A}{\pi}} \right]^{-0.11} \right) \qquad \text{Equation 5-6A}$$

where

ksv = COPC loss constant due to volatilization (yr^{-1})
3.1536×10^{7} = Units conversion factor (s/yr)
H = Henry’s Law constant ($\text{atm-m}^3\text{/mol}$)
Z_s = Soil mixing zone depth (cm)
Kd_s = Soil/water partition coefficient (cm^3 water/g soil)
R = Universal gas constant ($\text{atm-m}^3\text{/mol-K}$)
T_a = Ambient air temperature (K) = 298.1 K
BD = Soil bulk density (g soil/cm^3 soil)
0.482 = Empirical constant (unitless) Units conversion factor [$(3600 \text{ s/hr})^{0.78}$(100 cm/m)/(3600 s/hr)] · (empirical constant 0.0292)
W = Average annual wind speed (m/s)
0.78 = Empirical constant (unitless)
μ_a = Viscosity of air (g/cm-s)
ρ_a = Density of air (g/cm^3)
D_a = Diffusivity of COPC in air ($\text{cm}^2\text{/s}$)
-0.67 = Empirical constant (unitless)
A = Surface area of contaminated area (m^2)
-0.11 = Empirical constant (unitless)

U.S. EPA (1990e) recommended using Equation 5-7 to calculate *Ke* and Equation 5-8 to calculate *Kt*.

$$Ke = \frac{3.1536 \times 10^7 \cdot (H \times 10^3)}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \qquad \text{Equation 5-7}$$

$$Kt = 0.482 \cdot W^{0.78} \cdot Sc_a^{-0.67} \cdot d_e^{-0.11} \qquad \text{Equation 5-8}$$

where

Ke = Equilibrium coefficient (s/cm-yr)
3.1536×10^7 = Units conversion factor (s/yr)
H = Henry's Law constant (atm-L/mol)
10^3 = Units conversion factor (L/m^3)
Z_s = Soil mixing zone depth (cm)
Kd_s = Soil/water partition coefficient (cm^3 water/g soil)
R = Universal gas constant (atm-m^3/mol-K)
T_a = Ambient air temperature (K) = 298.1 K
BD = Soil bulk density (g soil/cm^3 soil)
Kt = Gas phase mass transfer coefficient (cm/s)
0.482 = Units conversion factor [(3600 s/hr)$^{0.78}$(100 cm/m)/(3600 s/hr)] · (empirical constant 0.0292)
W = Average annual wind speed (m/s)
Sc_a = Schmidt number for gas phase (unitless)
d_e = Effective diameter of contaminated media (m)

U.S. EPA (1990e) also recommended using Equation 5-9 to calculate the Schmidt number for gas phase (Sc_a), and Equation 5-10 to calculate the effective diameter of contaminated media (d_e).

$$Sc_a = \frac{\mu_a}{\rho_a \cdot D_a} \qquad \text{Equation 5-9}$$

$$d_e = \sqrt{\frac{4 \cdot A}{\pi}} \qquad \text{Equation 5-10}$$

where

Sc_a = Schmidt number for gas phase (unitless)
μ_a = Viscosity of air (g/cm-s)
ρ_a = Density of air (g/cm^3)
D_a = Diffusivity of COPC in air (cm^2/s)
d_e = Effective diameter of contaminated media (m)
A = Surface area of contaminated area (m^2)

As in U.S. EPA (1998c), we recommend using Equation 5-7A to calculate *ksv*, in cases where high concentrations of volatile organic compounds are expected to be present in the soil.

Recommended Equation for Calculating:
COPC Loss Constant Due to Volatilization (*ksv*)

$$ksv = \left(\frac{3.1536 \times 10^7 \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \right) \cdot \left(\frac{D_a}{Z_s} \right) \cdot \left[1 - \left(\frac{BD}{\rho_{soil}} \right) - \Theta_{sw} \right] \qquad \text{Equation 5-7A}$$

where

ksv = COPC loss constant due to volatilization (yr^{-1})
3.1536×10^7 = Units conversion factor (s/yr)
H = Henry's Law constant (atm-m^3/mol)
Z_s = Soil mixing zone depth (cm)
Kd_s = Soil/water partition coefficient (ml/g)
R = Universal gas constant (atm-m^3/mol-K)
T_a = Ambient air temperature (K) = 298.1 K
BD = Soil bulk density (g soil/cm^3 soil) = 1.5 g/cm^3
D_a = Diffusivity of COPC in air (cm^2/s)
ρ_{soil} = Solids particle density (g/cm^3) = 2.7 g/cm^3
θ_{sw} = Soil volumetric water content (ml/cm^3 soil) = 0.2 ml/cm^3

Henry's Law constants are compound-specific, and we supply recommended values in the HHRAP companion database. We describe the soil mixing depth (Z_s) in. Appendix A-2 describes how we recommend calculating the COPC-specific soil/water partition coefficient (Kd_s). The Universal gas constant (R) and ambient air temperature (T_a) are discussed further in Appendix B, Table B-1-6. Soil bulk density (*BD*) is described below, as well as in Section 5.2.4.2. Appendix A-2 discusses the diffusivity of a COPC in air (D_a). Solids particle density (ρ_{soil}) is discussed in this Section, below. Soil volumetric water content (θ_{sw}) is further described below, as well as in Section 5.2.4.4.

Equation 5-7A is based on gas equilibrium coefficients and gas phase mass transfer, and combines Equations 5-7, 5-7B, and 5-7C. You can derive *ksv* by adapting the Hwang and Falco (1986) equation for soil vapor phase diffusion, to obtain Equation 5-6, as previously reported by U.S. EPA (1990e). Based on general soil properties, you can also write the gas-phase mass transfer coefficient, K_t, as follows (Hillel 1980; Miller and Gardiner 1998):

$$K_t = \frac{D_a\ \theta_v}{Z_s} \qquad \text{Equation 5-7B}$$

where

K_t = Gas phase mass transfer coefficient (cm/s)
Z_s = Soil mixing zone depth (cm)
D_a = Diffusivity of COPC in air (cm^2/s)
θ_v = Soil void fraction (cm^3/cm^3)

We describe Soil mixing depth (Z_s) in Section 5.2.4.1. 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:

$$\theta_v = 1 - \left(\frac{BD}{\rho_s}\right) - \theta_{SW} \qquad \text{Equation 5-7C}$$

where

θ_v = Soil void fraction (cm^3/cm^3)
BD = Soil bulk density (g/cm^3) = 1.5 g/cm^3
ρ_{soil} = Solids particle density (g/cm^3) = 2.7 g/cm^3
θ_{sw} = Soil volumetric water content (ml water/cm^3 soil) = 0.2 ml/cm^3

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). Soil bulk density is affected by the soil structure, such as looseness or compactness of the soil, and depends on the water and clay content of the soil (Hillel 1980). A range for bulk density of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979). Blake and Hartge (1996) and Hillel (1980) both suggest that the mean density of solid particles is about 2.7 g/cm^3. We recommend a default soil bulk density of 1.5 g/cm^3, based on a mean value for loam soil from Carsel et al. (1988).

The soil water content (θ_{sw}) 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/cm^3 depending on soil type (Hoffman and Baes 1979). The lower values are typical of sandy soils, which can't retain much water; the higher values are typical of soils such as clay or loam soils which can retain water. If site-specific information isn't available, we recommend a mid-point default value of 0.2 ml water/cm^3 soil. However, since θ_{sw} is unique for each soil type, we highly recommend using site-specific information.

We discuss *ksv* further in Appendix B, Table B-1-6.

5.2.3 Calculating the Deposition Term (*Ds*)

We recommend using Equation 5-11 to calculate the deposition term *(Ds)*. This equation is further described in Appendix B, Table B-1-1. Using Equation 5-11 to calculate *Ds* is consistent with U.S. EPA (1994r) and NC DEHNR (1997), which both incorporate *Ds* into Equation 5-1C.

Recommended Equation for Calculating:
Deposition Term (*Ds*)

$$Ds = \left[\frac{100 \cdot Q}{Z_s \cdot BD}\right] \cdot [F_v \cdot (Dydv + Dywv) + (Dydp + Dywp) \cdot (1 - F_v)] \qquad \text{Equation 5-11}$$

where

Ds = Deposition term (mg COPC/kg soil/yr)
100 = Units conversion factor (mg-m^2/kg-cm^2)
Q = COPC emission rate (g/s)
Z_s = Soil mixing zone depth (cm)
BD = Soil bulk density (g soil/cm^3 soil) = 1.5 g/cm^3
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dydv$ = Unitized yearly average dry deposition from vapor phase (s/m^2-yr)
$Dywv$ = Unitized yearly average wet deposition from vapor phase (s/m^2-yr)
$Dydp$ = Unitized yearly average dry deposition from particle phase (s/m^2-yr)
$Dywp$ = Unitized yearly average wet deposition from particle phase (s/m^2-yr)

Chapters 2 and 3 explain how we suggest quantifying the COPC emission rate (*Q*). Chapter 3 describes generating modeled air parameters *Cyv*, *Dydv, Dywv*, *Dydp*, and *Dywp*. We describe the soil mixing depth (Z_s) in Section 5.2.4.1. Soil bulk density (*BD*) is described in Sections 5.2.2.5 and 5.2.4.2, as well as Appendix B. Appendix A-2 describes how we suggest determining the COPC-specific parameter *Fv*.

5.2.4 Site-Specific Parameters for Calculating Cumulative Soil Concentration

Calculating *Cs* requires the following site-specific parameters:

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

We discuss these parameters further in the following subsections, and in Appendix B.

5.2.4.1 Soil Mixing Zone Depth (Z_s)

When modeling exposures to COPCs in soils, the depth of contaminated soils is important in calculating the appropriate soil concentration. Tilling might mix deposited COPCs deeper into the soil, whether manually in a garden or mechanically in a large field. Increasing the volume of soil through which COPCs are mixed will tend to decrease (i.e. dilute) concentrations. The value of Z_s you choose 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:

- ingestion of plants contaminated by root uptake;
- direct ingestion of soil by humans, cattle, swine, or chickens; and
- surface runoff into water bodies.

For example, in calculations of exposures resulting from uptake through plant roots, the average concentration of COPCs over the depth of the plant root determines plant uptake.

In general, U.S. EPA (1992d, 1998c) estimated that if the area under consideration is likely to be tilled, soil depth is about 10 to 20 centimeters, depending on local conditions and the equipment used. If soil is not moved, COPCs were assumed to be retained in the shallower, upper soil layer. In this case, earlier Agency guidance (U.S. EPA 1990e; U.S. EPA 1998c) typically recommended a value of 1 centimeter.

U.S. EPA (1998c) recommended selecting Z_s as follows:

Soil Depth (Z_s)	Exposure	Description
1 cm	Direct ingestion of soil	Human exposure: in gardens, lawns, landscaped areas, parks, and recreational areas. Animal exposure: in pastures, lawns, and parks (untilled soils).
1 cm	Surface water runoff in nonagricultural areas	These areas are typically assumed to be untilled.
20 cm	Plant uptake for agricultural soils	The root depth is assumed to equal the tilling depth of 20 centimeters. In untilled soils, the root zone does not directly reflect tilling depth, although it is assumed that tilling depth is an adequate substitute for root zone depth.
20 cm	Surface water runoff in agricultural areas	These areas are typically assumed to be tilled.

We recommend the following values for Z_s:

Recommended Values for: Soil Mixing Zone Depth (Z_s)
2 cm - untilled 20 cm - tilled

We recommend a default Z_s of 2 cm for estimating surface soil concentrations in untilled soils, based on a study that profiled dioxin measurements within soil (Brzuzy et al. 1995). We recommend a default Z_s of 20 cm for estimating surface soil concentrations in tilled soils, as in U.S. EPA (1998c).

5.2.4.2 Soil Dry Bulk Density (*BD*)

BD is the ratio of the mass of soil to its total volume. This variable is affected by the soil structure, type, and moisture content (Hillel 1980).

U.S. EPA (1994r) recommended deriving wet soil bulk density by weighing a thin-walled, tube soil sample (e.g., a Shelby tube) of known volume and subtracting the tube weight (ASTM Method D2937). Moisture content can then be calculated (ASTM Method 2216) to convert wet soil bulk density to dry soil bulk density.

As in U.S. EPA (1994g; 1998c) and presented in Hoffman and Baes (1979), we recommend the following value for *BD*:

Recommended Value for: Soil Dry Bulk Density (*BD*)
1.50 g/cm^3

5.2.4.3 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 could apply in the various Agency regions.

The average annual precipitation (*P*), irrigation (*I*), runoff (*RO*), and evapotranspiration (E_v) rates and other climatological data are available 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*)—might also be found in resources such as Geraghty et al. (1973). You could also estimate surface runoff by using the Curve Number Equation developed by the U.S. Soil Conservation Service (NC DEHNR 1997). U.S. EPA (1985b) cited isopleths of mean annual cropland runoff corresponding to various curve numbers developed by Stewart et al. (1975). Curve numbers were assigned to an area on the basis of soil type, land use or cover, and the hydrologic conditions of the soil (NC DEHNR 1997).

The wide range of available values, however, demonstrates the uncertainties and limitations in our ability to estimate these parameters. For example, Geraghty et al. (1973) presented isopleths for annual surface water contributions that include interflow and ground water recharge. U.S. EPA (1994g) recommended reducing these values by 50 percent, to represent surface runoff only.

5.2.4.4 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 Agency regions. As in earlier guidance documents, (U.S. EPA 1993i; U.S. EPA 1994g; NC DEHNR 1997), we recommend using a default value of 0.2 ml/cm^3 for θ_{sw}.

Recommended Value for: **Soil Volumetric Water Content (θ_{sw})**
0.2 ml/cm^3

5.3 CALCULATING COPC CONCENTRATIONS IN PRODUCE

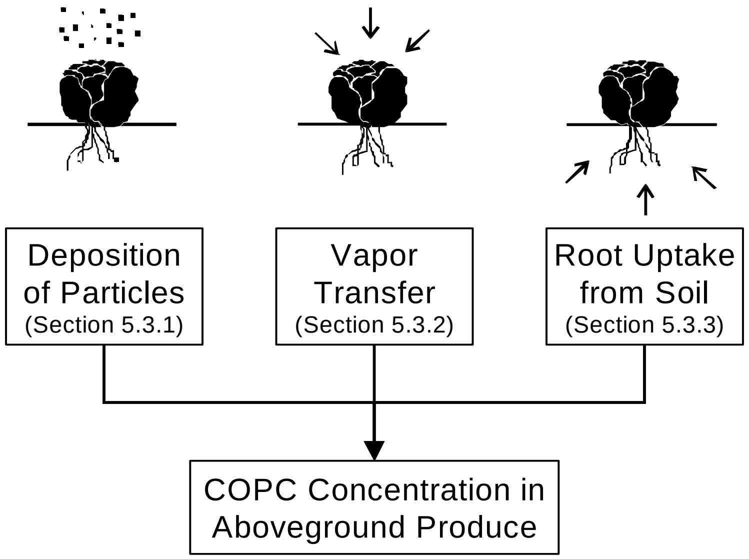
Indirect exposure resulting from ingestion of produce depends on the total concentration of COPCs in the leafy, fruit, and tuber portions of the plant. Because of general differences in contamination mechanisms, we recommend separating produce into two broad categories—aboveground produce and belowground produce. In addition, aboveground produce can be further subdivided into exposed and protected aboveground produce.

Aboveground Produce

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

- **Direct deposition of particles—**wet and dry deposition of particle phase COPCs on the leaves and fruits of plants (Section 5.3.1).
- **Vapor transfer—**uptake of vapor phase COPCs by plants through their foliage (Section 5.3.2).
- **Root uptake—**root uptake of COPCs available from the soil and their transfer to the aboveground portions of the plant (Section 5.3.3).

FIGURE 5-3
COPC CONCENTRATION IN PRODUCE



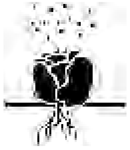
As in U.S.EPA (1998c), we recommend calculating the total COPC concentration in aboveground ***exposed*** produce as a sum of contamination occurring through all three of these mechanisms. However, edible portions of aboveground ***protected*** produce, such as peas, corn, and melons, are covered by a protective covering. They are therefore protected from contamination from deposition and vapor transfer. Root uptake of COPCs is the primary mechanism through which aboveground protected produce becomes contaminated (Section 5.3.3). Appendix B further describes the equations and parameters we recommend to calculate COPC concentrations in exposed and protected aboveground produce.

Belowground Produce

For belowground produce, we recommend assuming contamination occurs only through one mechanism—root uptake of COPCs available from soil (Section 5.3.3). The HHRAP doesn't address contamination of belowground produce via direct deposition of particles and vapor transfer because we assume that the root or tuber is protected from contact with contaminants in the vapor phase. Appendix B further describes the equations and parameters we recommend to calculate COPC concentrations in belowground produce.

Generally, we don't consider risks associated with exposure to VOCs via food-chain pathways significant. This is primarily because VOCs are typically low-molecular-weight COPCs that do not persist in the environment and do not bioaccumulate (U.S. EPA 1994r; U.S. EPA 1996g). However, as discussed in Chapter 2, we recommend evaluating all COPCs, including VOCs, for each exposure pathway.

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



Some earlier guidance documents (U.S. EPA 1990e; 1998c) recommended using Equation 5-13 to calculate COPC concentrations in aboveground vegetation resulting from wet and dry deposition onto plant surfaces of leafy plants and exposed produce (Pd):

$$Pd_i = \frac{1{,}000 \cdot [Dyd + (Fw \cdot Dywv)] \cdot Rp_i \cdot [1.0 - \exp(-kp \cdot Tp_i)]}{Yp_i \cdot kp} \qquad \text{Equation 5-13}$$

where

Pd_i = Concentration of pollutant due to direct deposition in the ith plant group (µg COPC/g plant tissue DW))
1,000 = Units conversion factor (kg/10^3 g and 10^6 µg/g pollutant)
Dyd = Yearly dry deposition from particle phase (g/m^2-yr)
Fw = Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
$Dywv$ = Yearly wet deposition from vapor phase (g/m^2-yr)
Rp_i = Interception fraction of the edible portion of plant tissue for the ith plant group (unitless)
kp = Plant surface loss coefficient (yr^{-1})

Tp_i = Length of plant's exposure to deposition per harvest of the edible portion of the *i*th plant group (yr)
Yp_i = Yield or standing crop biomass of edible portion of the *i*th plant group (kg DW/m^2)

U.S. EPA (1994r) modified Equation 5-13 to include stack emissions adjusted to remove the fraction of air concentration in vapor phase [Q (1 - F_v)] (Equation 5-14).

We recommend using Equation 5-14 to calculate *Pd*. We further discuss the use of this equation in Appendix B, Table B-2-7.

Recommended Equation for Calculating:
Aboveground Produce Concentration Due to Direct Deposition (*Pd*)

$$Pd = \frac{1{,}000 \cdot Q \cdot (1 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)]}{Yp \cdot kp} \qquad \text{Equation 5-14}$$

where
Pd = Plant (aboveground produce) concentration due to direct (wet and dry) deposition (mg COPC/kg DW)
1,000 = Units conversion factor (mg/g)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dydp$ = Unitized yearly average dry deposition from particle phase (s/m^2-yr)
Fw = 0.2 for anions, 0.6 for cations & most organics (unitless)
$Dywp$ = Unitized yearly wet deposition from particle phase (s/m^2-yr)
Rp = Interception fraction of the edible portion of plant (unitless)
kp = Plant surface loss coefficient (yr^{-1})
Tp = 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/m^2)

Chapters 2 and 3 explain how we recommend quantifying the COPC emission rate (*Q*). Appendix A-2 describes how we recommend determining the COPC-specific parameter *Fv*. Chapter 3 describes how the modeled air parameters *Dydp* and *Dywp* are generated. Appendix B explains our recommendations for *Fw*. *Rp*, *kp*, *Tp*, and *Yp* are neither site- nor COPC-specific, and are described in Sections 5.3.1.1 through 5.3.1.4.

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

U.S. EPA (1998c) stated that NRC models assumed a constant of 0.2 for *Rp* for dry and wet deposition of particles (Boone et al. 1981). However, Shor et al. (1982) suggested that diversity of plant growth necessitated vegetation-specific *Rp* values.

As summarized in Baes et al. (1984), experimental studies of pasture grasses identified a correlation between initial *Rp* values and productivity (standing crop biomass [*Yp*]) (Chamberlain 1970):

$$Rp = 1 - e^{-\gamma Yp} \qquad \text{Equation 5-14A}$$

where

Rp = Interception fraction of the edible portion of plant (unitless)
γ = Empirical constant (Chamberlain [1970] gives the range as 2.3 to 3.3 for pasture grasses; Baes et al. [1984] used the midpoint, 2.88, for pasture grasses.)
Yp = Standing crop biomass (productivity) (kg DW/m^2 for silage; kg WW/m^2 for exposed produce)

Baes et al. (1984) also developed methods for estimating *Rp* values for leafy vegetables, silage, and exposed produce. However, these vegetation class-specific calculations produced *Rp* values that were independent of productivity measurements. This independence led to potentially unreasonable estimates of surface plant concentrations. Therefore, Baes et al. (1984) proposed using the same empirical relationship developed by Chamberlain (1970) for other vegetation classes. Baes et al. (1984) developed class-specific estimates of the empirical constant (γ) by forcing an exponential regression equation through several points. Points included average and theoretical maximum estimates of *Rp* and *Yp*. The following class-specific empirical constants (γ) were developed:

- Exposed produce = 0.0324
- Leafy vegetables = 0.0846
- Silage = 0.769

U.S. EPA (1994r) and U.S. EPA (1995e) proposed a default aboveground produce *Rp* value of 0.05, based on a weighted average of class-specific *Rp* values. Specifically, class-specific *Rp* values were calculated using the equation developed by Chamberlain (1970) and the following empirical constants:

- Leafy vegetables were assigned the same empirical constant (0.0846) developed by Baes et al. (1984).

- Fruits, fruiting vegetables, and legumes were assigned the empirical constant (0.0324) originally developed by Baes et al. (1984) for "exposed produce."

Vegetables and fruits included in each class are as follows:

- Fruits—apple, apricot, berry, cherry, cranberry, grape, peach, pear, plum/prune, and strawberry
- Fruiting Vegetables—asparagus, cucumber, eggplant, sweet pepper, and tomato
- Legumes—snap beans
- Leafy Vegetables—broccoli, brussel sprouts, cauliflower, celery, lettuce, and spinach

The class-specific *Rp* values were then weighted by relative ingestion (by humans) of each class, to determine a weighted average *Rp* value of 0.05. However, the produce classes and relative ingestion values used by U.S. EPA (1994r) and U.S. EPA (1995e) to calculate and weight the *Rp* values are not current with the U.S. EPA *1997 Exposure Factors Handbook* (U.S. EPA 1997b). In addition, the overall *Rp* value presented in U.S. EPA (1994r; 1995e) was based on limited information; subsequent revision to U.S. EPA (1994r; 1995e) resulted in an overall *Rp* value of 0.2 (RTI 1997).

For purposes of consistency, we combined the produce classes into two groups—exposed fruit and exposed vegetables. We used the exposed produce empirical constant (γ) to calculate *Rp*. Since the exposed vegetable category includes leafy and fruiting vegetables, we calculated *Rp* for leafy and fruiting vegetables. We then calculated the exposed vegetable *Rp* by a weighted average based on productivity (*Yp*) of leafy and fruiting vegetables, respectively. The relative ingestion rates used to determine an average weighted *Rp* value we derived from the intake of homegrown produce discussion presented in the 1997 *Exposure Factors Handbook* (U.S. EPA 1997b). We recommend using the weighted average *Rp* value of 0.39 as a default *Rp* value, because it represents the most current parameters, including standing crop biomass and relative ingestion rates.

Recommended Value for: **Interception Fraction of the Edible Portion of Plant (*Rp*)**
0.39

Unweighted *Rp* and ingestion rates used for the weighting are as follows:

Aboveground Produce Class	***Rp***	**Ingestion Rate (g DW/kg-day)**
Exposed fruits	0.053	0.19
Exposed vegetables	0.982	0.11

One of the primary uncertainties associated with this variable is whether the algorithm developed by Chamberlain (1970) and the empirical constants developed by Baes et al. (1984) for use in this algorithm accurately represent aboveground produce. Specifically, Chamberlain (1970) based his algorithm on studies of pasture grass rather than aboveground produce. Baes et al. (1984) noted that their approach to developing class-specific *Rp* values is "at best *ad hoc,"* but stated that this approach was justified, because the consequences of using *Rp* estimates that are independent of productivity are "serious."

5.3.1.2 Plant Surface Loss Coefficient (*kp*)

U.S. EPA (1998c) identified several processes—including wind removal, water removal, and growth dilution—that reduce the amount of contaminant that has deposited on plant surfaces. The term *kp* is a measure of the amount of contaminant that is lost to these physical processes over time. U.S. EPA (1998c) cited Miller and Hoffman (1983) for the following equation:

$$kp = \left(\frac{\ln 2}{t_{1/2}}\right) \cdot 365 \qquad \text{Equation 5-15}$$

where

kp = Plant surface loss coefficient (yr^{-1})
$t_{1/2}$ = Half-life (days)
365 = Units conversion factor (days/yr)

Miller and Hoffman (1983) reported half-life values ranging from 2.8 to 34 days for a variety of contaminants on herbaceous vegetation. These half-life values converted to *kp* values of 7.44 to 90.36 (yr^{-1}). U.S. EPA (1994r; 1998c) recommended a *kp* value of 18, based on a generic 14-day half-life corresponding to physical processes only. The 14-day half-life is approximately the midpoint of the range (2.8 to 34 days) estimated by Miller and Hoffman (1983).

Lacking experimental data supporting chemical- and/or site-specific values, we recommend using a default *kp* value of 18. This *kp* value is the midpoint of Miller and Hoffman's (1983) range of values. Based on this range (7.44 to 90.36), plant concentrations could range from about 1.8 times higher to about 48 times lower than the plant concentrations, based on a *kp* value of 18. If chemical- or site-specific data is available, you could also calculate site- and chemical-specific *kp* values using the equation in Miller and Hoffman (1983).

Recommended Value for: **Plant Surface Loss Coefficient (*kp*)**
18 yr^{-1}

The primary uncertainty associated with *kp* relates to its position as the sole surface loss term in Equation 5-14. As defined by Miller and Hoffman (1983) and U.S. EPA (1998c), *kp* only represents potential losses from the physical processes listed above, not ***all*** potential losses (e.g. chemical degradation). However, information regarding chemical degradation of contaminants on plant surfaces is limited. Including chemical degradation processes would decrease half-life values and thereby increase *kp* values. Note that effective plant concentration decreases as *kp* increases. Therefore, using a *kp* value that does not consider chemical degradation processes is protective.

In addition, there are uncertainties associated with the half-life values reported by Miller and Hoffman (1983) with regard to how accurately these values represent the behavior of risk assessment COPCs on aboveground produce. However, the relative impact of this second uncertainty is less than the omission of chemical degradation processes.

5.3.1.3 Length of Plant Exposure to Deposition per Harvest of Edible Portion of Plant (*Tp*)

U.S. EPA (1990e; 1993f; 1994r; 1998c), and NC DEHNR (1997) recommended treating *Tp* as a constant, based on the average period between successive hay harvests. Belcher and Travis (1989) estimated this period at 60 days (0.164 years), which represents the length of time that aboveground vegetation (in this case, hay) is exposed to contaminant deposition before being harvested. Calculate *Tp* as follows:

$$Tp = \frac{60\ days}{365\ days/yr} = 0.164\ yr$$ Equation 5-16

where

Tp = Length of plant exposure to deposition per harvest of the edible portion of plant (yr)
60 = Average period between successive hay harvests (days)
365 = Units conversion factor (days/yr)

As in previous guidance, we recommend using a *Tp* value of 0.164 year.

Recommended Value for: **Length of Plant Exposure to Deposition per Harvest of Edible Portion of Plant (*Tp*)**
0.164 years

The primary uncertainty associated with using 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 could be appropriate to estimate a site-specific *Tp* value. The greater the difference between site-specific *Tp* and our recommended value, the greater the effect on plant concentration estimates.

5.3.1.4 Standing Crop Biomass (Productivity) (*Yp*)

U.S. EPA (1998c) recommended that the best estimate of *Yp* is productivity, which Baes et al. (1984) and Shor et al. (1982) define as follows:

$$Yp = \frac{Yh_i}{Ah_i}$$ Equation 5-17

where

Yh_i = Harvest yield of the *i*th crop (kg DW)
Ah_i = area planted to the *i*th crop (m^2)

U.S. EPA (1994r) and NC DEHNR (1997) recommended using this equation and calculated a *Yp* value of 1.6 for aboveground produce, based on weighted average *Yh* and *Ah* values for four aboveground produce classes (fruits, fruiting vegetables, legumes, and leafy vegetables). Vegetables and fruits included in each class were as follows:

- Fruits—apple, apricot, berry, cherry, cranberry, grape, peach, pear, plum/prune, and strawberry
- Fruiting Vegetables—asparagus, cucumber, eggplant, sweet pepper, and tomato
- Legumes—snap beans
- Leafy Vegetables—broccoli, brussel sprouts, cauliflower, celery, lettuce, and spinach.

Class-specific *Yp* values were estimated using U.S. average *Yh* and *Ah* values for a variety of fruits and vegetables for 1993 (USDA 1994a; USDA 1994b). *Yh* values were converted to dry weight using average class-specific conversion factors (Baes et al. 1984). U.S. EPA (1994r and 1995e) calculated class-specific *Yp* values and then used relative ingestion rates of each group to calculate the weighted average *Yp* value of 1.6. However, the produce classes and relative ingestion values used by U.S. EPA (1994r and1995e) to calculate and weight the *Yp* values are not current with the U.S. EPA 1997 *Exposure Factors Handbook*. In addition, overall *Yp* value presented in U.S. EPA (1994r and U.S. EPA 1995e) was based on limited information; subsequent revision to U.S. EPA (1994r and 1995e) has resulted in an overall *Yp* value of 1.7 (RTI 1997).

For consistency, we combined the produce classes into two groups—exposed fruit and exposed vegetables. We derived the exposed vegetable *Yp* summing *Yh* values for leafy and fruiting vegetables and dividing by the sum of *Ah* values for leafy and fruiting vegetables. We derived the relative ingestion rates used to calculate an overall average weighted *Yp* value from the homegrown produce discussions presented in the 1997 *Exposure Factors Handbook* (U.S. EPA 1997b). We recommend using the weighted average *Yp* value of 2.24 as a default *Yp* value, because this value represents the most complete and thorough information available.

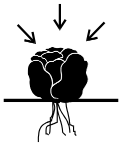
Recommended Value for: **Standing Crop Biomass (Productivity) (*Yp*)**
2.24

Unweighted *Yp* and ingestion rates used for the weighting are as follows:

Aboveground Produce Class	***Yp***	**Ingestion Rate (g DW/kg-day)**
Exposed fruits	0.25	0.19
Exposed vegetables	5.66	0.11

The primary uncertainty associated with this variable is that the harvest yield (*Yh*) and area planted (*Ah*) may not reflect site-specific conditions. To the extent to which site-specific information is available, you can estimate the magnitude of the uncertainty introduced by the default *Yp* value.

5.3.2 Aboveground Produce Concentration Due to Air-to-Plant Transfer (*Pv*)



The method we recommend for estimating COPC concentrations in exposed and aboveground produce due to air-to-plant transfer (*Pv*) was developed with consideration of items which might limit the transfer of COPC concentrations from plant surfaces to the inner portions of the plant. These limitations result from mechanisms responsible for

- inhibiting the transfer of lipophilic COPCs (e.g., the shape of the produce); and
- removing COPCs from the edible portion of the produce (e.g., washing, peeling, and cooking).

We recommend using Equation 5-18 to calculate *Pv*. We further discuss the use of this equation in Appendix B, Table B-2-8.

Recommended Equation for Calculating: Aboveground Produce Concentration Due to Air-to-Plant Transfer (*Pv*)

$$Pv = Q \cdot F_v \cdot \frac{Cyv \cdot Bv_{ag} \cdot VG_{ag}}{\rho_a} \qquad \text{Equation 5-18}$$

where

Pv = Concentration of COPC in the plant resulting from air-to-plant transfer (µg COPC/g DW)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
Cyv = Unitized yearly average air concentration from vapor phase (µg-s/g-m^3)
Bv_{ag} = COPC air-to-plant biotransfer factor ([mg COPC/g DW plant]/[mg COPC/g air]) (unitless)
VG_{ag} = Empirical correction factor for aboveground produce (unitless)
ρ_a = Density of air (g/m^3)

Chapters 2 and 3 explain how we recommend quantifying the COPC emission rate (Q). Appendix A-2 describes how we recommend determining the COPC-specific parameters Fv and Bv_{ag}. Chapter 3 describes generating the modeled air parameter Cyv. As discussed below in Section 5.3.2.1, the parameter VG_{ag} depends on the lipophilicity of the COPC. Appendix B further describes how we recommend using Equation 5-18, including calculating ρ_a.

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

The parameter VG_{ag} was incorporated into Equation 5-18 to address the potential to overestimate the transfer of lipophilic COPCs 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 COPCs (log K_{ow} greater than 4) to the center of the produce is not as likely as for non-lipophilic COPCs. As a result, the inner portions will be less affected.

To address this issue, U.S. EPA (1994m) recommended an empirical correction factor (VG_{ag}) of 0.01 for lipophilic COPCs to reduce estimated vegetable concentrations. The factor of 0.01 is based on a similar correction factor ($VG_{rootveg}$) for belowground produce. $VG_{rootveg}$ was estimated for unspecified vegetables as follows:

$$VG_{rootveg} = \frac{M_{skin}}{M_{vegetable}} \qquad \text{Equation 5-19}$$

where

$VG_{rootveg}$ = Correction factor for belowground produce (g/g)
M_{skin} = Mass of a thin (skin) layer of belowground vegetable (g)
$M_{vegetable}$ = Mass of the entire vegetable (g)

Assuming that the density of the skin and the whole vegetable are the same, this equation becomes a ratio of the volume of the skin to that of the whole vegetable. U.S. EPA (1994m) assumed that the vegetable skin is 0.03 centimeters, which is the leaf thickness of a broad-leaf tree, as was used in experiments conducted by Riederer (1990). Using this assumption, U.S. EPA (1994m) calculated $VG_{rootveg}$ values of 0.09 and 0.03 for carrots and potatoes, respectively.

Based on the work by Wipf et al. (1982), U.S. EPA (1994m) identified other processes—such as peeling, cooking, and cleaning—that further reduce the vegetable concentration. U.S. EPA (1994m) recommended a $VG_{rootveg}$ value of 0.01 for lipophilic COPCs. These are less than the estimates of 0.09 and 0.03 for the carrots and potatoes mentioned earlier, but greater than the estimate would be if the correction factor was adjusted for cleaning, washing, and peeling, as described by Wipf et al. (1982). Following this line of reasoning, U.S. EPA (1994m) recommended a lipophilic COPC VG_{ag} value of 0.01 for all aboveground produce except leafy vegetables. As with $VG_{rootveg}$, U.S. EPA (1994m) noted that assignment of this value is based on the consideration that it "should be less than estimated just based on surface volume to whole fruit volume ratios."

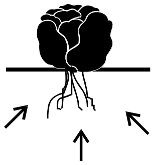
U.S. EPA (1994m) recommended a lipophilic COPC VG_{ag} of 1.0 for pasture grass because of a direct analogy to exposed azalea and grass leaves (for which data were available). Pasture grass is described as "leafy vegetation." However, the leafy vegetable group, as defined in Section 5.3.1.1, is composed of bulkier produce such as broccoli, brussel sprouts, cauliflower, celery, lettuce, and spinach. In addition, the outer leaves of most of the produce in this category are removed during preparation. Therefore, the VG_{ag} value of 1.0 for leafy vegetables is inappropriate and may overestimate COPC concentrations. A default lipophilic COPC VG_{ag} value of 0.01 for leafy vegetables is more appropriate for leafy vegetables, because the leafy vegetable category represents bulkier, more protected plants as compared to single leaves of grass blades. U.S. EPA (1994r) and NC DEHNR (1997) recommended a lipophilic COPC VG_{ag} value of 0.01, for all classes of aboveground produce.

For COPCs with a log K_{ow} greater than 4, we recommend using a lipophilic VG_{ag} value of 0.01 for all aboveground exposed produce. For COPCs with a log K_{ow} less than 4, we recommend using a VG_{ag} value of 1.0, because we assume these COPCs pass more easily through the skin of produce.

Recommended Values for: Empirical Correction Factor for Aboveground Produce (VG_{ag})
0.01 for COPCs with a log K_{ow} greater than 4
1.0 for COPCs with a log K_{ow} less than 4

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

5.3.3 Produce Concentration Due to Root Uptake (*Pr*)



Root uptake of contaminants from soil may contribute to COPC concentrations in aboveground exposed produce, aboveground protected produce, and belowground produce. As in previous guidance (U.S. EPA 1994m; U.S. EPA 1994r; and U.S. EPA 1995e), we recommend using Equations 5-20A and 5-20B to calculate *Pr*. We discuss the use of these equations further in Appendix B.

Recommended Equation for Calculating: Produce Concentration Due to Root Uptake (*Pr*)

Exposed and protected aboveground produce:

$$Pr = Cs \cdot Br \qquad \text{Equation 5-20A}$$

Belowground produce:

$$Pr = \frac{Cs \cdot RCF \cdot VG_{rootveg}}{Kd_s \cdot 1\ kg/L} \qquad \text{Equation 5-20B}$$

where

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

Appendix B and Section 5.2 explain how we recommend calculating Cs. Appendix A-2 describes how we recommend calculating the COPC-specific parameters Br, RCF, and Kd_s. Similar to VG_{ag} and as discussed in Section 5.3.2.1, $VG_{rootveg}$ is based on the lipophilicity of the COPC.

Equation 5-20A is based on the soil-to-aboveground plant transfer approach developed by Travis and Arms (1988). This approach is appropriate for evaluating exposed and protected aboveground produce; however, it might not be appropriate for soil-to-belowground plant transfers. For belowground produce, U.S. EPA (1994m) and U.S. EPA (1995e) recommended Equation 5-20B, which includes a root concentration factor (RCF) developed by Briggs et al. (1982). RCF is the ratio of COPC concentration in the edible root to the COPC concentration in the soil water. Since Briggs et al. (1982) conducted their experiments in a growth solution, in order to use this equation you must divide the COPC soil concentration (Cs) by the COPC-specific soil/water partition coefficient (Kd_s) (U.S. EPA 1994m).

As in U.S. EPA (1994m), we recommend using a $VG_{rootveg}$ value of 0.01 for lipophilic COPCs (log K_{ow} greater than 4) based on root vegetables like carrots and potatoes. A value of 0.01 appears to represent the most complete and thorough information available. For COPCs with a log K_{ow} less than 4, we recommend a $VG_{rootveg}$ value of 1.0.

Recommended Values for:
Empirical Correction Factor for Belowground Produce (*$VG_{rootveg}$*)

0.01 for COPCs with a log K_{ow} greater than 4

1.0 for COPCs with a log K_{ow} less than 4

5.4 CALCULATING COPC CONCENTRATIONS IN BEEF AND DAIRY PRODUCTS

We generally recommend that you estimate COPC concentrations in beef tissue and milk products on the basis of the amount of COPCs that cattle are assumed to consume through their diet. The HHRAP assumes the cattle's diet consists of:

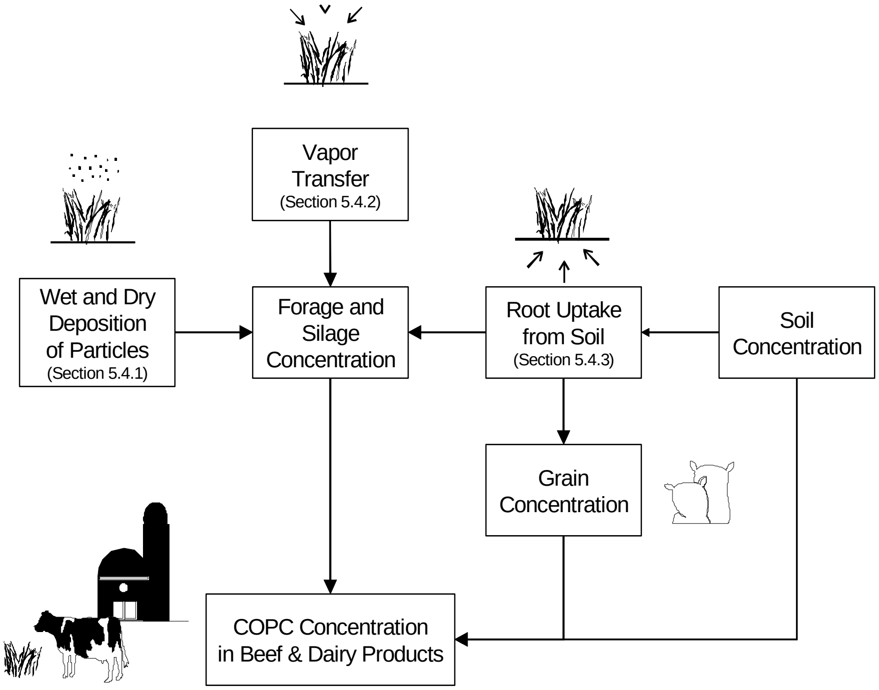
- forage (primarily pasture grass and hay),
- silage (forage that has been stored and fermented), and
- grain.

Additional contamination may occur through the cattle ingesting soil. The HHRAP calculates the total COPC concentration in the feed items (e.g., forage, silage, and grain) as a sum of contamination occurring through the following mechanisms:

- **Direct deposition of particles**—wet and dry deposition of particle phase COPCs onto forage and silage (Section 5.4.1).
- **Vapor transfer**—uptake of vapor phase COPCs by forage and silage through foliage (Section 5.4.2).
- **Root uptake**—root uptake of COPCs available from the soil and their transfer to the aboveground portions of forage, silage, and grain (Section 5.4.3).

Feed items consumed by animals can be classified as exposed or protected, depending on whether they have a protective outer covering. Because the outer covering on protected feed acts as a barrier, we assume that there is negligible contamination of protected feed through deposition of particles and vapor transfer. In the HHRAP, grain is classified as protected feed. As a result, we recommend that you assume grain contamination occurs only through root uptake. We also recommend assuming that contamination of exposed feed items, including forage and silage, occurs through all three mechanisms.

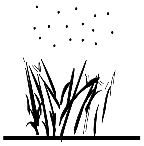
FIGURE 5-4
COPC CONCENTRATION IN BEEF AND DAIRY PRODUCTS



The HHRAP assumes that the amount of grain, silage, forage, and soil consumed varies between dairy and beef cattle. Sections 5.4.4 (beef) and 5.4.5 (dairy) describe the methods we recommend to estimate consumption rates and subsequent COPC concentrations in cattle. As in previous guidance (U.S. EPA 1990e and 1994a; NC DEHNR 1997), we recommend assuming that 100 percent of the plant materials eaten by cattle were grown on soil contaminated by emission sources. Therefore, we recommend assuming that 100 percent of the feed items are contaminated.

Appendix B, Tables B-3-1 through B-3-11, describe how we recommend calculating (1) the COPC concentrations in soil and feed items (forage, silage, and grain) consumed by beef and dairy cattle, and (2) the resulting COPC concentrations in beef and milk.

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



COPC concentrations in forage and silage result from wet and dry deposition onto exposed plant surfaces; similar to aboveground produce (Section 5.3.1). Therefore, we recommend also using Equation 5-14 to calculate *Pd* for forage and silage. We discuss calculating *Pd* for Forage and silage further in Appendix B. Appendix A-2 explains how we recommend calculating COPC-specific *Fv* values for forage and silage (i.e. exactly as they are calculated for aboveground produce). Sections 5.4.1.1 through 5.4.1.4 describe how we recommend calculating *Rp*, *kp*, *Tp*, and *Yp* for use in calculating forage and silage concentrations.

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

As discussed in Section 5.3.1.1, Chamberlain (1970) found a correlation between *Rp* and productivity, *Yp* (standing crop biomass). This correlation is expressed in Equation 5-14A.

Based on U.S. EPA (1994r and 1995b) and NC DEHNR (1997), we recommend using Equation 5-14 to calculate *Rp* values for forage and silage.

Substituting the Baes et al. (1984) empirical constant (() value of 2.88 for pasture grass, and the standing crop biomass value of 0.24 kg DW/m^2 (these variables are discussed in Section 5.3.1.1) into Equation 5-14, the forage-specific *Rp* is 0.5. Substituting the Baes et al. (1984) empirical constant (() value of 0.769 for silage, and the standing crop biomass value of 0.8 kg DW/m^2 into Equation 5-14, the silage-specific *Rp* value is 0.46.

Recommended Value for: Interception Fraction of the Edible Portion of Plant (*Rp*)
Forage = 0.5 Silage = 0.46

Several uncertainties are associated with the *Rp* variable:

- The empirical relationship developed by Chamberlain (1970) is based on a study of pasture grass, and therefore may not accurately represent site-specific silage types.
- The empirical constant for silage developed by Baes et al. (1984) used in Chamberlain's empirical relationship may also fail to accurately represent site-specific silage types.
- The range of empirical constants recommended by Baes et al. (1984) for pasture grass does not result in a significant range of estimated *Rp* values for forage (the calculated *Rp* range is 0.42 to 0.54). Therefore, using the empirical constant midpoint (2.88 for pasture grass) does not significantly affect the *Rp* value and the resulting estimate of plant COPC concentration.

5.4.1.2 Plant Surface Loss Coefficient (*kp*)

We recommend using Equation 5-15 (Section 5.3.1.2) to calculate the plant surface loss coefficient *kp* for aboveground produce. The *kp* factor is derived in the same manner for cattle forage and silage. The uncertainties of *kp* for cattle forage and silage are similar to the uncertainties for aboveground produce.

5.4.1.3 Length of Plant Exposure to Deposition per Harvest of the Edible Portion of Plant (*Tp*)

As discussed in Section 5.3.1.3, the HHRAP treats *Tp* as a constant, based on the average period between successive hay harvests. This period, which Belcher and Travis (1989) estimated at 60 days, represents the length of time that aboveground vegetation (in this case, hay) would be exposed to particle deposition before being harvested. We used Equation 5-16 (Section 5.3.1.3), to calculate a *Tp* of 0.16 year for cattle silage.

For cattle forage, we modified Equation 5-16 to consider the average of :

1. the average period between successive hay harvests, and
2. the average period between successive grazing.

Based on Belcher and Travis (1989), the we assumed the average period between hay harvests is 60 days, and the average period between successive grazing is 30 days. We therefore calculated *Tp* as follows:

$$Tp = \frac{0.5 \cdot (60\ days + 30\ days)}{365\ days/yr} = 0.12\ yr \qquad \text{Equation 5-21}$$

Recommended Value for: **Plant Exposure Length to Deposition per Harvest of the Edible Portion of Plant (*Tp*)**
Forage = 0.12 yr Silage = 0.16 yr

The primary uncertainties associated with *Tp* are similar to those for aboveground produce, as discussed in Section 5.3.1.3.

5.4.1.4 Standing Crop Biomass (Productivity) (*Yp*)

As discussed in Section 5.3.1.4, U.S. EPA (1998c) stated that the best estimate of *Yp* is productivity, as defined in Equation 5-17. Consequently, under this approach, you would consider dry harvest yield (*Yh*) and area harvested (*Ah*).

We calculated forage *Yp* as a weighted average of the calculated pasture grass and hay *Yp* values. We assumed weightings of 0.75 for forage and 0.25 for hay. The weightings are 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). We assumed an unweighted pasture grass *Yp* of 0.15 kg DW/m^2 (U.S. EPA 1994r; U.S. EPA 1994m). We then calculated an unweighted hay *Yp* of 0.5 kg DW/m^2 using Equation 5-17 and the following *Yh* and *Ah* values:

Yh = 1.22×10^{11} kg DW, calculated from the 1993 U.S. average wet weight *Yh* of 1.35×10^{11} kg (USDA 1994b) and a conversion factor of 0.9 (Fries 1994).

Ah = 2.45×10^{11} m^2, the 1993 U.S. average for hay (USDA 1994b).

The unweighted pasture grass and hay *Yp* values were multiplied by their weighting factors (0.75 and 0.25, respectively), and summed to calculate the recommended weighted forage *Yp* of 0.24 kg DW/m^2.

We recommend assuming a production-weighted U.S. average *Yp* of 0.8 kg DW/m^2 for silage (Shor, et al. 1982).

Recommended Values for: **Standing Crop Biomass (Productivity) (*Yp*)**
Forage = 0.24 kg DW/m^2 Silage = 0.8 kg DW/m^2

The primary uncertainty associated with this variable is that the harvest yield (*Yh*) and area planted (*Ah*) may not reflect site-specific conditions. To the extent that site-specific information is available, it's feasible to estimate the magnitude of the uncertainty introduced by the default *Yp* value. 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) could be adjusted to reflect site-specific conditions, as appropriate.

5.4.2 Forage and Silage Concentrations Due to Air-to-Plant Transfer (*Pv*)

We recommend using Equation 5-18 (Section 5.3.2) to calculate the COPC concentration in aboveground produce resulting from air-to-plant transfer (*Pv*). *Pv* is calculated for cattle forage and silage similarly to the way that it's calculated for aboveground produce. We provide a detailed discussion of *Pv* in Section 5.3.2. We present differences in VG_{ag} values for forage and silage, as compared to the values for aboveground produce described in Section 5.3.2.1, in Section 5.4.2.1. We discuss calculating *Pv* further in Appendix B. Appendix A-2 explains how we recommend calculating COPC-specific Bv values for forage and silage (i.e. the same as they are calculated for aboveground produce).

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

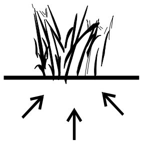
Please Section 5.3.2.1 for a detailed, general introduction to VG_{ag}. Using such a factor while estimating COPC concentrations specifically for forage and silage assumes that there is insignificant translocation of COPCs deposited on the surface of bulky silage to the inner parts of the vegetation. Applying a silage VG_{ag} would be relevant if the silage can't be characterized as leafy (e.g., if grain is used as silage). As a point of clarification, forage and silage are considered vegetative plant parts, and grains are considered reproductive plant parts.

U.S. EPA (1994m) didn't recommend a VG_{ag} value for silage. NC DEHNR (1997) recommended a VG_{ag} factor of 0.5 for bulky silage but didn't present a specific rationale for this value. U.S. EPA (1995b) noted that a volume ratio of outer whole surface area to volume of vegetation could be used to assign a silage VG_{ag} value, if one knew the proportions of each type of vegetation of which silage consisted. In the absence of specific data concerning the quantities of different silage material (e.g., hay and grain), U.S. EPA (1995b) recommended assuming a VG_{ag} of 0.5 for silage without rigorous justification.

We recommend using 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.

Recommended Values for: Empirical Correction Factor for Forage and Silage (VG_{ag})
Forage = 1 Silage = 0.5

5.4.3 Forage, Silage, and Grain Concentrations Due to Root Uptake (Pr)



We recommend using Equations 5-20A and 5-20B (Section 5.3.3) to calculate the COPC concentration in aboveground and belowground produce resulting from root uptake. Pr is calculated for cattle forage, silage, and grain in the same way that it is calculated for aboveground produce, except that we recommend using forage/silage- and grain-specific bioconcentration factors (Br_{forage} and Br_{grain} respectively). Appendix A-2 explains how we recommend calculating COPC-specific Br values for forage and silage (i.e. exactly as it's calculated for aboveground produce). We provide a detailed discussion on how we recommend calculating Pr in Section 5.3.3. We further discuss the calculation of Pr in Appendix B.

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

As in U.S. EPA (1995h), we recommend using Equation 5-22 to calculate COPC concentration in beef tissue (A_{beef}). The equation was modified from an equation presented in U.S. EPA (1990c), U.S. EPA (1994r), U.S. EPA (1995b), and NC DEHNR (1996) by introducing a metabolism factor (MF). Equation 5-22 calculates the daily amount of a COPC 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 COPC (mg/day) into an animal COPC tissue concentration (mg COPC/kg tissue). We further discuss using this equation in Appendix B, Table 3-10.

Recommended Equation for Calculating:
Concentration of COPC in Beef (A_{beef})

$$A_{beef} = \left(\Sigma(F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs\right) \cdot Ba_{beef} \cdot MF \qquad \text{Equation 5-22}$$

where

A_{beef} = Concentration of COPC in beef (mg COPC/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 COPC 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 COPC/kg soil)
Bs = Soil bioavailability factor (unitless)
Ba_{beef} = COPC biotransfer factor for beef (day/kg FW tissue)
MF = Metabolism factor (unitless)

Sections 5.4.4.1 through 5.4.4.7 describe the parameters F_i, Qp_i, P_i, Qs, Cs, Bs, and MF, respectively. Appendix A-2 explains how we recommend calculating the COPC-specific parameter Ba_{beef}.

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

As in U.S. EPA (1990e and 1994r), and NC DEHNR (1997), we recommend assuming that 100 percent of the plant materials eaten by cattle were grown on soil contaminated by the emission sources being evaluated. This assumption translates to a default value of 1.0 for F_i.

Recommended Value for: Fraction of Plant Type *i* Grown on Contaminated Soil and Eaten by the Animal (Cattle) (F_i)
1

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

The daily quantity of plants eaten by cattle can be estimated (kg DW/day) for each category of plant feed. U.S. EPA (1994r and 1998c) and NC DEHNR (1997) recommended including forage, silage, and grain feeds in this estimate.

NC DEHNR (1997) recommended plant ingestion rates for the cattle of either subsistence beef farmers or typical beef farmers. Subsistence beef farmers rely on a higher percentage of forage and silage to feed cattle, whereas typical beef farmers rely on greater amounts of grain to feed cattle. U.S. EPA (1990e) and U.S. EPA (1994r) identified plant ingestion rates only for subsistence farmers. The following daily quantities of forage, grain, and silage eaten by cattle were recommended by NC DEHNR (1997), U.S. EPA (1994r and 1990e), and Boone et al. (1981):

Source	Forage (kg DW/day)	Grain (kg DW/day)	Silage (kg DW/day)	References
NC DEHNR (1997) Subsistence Farmer Beef Cattle	8.8	0.47	2.5	Boone et al. (1981) NAS (1987)
NC DEHNR (1997) Typical Farmer Beef Cattle	3.8	3.8	1.0	Rice (1994)
U.S. EPA (1994r) Subsistence Farmer Beef Cattle	8.8	Not reported	Not reported	Boone et al. (1981) NAS (1987)
U.S. EPA (1990e) Subsistence Farmer Beef Cattle	8.8	0.47	2.5	Boone et al. (1981) McKone and Ryan (1989)
Boone et al. (1981)	8.87	1.9	2.5	Boone et al. (1981)

With the exception of a higher grain ingestion rate, Boone et al. (1981) rates are consistent with those recommended by U.S. EPA (1990e and 1994r), and NC DEHNR (1997). For typical farmer beef cattle, NC DEHNR (1997) cites Rice (1994) as a reference for the Qp_i variables and notes that the values include grain supplemented during the growing phase for beef cattle.

U.S. EPA (1990e) noted that McKone and Ryan (1989) reported an average total ingestion rate of 12 kg DW/day for the three plant feeds, which is consistent with the total recommended by U.S. EPA (1990e) and NC DEHNR (1997) (forage, grain, and silage total of 11.8 kg DW/day). U.S. EPA (1994r) and NC DEHNR (1997) also noted that NAS (1987) reported a daily dry matter intake that is 2 percent of an average beef cattle body weight of 590 kilograms. This results in a daily total intake rate of 11.8 kg DW/day. NAS (1987) reported that a nonlactating cow eats dry matter equivalent to 2 percent of its body weight.

We recommend using 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.

Recommended Values for:
Quantity of Plant Type *i* Eaten by the Animal (Cattle) Each Day (Qp_i)

Forage = 8.8 kg DW/day

Silage = 2.5 kg DW/day

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.

5.4.4.3 Concentration of COPC in Plant Type *i* Eaten by the Animal (Cattle) (P_i)

We generally recommend using Equation 5-23 to calculate the total COPC concentration in forage, silage, and grain. We recommend deriving values for *Pd*, *Pv*, and *Pr* for each type of feed by using Equations 5-14, 5-18, and 5-20, respectively.

Recommended Equation for Calculating:
Concentration of COPC in Plant Type *i* Eaten by the Animal (Cattle) (P_i)

$$P_i = \Sigma_i (Pd + Pv + Pr) \qquad \text{Equation 5-23}$$

where

P_i = Concentration of COPC in each plant type *i* eaten by the animal (mg COPC/kg DW)
Pd = Plant concentration due to direct deposition (mg COPC/kg DW)
Pv = Plant concentration due to air-to-plant transfer (mg COPC/kg DW)
Pr = Plant concentration due to root uptake (mg COPC/kg DW)

This equation is further described in Appendix B.

5.4.4.4 Quantity of Soil Eaten by the Animal (Cattle) Per Day (Qs)

Additional cattle contamination occurs through ingestion of soil.

NC DEHNR (1997) and U.S. EPA (1994r) recommended a soil ingestion rate for subsistence beef cattle of 0.5 kg/day. This rate is based on Fries (1994). U.S. EPA (1994r) and NC DEHNR (1997) noted that

Fries (1994) reported soil ingestion to be 4 percent of the total dry matter intake. NAS (1987) was also referenced. NAS (1987) cited an average beef cattle weight of 590 kg, and a daily dry matter intake rate (nonlactating cows) of 2 percent of body weight. This results in a daily dry matter intake rate of 11.8 kg DW/day and a daily soil ingestion rate of about 0.5 kg/day. U.S. EPA (1990e) reported a soil ingestion rate that is 3 percent of the forage intake rate of 8.8 kg DW/day, resulting in a daily soil ingestion rate of approximately 0.3 kg/day. Simmonds and Linsley (1981) and Thornton and Abrams (1983) were cited as the references for this assumption.

We recommend using 0.5 kg/day for the quantity of soil ingested by the animal (cattle).

Recommended Value for: **Quantity of Soil Ingested by the Animal (Cattle) Per Day (*Qs*)**
0.5 kg/day

5.4.4.5 Average Soil Concentration Over Exposure Duration (*Cs*)

We recommend using Equations 5-1C, 5-1D, and 5-1E to calculate the COPC concentration in soil as discussed in Section 5.2.1. Also, Appendix B further describes how we recommend calculating the soil concentration.

> ***Please Note:*** You might need to generate soil concentration estimates for grain separate from those for forage and silage. Currently, the HHRAP assumes that forage and silage are grown on untilled land, and grain is grown on tilled land. We highly recommend that your C_s calculations include the appropriate Z_s (1 for untilled land, 20 for tilled land).

5.4.4.6 Soil Bioavailability Factor (*Bs*)

The efficiency of transfer from soil may differ from the efficiency of transfer from plant material for some COPCs. If the transfer efficiency is lower for soils, then the ratio would be less than 1.0. If it is equal to or greater than that of vegetation, the *Bs* value would be equal to or greater than 1.0.

Until more COPC-specific data becomes available for this parameter, we recommend a default value of 1 for *Bs*.

Recommended Values for: **Soil Bioavailability Factor (*Bs*)**
1.0

5.4.4.7 Metabolism Factor (*MF*)

The metabolism factor (*MF*) estimates the amount of COPC that remains in fat and muscle. Based on a study by Ikeda et al. (1980), U.S. EPA (1995h) used a COPC-specific *MF* to account for metabolism in animals and humans. Evidence indicates BEHP is more readily metabolized and excreted by mammalian species than other contaminants (ATSDR 1987). As in U.S. EPA (1995h), we recommend a *MF* of 0.01 for bis(2-ethylhexyl)phthalate (BEHP). Lacking data to support derivation of other chemical-specific *MF*s, we recommend using a *MF* of 1.0 for all chemicals other than BEHP. Using the recommended values for this variable, *MF* has no quantitative effect on A_{beef} (with the exception of BEHP).

Recommended Values for: **Metabolism Factor (*MF*)**
bis(2-ethylhexyl)phthalate (BEHP) = 0.01 All other COPCs = 1.0

The *MF* presented above for BEHP 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 guidance are intake driven, using an MF applies only to estimating COPC concentrations in food sources used in evaluating indirect human exposure, including ingestion of beef, milk, and pork. In summary, an *MF* is not applicable for direct exposures to air, soil, or water, or to ingestion of produce, chicken, or fish.

5.4.5 COPC Concentration In Milk Due to Plant and Soil Ingestion (A_{milk})

We recommend modifying Equation 5-22 (Section 5.4.4) to calculate COPC milk concentrations (A_{milk}), as follows:

Recommended Equation for Calculating:
Concentration of COPC in Milk (A_{milk})

$$A_{milk} = \left(\Sigma(F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs\right) \cdot Ba_{milk} \cdot MF \qquad \text{Equation 5-24}$$

where

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

Appendix A-2 explains how we recommend calculating the COPC-specific parameter Ba_{milk}. The discussion in Section 5.4.4 of the variables F_i, Qp_i, P_i, Qs, Cs, 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.

We recommend using Equation 5-24 to estimate A_{milk}. Using Equation 5-24 is described further in Appendix B, Table B-3-11.

5.4.5.1 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 5.4.4.1).

5.4.5.2 Quantity of Plant Type *i* Eaten by the Animal (Dairy Cattle) Per Day (Qp_i)

As discussed in Section 5.4.4.2, 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. We generally recommend estimating the daily quantity of feed consumed by cattle on a dry weight basis for each category of plant feed.

NC DEHNR (1997) recommended using plant ingestion rates for either subsistence dairy farmer or typical dairy farmer cattle. In addition, subsistence dairy farmers rely on a higher percentage of forage and silage to feed cattle, whereas typical dairy farmers rely on greater amounts of grain to feed cattle. U.S. EPA (1990e and 1994r) identified plant ingestion rates only for subsistence farmers.

The following daily quantities of forage, grain, and silage eaten by dairy cattle were recommended by NC DEHNR (1997), U.S. EPA (1994r), U.S. EPA (1990e), and Boone et al. (1981):

Source	Forage (kg/day DW)	Grain (kg/day DW)	Silage (kg/day DW)	References
NC DEHNR (1997) Subsistence Dairy Farmer Cattle	13.2	3.0	4.1	Boone et al. (1981) NAS (1987)
NC DEHNR (1997) Typical Dairy Farmer Cattle	6.2	12.2	1.9	Rice (1994)
U.S. EPA (1994r) Subsistence Dairy Farmer Cattle	13.2	Not reported	Not reported	Boone et al. (1981) NAS (1987)
U.S. EPA (1990e) Subsistence Dairy Farmer Cattle	11.0	2.6	3.3	Boone et al. (1981) McKone and Ryan (1989)
Boone et al. (1981)	11.0	2.6	3.3	Boone et al. (1981)

U.S. EPA (1990e) noted that McKone and Ryan (1989) reports an average total ingestion rate of 17 kg/day DW for the three plant feeds, which is consistent with the total ingestion rate recommended by U.S. EPA (1990e). U.S. EPA (1994r) and NC DEHNR (1997) noted that NAS (1987) reports a daily dry matter intake that is 3.2 percent of an average dairy cattle body weight of 630 kilograms. This results in a daily total intake rate of approximately 20 kg/day DW, which is consistent with the average total ingestion rates for the three plant feeds recommended by U.S. EPA (1994r) and NC DEHNR (1997) . NAS (1987) reported that dairy cows eat dry matter equivalent to 3.2 percent of their body weight; the

630-kilogram average dairy cow body weight was not confirmed. U.S. EPA (1995b) also cited a feed ingestion rate of 20 kg/day DW, citing U.S. EPA (1993c).

Based on more recent references (NAS 1987; U.S. EPA 1993c) which recommend a feed ingestion rate of 20 kg/day DW, we recommend a default total ingestion rate of 20 kg DW/day for dairy cattle.

Recommended Values for: **Quantity of Plant Type *i* Eaten by the Animal (Dairy Cattle) Per Day (Qp_i)**
Forage = 13.2 kg DW/day
Silage = 4.1 kg DW/day
Grain = 3.0 kg DW/day

Uncertainties associated with estimating Qp_i include estimating forage, grain, and silage ingestion rates, which will vary from site to site. Assuming uniform contamination of plant materials consumed by cattle also introduces uncertainty.

5.4.5.3 Concentration of COPC 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 5.4.4.3).

5.4.5.4 Quantity of Soil Eaten by the Animal (Dairy Cattle) Per Day (Qs)

As discussed in Section 5.4.4.4, contamination of dairy cattle also results from the ingestion of soil. We generally recommend the following soil ingestion rate for dairy cattle:

Recommended Values for: **Quantity of Soil Eaten by the Animal (Dairy Cattle) Per Day (Qs)**
0.4 kg/day

U.S. EPA (1994r) and NC DEHNR (1997) recommended a soil ingestion rate of 0.4 kg/day for dairy cattle, based on Fries (1994). U.S. EPA (1994r) and NC DEHNR (1997) noted that Fries (1994) reported soil ingestion rates as 2 percent of the total dry matter intake. NAS (1987) was also referenced, which reported an average dairy cattle weight of 630 kilograms and a daily dry matter intake rate (nonlactating cows) of 3.2 percent of body weight. This resulted in a daily dry matter intake rate of 20 kg/day DW, and a daily soil ingestion rate of approximately 0.4 kg/day. NC DEHNR (1997) recommended a soil ingestion rate of 0.2 kg/day for the cattle of typical dairy farmers, citing Rice (1994). U.S. EPA (1990e) reported soil ingestion rates as 3 percent of the forage intake rate. U.S. EPA (1990e) assumed that the more protective forage intake rate of 13.2 kg/day DW results in a daily soil ingestion rate of about 0.4 kg/day. Simmonds and Linsley (1981) and Thornton and Abrams (1983) were cited as the references for this assumption.

Uncertainties associated with *Qs* include the lack of current empirical data to support soil ingestion rates for dairy cattle. Assuming uniform contamination of soil ingested by cattle also adds uncertainty.

5.4.5.5 Average Soil Concentration Over Exposure Duration (*Cs*)

The calculation of *Cs* for dairy cattle is the same as for beef cattle (Section 5.4.4.5).

> ***Please Note:*** You might need to generate soil concentration estimates for grain separate from those for forage and silage. Currently, the HHRAP assumes that forage and silage are grown on untilled land, and grain is grown on tilled land. We highly recommend making sure that your C_s calculations include the appropriate Z_s (2 for untilled land, 20 for tilled land).

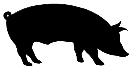
5.4.5.6 Soil Bioavailability Factor (*Bs*)

The calculation of *Bs* for dairy cattle is the same as for beef cattle (Section 5.4.4.6).

5.4.5.7 Metabolism Factor (*MF*)

The recommended values for *MF* are identical to those we recommend for beef cattle (Section 5.4.4.7).

5.5 CALCULATING COPC CONCENTRATIONS IN PORK

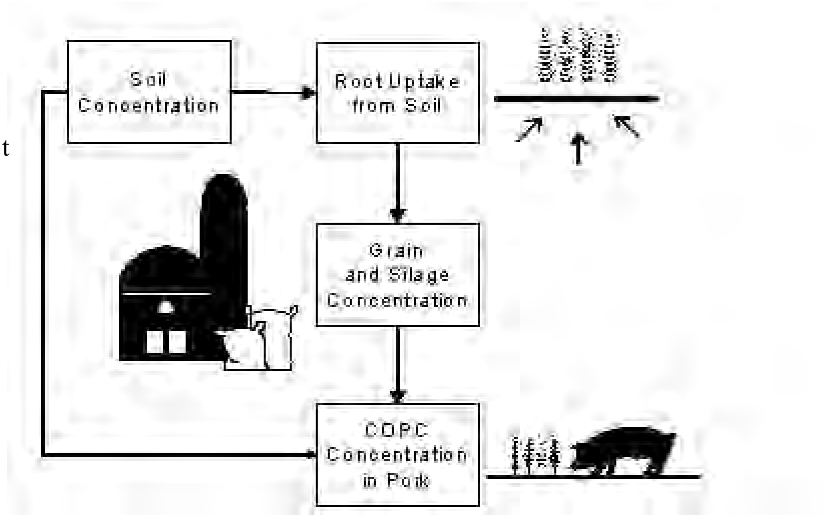


Under the approach recommended in this guidance, COPC concentrations in pork tissue are estimated on the basis of the amount of COPCs that swine consume through a diet consisting of silage and grain. Additional COPC contamination of pork tissue may occur through their ingestion of soil.

Equation 5-22 (Section 5.4.4) describes how we recommend calculating COPC concentration in beef cattle (A_{beef}). We suggest modifying Equation 5-22 to calculate COPC concentrations in swine (A_{pork}), as follows:

FIGURE 5-5

COPC CONCENTRATION IN PORK



Recommended Equation for Calculating:

Concentration of COPC in Pork (A_{pork})

$$A_{pork} = \left(\sum (F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs\right) \cdot Ba_{pork} \cdot MF \qquad \text{Equation 5-25}$$

where

A_{pork} = Concentration of COPC in pork (mg COPC/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 COPC 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 COPC/kg soil)
Bs = Soil bioavailability factor (unitless)
Ba_{pork} = COPC biotransfer factor for pork (day/kg FW tissue)
MF = Metabolism factor (unitless)

Appendix A-2 explains how we recommend calculating the COPC-specific parameter Ba_{pork}. The discussions in Section 5.4.5 of the variables F_i, Qp_i, P_i, Qs, Cs and MF for beef cattle generally apply to the corresponding variables for pork. However, some different assumptions are made for pork. These differences are summarized in the following subsections.

We generally recommend using Equation 5-25 to calculate COPC pork concentrations (A_{pork}). This equation is further described in Appendix B, Table B-3-12.

5.5.1 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 5.4.4.1).

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

Section 5.4.4.2 discusses estimating the daily quantity of forage, silage, and grain feed consumed by beef cattle for each feed category. However, daily ingestion rates for pork are estimated differently than for beef cattle. U.S. EPA (1994r and 1998c), and NC DEHNR (1997) recommended only including silage and grain feeds to estimate daily plant quantity eaten by swine. Because swine are not grazing animals, they are assumed not to eat forage (U.S. EPA 1998c). We therefore generally recommend estimating the daily quantity of plant feeds (kilograms of DW) consumed by swine for each category of plant feed.

U.S. EPA (1990e) and NC DEHNR (1997) recommended grain and silage ingestion rates for swine of 3.0 and 1.3 kg DW/day, respectively. NC DEHNR (1997) references U.S. EPA (1990e) as the source of these ingestion rates. U.S. EPA (1990e) reported total dry matter ingestion rates for hogs and lactating sows as 3.4 and 5.2 kg DW/day, respectively. U.S. EPA (1990e) cites Boone et al. (1981) as the source of the ingestion rate for hogs, and NAS (1987) as the source of the ingestion rate for a lactating sow. Boone et al. (1981) reported a grain ingestion rate of 3.4 kg DW/day for a hog. NAS (1987) reported an average ingestion rate of 5.2 kg DW/day for a lactating sow. U.S. EPA (1990e) recommended using the average of these two rates (4.3 kg DW/day).

U.S. EPA (1990e) 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. U.S. EPA (1990e) cited U.S. EPA (1982b) as the source of the grain and silage dietary fractions. U.S. EPA (1995b) recommended an ingestion rate of 4.7 kg DW/day for a swine, referencing NAS (1987). NAS (1987) 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.

Recommended Values for: Quantity of Plant Type *i* Eaten by the Animal (Swine) Each Day (Qp_i)
Grain = 3.3 kg DW/day 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. You could use site-specific data to mitigate this uncertainty. In addition, assuming uniform contamination of the plant materials consumed by swine produces some uncertainty.

5.5.3 Concentration of COPC in Plant Type *i* Eaten by the Animal (Swine) (P_i)

The suggested calculation of P_i for pork is identical to that for beef cattle (Section 5.4.4.3).

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

As discussed in Section 5.4.4.4, additional contamination of swine results from ingestion of soil. The following Q_s values were recommended by earlier guidance:

Guidance	Quantity of Soil Eaten by Swine Each Day (Q_s)
U.S. EPA (1990e)	Stated that sufficient data are not available to estimate swine soil ingestion rates.
NC DEHNR (1997)	0.37 kg/day Estimated by assuming a soil intake that is 8% of the plant ingestion rate of 4.3 kg DW/day). U.S. EPA (1993f) was cited as the reference for the soil ingestion rate of 8 percent of dry matter intake.
U.S. EPA (1998c)	Cites a companion “Parameters Guidance Document” for detailed recommendations on Q. The “Parameters” document has not been published.

As in NC DEHNR (1997), we recommend the following soil ingestion rate for swine:

Recommended Value for: Quantity of Soil Eaten by the Animal (Swine) Each Day (Q_s)
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 assuming uniform contamination of the soil ingested by swine.

5.5.5 Average Soil Concentration Over Exposure Duration (*Cs*)

Our suggested calculation of *Cs* for pork is the same as for beef cattle (Section 5.4.4.5).

> ***Please Note:*** You might need to generate soil concentration estimates for grain separate from those for silage. We recommend assuming that silage is grown on untilled land, and grain is grown on tilled land. We highly recommend that you make sure that your C_s calculations include the appropriate Z_s (2 for untilled land, 20 for tilled land).

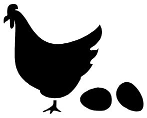
5.5.6 Soil Bioavailability Factor (*Bs*)

Our suggested calculation of *Bs* for pork is the same as for beef cattle (Section 5.4.4.6)

5.5.7 Metabolism Factor (*MF*)

Our recommended values for MF are identical to those we recommended for beef cattle (Section 5.4.4.7).

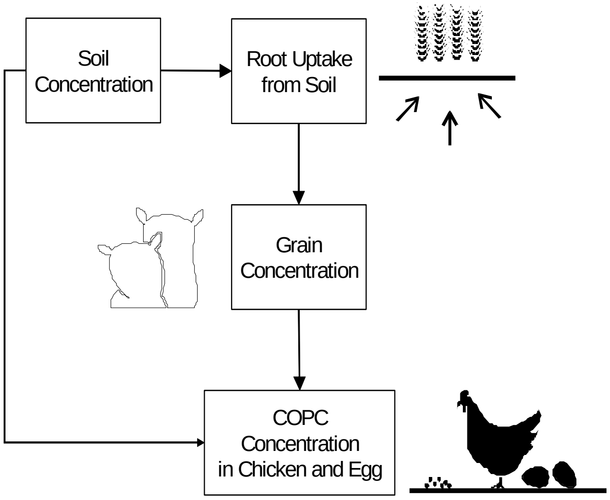
5.6 CALCULATING COPC CONCENTRATIONS IN CHICKEN AND EGGS



Under the approach outlined in this guidance document, estimates of the COPC concentrations in chicken and eggs are based on the amount of COPCs that chickens consume through ingestion of grain and soil. We recommend assuming that the uptake of COPCs via inhalation and via ingestion of water are insignificant relative to other pathways. The HHRAP assumes that chickens are housed in a typical manner that allows contact with soil. Because of this, chickens are assumed to consume 10 percent of their diet as soil. Assuming 10 percent is consistent with the study from which the biotransfer factors were obtained (Stephens et al. 1995). We recommend assuming that the remainder of the diet (90 percent) consists of grain grown at the exposure scenario location. Therefore, it's appropriate to assume 100 percent of the grain consumed is contaminated. The equations don't account for the uptake of COPCs via ingestion of contaminated insects and other organisms (e.g., worms, etc.), which may also contribute to the ingestion of COPCs. This may be a limitation, depending on the site-specific conditions under which the chickens are raised.

We generally recommend using the algorithm for aboveground produce described in Section 5.3 to estimate the COPC concentration in grain. Grain is considered to be protected from direct deposition of particles, and vapor transfer. This approach considers only contamination due to root uptake of COPCs in calculating COPC concentrations in grain. Our recommended equations for calculating concentrations in chicken and eggs are presented in Appendix B. The method we used to derive biotransfer factors, and the COPC-specific values for chicken and eggs are presented in Appendix A-2.

FIGURE 5-6
COPC CONCENTRATION IN CHICKEN & EGGS



As in NC DEHNR (1997), we recommend using Equation 5-26 to calculate COPC concentrations in chicken and eggs (Stephens et al. 1995). We generally recommend calculating COPC concentrations in chicken and eggs separately. Parameters and variables in Equation 5-26 are further described in Appendix B, Tables B-3-13 and B-3-14.

Recommended Equation for Calculating:
Concentration of COPC in Chicken and Eggs ($A_{chicken}$ or A_{egg})

$$A_{chicken} \; or \; A_{egg} = (\Sigma[F_i \cdot Qp_i \cdot Pi] + Qs \cdot Cs \cdot Bs) \cdot (Ba_{egg} \; or \; Ba_{chicken}) \qquad \text{Equation 5-26}$$

where

$A_{chicken}$ = Concentration of COPC in chicken (mg COPC/kg FW tissue)
A_{egg} = Concentration of COPC in eggs (mg COPC/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 COPC 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 COPC/kg soil)
Bs = Soil bioavailability factor (unitless)
$Ba_{chicken}$ = COPC biotransfer factor for chicken (day/kg FW tissue)
Ba_{egg} = COPC biotransfer factor for eggs (day/kg FW tissue)

Appendix A-2 explains how we recommend determining the COPC-specific parameters $Ba_{chicken}$ and Ba_{egg}. The remaining parameters are discussed in Appendix B and in the following subsections.

5.6.1 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 5.4.4.1).

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

Section 5.4.4.2 discusses estimating the daily quantity of forage, silage, and grain feed consumed by beef cattle for each feed category. However, daily ingestion rates for chicken are estimated differently than for beef cattle. NC DEHNR (1997) recommended that only grain feeds be included in this estimate. Because chickens are not grazing animals, they are assumed not to eat forage (U.S. EPA 1998c). Chickens are similarly assumed not to consume any silage. We recommend only estimating the daily quantity of plant feeds (kilograms of DW) consumed by chicken (*Qp*) for grain feed.

As in Ensminger (1980), Fries (1982), and NAS (1987), we recommend using the following ingestion rate:

Recommended Value for: **Quantity of Plant Type *i* Eaten by the Animal (Chicken) Each Day (Qp_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, assuming uniform contamination of plant materials consumed by chicken produces some uncertainty.

5.6.3 Concentration of COPC in Plant Type *i* Eaten by the Animal (Chicken) (P_i)

The total COPC concentration is the COPC concentration in grain. We recommend using Equation 5-27 to calculate P_i. This equation is further described in Appendix B.

Recommended Equation for Calculating:
Concentration of COPC in Plant Type *i* Eaten by the Animal (Chicken) (P_i)

$$P_i = \sum_i (Pr) \qquad \text{Equation 5-27}$$

where

P_i = Concentration of COPC in each plant type *i* eaten by the animal (mg COPC/kg DW)
Pr = Plant concentration due to root uptake (mg COPC/kg DW)

We generally recommend calculating plant concentration due to root uptake (*Pr*) using Equation 5-20, as discussed in Section 5.3.3.

5.6.4 Quantity of Soil Eaten by the Animal (Chicken) Each Day (Qs)

COPC concentration in chickens also results from intake of soil. As discussed earlier, The HHRAP assumes that chickens consume 10 percent of their total diet as soil, a percentage that is consistent with the study from Stephens et al. (1995). We recommend the following soil ingestion rate for chicken:

Recommended Value for: **Quantity of Soil Eaten by the Animal (Chicken) Each Day (*Qs*)**
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 assuming uniform contamination of soil ingested by chicken.

5.6.5 Average Soil Concentration Over Exposure Duration (*Cs*)

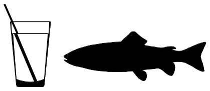
The calculation of *Cs* for chicken is the same as for beef cattle (Section 5.4.4.5).

> ***Please Note:*** We recommend assuming that forage and silage are grown on untilled land, and grain is grown on tilled land. We highly recommend making sure that your C_s calculations include the appropriate Z_s (20 for tilled land).

5.6.6 Soil Bioavailability Factor (*Bs*)

The calculation of *Bs* for chicken is the same as for beef cattle (Section 5.4.4.6)

5.7 CALCULATING COPC CONCENTRATIONS IN DRINKING WATER AND FISH

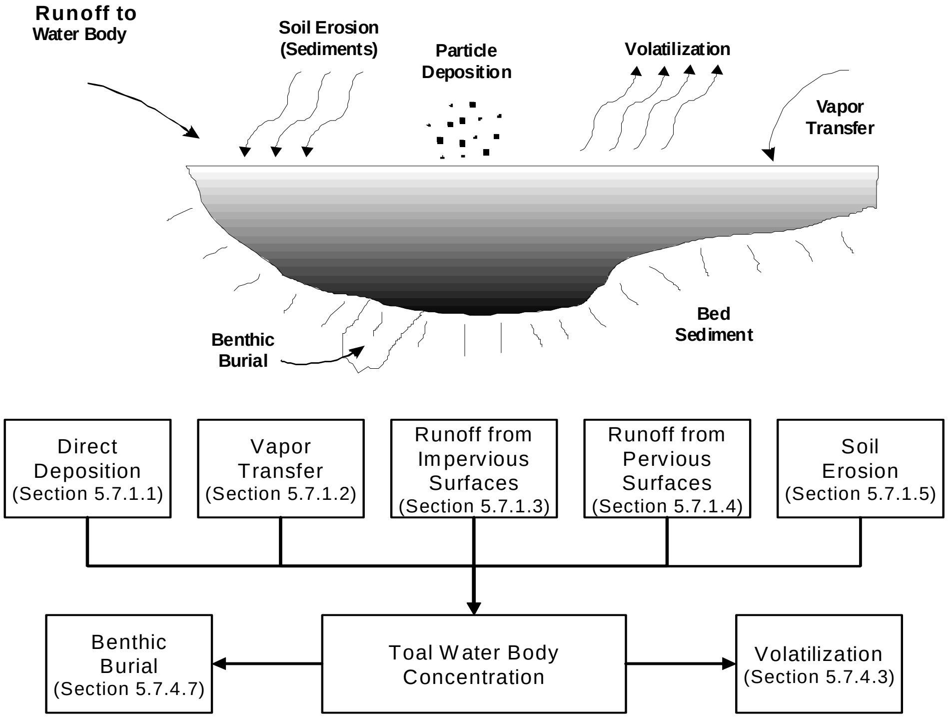


We generally recommend calculating COPC concentrations in surface water for all water bodies you selected to evaluate in the risk assessment. Specifically, those waterbodies selected as potential sources for the drinking water and/or fish ingestion exposure pathways. Mechanisms we suggest considering in determining COPC loading of the water column include:

- Direct deposition,
- Runoff from impervious surfaces within the watershed,
- Runoff from pervious surfaces within the watershed,
- Soil erosion over the total watershed,
- Direct diffusion of vapor phase COPCs into the surface water, and
- Internal transformation of compounds chemically or biologically.

Considering other potential mechanisms may be appropriate, due to site-specific conditions (e.g., tidal influences). Typically, though, we assume that contributions from other potential mechanisms are negligible compared to those evaluated in the HHRAP.

FIGURE 5-7
COPC LOADING TO THE WATER BODY



The total concentration of each COPC partitions between the sediment and the water column. Partitioning between water and sediment varies with the COPC. The HHRAP uses the Universal Soil Loss Equation (USLE) and a sediment delivery ratio to estimate the rate of soil erosion from the watershed. The equations we recommend for estimating surface water concentrations 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, we typically assume 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 COPC concentration is the sum of the COPC concentration dissolved in water and the COPC concentration associated with suspended solids. Appendix B-4 presents the equations we recommend using to estimate surface water concentrations.

To evaluate the COPC loading to a water body from its associated watershed, we generally recommend calculating watershed soil-specific COPC concentrations. The equation in Section 5.2 for estimating COPC 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. Appendix B (Tables B-4-1 through B-4-28) provides the equations we recommend for calculating COPC concentrations in watershed soils and in the water body.

The equations presented in Appendix B for modeling COPC loading to a water body represent a simple steady-state model to solve for a water column in equilibrium with the upper sediment layer. These equations (Appendix B) predict the steady-state mass of contaminants in the water column and underlying sediments, and don't address 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, evaluating complex water bodies or shorter term loading scenarios might be improved by using a dynamic modeling framework [e.g., Exposure Analysis Modeling System (EXAMS), or Water Quality Analysis Simulation Program (WASP), both of which can be downloaded from the EPA Center for Exposure Assessment Modeling]. Although typically more resource intensive, such analysis may be able to refine modeling of contaminant loading to a water body. Also, the computations may better represent the exposure scenario you are evaluating.

For example, EXAMS allows performing computations 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 evaluating exposure is of greatest interest.

The following are some considerations regarding the selection and use of a dynamic modeling framework or simulation model to evaluate water bodies:

- Will a complex surface water modeling effort provide enhanced results over the use of the more simplistic steady-state equations presented in Appendix B?
- Are the resources needed to conduct, as well as review, a more complex modeling effort justified compared to the more refined results?
- 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?

As mentioned previously in Chapter 2 (Section 2.3.5.3 - “Mercury”), the SERAFM model offers a dynamic modeling framework for mercury that enables the user to model specific water body mercury transformation processes in lieu of applying default speciation assumptions.

5.7.1 Total COPC Load to the Water Body (L_T)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-28 to calculate the total COPC load to a water body (L_T). This equation is described in detail in Appendix B, Table B-4-7.

Recommended Equation for Calculating:
Total COPC Load to the Water Body (L_T)

$$L_T = L_{DEP} + L_{dif} + L_{RI} + L_R + L_E + L_I \qquad \text{Equation 5-28}$$

where

L_T = Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
L_{DEP} = Total (wet and dry) particle phase and vapor phase COPC direct deposition load to water body (g/yr)
L_{dif} = Vapor phase COPC 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 degradation products, we generally recommend a default value for this variable of zero. However, if a permitting authority determines that site-specific conditions indicate calculating internal transfer may need to be considered, we recommend following the methods described in U.S. EPA (1998c). The remaining variables (L_{DEP}, L_{dif}, L_{RI}, L_R, and L_E) are discussed in the following subsections.

5.7.1.1 Total (Wet and Dry) Particle Phase and Vapor Phase COPC Direct Deposition Load to Water Body (L_{DEP})

As in U.S. EPA (1994r) and NC DEHNR (1997), with the inclusion of the direct deposition of total vapor, we recommend using Equation 5-29 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}). The equation is described in detail in Appendix B, Table B-4-8.

Recommended Equation for Calculating:
Total Particle Phase and Vapor Phase Direct Deposition Load to Water Body (L_{DEP})

$$L_{DEP} = Q \cdot [\, F_v \cdot Dytwv + (1 - F_v) \cdot Dytwp \,] \cdot A_W \qquad \text{Equation 5-29}$$

where

L_{DEP} = Total (wet and dry) particle phase and vapor phase COPC direct deposition load to water body (g/yr)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dytwv$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
$Dytwp$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase (s/m^2-yr)
A_W = Water body surface area (m^2)

Appendix A-2 describes how we recommend determining the COPC-specific parameter F_v. Chapter 3 describes generating the modeled air parameters, *Dytwv* and *Dytwp*. Methods for determining the water body surface area, A_w, are described in Chapter 4 and Appendix B.

5.7.1.2 Vapor Phase COPC Diffusion Load to Water Body (L_{dif})

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-30 to calculate L_{dif}. The equation is described in detail in Appendix B, Table B-4-12.

Recommended Equation for Calculating:
Vapor Phase COPC Diffusion Load to Water Body (L_{Dif})

$$L_{dif} = \frac{K_v \cdot Q \cdot F_v \cdot Cywv \cdot A_W \cdot 1 \times 10^{-6}}{\frac{H}{R \cdot T_{wk}}} \qquad \text{Equation 5-30}$$

where

L_{dif} = Vapor phase COPC diffusion load to water body (g/yr)
K_v = Overall COPC transfer rate coefficient (m/yr)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Cywv$ = Unitized yearly (water body or watershed) average air concentration from vapor phase (µg-s/g-m^3)
A_W = Water body surface area (m^2)
10^{-6} = Units conversion factor (g/µg)
H = Henry's Law constant (atm-m^3/mol)
R = Universal gas constant (atm-m^3/mol-K)
T_{wk} = Water body temperature (K)

Calculating the overall COPC transfer rate coefficient (K_v) is described in Section 5.7.4.4, as well as in Appendix B, Table B-4-19. Chapters 2 and 3 explain how we recommend quantifying the COPC emission rate (Q). Appendix A-2 describes how we recommend determining the COPC-specific parameters F_v, H, and R. Chapter 3 describes generating the modeled air parameter, *Cywv*. Methods for determining the water body surface area, A_w, are described in Chapter 4 and Appendix B. Consistent with U.S. EPA (1994r) and U.S. EPA (1998c), we recommend a default water body temperature (T_{wk}) of 298 K (or 25°C).

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

In some watershed soils, a portion 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. As in U.S. EPA (1994r) and NC DEHNR (1997), with the inclusion of total (wet and dry) vapor phase deposition, we recommend using Equation 5-31 to calculate impervious runoff load to a water body (L_{RI}). The equation is also presented in Appendix B, Table B-4-9.

Recommended Equation for Calculating:
Runoff Load from Impervious Surfaces (L_{RI})

$$L_{RI} = Q \cdot [\, F_v \cdot Dytwv + (1.0 - F_v) \cdot Dytwp \,] \cdot A_I \qquad \text{Equation 5-31}$$

where

L_{RI} = Runoff load from impervious surfaces (g/yr)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dytwv$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
$Dytwp$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase (s/m^2-yr)
A_I = Impervious watershed area receiving COPC deposition (m^2)

Chapters 2 and 3 explain how we recommend quantifying the COPC emission rate (Q). Appendix A-2 describes how we recommend determining the COPC-specific parameter F_v. Chapter 3 describes a method for generating the modeled air parameters, $Dytwv$ and $Dytwp$. Impervious watershed area receiving COPC 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. Our recommended method for determining A_I is described in Chapter 4 and Appendix B.

5.7.1.4 Runoff Load from Pervious Surfaces (L_R)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-32 to calculate the runoff dissolved COPC load to the water body from pervious soil surfaces in the watershed (L_R). The equation is also presented in Appendix B, Table B-4-10.

Recommended Equation for Calculating:
Runoff Load from Pervious Surfaces (L_R)

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

Equation 5-32

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 COPC deposition (m^2)
A_I = Impervious watershed area receiving COPC deposition (m^2)
Cs = Average soil concentration over exposure duration (in watershed soils) (mg COPC/kg soil)
BD = Soil bulk density (g soil/cm^3 soil) = 1.5 g/cm^3
θ_{sw} = Soil volumetric water content (ml water/cm^3 soil) = 0.2 ml/cm^3
Kd_s = Soil-water partition coefficient (cm^3 water/g soil)
0.01 = Units conversion factor (kg-cm^2/mg-m^2)

Appendix B describes how we recommend determining the site-specific parameters RO, A_L, A_I, BD, and θ_{sw}. We also address soil bulk density (BD) in Section 5.2.4.2. We also address soil water content (θ_{sw}) in Section 5.2.4.4. Our recommended method for calculating the COPC concentration in watershed soils (Cs) is discussed in Section 5.2.1 and Appendix B, Table B-4-1. Appendix A-2 describes how we recommend calculating the COPC-specific soil/water partition coefficient (Kd_s).

5.7.1.5 Soil Erosion Load (L_E)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-33 to calculate soil erosion load (L_E). The equation is also presented in Appendix B, Table B-4-11.

Recommended Equation for Calculating:
Soil Erosion Load (L_E)

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001 \qquad \text{Equation 5-33}$$

where

L_E = Soil erosion load (g/yr)
X_e = Unit soil loss (kg/m^2-yr)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I = Impervious watershed area receiving COPC deposition (m^2)
SD = Sediment delivery ratio (watershed) (unitless)
ER = Soil enrichment ratio (unitless)
Cs = Average soil concentration over exposure duration (in watershed soils) (mg COPC/kg soil)
BD = Soil bulk density (g soil/cm^3 soil) = 1.5 g/cm^3
2_{sw} = Soil volumetric water content (ml water/cm^3 soil) = 0.2 ml/cm^3
Kd_s = Soil-water partition coefficient (ml water/g soil)
0.001 = Units conversion factor (k-cm^2/mg-m^2)

Section 5.7.2 describes unit soil loss (X_e). Chapter 4 and Appendix B describe how we recommend determining the site-specific parameters A_L and A_I. We generally recommend calculating the watershed sediment delivery ratio (SD) as described in Section 5.7.3 and in Appendix B, Table B-4-14. COPC concentration in soils (Cs) is described in Section 5.2.1, and Appendix B, Table B-4-1. Soil bulk density (BD) is described in Section 5.2.4.2. Soil water content (2_{sw}) is described in Section 5.2.4.4. Appendix B, Table B-4-11 describes how we recommend determining the COPC-specific soil enrichment ration (ER).

5.7.2 Universal Soil Loss Equation - USLE

As in U.S. EPA (1994g and 1994r), we generally recommend using the universal soil loss equation (USLE), Equation 5-33A, to calculate the unit soil loss (X_e) specific to each watershed. This equation is further described in Appendix B, Table B-4-13. Appendix B also describes how we suggest determining the site- and watershed-specific values for each of the variables associated with Equation 5-33A.

Recommended Equation for Calculating:
Unit Soil Loss (X_e)

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047} \qquad \text{Equation 5-33A}$$

where

X_e = Unit soil loss (kg/m^2-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 (m^2/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). 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) and U.S. EPA guidance (U.S. EPA 1985b).
Refer to Appendix B, Table B-4-13 for additional discussion of the USLE.

5.7.3 Sediment Delivery Ratio (*SD*)

We recommend using Equation 5-34 to calculate the sediment delivery ratio (*SD*). The use of this equation is further described in Appendix B, Table B-4-14.

Recommended Equation for Calculating:
Sediment Delivery Ratio *(SD)*

$$SD = a \cdot (A_L)^{-b} \qquad \text{Equation 5-34}$$

where

SD = Sediment delivery ratio (watershed) (unitless)
a = Empirical intercept coefficient (unitless)
b = Empirical slope coefficient (unitless)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)

The sediment delivery ratio (*SD*) for a large land area (i.e. a watershed or part of a watershed) can be calculated, on the basis of the area of the watershed, by using an approach proposed by Vanoni (1975). Accordingly, U.S. EPA (1998c) recommended using Equation 5-34 to calculate the *SD*.

According to Vanoni (1975), sediment delivery ratios vary approximately with the -0.125 power of the drainage area. Therefore, the empirical slope coefficient is assumed to be equal to 0.125. An inspection of the data presented by Vanoni (1975) indicates that the empirical intercept coefficient varies with the size of the watershed, as illustrated in Appendix B, Table B-4-14.

A_L is the total watershed surface area evaluated that is affected by deposition and drains to the body of water (see Chapter 4). In assigning values to the watershed surface area affected by deposition, we generally consider the following relevant:

- the distance from the emission source,
- the location of the area affected by deposition fallout with respect to the point at which drinking water is extracted or fishing occurs
- the watershed hydrology.

5.7.4 Total Water Body COPC Concentration (C_{wtot})

We recommend using Equation 5-35 to calculate the total water body COPC concentration (C_{wtot}). C_{wtot} includes both the water column and the bed sediment. The equation is also presented in Appendix B, Table B-4-15.

Recommended Equation for Calculating: Total Water Body COPC Concentration (C_{wtot})

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} + k_{wt} \cdot A_W \cdot (d_{wc} + d_{bs})} \qquad \text{Equation 5-35}$$

where

C_{wtot} = Total water body COPC concentration (including water column and bed sediment) (g COPC/m^3 water body)
L_T = Total COPC 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 COPC concentration in the water column (unitless)
k_{wt} = Overall total water body COPC dissipation rate constant (yr^{-1})
A_W = Water body surface area (m^2)
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

The total COPC load to the water body (L_T)—including deposition, runoff, and erosion—is described in Section 5.7.1 and Appendix B, Table B-4-7. Average volumetric flow rate through the water body (Vf_x) and water body surface area (A_w) are discussed in Appendix B. Section 5.7.4.1 discusses the fraction of total COPC concentration in the water column (f_{wc}). Section 5.7.4.2 discusses the COPC dissipation rate constant (k_{wt}). Chapter 4 discusses the water body-specific d_{wc}. We discuss the depth of the upper benthic sediment layer (d_{bs}) below.

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, U.S. EPA (1998c) recommended values ranging from 0.01 to 0.05. As in U.S. EPA (1994r), we recommend a default value of 0.03, which represents the midpoint of the specified range. Issues related to the remaining parameters are summarized in the following subsections.

Recommended Default Value for: Depth of Upper Benthic Sediment Layer (d_{bs})

0.03 m

5.7.4.1 Fraction of Total Water Body COPC Concentration in the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

We generally recommend using Equation 5-36A to calculate the fraction of total water body COPC concentration in the water column (f_{wc}), and Equation 5-36B to calculate the total water body contaminant concentration in benthic sediment (f_{bs}). The equations are also presented in Appendix B, Table B-4-16.

Recommended Equation for Calculating:
Fraction of Total Water Body COPC Concentration in
the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

$$f_{wc} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z}{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z + (\theta_{bs} + Kd_{bs} \cdot C_{BS}) \cdot d_{bs} / d_z} \qquad \text{Equation 5-36A}$$

$$f_{bs} = 1 - f_{wc} \qquad \text{Equation 5-36B}$$

where

f_{wc} = Fraction of total water body COPC concentration in the water column (unitless)
f_{bs} = Fraction of total water body COPC 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/cm^3 [equivalent to kg/L])
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

The COPC-specific partition coefficient (Kd_{sw}) describes the partitioning of a contaminant between sorbing material, such as soil, surface water, suspended solids, and bed sediments (see Appendix A-2). Total suspended solids (TSS), total water body depth (d_z), bed sediment porosity (θ_{bs}) and bed sediment concentration (C_{BS}) are addressed below. Bed sediment and sediment pore water partition coefficient

(Kd_{bs}) is discussed in Appendix A-2. Depth of water column (d_{wc}) and depth of upper benthic layer (d_{bs}) are discussed in Section 5.7.4.

U.S. EPA (1998c) and NC DEHNR (1997) recommended using Equations 5-36A and 5-36B to calculate f_{wc} and f_{bs}. NC DEHNR (1997) also recommended adding the depth of the water column to the depth of the upper benthic layer ($d_{wc} + d_{bs}$) to calculate the total water body depth (d_z).

NC DEHNR (1997) recommended a default total suspended solids (*TSS*) concentration of 10 mg/L, which was adapted from U.S. EPA (1993e). However, due to variability in water body specific values for this variable, we recommend using water body-specific measured *TSS* values representative of long-term average annual values. Average annual values for *TSS* are generally expected to be in the range of 2 to 300 mg/L. Additional information on anticipated *TSS* values is available in U.S. EPA (1998c).

If measured data are not available, or of unacceptable quality, it's possible to calculate a *TSS* value for non-flowing water bodies using Equation 5-36C.

$$TSS = \frac{X_e \cdot (A_L - A_I) \cdot SD \cdot 1x10^3}{Vf_x + D_{ss} \cdot A_W} \qquad \text{Equation 5-36C}$$

where

TSS = Total suspended solids concentration (mg/L)
X_e = Unit soil loss (kg/m^2-yr)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I = Impervious watershed area receiving COPC deposition (m^2)
SD = Sediment delivery ratio (watershed) (unitless)
Vf_x = Average volumetric flow rate through water body (value should be 0 for quiescent lakes or ponds) (m^3/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 (m^2)

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, it's possible to evaluate the appropriateness of watershed-specific values used in calculating the unit soil loss (X_e), as described in Section 5.7.2 and Appendix B, by comparing the water-body specific measured *TSS* value to the estimated *TSS* value obtained using Equation 5-36C. If the measured and calculated *TSS* values differ significantly, we recommend re-evaluating the parameter values used to calculate X_e. You might also re-evaluate *TSS* and X_e if the calculated *TSS* value is outside of the normal range expected for average annual measured values, as discussed above.

One approach to calculating bed sediment porosity (θ_{bs}) from the bed sediment concentration is by using the following equation (U.S. EPA 1998c):

$$\theta_{bs} = 1 - \frac{C_{BS}}{\rho_s} \qquad \text{Equation 5-37}$$

where

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

We recommend the following default value for bed sediment porosity (θ_{bs}), adapted from NC DEHNR (1997):

Recommended Value for: **Bed Sediment Porosity (θ_{bs})**
$\theta_{bs} = 0.6\ L_{water}/L_{sediment}$ assuming ρ_s = 2.65 kg/L [bed sediment density] and C_{BS}= 1.0 kg/L [bed sediment concentration])

U.S. EPA (1994r) and NC DEHNR (1997) recommended a benthic solids concentration (C_{BS}) ranging from 0.5 to 1.5 kg/L, which was adapted from U.S. EPA (1993e). We recommend the following default value for bed sediment concentration (C_{BS}):

Recommended Default Value for: **Bed Sediment Concentration (C_{BS})**
1.0 kg/L

5.7.4.2 Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-38 to calculate the overall dissipation rate of COPCs in surface water, resulting from volatilization and benthic burial. The equation is also presented in Appendix B, Table B-4-17.

Recommended Equation for Calculating:
Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b \qquad \text{Equation 5-38}$$

where

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

The variables f_{wc} and f_{bs} are discussed in Section 5.7.4.1. The water column volatilization rate constant (k_v) is discussed in Section 5.7.4.3. The benthic burial rate constant (k_b)is discussed in Section 5.7.4.7.

5.7.4.3 Water Column Volatilization Rate Constant (k_v)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-39 to calculate k_v. The equation is also presented in Appendix B, Table B-4-18.

Recommended Equation for Calculating: Water Column Volatilization Rate Constant (k_v)

$$k_v = \frac{K_v}{d_z \cdot (1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6})} \qquad \text{Equation 5-39}$$

where

k_v = Water column volatilization rate constant (yr^{-1})
K_v = Overall COPC 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)

The overall transfer rate coefficient (K_v) is discussed in Section 5.7.4.4. 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 5.7.4.1. Kd_{sw} is also discussed in Appendix A-2.

5.7.4.4 Overall COPC 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.

As in U.S. EPA (1993f; 1993e; 1998c), and NC DEHNR (1997), we recommend using Equation 5-40 to calculate K_v. The equation is also presented in Appendix B, Table B-4-19.

Recommended Equation for Calculating:
Overall COPC Transfer Rate Coefficient (K_v)

$$K_v = \left(K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right)^{-1} \cdot \theta^{T_{wk} - 293} \qquad \text{Equation 5-40}$$

where

K_v = Overall COPC 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-m^3/mol)
R = Universal gas constant (atm-m^3/mol-K)
T_{wk} = Water body temperature (K)
θ = Temperature correction factor (unitless)

The liquid and gas phase transfer coefficients, K_L and K_G, respectively, vary with the type of water body. We discuss the liquid phase transfer coefficient (K_L) in Section 5.7.4.5, and the gas phase transfer coefficient (K_G) in Section 5.7.4.6.

Henry's Law constants generally increase with increasing vapor pressure of a COPC and generally decrease with increasing solubility of a COPC. Henry's Law constants are COPC-specific and we offer recommended default values in the HHRAP companion database. The universal ideal gas constant, R, is 8.205×10^{-5} atm-m^3/mol-K, at 20°C. The temperature correction factor (θ), which is equal to 1.026, adjusts for the actual water temperature. Equation 5-40 assumes that volatilization occurs much less readily in lakes and reservoirs than in moving water bodies.

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.

5.7.4.5 Liquid Phase Transfer Coefficient (K_L)

We generally recommend using Equations 5-41A and 5-41B to calculate liquid phase transfer coefficient. (K_L). The use of these equations is further described in Appendix B, Table B-4-20.

Recommended Equation for Calculating:
Liquid Phase Transfer Coefficient (K_L)

For flowing streams or rivers:

$$K_L = \sqrt{\frac{(1 \times 10^{-4}) \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7 \qquad \text{Equation 5-41A}$$

For quiescent lakes or ponds:

$$K_L = (C_d^{0.5} \cdot W) \cdot (\frac{\rho_a}{\rho_w})^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot (\frac{\mu_w}{\rho_w \cdot D_w})^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 5-41B}$$

where

K_L = Liquid phase transfer coefficient (m/yr)
D_w = Diffusivity of COPC 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)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using the following default values:

- a diffusivity of chemical in water ranging (D_w) from 1.0×10^{-5} to 8.5×10^{-2} cm^2/s,
- a drag coefficient (C_d) of 0.0011 which was adapted from U.S. EPA (1998c),
- a density of air (ρ_a) of 0.0012 g/cm^3 at standard conditions (temperature = 20°C or 293 K, pressure = 1 atm or 760 millimeters of mercury) (Weast 1986),
- a density of water (ρ_w) of 1 g/cm^3 (Weast 1986),
- a von Karman's constant (k) of 0.4,
- a dimensionless viscous sublayer thickness (λ_z) of 4,
- a viscosity of water (μ_w) of a 0.0169 g/cm-s corresponding to water temperature (Weast 1986).

The values above are further discussed in Appendix A-2. Chapter 4 discusses the current velocity (u). Chapter 3 describes methods for determining the average annual wind speed (W). Section 5.7.4.1 discusses the total water body depth (d_z) for liquid phase transfer coefficients.

For a flowing stream or river, the transfer coefficients are controlled by flow-induced turbulence. For these systems, we recommend calculating K_L using Equation 5-41A, which is the O'Connor and Dobbins (1958) formula, as presented in U.S. EPA (1998c).

For a stagnant system (quiescent lake or pond), the transfer coefficient is controlled by wind-induced turbulence. For quiescent lakes or ponds, we recommend calculating K_L using Equation 5-41B (O'Connor 1983; U.S. EPA 1998c).

5.7.4.6 Gas Phase Transfer Coefficient (K_G)

We generally recommend using Equations 5-42A and 5-42B to calculate gas phase transfer coefficient (K_G). The equation is also discussed in Appendix B, Table B-4-21.

Recommended Equation for Calculating:
Gas Phase Transfer Coefficient (K_G)

For flowing streams or rivers:

$$K_G = 36500 \text{ m/yr} \qquad \text{Equation 5-42A}$$

For quiescent lakes or ponds:

$$K_G = (C_d^{0.5} \cdot W) \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_a}{\rho_a \cdot D_a}\right)^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 5-42B}$$

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/cm^3)
D_a = Diffusivity of COPC in air (cm^2/s)
3.1536×10^7 = Units conversion factor (s/yr)

The following parameters, including default values, are discussed in Section 5.7.4.5, and in Appendix A-2: C_d, k, λ_z, and ρ_a. Chapter 3 describes methods for determining the average annual wind speed (W). As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using a value of 1.81 x 10^{-4} g/cm-s for the viscosity of air corresponding to air temperature (μ_a). Appendix A-2 discusses the COPC-specific parameter D_a.

U.S. EPA (1998c) indicated that the rate of transfer of a COPC from the gas phase for a flowing stream or river is assumed to be constant, in accordance with O'Connor and Dobbins (1958) (Equation 5-42A).

For a stagnant system (quiescent lake or pond), the transfer coefficients are controlled by wind-induced turbulence. For quiescent lakes or ponds, we recommend calculating the gas phase transfer coefficient using the equation presented in O'Connor (1983) (Equation 5-42B).

5.7.4.7 Benthic Burial Rate Constant (k_b)

We generally recommend using Equation 5-43 to calculate benthic burial rate (k_b). The equation is also discussed in Appendix B, Table B-4-22.

Recommended Equation for Calculating:
Benthic Burial Rate Constant (k_b)

$$k_b = \left(\frac{X_e \cdot A_L \cdot SD \cdot 1 \times 10^3 - Vf_x \cdot TSS}{A_W \cdot TSS} \right) \cdot \left(\frac{TSS \cdot 1 \times 10^{-6}}{C_{BS} \cdot d_{bs}} \right) \qquad \text{Equation 5-43}$$

where

k_b = Benthic burial rate constant (yr^{-1})
X_e = Unit soil loss (kg/m^2-yr)
A_L = Total watershed area (evaluated) receiving deposition (m^2)
SD = Sediment delivery ratio (watershed) (unitless)
Vf_x = Average volumetric flow rate through water body (m^3/yr)
TSS = Total suspended solids concentration (mg/L)
A_W = Water body surface area (m^2)
C_{BS} = Bed sediment concentration (g/cm^3)
d_{bs} = Depth of upper benthic sediment layer (m)
1 x 10^{-6} = Units conversion factor (kg/mg)
1 x 10^3 = Units conversion factor (g/kg)

Section 5.7.2 discusses the unit soil loss (X_e). Section 5.7.3 discusses watershed area evaluated receiving COPC deposition (A_L) and sediment delivery ratio (SD). Average volumetric flow rate through the water body (Vf_x) and water body surface area (A_w) are discussed in Appendix B. A_w is also discussed in Appendix A-2. Section 5.7.4.1 discusses total suspended solids concentration (TSS) and bed sediment concentration (C_{BS}). Section 5.7.4 discusses the depth of the upper benthic sediment layer (d_{bs}).

It's possible to express the benthic burial rate constant (k_b), which is calculated in Equation 5-43, in terms of the rate of burial (Wb):

$$Wb = k_b \cdot d_{bs} \qquad \text{Equation 5-44}$$

where

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

According to U.S. EPA (1994r) and NC DEHNR (1997), COPC loss from the water column resulting from burial in benthic sediment can be calculated using Equation 5-43.

We expect k_b values to range from 0 to 1.0: Low k_b values for water bodies with limited or no sedimentation (rivers and fast flowing streams), and k_b values closer to 1.0 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 5-44; with the depth of upper benthic sediment layer held constant. If you calculate a negative k_b value (water bodies with high average annual volumetric flow rates in comparison to watershed area evaluated), we recommend using a k_b value of 0 in calculating the total water body COPC concentration (C_{wtot}) in Equation 5-35. If the calculated k_b value exceeds 1.0, we recommend re-evaluating the parameter values used in calculating X_e. Our experience has shown that the value calculated for X_e is the most likely reason for estimating a large and potentially unrealistic benthic burial rate. Information about determining site-specific values and variables for calculating Xe are in the references cited in Section 5.7.2.

5.7.4.8 Total COPC Concentration in Water Column (C_{wctot})

As in U.S. EPA (1994r) and NC DEHNR (1997), we generally recommend using Equation 5-45 to calculate total COPC concentration in water column (C_{wctot}). The equation is also discussed in Appendix B, Table B-4-23.

Recommended Equation for Calculating:
Total COPC Concentration in Water Column (C_{wctot})

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}} \qquad \text{Equation 5-45}$$

where

C_{wctot} = Total COPC concentration in water column (mg COPC/L water column)
f_{wc} = Fraction of total water body COPC concentration in the water column (unitless)
C_{wtot} = Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

We discussed the fraction of total water body COPC concentration in the water column (f_{wc}) in Section 5.7.4.1. We discussed the total COPC Concentration in the water column (C_{wctot}), as well as depth of the water column (d_{wc}) and benthic sediment layer (d_{bs}) in Section 5.7.4.

5.7.4.9 Dissolved Phase Water Concentration (C_{dw})

We recommend using Equation 5-46 to calculate the concentration of COPC dissolved in the water column (C_{dw}). The equation is discussed in detail in Appendix B, Table B-4-24.

Recommended Equation for Calculating:
Dissolved Phase Water Concentration (C_{dw})

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}} \qquad \text{Equation 5-46}$$

where

C_{dw} = Dissolved phase water concentration (mg COPC/L water)
C_{wctot} = Total COPC concentration in water column (mg COPC/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)

We discussed C_{wctot} in Section 5.7.4.8. We discussed Kd_{sw} and TSS in Section 5.7.4.1.

Using Equation 5-46 to calculate the concentration of COPC dissolved in the water column is consistent with recommendations in U.S. EPA (1994r) and NC DEHNR (1997).

5.7.4.10 COPC Concentration Sorbed to Bed Sediment (C_{sb})

We recommend using Equation 5-47 to calculate COPC concentration sorbed to bed sediment (C_{sb}). The equation is also presented in Appendix B, Table B-4-25.

Recommended Equation for Calculating:
COPC Concentration Sorbed to Bed Sediment (C_{sb})

$$C_{sb} = f_{bs} \cdot C_{wtot} \cdot \left(\frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot C_{BS}} \right) \cdot \left(\frac{d_{wc} + d_{bs}}{d_{bs}} \right) \qquad \text{Equation 5-47}$$

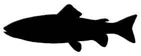
where

C_{sb} = COPC concentration sorbed to bed sediment (mg COPC/kg sediment)
f_{bs} = Fraction of total water body COPC concentration in benthic sediment (unitless)
C_{wtot} = Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
Kd_{bs} = Bed sediment/sediment pore water partition coefficient (L COPC/kg water body)
2_{bs} = Bed sediment porosity ($L_{pore\ water}/L_{sediment}$)
C_{BS} = Bed sediment concentration (g/cm^3)
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

We discussed f_{bs}, 2_{bs}, and C_{BS} in Section 5.7.4.1. We discussed C_{wtot}, d_{wc}, and d_{bs} in Section 5.7.4. We discuss Kd_{bs} in Appendix A-2.

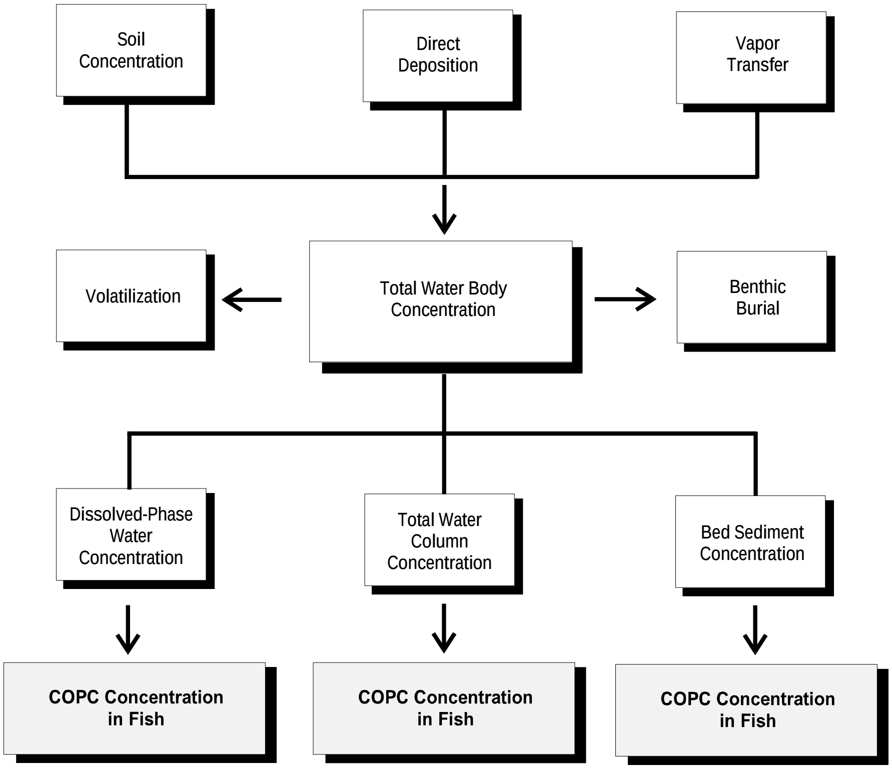
As in U.S. EPA (1994r) and NC DEHNR (1997), we continue to recommend using Equation 5-47 to calculate the COPC concentration sorbed to bed sediment.

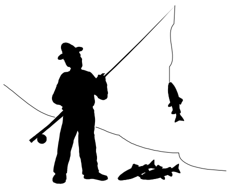
5.7.5 Concentration of COPC in Fish (C_{fish})



We generally recommend calculating the COPC concentration in fish using either a COPC-specific bioconcentration factor (*BCF*), a COPC-specific bioaccumulation factor (*BAF*), or a COPC-specific biota-sediment accumulation factor (*BSAF*). Under this approach you would use *BCFs* for COPCs with a $log\ K_{ow}$ less than 4.0. We assume that COPCs with a $log\ K_{ow}$ greater than 4.0 (except for extremely hydrophobic compounds such as dioxins, furans, and PCBs), have a high tendency to bioaccumulate. As a result, *BAF*s are used. While we assume that extremely hydrophobic COPCs like dioxins, furans, and PCBs also have a high tendency to bioaccumulate, they are expected to be sorbed to the bed sediments more than associated with the water phase. Therefore, we recommend using *BSAF*s to calculate concentrations of dioxins, furans, and PCBs in fish. Appendix A-2 provides a detailed discussion on the sources of the COPC-specific *BCF*, *BAF*, and *BSAF* values, and the method we used to derive them.

FIGURE 5-8
COPC CONCENTRATION IN FISH





BCF and *BAF* values are generally based on dissolved water concentrations. Therefore, when you use *BCF* or *BAF* values, it's appropriate to calculate the COPC concentration in fish using dissolved water concentrations. *BSAF* values are based on benthic sediment concentrations. Therefore, when using *BSAF* values, we recommend calculating COPC concentrations in fish using benthic sediment concentrations. We describe our recommended equations for calculating fish concentrations in the subsequent subsections.

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

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-48 to calculate fish concentration from *BCF*s using dissolved phase water concentration. Using this equation is further described in Appendix B, Table B-4-26.

Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Bioconcentration Factors (BCF_{fish})
Using Dissolved Phase Water Concentration

$$C_{fish} = C_{dw} \cdot BCF_{fish} \qquad \text{Equation 5-48}$$

where

C_{fish} = Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{dw} = Dissolved phase water concentration (mg COPC/L)
BCF_{fish} = Bioconcentration factor for COPC in fish (L/kg)

We discussed C_{dw} in Section 5.7.4.9. COPC-specific BCF_{fish} values are presented in the HHRAP companion database.

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

We recommend using Equation 5-49 to calculate fish concentration from *BAF*s using dissolved phase water concentration. The equation is also presented in Appendix B, Table B-4-27.

Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Bioaccumulation Factors (BAF_{fish})
Using Dissolved Phase Water Concentration

$$C_{fish} = C_{dw} \cdot BAF_{fish} \qquad \text{Equation 5-49}$$

where

C_{fish} = Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{dw} = Dissolved phase water concentration (mg COPC/L)
BAF_{fish} = Bioaccumulation factor for COPC in fish (L/kg FW tissue)

We discussed C_{dw} in Section 5.7.4.9. COPC-specific bioaccumulation factor (BAF_{fish}) values are presented in the HHRAP companion database.

5.7.5.3 Fish Concentration (C_{fish}) from Biota-To-Sediment Accumulation Factors Using COPC Sorbed to Bed Sediment

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-50 to calculate fish concentration from *BSAF*s using COPC concentrations sorbed to bed sediment. We recommend using *BSAFs* for very hydrophobic compounds such as dioxins, furans, and PCBs. The equation is also presented in Appendix B, Table B-4-28.

Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Biota-To-Sediment Accumulation Factors *(BSAF)*
Using COPC Sorbed to Bed Sediment

$$C_{fish} = \frac{C_{sb} \cdot f_{lipid} \cdot BSAF}{OC_{sed}} \qquad \text{Equation 5-50}$$

where

C_{fish} = Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{sb} = Concentration of COPC sorbed to bed sediment (mg COPC/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)

We discussed C_{sb} in Section 5.7.4.10. We discuss f_{lipid} and OC_{sed} below. Our recommended default values for f_{lipid} and OC_{sed} are given in Appendix B, Table B-4-28. We offer biota-to-sediment accumulation factors (*BSAF*), which are applied only to dioxins, furans, and PCBs, in the HHRAP companion database.

Values recommended by U.S. EPA (1998c) range from 0.03 to 0.05 for $_{OCSED}$. These values are based on an assumption of a surface soil organic carbon (OC) content of 0.01. U.S. EPA (1998c) 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 consumed. As stated in Appendix B, Table B-4-28, we recommend a default range of 0.03 to 0.07 specific to warm or cold water fish species. U.S. EPA (2000c) provides information supporting a value of 0.03 (3 percent lipid content of the edible portion). U.S. EPA (1993e) recommended a default value of 0.04 for $_{OCSED}$, which is the midpoint of the specified range. U.S. EPA (1993f; 1993e) recommended using 0.07, which was originally cited in Cook et al. (1991).

5.8 USING SITE-SPECIFIC vs. DEFAULT PARAMETER VALUES

As initially discussed in Chapter 1, many of the parameter values we recommend in the HHRAP are not site-specific. After completing a risk assessment using HHRAP default values, you might choose to investigate using site-specific parameter values. More site-specific values might provide a more representative estimate of site-specific risk. If you use parameter values other than those specified in the HHRAP, we recommend that you clearly described them in the risk assessment report. We also recommend that you discuss them with the permitting authority prior to using them. We recommend that requests to change default parameter values include the following information, as appropriate:

1. An explanation of why using a more site-specific parameter value is warranted (e.g., the default parameter is based on data or studies at sites in the northwestern U.S., but the facility is located in the southeast);
2. The technical basis of the site-specific parameter value, including readable copies of any relevant technical literature or studies;

3. A comparison of the weight-of-evidence between the competing studies (e.g., the site-specific parameter value is based on a study that is more representative of site conditions, a specific exposure setting being evaluated, or a more scientifically valid study than the default parameter, the site-specific parameter is based on the analysis of 15 samples as opposed to 5 for the default parameter, or the site-specific study used more stringent quality control/quality assurance procedures than the study upon which the default parameter is based);

4. A description of other risk assessments or projects that used the site-specific parameter value, and how such risk assessments or projects are similar to the current risk assessment.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

C Identification of site-specific or alternate default media equations and/or inputs; including justification and full referencing

C Media concentration calculations