TERRESTRIAL FOOD WEB MODULE: BACKGROUND AND IMPLEMENTATION FOR THE MULTIMEDIA, MULTIPATHWAY, AND MULTIRECEPTOR RISK ASSESSMENT (3MRA) FOR HWIR99

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DISCLAIMER

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1.1 Overview

The Terrestrial Food Web module (TerFW) calculates chemical concentrations in soil, terrestrial plants, and various prey items consumed by ecological receptors, including earthworms, other soil invertebrates, and vertebrates. These concentrations are used as input to the Ecological Exposure (EcoEx) module to determine the applied dose to each receptor of interest (e.g., deer, kestrel). The module is designed to calculate spatially-averaged soil concentrations in the top layer of soil (i.e., surficial soil) as well as deeper soil horizons (i.e., depth-averaged over approximately 5 cm). The spatial averages are defined by the home ranges and habitats that are delineated within the area of interest (AOI) at each site. Once the average soil concentrations are calculated, these values are multiplied by empirical bioconcentration factors (for animals) and biotransfer factors (for plants) to predict the tissue concentrations for items in the terrestrial food web.

The conceptual approach used in developing the TerFW module was designed to predict a range of concentrations in plants and prey items to which a given receptor may be exposed. For example, the dietary data for a fox assigned to a terrestrial habitat indicates that part of its diet will consist of small mammals (e.g., rabbits, shrews, mice). The spatial linkages between the fox (predator) and various small mammals (prey) are represented in the site layout by allowing the respective home ranges to overlap. However, the proportion of each species consumed by the fox is unknown; the fox may consume any combination of these animals depending on prey availability, dietary preferences, and numerous other factors that affect prey availability. To address this uncertainty, the TerFW estimates the tissue concentrations in each of the species within the fox's home range and reports the minimum and maximum values. These values are used by the EcoEx module to select, at random, an effective tissue concentration in small mammals that represents the full range of concentrations to which the fox may be exposed.

For plants and soil fauna, the TerFW estimates concentrations based on the spatially-averaged soil and air concentrations across each home range. Receptors that ingest plants and soil invertebrates as part of the diet are presumed to forage only within that part of the home range that is contained within the AOI at a given site. Consequently, home range defines the spatial scale for concentrations in soil, plants, and prey (both mobile and relatively immobile) to which a given receptor is exposed.[1]

[1] As noted in the Ecological Exposure module documentation, exposures are prorated depending upon the relationship of the home range to the habitat contained within the area of interest.

As with the Farm Food Chain (FFC) module, the TerFW contains subroutines to estimate contaminant uptake in edible parts of plants for six main categories of vegetation relevant to omnivorous and herbivorous animals: exposed vegetables (e.g., ferns, dicot and monocot shoots, fungi), exposed fruits, forage (e.g., forbs, grasses, shrubs, woody plants), silage (i.e., crops), grains (e.g., nuts and seeds), and root vegetables (e.g., tubers). The modeling construct for estimating concentrations in plants consumed by wildlife is based on recent and on-going research conducted by the U.S. EPA Office of Research and Development and presented in *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (EPA, U.S. EPA, in press). As described in Section 3.0, the subroutine distinguishes among different types of chemicals, using empirically-derived algorithms for some chemicals and biouptake data from field or greenhouse studies for other chemicals. The TerFW module accounts for uptake via root-to-plant translocation, air-to-plant transfer for volatile and semi-volatile chemicals, and particle-bound deposition to edible plant surfaces. Specific differences between the FFC module and the TerFW module in predicting plant concentrations are noted in the methodology section below.

To estimate the concentrations in other categories of terrestrial prey items (e.g., earthworms, small birds), the TerFW relies on soil-to-organism bioconcentration factors (BCFs) identified from empirical studies and/or generated using regression methods developed by the Oak Ridge National Laboratory (see, for example, Sample et al., 1998). A thorough discussion of these data is provided in the data collection documentation for the FFC and TerFW modules.

The concentration inputs required by the TerFW module are provided by the Air module , the Regional Watershed (RW) module, and two source modules: the Wastepile and Land Application Unit. The Air (Ar) module provides air concentrations and deposition rates relevant to plant loadings. The RW module provides surficial and depth-averaged soil concentrations for watersheds within the AOI, and the source modules provide soil concentrations within the drainage sub-basin that includes the source. The average chemical concentration in soil calculated for a given home range may include contributions from regional watersheds as well as from a source-related drainage sub-basin (referred to as the local watershed). These inputs are described in Appendix A and include:

Air Module

- vapor concentration for each home range and habitat within the AOI
- wet vapor deposition rate for each home range and habitat within the AOI
- dry particle deposition rate for each home range and habitat within the AOI
- wet particle deposition rate for each home range and habitat within the AOI

Regional Watershed

- surficial soil concentration for each watershed within the AOI
- depth-averaged soil concentration for each watershed within the AOI

Source Modules

- surficial soil concentration for the each local watershed within the AOI
- depth-averaged soil concentration for each local watershed within the AOI

1.2 Summary of Functionality

The major computational functions performed by the Terrestrial Food Web Module are the following:

- *Time series management*. The TerFW module determines the overall duration of the time period to be simulated (including concentration data from discontinuous time periods), and identifies the individual years within the overall duration that will be simulated.

- *Module loops over the time series, through habitats and home ranges.* The TerFW module has three basic loops: (1) over the time series, (2) over each habitat delineated at the site, and (3) over the four home range areas delineated within each habitat.

- *Calculation of time series soil and plant concentrations, and minimum and maximum concentrations in terrestrial prey types (e.g., small mammals).* This is the fundamental structure of the TerFW module, namely, to develop soil and tissue concentrations for each year of the simulation that reflect the range of potential exposure concentrations. These concentrations are spatially explicit with regard to the home range for each ecological receptor.

The major steps performed by the Terrestrial Food Web module that are required to predict concentrations in soil (surficial and depth-averaged), plants, and other prey types may be summarized as follows:

- Select terrestrial habitat of interest (i.e., cropland, residential area, grassland, forest, shrub/scrub).

- Select home range within habitat (i.e., one of four home range areas).

- Calculate average soil concentration within home range for surficial soil and depth-averaged soil.

- Calculate concentration for all categories of terrestrial plants within home range.

- Calculate tissue concentration in soil fauna within home range (i.e., earthworms and other soil invertebrates).

- Calculate tissue concentrations in receptors assigned to home range (e.g., small mammals, omnivores).

- Loop through all home ranges within habitat of interest and repeat calculations of soil and tissue concentrations.

- Report minimum and maximum values for tissue concentrations in prey types other than terrestrial plants and soil fauna.

The calculation of time series concentrations is described in detail in Section 3.0.

2.0 Assumptions and Limitations

The contaminant concentration calculations used in the Terrestrial Food Web module reflect a number of assumptions and/or limitations, which are listed below.

Assumptions

- *Study area is bounded at 2 km.* EPA assumed that significant exposures to source-related contaminants do not occur for ecological receptors that are beyond 2 km of the source. Consequently, tissue concentrations in food items located outside of the study (measured from the edge of the source to a point 2 km away) are presumed to be zero.

- *Uptake and accumulation of chemicals within categories of plants (e.g., exposed vegetables) is assumed to be similar.* The algorithms used to estimate biotransfer factors do not distinguish physiological differences across various kinds of plants. For example, the category "forage" includes forbs, grasses, fungi, shrubs, trees, and unclassified plants. Therefore, in estimating biotransfer factors for this category, it is implicitly assumed that the physiological differences in different plant species do not significantly affect chemical loadings in plant tissues. The use of empirical data on selected plant species (typically crops) also assumes similar mechanisms of uptake and accumulation.

- *No less than 10 percent of the diet is attributed to the study area.* In many instances, the home range for a given receptor exceeds the size of the habitat. In general we assumed that the percent of the home range that "fits" into the habitat is a suitable surrogate with which to scale exposure and predict tissue concentration. However, the purpose of this analysis is to determine acceptable waste concentrations assuming that the study area (e.g., forests) would be used as habitat by wildlife. Therefore, we assumed that no less than 10 percent of the diet originated from the study area, even if the fraction of the home range inside the habitat fell below 10 percent.

- *A reasonable averaging depth for soil concentrations is 5 cm.* In view of the multiple purposes of this soil concentration (e.g., evaluate risks to soil fauna; predict tissue concentrations in prey using soil-based bioaccumulation factors), this was selected as a depth that was ecologically meaningful (with regard to organisms occupying different soil horizons) and consistent with the goals for the ecological risk analysis. However, this assumption carries with it some uncertainty in its application within the exposure and risk modules.

Limitations

- *Concentrations in terrestrial prey are based on soil-to-prey bioaccumulation factors (BAFs).* The most significant limitation in predicting tissue concentrations in terrestrial prey is the paucity of mechanistic models and data sources with which to estimate food web dynamics. For instance, the tissue concentration in small birds is generally predicted using a BAF for soil rather than a biotransfer factor (or BAF) from earthworms and insects into birds. As a result, the TerFW can not rely on the matrix solution technique used by the Aquatic Food Web module to solve for concentrations in various prey items.

- *Some chemicals rely heavily on empirical uptake data.* This limitation is similar to that noted for the Farm Food Chain module. In essence, the paucity of data on uptake and accumulation of constituents in terrestrial food items introduces significant uncertainty into this module. This limitation was explained in some detail in the proposed HWIR95 (RTI, 1995); however, little progress has been made in developing terrestrial data for most chemical classes.

- *Estimates of tissue concentrations reflect a single home range setting.* The TerFW module calculates tissue concentrations in prey items for a single random placement of four home range sizes.[2] As a result, the four home ranges in the site layout may not reflect the spatial variability in soil contamination, particularly for large habitats (i.e., habitats that cover substantially greater areas than most of the home ranges).

- *Resuspension and redeposition on plants are not considered.* Plant concentrations are a function of the deposition on plants of the contaminants that have been emitted from the waste management unit. Plant concentrations do not reflect resuspension and redeposition, which can occur due to tillage, wind erosion, vehicular resuspension, and rainsplash

[2] As described in Section 13 of the data collection documentation on Ecological Receptors and Habitats, each receptor is assigned to one of four discrete home range sizes, depending on the receptor-specific home range size. The four home ranges overlap in a manner that reflects the predator-prey relationships. Examples of this scheme are provided in Section 13.

3.0 Methodology

Once chemical constituents are released from waste management units (WMUs), they can be introduced onto soils and plant surfaces through a variety of mechanisms, including wet and dry deposition (particles and vapors) and overland erosion and runoff. The methodology developed to predict concentrations in plants and prey items in terrestrial habitats uses input from the Regional Watershed module and source modules to predict both surficial and depth-averaged soil concentrations. The TerFW uses outputs from the Air module (Ar) to predict the direct contribution to plant loadings from airborne chemical constituents. The architecture of the TerFW can be thought of in three parts: (1) calculating chemical concentrations in surficial and depth-averaged soils for each home range, (2) calculating chemical concentrations in the tissues of terrestrial prey found in each home range, and (3) calculating chemical concentrations in plants presumed to be in each home range. Each of these components is discussed in detail below.

3.1 Calculating Chemical Concentrations in Soil

The TerFW calculates soil concentrations for surficial soils and depth-averaged soils for each home range. Because the difference between surficial and depth-averaged soils simply depends on the depth of the soil horizon, the same equations are used to calculate the average concentration in each home range. The surficial soil, or top layer (~ 1 cm), is relevant to incidental soil ingestion to foraging animals, thus, the surficial soil concentration is used only by the Ecological Exposure (EcoEx) module to calculate the applied dose to terrestrial receptors. The depth-averaged soils (~ 10 cm) represent deeper soil horizons that are relevant to plant uptake through root-to-plant translocation and to direct exposures of soil fauna (e.g., earthworms). Hence, the depth-averaged soil concentrations are used both internally by the TerFW module to predict plant and prey concentrations, and are passed to the Ecological Risk (EcoRisk) module for use in evaluating risks to the soil community and terrestrial plants (as receptors).

As suggested in Section 1.0, the average soil concentration for each home range is a function of the chemical contribution from both the local and regional watersheds. However, erosion and runoff within the local watershed is only relevant to certain types of waste management units (WMU). For Aerated Tanks (AT) and Surface Impoundments (SI), it is assumed that controls are sufficient to prevent erosion and runoff releases within the drainage subbasin that contains the unit (i.e., there is no erosion or runoff directly from the AT or SI) . Consequently, the contribution to the soil concentration is predicted exclusively with the Regional Watershed module and the contribution from the local watershed is effectively set at

zero. For the Land Application Unit (LAU), Landfill (LF)[3], and Wastepile (WP), the average soil concentration in each home range may include contributions from both the local and regional watersheds, depending upon the placement of the home range with respect to the WMU. We assumed that wildlife could use parts of the LAU and LF as habitat; however, the WP is not considered suitable habitat and was excluded from habitat and home range delineation (i.e., animals can not ingest soil or contaminated prey in the wastepile). Equations 3-1 through 3-3 describe the calculations of watershed-weighted average soil concentrations for each home range (equations apply to both surficial soils and depth-averaged soils).

Soil concentration from regional watershed

$$C_{soil}{}^{WS}{}_{HomeRange\,j} = \sum \left(C_{soil}^{WS\,i} \cdot Frac_{HomeRange\,j}^{WS\,i}\right) \qquad (3\text{-}1)$$

where

$C_{soil}{}^{WS}{}_{HomeRange}{}^{j}$ = average soil concentration for home range j from regional watershed (mg/kg soil)

$C_{soil}{}^{WSi}$ = annual average soil concentration from regional watershed i (mg/kg soil)

$Frac^{WSi}{}_{HomeRange}{}^{j}$ = fraction of home range j impacted by regional watershed i (unitless)

Soil concentration from local watershed

$$C_{soil}{}^{LWS}{}_{HomeRange\,j} = \sum \left(C_{soil}^{LWS\,i} \cdot Frac_{HomeRange\,j}^{LWS\,i}\right) \qquad (3\text{-}2)$$

where

$C_{soil}{}^{LWS}{}_{HomeRange}{}^{j}$ = average soil concentration for home range j from local watershed (mg/kg soil)

$C_{soil}{}^{LWSi}$ = annual average soil concentration from local watershed i (mg/kg soil)

$Frac^{LWSi}{}_{HomeRange}{}^{j}$ = fraction of home range j impacted by local watershed i (unitless)

[3] It should be noted that, in the case of the landfill, there is only one subarea included in the local watershed. In other words, the landfill is itself the drainage subbasin. Because it was assumed that wildlife might

The average soil concentration for the home range is calculated by summing the contributions from the regional and local watershed models, as shown in Equation 3-3.

Average soil concentration in home range

$$C_{soil}{}^{AVE}{}_{HomeRange^j} = C_{soil}{}^{LWS}{}_{HomeRange^j} + C_{soil}{}^{WS}{}_{HomeRange^j} \quad (3\text{-}3)$$

where

$C_{soil}{}^{AVE}{}_{HomeRange}{}^{j}$ = average soil concentration for home range j (mg/kg soil)

$C_{soil}{}^{LWS}{}_{HomeRange}{}^{j}$ = average soil concentration for home range j from local watershed (mg/kg soil)

$C_{soil}{}^{WS}{}_{HomeRange}{}^{j}$ = average soil concentration for home range j from regional watershed (mg/kg soil)

3.2 Calculating Chemical Concentrations in Terrestrial Prey

Chemical concentrations in terrestrial prey are estimated as a function of depth-averaged soil concentrations[4] in each home range, chemical-specific bioaccumulation factors[5] for each prey type (e.g., small mammals, small birds), and the fraction of each prey species home range that is contained within the habitat (i.e., the fraction that does not extend beyond the 2 km radius of the AOI). Prey types considered in the module include earthworms, invertebrates, small mammals, small birds, omniverts (larger omniverous vertebrates such as raccoons), herbiverts (larger herbivorous vertebrates such as deer), and small herpetafauna. Because these prey types consist of a variety of species (e.g., a Cerulean Warbler, Marsh Wren, and Northern Bobwhite are all considered small birds), the module calculates the tissue concentration for species within each prey type and then selects the maximum and minimum values from that range. The maxima and minima are reported to the TerFW output file (tf.grf), and the EcoEx module selects the concentration for each prey type at random from this range, assuming a uniform distribution (see Ecological Exposure module documentation for additional detail). For each home range, the tissue concentrations in earthworms and terrestrial invertebrates are calculated as shown below in Equation 3-4. Note that in reporting only the minimum and maximum tissue concentrations for each prey type the TerFW module reports concentrations that allow the EcoEx module to represent the variability in wildlife diets. Predatory animals may consume prey in different areas

[4] Depth-averaged, rather than surficial, soil concentrations were used to be more representative of the types of exposures likely to be reflected in soil-to-organism bioaccumulation factors (e..g., direct ingestion of soil invertebrates from deeper soil horizons; ingestion of prey that feed primarily on plant matter).

[5] Bioaccumulation factors (BAFs) for terrestrial prey are defined as the ratio of the chemical concentration in the animal to the chemical concentration in soil; BAFs are intended to reflect relevant exposure pathways to the study species (e.g., ingestion of contaminated soil and food).

of the habitat (changes in foraging patterns) and are highly likely to be opportunistic in their feeding habits (altering diet due to prey availability).

$$Cprey^{i}_{terr} = C_{soil}^{AVE}{}_{HomeRange^{j}} \cdot BAF_{prey}^{i} \quad (3\text{-}4)$$

where

$Cprey^{i}_{terr}$	=	tissue concentration in prey type i (mg/kg tissue)
$C_{soil}^{AVE}{}_{HomeRange}^{j}$	=	average soil concentration for home range j (mg/kg soil)
BAF_{prey}^{i}	=	bioaccumulation factor for prey type i from soil (kg soil / kg tissue)

The tissue concentrations in other terrestrial prey items (for each home range) are calculated as in Equation 3-5:

$$Cprey^{i}_{terr} = C_{soil}^{AVE}{}_{HomeRange^{j}} \cdot BAF_{prey}^{i} \cdot HabitatFrac_{HomeRange} \quad (3\text{-}5)$$

where

$Cprey^{i}_{terr}$	=	tissue concentration in prey type i (mg/kg tissue)
$C_{soil}^{AVE}{}_{HomeRange}^{j}$	=	average soil concentration for home range j (mg/kg soil)
BAF_{prey}^{i}	=	bioaccumulation factor for prey type i from soil (kg soil / kg tissue)
$HabitatFrac_{HomeRange}$	=	fraction of home range size (one of four) within habitat (unitless)

It is important to point out that each of the four home range sizes represents a range of species-specific home range sizes. Therefore, the $HabitatFrac_{HomeRange}$ - defined as the ratio of one of the four home range sizes to the habitat - does not reflect the specific home ranges for each of the prey species. As a result, the values for $HabitatFrac_{HomeRange}$ may be smaller than the fraction calculated using the individual home ranges for each species. Given the level of resolution inherent in deriving homogenous soil concentrations in watershed subbasins, we considered this to be a reasonable method to adjust exposure to allow for wildlife feeding in habitat areas outside the AOI. This prorating scheme is also employed in the Ecological Exposure module and is intended to prevent an overly conservative estimate of exposure.

3.3 Calculating Chemical Concentrations in Plants

The modeling construct to estimate plant concentrations in both the TerFW and Farm Food Chain (FFC) modules is based on recent and on-going research conducted by the U.S. EPA

Office of Research and Development and presented in *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (referred to as the Indirect Exposure Methodology, or IEM, U.S. EPA, in press).

In application to the 3MRA system, the spatial averaging of media concentrations performed for farms in the FFC module was virtually identical to the method used for home ranges delineated within the AOI. The primary difference in implementation is with regard to the categories of plants assumed by the modules. Protected fruits and vegetables are not considered by the TerFW module; it was assumed that animals will generally eat some portion (if not all) of the outer portions of plants that are typically discarded by humans. In addition, the plant categories for the TerFW include a much broader array of plant species than the crop species identified for human exposures. For instance, the category of exposed vegetables includes ferns and shoots that are not considered in the human diet. Because of the similarities in calculating plant concentrations between the two modules, some of the following discussion is intentionally brief. The reader may refer to the FFC module documentation (U.S. EPA, 1999) for additional detail.

The module simulates uptake by plants through three mechanisms: (1) wet and dry deposition of vapor-phase contaminants,[6] (2) wet and dry deposition of particle-bound contaminants, (3) soil-to-plant uptake and translocation of contaminants in soil. The module recognizes the chemical type of each constituent - dioxin-like (D), mercury (Hg), metal (M), organic (O), or special (S) - and executes the appropriate subroutines to predict the chemical concentration in plants. As with the FFC module, the TerFW module produces biotransfer factors for air-to-plant and soil-to-plant uptake and then sums the contributions from deposition and uptake, as appropriate, for the different categories of plants. For organic chemicals, these biotransfer factors are generally estimated using algorithms presented in the IEM (U.S. EPA, in press). The biotransfer factors for other chemical types are generally derived from empirical data. For convenience and consistency with the FFC module documentation, the presentation of model calculations is organized around aboveground plants (e.g., exposed vegetables, silage) and below ground vegetation (e.g., tubers, root vegetables).

3.3.1 Aboveground Plants

Chemical loadings to aboveground plants occur through deposition of particle-bound and vapor-phase contaminants (wet and dry) and through soil-to-plant uptake and accumulation. To predict plant concentrations relevant to wildlife, aboveground plants include exposed fruits and vegetables, forage, and silage. For each home range delineated within the AOI, the total concentration in aboveground plants is calculated using Equation 3-6 (the subscript "xxx" refers to the plant categories such as forage and exposed vegetables):

$$P_{xxx\,DW} = PD_{xxx\,DW} + PV_{xxx\,DW} + PR_{xxx\,DW} \qquad (3\text{-}6)$$

[6] The IEM (U.S. EPA, in press) points out that, for highly hydrophobic constituents such as dioxin, the dry deposition from the vapor phase is misleading with respect to the mechanism of uptake. ORD scientists have asserted that these types of constituents are, in essence, actively stripped from the air by vegetation.

where

P_{xxx_DW} = total concentration in plant (mg/kg DW)
PD_{xxx_DW} = plant concentration due to particle-bound deposition (mg/kg DW).
PV_{xxx_DW} = plant concentration due to vapor-phase deposition (mg/kg DW)
PR_{xxx_DW} = plant concentration due to root uptake and translocation (mg/kg DW).

3.3.1.1 Plant Concentration Due to Deposition of Particle-bound Contaminants

Calculating the contribution to plant concentrations from the wet and dry deposition of particle-bound contaminants relies on deposition rates provided by the Air module. For all constituents, this calculation is given by Equation 3-7:

$$PD_{xxx\,DW} = \frac{1000 \cdot 365 \cdot [ParDDepAve + (Fw_{xxx} \cdot ParWDepAve) \cdot Rp_{xxx}(1.0 - \exp^{(-kpPar_{xxx} \cdot Tp_{xxx})})]}{Yp_{xxx} \cdot kpPar_{xxx}} \quad (3\text{-}7)$$

where

PD_{xxx_DW} = plant concentration due to direct deposition of particle-bound contaminants (mg/kg DW)

1,000 = units conversion factor (1,000 mg/g)

365 = units conversion factor (365 d/yr)

ParDDepAve = average dry deposition rate (g/m^2-yr)

Fw_{xxx} = fraction of wet deposition that sticks to plant (unitless)

ParWDepAve = average wet deposition rate (g/m^2-yr)

Rp_{xxx} = interception fraction (unitless)

$kpPar_{xxx}$ = plant surface loss of particulate-bound constituent (1/yr)

Tp_{xxx} = length of plant exposure (yr)

Yp_{xxx} = yield or standing crop biomass (kg DW/m^2).

3.3.1.2 Plant Concentration Due to Dry Deposition of Vapor-phase Contaminants

For organic contaminants with a $K_{ow} < 100{,}000$ (or $\log K_{ow} < 5$), the contribution to the plant concentration due to wet and dry deposition of vapor-phase contaminants is given by:

$$PV_{xxx\,DW} = \frac{1000 \cdot 365 \cdot [VapDDepAve + (Fw_{xxx} \cdot VapWDepAve) \cdot Rp_{xxx}(1.0 - \exp^{(-kpVap_{xxx} \cdot Tp_{xxx})})]}{Yp_{xxx} \cdot kpVap_{xxx}} \quad (3\text{-}8)$$

where

$PV_{xxx\_farm\_DW}$	=	plant concentration due to deposition of vapor-phase contaminants (mg/kg DW)
1,000	=	units conversion factor (1,000 mg/g)
365	=	units conversion factor (365 d/yr)
VapDDepAve	=	average dry deposition rate (g/m^2-yr)
Fw_{xxx}	=	fraction of wet deposition that sticks to plant (unitless)
VapWDepAve	=	average wet deposition rate (g/m^2-yr)
Rp_{xxx}	=	interception fraction (unitless)
$kpVap_{xxx}$	=	degradation loss of vapor phase constituents (1/yr)
Tp_{xxx}	=	length of plant exposure (yr)
Yp_{xxx}	=	yield or standing crop biomass (kg DW/m^2)

and

VapDDepAve is estimated using vapor-phase concentration averaged generated by the Air module for the home range of interest:

$$VapDDepAve = 0.31536 \cdot CvAve \cdot VapDdv \quad (3\text{-}9)$$

where

VapDDepAve	=	areal average yearly dry deposition rate (g constituent/m^2-yr)
0.31536	=	units conversion factor ((m/yr)/cm/s and (g/µg))
CvAve	=	average vapor-phase concentration (µg/m^3)
VapDdv	=	default factor of 1 for vapor phase dry deposition velocity (cm/s).

For organic contaminants with a $K_{ow} \geq 100{,}000$ (or $\log K_{ow} \geq 5$), the contribution to the plant concentration from vapor-phase contaminants that are stripped from the air is calculated as shown in Equation 3-10:

$$PV_{xxx\,DW} = \frac{CvAve \cdot Bv_{xxx} \cdot VG_{ag\,xxx}}{1{,}000 \cdot \rho_{air}} \qquad (3\text{-}10)$$

where

PV_{xxx_DW} = plant concentration due to deposition of vapor-phase contaminants (mg/kg DW)

CvAve = average vapor-phase concentration in air ($\mu g/m^3$)

Bv_{xxx} = mass-based air-to-plant biotransfer factor ([µg/g DW]/[µg/g air])

VG_{ag_xxx} = empirical correction factor (unitless)

1,000 = units conversion factor (g/m^3)

ρ_{air} = density of air (constant at 1.19 g/L).

Mass-based air-to-plant biotransfer factor (Bv)

The mass-based air-to-plant biotransfer factor is calculated for constituents designated as ChemType "O" (organic) with $\log K_{ow} \geq 5$ as in Equation 3-10:

$$Bv = \left(\frac{\rho_{air} \cdot Bvol}{\left(\frac{(100 - MAF_{leaf})}{100} \right) \cdot \rho_{leaf}} \right) \cdot \frac{1}{Bv_{ecf_{plant}}} \qquad (3\text{-}11)$$

where

Bv = biotransfer factor ([µg/g DW plant]/[µg/g air])
ρ_{air} = density of air (constant at 1.19 g/L)
Bvol = volume-based biotransfer factor ([µg/L FW leaf]/[µg/L air])
MAF_{leaf} = moisture content in leaf (percentage)
ρ_{leaf} = density of the leaf (g/L FW)
Bv_{ecf_plant} = empirical correction factor for Bv (unitless).

Volume-based air-to-plant biotransfer factor

The calculation of the mass-based biotransfer factor (Bv) is based on the volume-based biotransfer factor (Bvol) calculation in Equation 3-12:

$$\log Bvol = 1.065 \log K_{ow} - \log\left[\frac{HLC}{RT}\right] - 1.654$$
$$Bvol = antilog\ [\log Bvol] \qquad (3\text{-}12)$$

where

Bvol	=	biotransfer factor ([µg/L FW leaf]/[µg/L air])
K_{ow}	=	octanol/water partition coefficient (unitless)
HLC	=	Henry's law constant (atm-m^3/mol)
R	=	universal gas constant (constant at 8.205E-05 atm-m^3/mol-K)
T	=	air temperature (constant at 298.1 K).

For contaminants with ChemType "D" (dioxin-like), "S" (special), and "Hg" (mercury), the air-to-plant biotransfer factor is not calculated; rather, it is based on empirical data (see documentation on data collection for TerFW module). Vapor-phase deposition is not modeled for metal contaminants.

3.3.1.3 Plant Concentration Due to Root Uptake and Translocation

The contribution to the plant concentration from soil-to-plant uptake is a function of the depth-averaged soil concentration and the biotransfer factor (Br). As with other mechanisms of uptake and accumulation, the TerFW includes chemical-specific switches that "turn on" appropriate subroutines and read from chemical properties files when needed. For all chemical types, Equation 3-13 is used to calculate the plant concentration from root uptake:

$$PR_{xxx\_DW} = C_{soil}^{\ AVE}{}_{HomeRange\ j} \cdot Br_{xxx} \qquad (3\text{-}13)$$

where

PR_{xxx_DW}	=	plant concentration due to root uptake and translocation (mg/kg DW)
$C_{soil}^{\ AVE}{}_{HomeRange\ j}$	=	average soil concentration for home range j (µg/g soil)
Br_{xxx}	=	soil-to-plant biotransfer factor ([µg/g DW]/[µg/g soil]).

Soil-to-plant biotransfer factor (Br)

For organic constituents (ChemType "O") and special constituents (ChemType "S") lacking empirical data, the biotransfer factor for soil-to-plant is given by Equation 3-14:

$$\log Br = 1.588 - 0.578 \log K_{ow}$$
$$Br = antilog\ [\log Br] \qquad (3\text{-}14)$$

where

Br = soil-to-plant biotransfer factor ([µg/g DW plant]/[(µg/g soil])
K_{ow} = octanol/water partition coefficient (unitless).

For other chemical types, the TerFW reads empirical values from the chemical properties file (i.e., the chemical/physical properties database, or CPP) and uses those values in Equation 3-13 to calculate the plant concentration related to root uptake and translocation. It should be noted that, for dioxin-like constituents (ChemType "D"), this uptake mechanism is considered to be negligible, and the empirical values for Br are set to zero.

3.3.2 Belowground Plants

Chemical uptake in belowground plants (e.g., root vegetables) results in uptake and accumulation of constituents in the outer "skin" of the plant and some translocation to the inner plant parts considered edible by humans and wildlife. The TerFW executes one subroutine for ChemTypes "O" (organic), "D" (dioxin-like), and "S" (special) chemicals, and a second subroutine for mercury and metals.

3.3.2.1 Plant Concentration for Organic, Dioxin-like, and Special Chemicals

The concentration in belowground plants for ChemTypes O, D, and S is calculated as shown in Equation 3-15. Depending on the chemical type, the input variables RCF concentration and K_dS_{Ave} (defined below) may be calculated or read from the database on chemical properties.

$$Proot_{DW} = \frac{C_{soil}^{AVE}{}_{HomeRange^j} \cdot RCF \cdot VG_{bg}}{\frac{(100 - MAFroot)}{100} K_d S^{Ave}{}_{HomeRange^j}} \qquad (3\text{-}15)$$

where

$Proot_{DW}$ = concentration in root vegetables (mg/kg DW)
$C_{soil}^{AVE}{}_{HomeRange}{}^{j}$ = average soil concentration for home range j (µg/g soil)

RCF	=	root concentration factor ([µg/g WW plant]/[µg/ml soil water])
VG_{bg}	=	empirical correction factor (unitless)
MAFroot	=	percent of moisture in belowground vegetation (unitless)
$K_dS^{Ave}{}_{HomeRange}{}^{j}$	=	average soil-water partition coefficient for home range j (mL/g)

with $K_dS^{Ave}{}_{HomeRange}{}^{j}$ defined by

$$K_dS^{Ave}{}_{HomeRange}{}^{j} = K_{oc} \cdot focS^{Ave}{}_{HomeRange}{}^{j} \quad (3\text{-}16)$$

where

K_{oc}	=	organic carbon partition coefficient (mL/g)
$focS^{Ave}{}_{HomeRange}{}^{j}$	=	average fraction of organic carbon in depth-averaged soil for home range j (unitless)

The average partition coefficient ($K_dS^{Ave}{}_{HomeRange}{}^{j}$) and fraction organic carbon ($focS^{Ave}{}_{HomeRange}{}^{j}$) are calculated in exactly the same manner as the average soil concentration ($C_{soil}{}^{AVE}{}_{HomeRange}{}^{j}$) for each home range (see Equations 3-1 through 3-3).

In addition to accounting for volumetric differences among roots of different types of plants, the empirical correction factor, VG_{bg}, also adjusts for peeling, cooking, and cleaning, which can all reduce the contaminant concentration. As discussed in the FFC module documentation and the IEM (U.S. EPA, in press), the correction factor was developed as part of the exposure methodology that accounts for root vegetable ingestion. Because the correction factor does not quantify the fraction that is based on food preparation, application in the TerFW module introduces some uncertainty into the root vegetable calculation. However, data were not identified to refine the estimate of VG_{bg} provided by ORD and, therefore, the same default value was used in the TerFW module as with the FFC module. Relative to other sources of uncertainty (e.g., estimating an RCF that is appropriate for all types of roots eaten by wildlife), the use of the default value for VG_{bg} is not considered to be significant.

For dioxin-like constituents, the RCF is based on empirical data from the chemical properties database. For organic and special constituents with log K_{ow} values $\leq$ 2.0 , the RCF is estimated using Equation 3-17:

$$\log(RCF - 0.82) = 0.77 \log K_{ow} - 1.52$$
$$RCF = antilog[\log RCF] \quad (3\text{-}17)$$

where

RCF	=	root concentration factor ([µg/g WW plant]/[µg/ml soil water])
K_{ow}	=	octanol/water partition coefficient (unitless).

For organic and special constituents with log K_{ow} values > 2.0, the RCF is estimated using Equation 3-18:

$$\log RCF = 0.77 \log K_{ow} - 1.52$$
$$RCF = antilog[\log RCF] \quad (3\text{-}18)$$

where

RCF = root concentration factor ([µg/g WW plant]/[µg/ml soil water])
K_{ow} = octanol/water partition coefficient (unitless).

3.3.2.2 Plant Concentration for Metals and Mercury

For the chemical types "M" (metal) and "Hg" (mercury), the concentration in belowground plants for is calculated as shown in Equation 3-19 using an empirical soil-to-root uptake factor.

$$Proot_{DW} = CTdaAve \cdot Broot \quad (3\text{-}19)$$

where

$Proot_{DW}$ = concentration in root vegetables (mg/kg DW)
$C_{soil}^{\overline{AVE}}{}_{HomeRange}^{j}$ = average soil concentration for home range j (µg/g soil)
Broot = soil-to-root uptake factor ([µg/g WW plant]/[µg/mL soil water]).

3.3.3 Conversion of Dry Weight Concentrations to Wet Weight Concentrations

The Human and Ecological Exposure modules are based on wet weight exposures to contaminated food items and, therefore, it is necessary to convert the dry weight concentrations to wet weight concentrations for the TerFW output file (tf.grf). This calculation is given by Equation 3-20:

$$P_{xxx} = \left(\frac{100 - MAF_{xxx}}{100}\right) \cdot P_{xxx\,DW} \qquad (3\text{-}20)$$

where

P_{xxx} = plant concentration for category xxx (mg/kg WW)
MAF_{xxx} = plant-specific moisture adjustment factor to convert DW concentration into WW (percent)
P_{xxx_DW} = plant concentration for category xxx (mg/kg DW)

4.0 Implementation

The flowchart shown in Figure 4-1 illustrates the generalized structure of the Terrestrial Food Web Module.

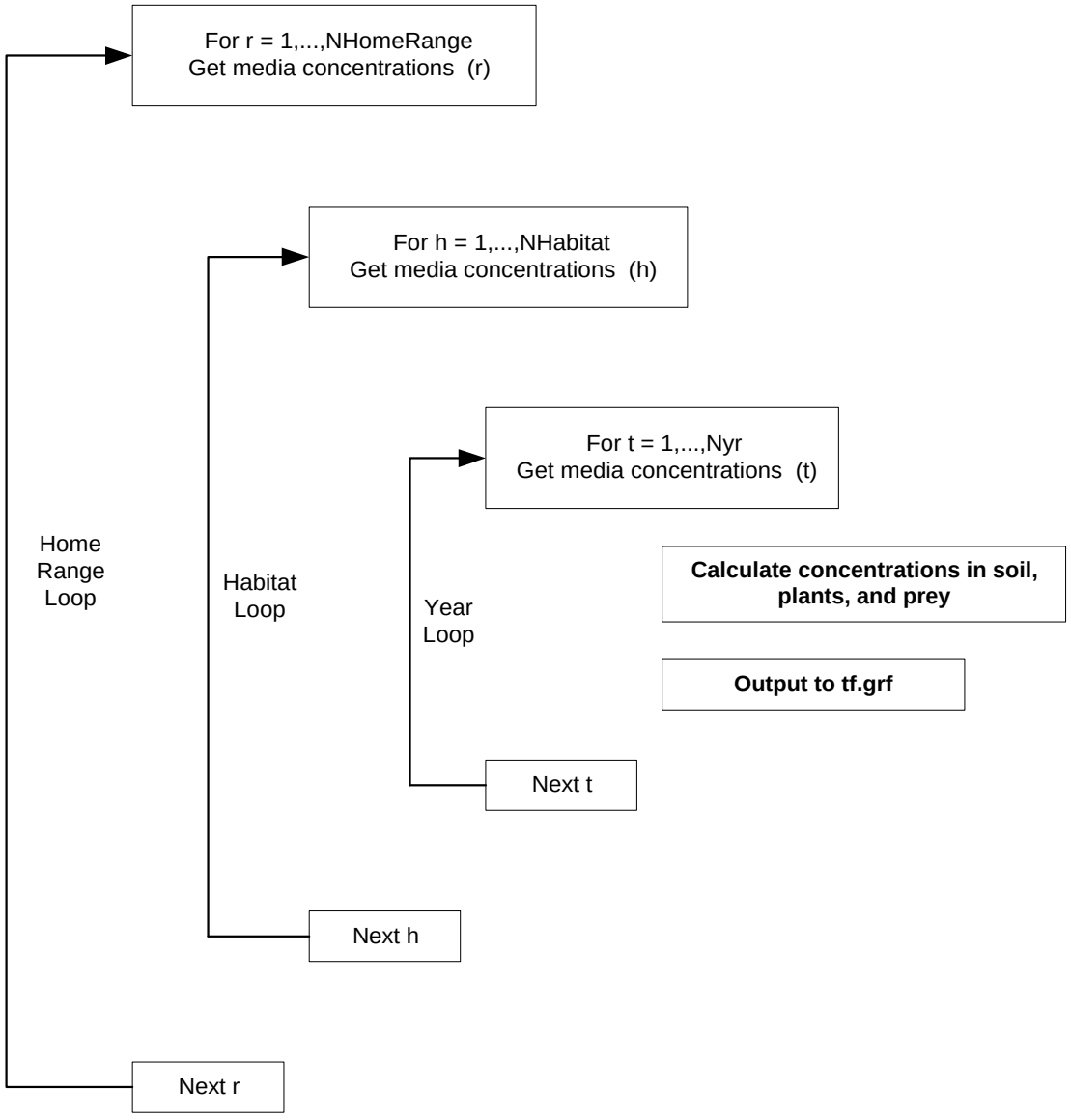

Figure 4-1. Conceptual flow diagram of major functionality of Terrestrial Food Web Module.

5.0 References

RTI (Research Triangle Institute). 1995. *Technical Support Document for the Hazardous Waste Identification Rule: Risk Assessment for Human and Ecological Receptors - Volumes I and II.* Prepared for the Office of Solid Waste, U.S. Environmental Protection Agency under Subcontract No. 801-01.

Sample, B.E., J.J. Beauchamp, R.A. Efroymson, and G.W. Suter, II. 1998. *Development and Validation of Bioaccumulation Models for Small Mammals.* Prepared for the U.S. Department of Energy under contrct DE-AC05-84OR21400.

U.S. EPA (Environmental Protection Agency). In press. *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions*. EPA/600/6-90/003. National Center for Environmental Assessment. Cincinnati, OH.

U.S. EPA (Environmental Protection Agency). 1999. *Data Collection for the Hazardous Waste Identification Rule. Section 10. Farm Food Chain and Terrestrial Food Web Data.* U.S EPA. July 1999.

Appendix A

Inputs and Outputs

Appendix A

Inputs and Outputs

The Terrestrial Food Web module receives inputs from its module-specific input file (tf.ssf), the generic site layout file (sl.ssf), the generic chemical properties file (cp.ssf), and modeled inputs from the following other modules: Air Module (ar.grf), Watershed Module (ws.grf), and those source modules outputting to a common grf file (sr.grf) a "true" for the soil-presence logical flag, SrcSoil. These sources are the Land Application Unit, Landfill, Wastepile, and Surface Impoundment. The Terrestrial Food Web module outputs are written to the tf.grf file. The soil, plant, invertebrate, and worm concentration outputs are three-dimensional arrays indexed on time, space, and receptor. The small birds, small herpetofauna, small mammals, herbiverts, and omniverts are two-dimensional arrays indexed on time and space.

All input and output variables are listed and described in Tables A-1 through A-7.

Table A-1. Tf.ssf Input Parameters (Module-Specific Inputs)

Input Parameters	Units	Description
Bv_ecf_plant	unitless	Empirical correction factor for Bv.
Fw_<plant type>	unitless	Fraction of wet deposition that adheres to the plant. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
MAF<plant type>	percent	Moisture adjustment factor to convert DW into WW. (Note: "<plant type>" is replaced with exfruit, exveg, leaf, profruit, proveg, and root.)
MAFleaf	percent	Moisture content in leaf.
rho_leaf	g/L	Density of the leaf.
Rp_<plant type>	unitless	Interception fraction. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
tp_<plant type>	year	Length of plant exposure to deposition. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
VapDdv	cen/sec	Vapor phase dry deposition velocity.
VGag_<plant type>	unitless	Empirical correction factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
VGbg_root	unitless	Empirical correction factor for roots.
Yp_<plant type>	kg DW/m^2	Yield or standing crop biomass. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)

Table A-2. SL.ssf Input Parameters (Module-Specific Site Layout Inputs)

Input Parameters	Units	Description
focS	mass fraction	Fraction organic carbon (soil).
HabRangeAirIndex	NA	Index of air points that impacts a home range.
HabRangeAirFrac	fraction	Fraction of home range impacted by air points.
HabRangeNumWSSub	unitless	Number of watersheds that impact a home range.
HabRangeLWSSubAFrac	fraction	Fraction of contributing local watershed subarea.
HabRangeWSSubFrac	fraction	Fraction of home range impacted by watershed.

Table A-3. CP.ssf Input Parameters (Module-Specific Chemical Inputs)

Input Parameters	Units	Description
ChemBAF<animal>	unitless	Bioaccumulation factor for small birds, herbiverts, small herpetofauna, invertebrates, small mammals, omniverts, and worms.
ChemBr_<plant type>	(μg/g DW plant) / (μg/g soil)	Soil-to-plant bioconcentration factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, grain, profruit, proveg, root, and silage.)
ChemBv_ecf_plant	unitless	Empirical correction factor for Bv.
ChemBv_<plant type>	(μg/g DW plant) / (μg/g air)	Mass-based air-to-plant biotransfer factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
ChemHLC	(atm-m^3) / mol	Henry's law constant.
ChemKoc	mL/g	Organic carbon partition coefficient
ChemKow	unitless	Octanol/water partition coefficient
ChemkpPar_<plant type>	1/ year	Plant surface loss of particulate-bound constituent. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
ChemkpVap_<plant type>	1/ year	Degradation loss of vapor phase constituents. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
ChemRCF	(μg/g WW plant) / (μg/mL sl water)	Root concentration factor.
ChemType	NA	Chemical type (O, M, Hg, S, or D)

Table A-4. Ar.grf Input Parameters (Air Module Inputs)

Input Parameters	Units	Description
CVap	μg/m3	Concentration of chemical in air vapor.
CVapNY	unitless	Number of years in the time series corresponding to this variable.
CVapYR	year	Time series of years corresponding to this variable.
ParDDep	g/m2/d	Particle dry deposition rate.
ParDDepNY	unitless	Number of years in the time series corresponding to this variable.
ParDDepYR	year	Time series of years corresponding to this variable.
ParWDep	g/m2/d	Particle wet deposition rate.
ParWDepNY	unitless	Number of years in the time series corresponding to this variable.
ParWDepYR	year	Time series of years corresponding to this variable.
VapWDep	g/m2/d	Vapor wet deposition rate.
VapWDepNY	unitless	Number of years in the time series corresponding to this variable.
VapWDepYR	year	Time series of years corresponding to this variable.

Table A-5. Sr.grf Input Parameters (Source Module Inputs)

Input Parameters	Units	Description
CTda	μg/g	Depth-averaged soil concentration across farm area.
CTdaNY	year	Number of years in the time series corresponding to this variable.
CTdaYR	unitless	Time series of years corresponding to this variable.
CTss	μg/g	Surficial soil concentration across farm area.
CTssNY	year	Number of years in the time series corresponding to this variable.
CTssYR	unitless	Time series of years corresponding to this variable.

Table A-6. Ws.grf Input Parameters (Watershed Module Inputs)

Input Parameters	Units	Description
CTdaR	μg/g	Depth-averaged soil concentration for the regional watershed area.
CTdaRNY	year	Number of years in the time series corresponding to this variable.
CTdaRYR	unitless	Time series of years corresponding to this variable.
CTssR	μg/g	Surface soil concentration for the regional watershed area.
CTssRNY	year	Number of years in the time series corresponding to this variable.
CTssRYR	unitless	Time series of years corresponding to this variable.

Table A-7. Tf.grf Output Parameters (Terrestrial Food Web Module Outputs)

Output Parameters	Units	Description
C<animals>_<max or min>NY	unitless	Number of years in the time series corresponding to this variable.
C<animals>_<max or min>	mg/kg	Concentration of contaminant found in herbiverts and omniverts.
C<animals>_<max or min>YR	year	Time series of years corresponding to this variable.
C<animals>_HabRange	mg/kg	Concentration of contaminant found in invertebrates and worms.
C<animals>_HabRangeNY	unitless	Number of years in the time series corresponding to this variable.
C<animals>_HabRangeYR	year	Time series of years corresponding to this variable.
C<animals>_sm_<max or min>	mg/kg	Concentration of contaminant found in small birds, herpetofauna, and mammals.
C<animals>_sm_<max or min>YR	year	Time series of years corresponding to this variable.
C<animals>_sm_<max or min>NY	unitless	Number of years in the time series corresponding to this variable.
CTdaAveHabRange	μg/g	Average depth average soil concentration in each home range.
CtdaAveHabRangeNY	unitless	Number of years in the time series corresponding to this variable.
CTdaAveHabRangeYR	year	Time series of years corresponding to this variable.
CTssAveHabRange	μg/g	Average depth average soil concentration in each home range.
CTssAveHabRangeNY	unitless	Number of years in the time series corresponding to this variable.
CTssAveHabRangeYR	year	Time series of years corresponding to this variable.
P<plant type>_HabRangeNY	unitless	Number of years in the time series corresponding to this variable.
P<plant type>_HabRangeYR	year	Time series of years corresponding to this variable.
P<plant type>_HabRange	mg/kg	Concentration of contaminant found in exfruit, exveg, forage, grain, root, and silage.