ATTACHMENT 1-1. Methodology for Estimating Exposures to Terrestrial Animals (mammals, birds, reptiles, amphibians and invertebrates)

1. Introduction

Two types of exposures are estimated for terrestrial vertebrates: concentration (dietary) based and dose-based. Dose-based exposures include dietary, drinking water, dermal and inhalation routes. This attachment describes the method for estimating dietary-based and dose-based exposures to listed terrestrial vertebrates located on the treated field, as well as in adjacent areas receiving spray drift. All of the dose-based exposures are estimated using allometric equations that are dependent upon body weight. Dietary requirements as well as body weights of specific species are provided within the MAGtool model. All information on species traits, including dietary items and body weights, are based on data gathered from Fish and Wildlife Services (FWS) species documents (*e.g.,* Recovery Plans, 5-year review, etc.).

This attachment also summarizes the methodology that is used to estimate exposures to terrestrial invertebrates. Available toxicity data is expressed as a wide variety of units. Those that can be translated into an application rate (*i.e.,* lb a.i./A), a direct exposure (*e.g.*, mg/kg-bw), or a concentration in a relevant medium (*e.g.*, food, soil) can be used to estimate exposures to terrestrial invertebrates. Toxicity data that are expressed as lb a.i./A combine multiple exposure routes, while concentration-based endpoints may represent contact or dietary exposure routes.

The methods described in this attachment may also be used to assess potential exposures to animals that represent the prey of listed species. These exposures can be used to assess potential effects to prey, pollination, habitat, and/or dispersal (PPHD) of a listed species.

Since this approach applies to Steps 1 and 2, the scale of these models is focused on the field level. The intention of this approach is to assess exposures to individuals of a listed species. Estimated exposures to individuals are intended to be conservative, representing potential “high-end” exposures to an individual animal.

1. Exposures expressed as application rate (lb a.i./A)

Application rates are taken directly from registered labels and can be used to determine whether or not the rate is above the available toxicity endpoints expressed as lb a.i./A. The AgDRIFT model is used to determine the distance from the edge of the field where the deposition (in lb a.i./A) is equivalent to the endpoints and thresholds of concern.

1. Spray Drift

According to **Equation 1**, the fraction of the application rate (FAR) that is equivalent to the threshold is used to determine the distance where the risk extends (dt; units: ft). Spray drift deposition differs by application method, droplet spectra and release height. An analysis of the deposition curves generated from AgDRIFT (v. 2.1.1)[[1]](#footnote-2) yielded the parameters included in **Table 1** that are used by **Equation 1**.

**Equation 1**.

**Table 1. Parameters for Spray Drift Equation, Based on Application Method.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Application method** | **Boom height** | **Droplet spectrum** | **a5** | **b5** | **c5** |
| Aerial | NA | Very Fine to Fine | 0.0292 | 0.822 | 0.6539 |
| Fine to Medium | 0.043 | 1.03 | 0.5 |
| Medium to Coarse | 0.0721 | 1.0977 | 0.4999 |
| Coarse to Very Coarse | 0.1014 | 1.1344 | 0.4999 |
| Ground | High | Very Fine to Fine | 0.1913 | 1.2366 | 1.0552 |
| Fine to Medium/Coarse | 2.4154 | 0.9077 | 1.0128 |
| Low | Very Fine to Fine | 1.0063 | 0.9998 | 1.0193 |
| Fine to Medium Coarse | 5.5513 | 0.8523 | 1.0079 |
| Airblast (sparse) | NA | NA | 0.0351 | 2.4586 | 0.4763 |

1. Concentrations on and in food of terrestrial diet of animals and direct exposures to listed invertebrates

Concentration based exposures (units: mg a.i./kg-ww) are reliant upon the amount of pesticide in/on a dietary item. As discussed in the appendices that describe the specific listed birds, mammals, amphibians and reptiles, the diets of listed vertebrates include plants (seeds, leaves, grass, fruit, flowers, nectar), invertebrates (above and below ground in terrestrial areas) and other vertebrates (mammals, birds, reptiles, amphibians, and carrion). Food items of listed terrestrial invertebrates include: grass, broadleaf plants, arthropods, fruit, seeds, carrion and nectar.

The methods for estimating concentrations on these food items are based on existing models, *i.e.,* T-REX and T-HERPS, both of which are described in detail at: <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment#terrestrial>. In this approach, upper-bound and mean concentrations are estimated. The upper bound concentrations on plants represent high-end exposures that are based on empirical data from Hoerger and Kenaga 1972[[2]](#footnote-3) and Fletcher et al. 1994[[3]](#footnote-4). The mean values represent the mean concentrations across many different fields, crops, locations throughout the US and pesticides.

* 1. Plants

The method for estimating upper-bound and mean concentrations of pesticides on seeds, grass (short and tall), broadleaves and fruit is described in detail in the T-REX manual. Direct estimates of pesticides are not available for some food items; therefore, surrogates are used as follows:

* For nectar and pollen, tall grass is used as a surrogate (based on honeybee risk assessment methodology[[4]](#footnote-5)).
* For pine needles and twigs, short grass is used.
* Broadleaves are used for flowers, fungi, and lichens.
  1. Invertebrates

Concentrations are estimated in units of mg a.i./kg-ww. For direct effects to listed invertebrates, these concentrations can be compared to thresholds that are in the same units. Note that these concentrations may be compared to toxicity data from contact or dietary based exposure toxicity studies.

* + 1. Above ground

The method for estimating upper-bound and mean concentrations of pesticides on above-ground arthropods is described in detail in the T-REX manual. These residues represent values from a 90th percentile field. These values are used to assess exposures for direct effects to listed invertebrates as well as insect prey.

The original dataset used to estimate residues on arthropods is based on empirical residues from larvae, beetles, crickets, grasshoppers and wild caught invertebrates. This method may not account for the increased surface area of species with large wings (*e.g.*, butterflies) and therefore may underestimate exposure to large winged species.

The contact-based exposure approach integrated into the BeeREX model was not used because that approach includes residues that are specific to honeybees. It is assumed here that the arthropod residue values in the T-REX model generally apply to more species. Resides from the two approaches are generally similar.

* + 1. Soil dwelling

A simple partitioning approach is employed in this analysis to estimate concentrations of the pesticide of interest in earthworms using the earthworm fugacity model. Earthworms are used to represent soil dwelling invertebrate prey (*e.g.,* worms, snails) of listed species, as well as listed invertebrates that inhabit soil, for instance, snails.

In this approach, it is assumed that a pesticide partitions between the soil and the pore water of the treatment site. It is assumed that earthworms dwelling within the soil are exposed to a pesticide via ingestion of and contact with contaminated soil. The concentration of a pesticide in earthworm tissues can be calculated according to **Equation 2**. In this approach, the octanol water partitioning coefficient (Kow) of a chemical and the lipid content of the worm is used to predict the partitioning of the chemical between the worm and pore water. L is based on the lipid content of earthworms, which was assumed to be 0.01 (Cobb et al. 1995[[5]](#footnote-6)). The density of the earthworm (ρE) is assumed to be 1 kg/L(equivalent to density of water).

**Equation 2**.

Pesticide concentrations in pore water are estimated using a simple partitioning approach (**Equation 3; Table 2**) that is based on modifications to the Tier I rice model (USEPA, 2007b). In this equation, the pesticide concentration in pore water is dependent upon the pesticide application rate (Arate), mean organic carbon-water partitioning coefficient of the pesticide (Koc; L/kg), and the puddle depth and soil properties. A factor of 11.2 is used to convert the units of the application rate, which are lb a.i./A, to the metric units needed to generate a concentration value expressed in µg a.i./mL. Water depth (dw) is assumed to be 0 cm. The soil depth (dsoil) is set to 2.6 cm (1 inch). Default parameter values for soil properties, including bulk density (ρb) and fraction of organic carbon (foc(soil)), are based on EFED scenarios for the Pesticide Root Zone Model (PRZM). The default values of 1.5 kg/L for ρb and 0.015 for foc(soil) are based on the mean values from the field crop and orchard scenarios. Porosity (θsoil) and bulk density are related (**Equation 4**), where ρp is the density of soil particles (kg/L). A typical value of 2.65 (Smettem 2006[[6]](#footnote-7)) is used for soil particle density.

**Equation 3.**

**Equation 4.**

It should be noted that the estimated exposure generated using this approach is based on the pesticide concentration in the tissue of the worm. It does not include the pesticide that is in the gut of the worm (*e.g.,* sorbed to soil). In addition, metabolism of the chemical by the worm is not accounted for, potentially resulting in an overestimate of exposure. Finally, it is assumed that the partitioning of the chemical between worms and pore water is comparable to the chemical’s partitioning between octanol and water. This is a common assumption when predicting chemical uptake by organisms (*e.g.,* in aquatic bioaccumulation modeling).

**Table 2. Summary of parameters used to estimate pesticide concentrations in soil dwelling invertebrates.**

|  |  |  |
| --- | --- | --- |
| **Symbol** | **Definition** | **Units** |
| Arate | Application rate from label | lb a.i./A |
| CE | Chemical concentration in earthworm tissue | mg a.i./kg |
| Cw(pore) | Concentration of the pesticide in pore water | mg/L = µg/mL |
| dsoil | Depth of soil at equilibrium with water | cm |
| dw | Depth of puddle water | cm |
| foc(soil) | Fraction of organic carbon in soil | none |
| Koc | Organic carbon:water partition coefficient | L/kg-oc |
| KOW | Octanol to water partition coefficient | none |
| L | Lipid fraction of earthworm | none |
| θsoil | Porosity of soil | none |
| ρb | Bulk density of soil | kg/L |
| ρE | density of earthworm | kg/L |
| ρp | Density of soil particles | kg/L |

* 1. Vertebrates

The method for estimating upper-bound and mean concentrations of pesticides in mammals, birds, reptiles and amphibians is described in detail in the T-HERPS manual. For mammals serving as prey, the 15 g mammal that consumes short grass was chosen because it is conservative and representative of prey species expected to be commonly found. For birds, the small bird (20 g) that consumes 100% arthropods was selected because this is the most common dietary item among birds (**Appendix D** of TIM manual[[7]](#footnote-8)). A 2 g animal that consumes 100% arthropods is selected to represent reptile and amphibian prey. For carrion, residues in large mammals (1000 g) consuming short grass are used as a surrogate.

In this approach, concentrations in mammals and birds are decreased on a daily basis based on elimination or metabolism. The amount of chemical that is retained from one day to the next is based on chemical-specific magnitude of the residue studies with chickens and rats.

1. Concentrations in soil

The pesticide concentration in soil can be calculated using the pore water concentration used in the earthworm fugacity model. In this approach, Cw(pore) (units: mg a.i./L-water) is multiplied by the Koc (L-water/kg-oc) and the foc (fraction of organic carbon in soil). The default foc value is 0.015. The result is the mg a.i./kg-dw (soil). This value is used to estimate exposures to terrestrial invertebrates.

For species that consume decaying organic matter that is likely associated with soil (*e.g.*, decaying leaves and bark), estimated concentrations in soil will be used to represent concentration-based EECs. This will be applied to some species of soil-dwelling invertebrates.

1. Concentrations in aquatic organisms

Many species of listed vertebrates also consume aquatic organisms *(e.g.,* plants, benthic invertebrates, fish). Typically, EFED would run the Kow (based) Aquatic BioAccumulation Model (KABAM)[[8]](#footnote-9) for a pesticide with Log Kow values ≥4 to estimate concentrations of the pesticide in the tissues of aquatic organisms. Unless a chemical-specific metabolism rate constant can be derived, KABAM estimates concentrations of the chemical in aquatic organisms assuming that the chemical is at steady state and that there is no metabolism of the chemical. Although part of the analyses in the model, for carbaryl and methomyl, based on their low Kow values, bioaccumulation is not expected.

This attachment is focused on methods for estimating exposures to birds, mammals, reptiles and terrestrial-phase amphibians. Exposures to aquatic-phase amphibians (*i.e.,* tadpole life stages and aquatic-obligate species) will be assessed using PWC. Dietary exposures to aquatic-phase amphibians (that consume algae, aquatic invertebrates, fish and amphibians) will not be quantified because the major uptake route of carbaryl and methomyl for aquatic organisms is expected to be through respiration. In addition, since the available toxicity data representative of aquatic-phase amphibians is expressed as aqueous concentrations, dietary-based exposures cannot be evaluated.

1. Doses received by birds, mammals, reptiles and terrestrial-phase amphibians

Dose-based exposures (units: mg a.i./kg-bw = µg a.i./g-bw) include four different routes: diet, drinking water, dermal and inhalation. Essentially, a dose-based exposure is calculated by multiplying the relevant ingestion rate by the concentration in the relevant medium. Ingestion rates are heavily dependent upon the body weight of the assessed animal because they are calculated using allometric equations. In general, the smaller the animal, the larger the dose. The methods for estimating dose-based exposures from different routes are described below.

Doses estimated using the MAGtool for each exposure route are evaluated independently by comparing the estimated dose to the appropriate toxicity endpoint. Individual doses are not added together due to their conservative nature. In the MAGtool, drinking water, inhalation and dermal based exposure values are calculated and used in the determination of off-site transport distances in both Step 1 and Step 2, if they represent the most sensitive exposure value. In the Step 2 probabilistic analyses, as outlined in the MAGtool documentation, the exposure analysis is focused on dietary exposures. As discussed below, exposure can be assessed directly on the field or in areas that receive spray drift.

* 1. Diet

Concentration based values in the appropriate food item of a species are multiplied by the food ingestion rate and then divided by the body weight of the assessed species (**Equation 5; Table 3**). Food ingestion rates vary by type of vertebrate and the water content of the diet (**Table 4**). **Equation 6** is the allometric equation that is used to estimate the daily food ingestion rate (g food per day, wet weight) for an animal. The taxa-specific parameters used by **Equation 6** are provided in **Table 5**. Based on the available data from USEPA 1993[[9]](#footnote-10), food ingestion rates can be estimated for birds in the Passeriformes order (“passerines”) and non-passerine birds as well as mammals in the Rodentia order (“rodents”) and non-rodent species. One set of parameters is available for a reptile (iguana), which are used to estimate the food intake rate of reptiles and terrestrial-phase amphibians.

**Equation 5**.

**Equation 6.**

**Table 3. Parameters used to calculate dietary-doses.**

|  |  |  |
| --- | --- | --- |
| **Symbol** | **Description** | **Units** |
| BW | Body weight (of species) | g |
| Cfood | Pesticide concentration on a food item | mg a.i./kg = ug a.i./g |
| FWk | Fraction of water in dietary item k | none |
| IRfood | Food intake rate | g per day (WW) |

**Table 4. Fraction of Water in Fresh Food Items (FWk) (from USEPA 1993).**

|  |  |
| --- | --- |
| **Food Item (k)** | **FWk** |
| Amphibians | 0.85 |
| Arthropods | 0.69 |
| Aquatic plants | 0.80\* |
| Benthic invertebrates | 0.78\*\* |
| Birds, mammals, carrion | 0.68 |
| Broadleaves (and surrogates) | 0.85 |
| Fruit | 0.77 |
| Fish | 0.75 |
| Grasses | 0.79 |
| Filter feeders | 0.82 |
| Nectar | 0.70+ |
| Pollen | 0.063++ |
| Soil-dwelling invertebrates (earthworms) | 0.84 |
| Reptiles | 0.66 |
| Seeds (assumed to also represent pine needles) | 0.093 |
| zooplankton | 0.83# |

\*Although a range of values is available, 0.8 was chosen to represent the upper end of “emergent vegetation”. This value is also consistent with those available for algae (0.84±0.047) and aquatic macrophytes (0.87±0.031).

\*\*Value for shrimp used.

+Average sugar content of nectar is 0.3 (from bee risk assessment method), remainder is assumed to be water.

++From Morgano et al 2011[[10]](#footnote-11)

#Midpoint of range of values for cladocerans used (*i.e.,* 0.79-0.87).

**Table 5. Parameters used to calculate food intake rate for vertebrates (from USEPA 1993).**

|  |  |  |
| --- | --- | --- |
| **Taxa** | **a1** | **b1** |
| Birds in Passeriformes order | 0.398 | 0.850 |
| All Birds (applied to species not in Passeriformes order) | 0.301 | 0.751 |
| Mammals in Rodentia order | 0.621 | 0.564 |
| All mammals (applied to mammal species not in Rodentia order) | 0.235 | 0.822 |
| Reptiles and amphibians\* | 0.013 | 0.773 |

\*No amphibian-specific values are available, therefore, reptile values are used as a surrogate.

* 1. Drinking water

The pesticide dose received through a day’s worth of drinking contaminated water is calculated using **Equation 7**. Like with food, drinking water ingestion rates vary by type of vertebrate and the water content of the diet. As indicated by **Equation 8**, the daily water drinking water rate is based on the difference between an animal’s daily flux and the amount of water consumed through the diet. The daily water flux rate, which represents the total daily water requirement from all sources is estimated according to **Equation 9**, with the parameters in **Table 6.** If all of an animal’s daily water need (*i.e.,* flux) is met through the diet, then that animal does not drink water. Two different types of drinking water are assessed independent of each other: puddles and dew. **Equations 3 and 11** are used to generate CW values for puddles and dew, respectively.

**Equation 7.**

**Equation 8.** 

**Equation 9.** 

**Equation 10.** 

**Equation 11.**

Pesticide concentrations in puddles are estimated using a simple partitioning approach (**Equation 3; Table 6**) that is based on the Tier I rice model (USEPA, 2007b), with modifications. The approach for estimating pesticide concentrations in puddle water is the same as the one discussed above for pore water, with the following exception: puddle depth (dw) is assumed to be 1.3 cm (0.5 in).

**Table 6. Parameters used to calculate drinking water-doses.**

|  |  |  |
| --- | --- | --- |
| **Symbol** | **Description** | **Units** |
| BW | Body weight (of species) | g |
| Cw(dew) | Concentration of the pesticide in dew | mg/L = µg/mL |
| Cplant | Concentration of the pesticide in crop foliage | mg/kg = µg/g |
| Cw(puddle) | Concentration of the pesticide in puddle | mg/L = µg/mL |
| dsoil | Depth of soil at equilibrium with water (in puddle) | Cm |
| dw | Depth of puddle water | cm |
| Fdfr | Dislodgeable foliar residue adjustment factor | kg/m2 |
| Fluxwater | Total daily water flux rate | mL/day |
| foc(soil) | Fraction of organic carbon in soil | none |
| FWk | Fraction of water in a fresh food item k | none |
| IRdw | Drinking water intake rate | mL/day |
| IRfood | Food intake rate | g per day (WW) |
| Koc | Organic carbon:water partition coefficient | L/kg-oc |
| mwax | Mass of wax per surface area of leaf cuticle | kg/m2 |
| ρb | Bulk density of soil | kg/L |
| ρp | Density of soil particles | kg/L |
| ρwater | Density of water (1) | kg/L |
| θsoil | Porosity of soil | none |

**Table 7. Parameters used to calculate water intake rate for vertebrates (from Nagy and Peterson 1988[[11]](#footnote-12)).**

|  |  |  |  |
| --- | --- | --- | --- |
| **Taxa** | **a2** | **b2** | **c2** |
| Birds in Passeriformes order | 1.18 | 0.874 | 1 |
| Other birds not in Passeriformes order | 1.18 | 0.874 | 3.7 |
| Mammals | 0.326 | 0.818 | 1 |
| Reptiles and amphibians\* | 0.065 | 0.726 | 1 |

\*No amphibian-specific values are available, therefore, reptile values are used as a surrogate.

Pesticide concentrations in dew are estimated through the use of a simple equilibrium partitioning model. This model assumes two compartments, water and leaf cuticle, into which the pesticide may associate. **Equation 11** is used to estimate the pesticide concentration in dew (Cw(dew)(t)). Partitioning between the two compartments is based on the octanol-water partition coefficient of the chemical (Kow), where octanol is a surrogate for the waxy, external (epicuticular) layer of the leaf cuticle. Cplant is the total concentration of pesticide in broadleaf forage leaves (mg/kg-ww). Fdfr is used to account for the amount of pesticide that is present on the surface of the leaf, and thus may partition between the waxy layer of the leaf cuticle and dew.This approach establishes a distribution of pesticide concentrations in dew that is correlated with random selection of pesticide concentrations on broadleaf forage. The pesticide partitions into the epicuticular layer of the cuticle, which is influenced by the mass of wax (mwax). Available data indicate that the mass of wax in the epicuticular layer varies by species, with ranges of 5-30 µg/cm2 (Buschhaus and Jetter, 2011[[12]](#footnote-13)). Therefore, a default value of 0.012 kg/m2 is selected for mwax to represent the central tendency of this parameter. The density of water is used to generate an estimate of the pesticide concentration in water. It is assumed that the density of water is 1 kg/L.

In this approach, drinking water is estimated under the assumption that the animal is consuming 100% of its daily diet from an individual food item and 100% of the remaining water need from either puddles or dew. If the diet of a species includes multiple food items (*e.g.,* yellow-billed cuckoo), the model automatically calculates the drinking water rates for each of these food items, for dew and for puddles, independent of each other. This is a kind of “what-if” approach, where the question is: “What is the dose if the animal is consuming 100% of its diet as this single food item with residues representative of the treated field and 100% of its remaining water from either dew or puddles on the treated field?”

* 1. Dermal

Two different types of dermal dose are calculated here: direct spray at the time of application and contact with contaminated foliage. Because most toxicity data for terrestrial vertebrates are based on oral exposure studies, it is necessary to convert dermal doses to oral equivalents so that these exposures can be evaluated by existing toxicity data. This method is described below.

These methods were originally developed for assessing dermal exposures to birds. For amphibians and reptiles, which are expected to be lower to the ground than birds and mammals, contact with contaminated foliage seems less likely. Therefore, dermal exposures for reptiles and amphibians are only estimated considering direct spray of the pesticide.

Dermal exposure estimates rely upon the estimated surface area of the assessed species, which is calculated using an allometric equation that differs by taxon (**Equation 12, Table 8**).

**Equation 12.** 

**Table 8. Parameters used to calculate surface area for vertebrates.**

|  |  |  |  |
| --- | --- | --- | --- |
| **Taxon** | **a3** | **b3** | **Source** |
| Birds | 10 | 0.667 | USEPA 1993 |
| Mammals | 12.3 | 0.65 | USEPA 1993 |
| Amphibians: frogs and toads | 1.131 | 0.579 | USEPA 1993 |
| Amphibians: salamanders | 8.42 | 0.694 | USEPA 1993 |
| Reptiles: turtles and tortoises | 16.61 | 0.61 | For soft-shelled turtle; Stone et al. 1992[[13]](#footnote-14) |
| Reptiles - snakes | 25.05 | 0.63 | Gans et al. 1968[[14]](#footnote-15) |

* + 1. Dermal dose through direct spray

Dermal exposure from applied pesticide droplets is considered for the day of application (**Equation 13, Table 9**). The dermal interception model assumes that pesticide deposition occurs in a manner consistent with a horizontal surface in the treatment area. It is assumed that the upper half of the animal in the field is exposed as a result of either ground or aerial spray applications. Therefore, the total surface area of the animal is multiplied by 0.5. The dermal adsorption fraction (DAF) is used to account for pesticide specific data that define a fraction of the pesticide mass present on the animal that is actually absorbed. These data may be submitted by the registrant (non-guideline study) or obtained from the literature. When no data are available to parameterize DAF, the default value is 1. In this equation, a factor of 11.2 is used to convert the units of the application rate, which are lb a.i./A, to the metric units needed to generate a concentration value expressed in µg a.i./g-bw. The dermal equivalency factor (Fred) is described below.

Equation 13.

**Table 9. Parameters Used to Estimate Pesticide dose through Dermal Exposure.**

|  |  |  |
| --- | --- | --- |
| **Symbol** | **Parameter Description** | **Units** |
| Arate | Application rate from label | lb a.i./A |
| BW | Body weight | g/bird |
| Cplant(t) | Concentration of the pesticide in crop foliage at time t | mg/kg |
| DAF | Dermal absorption fraction | none |
| Fdfr | Dislodgeable foliar residue adjustment factor | kg/m2 |
| Fred | Dermal route equivalency factor | none |
| Rfoliar contact | Rate of foliar contact (6.01) | cm2foliage/cm2body surface (per hour) |
| SAtotal | Total surface area of bird | cm2 |

* + 1. Dermal equivalency factor

The dermal route equivalency factor (Fred) is applied to estimated dermal exposures in order to derive an estimate of the equivalent oral dose (**Equation 14**). Chemical-specific dermal LD50 values are rarely available.

For birds, a dermal LD50 can be estimated using **Equation 15** (see **Appendix H** of TIM manual). This equation was derived using relationships between avian dermal and oral toxicity data for 25 chemicals (primarily organophosphate insecticides). Effectively, this equation generates a dermal LD50 that is greater than the oral LD50 (indicating that the dermal route is less toxic). Since avian toxicity data is used as a surrogate for reptiles, this equation will also be applied to reptiles. Since the skin of birds and amphibians is remarkably different (in terms of assumed permeability), this approach will not be applied to amphibians. Instead, it will be assumed that the toxicity of the assessed chemical is equivalent through the dermal and oral routes for terrestrial-phase amphibians (since only avian toxicity data are available, it will be assumed that the oral and dermal toxicity endpoints of a chemical for amphibians are equivalent to the endpoints available for birds). For mammals, dermal toxicity data for rats will be used if available. If not, it will also be assumed that the oral and dermal routes are equivalent.

**Equation 14**.

**Equation 15.**

* + 1. Dermal contact dose

For birds and mammals, dermal contact with foliage is modeled using **Equation 16.** The dermal exposure doses from contact with dislodgeable pesticide residues on treated foliage (*i.e.,* incidental dermal contact dose) is calculated by considering the concentration of pesticide on treated foliage, fraction of total residues that are dislodgeable, the rate of foliar contact of the bird or mammal, the surface area of the bird or mammal that is contacted by dislodgeable foliar residues, and BW of the animal. Cplant is the same residue value used for the broadleaf foliage concentration in the assessment of dietary exposure**.** In this equation, a factor of 0.1 is used to generate Dcontact(t) value with units in µg a.i./g-bw. A default value of 0.62 can be used for the Fdfr (details in TIM manual). The default value for Rfoliar contact is 6.01 cm2 foliage/cm2 body surface (TIM manual). Since this value is on an hourly basis, it is multiplied by 8 in order to generate a dermal dose on a daily time step (assuming that the animal is active for 8 hours a day).The value of 0.079 is used to represent the fraction of the animal that is contacting foliage. This value is based on the fraction of a bird that is represented by its unfeathered feet. It is assumed that this fraction can also be applied to mammals.

Equation 16.

* 1. Inhalation

Similar to dermal exposure, two different routes of exposure through inhalation are considered: inhalation of spray droplets at the time of the application and inhalation of volatilized residues under the crop’s canopy. Also, these does are converted to an oral-equivalent for comparison to oral-based thresholds and toxicity data. This section describes the methods for estimating pesticide doses through inhalation.

* + 1. Spray dose

Inhalation exposure from applied pesticide droplets is considered on the day of the application. The pesticide dose inhaled by the animal in airborne droplets from a spray application is estimated using **Equation 17 (Table 10).** This equation accounts for the pesticide concentration in the volume of air under the release height (Cair(drops)), the volume of air respired by the animal during the time step (Vinhalation) and the fraction of droplets that can be respired (Frespired). These factors considered together result in a mass of pesticide respired by the animal on the day of the application. This number is converted to a dose basis by dividing by the BW of the assessed animal. It is assumed that a suspended droplet will have either settled or cleared from the application area by 60 minutes after application. Therefore, only one hour of inhalation is considered.

**Equation 17.**

**Table 10. Parameters Used to Estimate Pesticide Dose through Inhalation Exposure.**

|  |  |  |
| --- | --- | --- |
| **Symbol** | **Parameter Description** | **Units** |
| Arate | Application rate from label | lb a.i./A |
| Bvol | The volume-based biotransfer factor; function of Henry’s law constant and Log Kow | μg/L fresh weight leaf/ μg/L air |
| BW | Body weight | g/bird |
| Cair(drops) | Pesticide concentration in a volume of air for the time step immediately following the pesticide application | µg/mL |
| Cair(t)(vol) | Concentration of the pesticide in air at time t (resulting from volatilization); function of Mpesticide, mplant, and Bvol | µg/mL |
| CH | Height of crop | m |
| D | Fraction of hour where pesticide is applied | none |
| Dinhalation(t) | Dose through inhalation for a pesticide at time t | µg pesticide/g-bw |
| Dspray(t) | Droplet Inhalation Dose | µg pesticide/g-bw |
| Dvapor(t) | Volatilization inhalation dose; function of pesticide concentration in air, volume of inhaled air, and body weight of the bird | µg pesticide/g-bw |
| FAM | The ratio of avian to mammalian pulmonary membrane diffusion rates from USEPA 2004 | none |
| Fre | The avian route equivalency factor | none |
| Frespired | Volumetric fraction of droplet spectrum not exceeding the upper size limit of respired particles for birds | none |
| H | Henry’s law constant | atm-m3/mol |
| Kow | Octanol-water partition coefficient | none |
| LD50 | Lethal dose sufficient to kill 50% of exposed individuals | mg/kg= µg/g |
| Mpesticide | The pesticide concentration on the treated field at time t (accounting for dissipation); function of application rate | mg |
| mplant | The mass of plant (crop) per hectare based on user input | kg |
| R | Universal gas constant (8.205 e-5) | atm-m3/mol-K |
| RH | Height of spray release | m |
| Rrate | Respiration rate (during a toxicity test) | mL/h |
| T | Air temperature | K |
| Vair | The volume of air in 1 ha to a height equal to the height of the crop canopy | L |
| Vinhalation | Volume of air respired | mL |
| ρplant | The density of the crop tissue assumed as fresh leaf (0.77) | kg/L |

The pesticide concentration in a volume of air (Cair(drops)) for the day of the pesticide application is calculated according to **Equation 18.** This equation uses the application rate of the pesticide (Arate), the release height (RH) of the application and the fraction of the time step where the pesticide is being applied (D). For aerial applications, it is assumed that D = 0.025 based on 90 s duration of direct spray inhalation and for ground spray applications, D = 0.0083 based on 30 s duration of direct spray applications. For ground and aerial applications, RH is assumed to be a constant value of 1 m and 3.3 m, respectively. D (hours) is calculated by dividing the duration of the application (in minutes) by 60 minutes to give a fraction in hours, which is the duration of the time step of interest. In this equation, the factor of 0.112 is used to convert the units of the application rate, which are lb a.i./A, to the metric units needed to generate a concentration value expressed in µg a.i./mL of air.

**Equation 18**.

The size of the spray droplet spectrum that can be inhaled into the lungs is conservatively assumed to be up to 100 μm in diameter. Therefore, the fraction of applied pesticide spray (Frespired) is assumed to be the fraction of the spray droplet spectrum that is ≤100μm. This value varies based on the application scenario of the pesticide being modeled, with variability attributed to nozzle types. **Table 11** includes the default values for Frespired that were determined using the Tier III aerial module of AgDRIFT for aerial and ground spray applications (Teske *et al*., 2001). For airblast applications, droplet spectra are not available in AgDRIFT. Therefore, for airblast applications, a default value of 0.28 is used for Frespired, which is the most conservative value of the droplet spectra included in **Table 11**.

**Table 11. Frespired Values for Different Droplet Spectra for Ground and Aerial Applications.**

|  |  |
| --- | --- |
| **Droplet spectra** | **Frespired** |
| Very fine to fine | 0.28 |
| Fine to medium | 0.067 |
| Medium to coarse | 0.028 |
| Coarse to very coarse | 0.02 |

* + 1. Inhaled air volume (V*inhalation)*

The volume of inhaled air (Vinhalation) in an hour is determined according to **Equation 19.** This incorporates an allometric equation that estimates a respiration rate. Taxa specific parameters are included in **Table 12.** Based on the recommendation of USEPA (1993), this equation includes a factor of three that allows for adjustment of the laboratory derived respiration rate to represent a field respiration rate. Since this equation uses BW values that are in kg, the BW of an animal is divided by 1000 to convert from g to kg. The original equation for respiration rate, as provided in USEPA (1993), generates values in units of mL/minute, which are in turn converted to an hourly time step by multiplying by 60 (min/hour).

**Equation 19**.

**Table 12. Parameters used to calculate inhalation rate for vertebrates (from USEPA 1993).**

|  |  |  |
| --- | --- | --- |
| **Taxa** | **a4** | **b4** |
| Birds | 284 | 0.77 |
| Mammals | 379 | 0.80 |
| Reptiles and amphibians\* | 76.9 | 0.76 |

\*No value is available for amphibians. Parameters for lizards published by Bennett 1973[[15]](#footnote-16) are used.

According to USEPA 1993, amphibians and reptiles have irregular breathing patterns over the course of a day. Variability is due to activity level. Gas exchange also occurs through skin. An equation for an iguanid (from Bennett 1973) is used here. According to the authors, this equation generates higher inhalation rates (and thus more conservative exposures through this route) compared to other reptiles (snakes and turtles).

* + 1. Relating External Inhalation Dose to Oral Dose Equivalents

In cases where inhalation toxicity data are available for the same species for a specific chemical, they may be used to derive the oral dose equivalence factor (Fre) for a taxon using **Equation 20.** Typically, these data will be available for rats, therefore, this approach can be used for mammals.

**Equation 20.** 

Generally, mammalian or avian inhalation toxicity endpoints are expressed as concentration and specific duration based on the exposure period of the test (*e.g.,* 4-hour LC50 in mg a.i./L). The user must convert the LC50 to a dose-based endpoint (*i.e.,* LD50 in mg a.i./kg-bw) using **Equation 21.** It should be noted that the BW and respiration rate used in this equation should be derived based on the test species (BWtest and Rrate(test)). The variable h represents the duration of the exposure period (in hours) and is used to derive the total volume of contaminated air inhaled by the bird during the study. This approach assumes that the animals that died during the study did so after the 4-hour exposure period.

**Equation 21.**

When taxon-specific inhalation toxicity data are not available for birds, the relationship between rat acute oral and acute inhalation LD50 values can be used to establish a route equivalency factor. This factor is applied to avian inhalation dose estimates to calculate an oral dose equivalent exposure for subsequent comparison with oral dose acute toxicity endpoints. Based on pulmonary membrane diffusion rate estimates for birds and mammals, the relative diffusion rates across the pulmonary membrane (FAM) is between 2.4 and 3.4 times greater in birds than in mammals of similar BWs (weight range 1 to 2,000 g; **Table 13**). These differences in diffusion rate can be used to modify the relationship of oral to inhalation toxicity endpoints in mammals to produce a route equivalency factor Fre that would at least account for the expected higher diffusion rates across avian pulmonary membranes (**Equation 22).** Using the oral equivalent dose to describe inhalation exposure allows the available oral toxicity studies to describe potential risks resulting from estimated inhalation exposures. To simplify this approach, the maximum available FAM value (3.4), which generates the most conservative dose, is used for all avian species, regardless of their body weights.

**Equation 22.** 

**Table 13. Respiratory physiology adjustment factors based on BW of assessed species.**

| **Approximate BW (g)** | **FAM** |
| --- | --- |
| 10 | 2.6 |
| 20 | 2.7 |
| 30-50 | 2.8 |
| 60-110 | 2.9 |
| 120-220 | 3.0 |
| 250-500 | 3.1 |
| 550-900 | 3.2 |
| 1000 | 3.3 |
| 2000 | 3.4 |

For reptiles and terrestrial-phase amphibians, the difference in toxicity when comparing the inhalation and oral routes has not been established. Given this lack of knowledge relating reptiles and amphibians to mammals, it will be assumed that the oral and inhalation routes of exposure are equivalent for reptiles and terrestrial-phase amphibians. Therefore, a value of 1 will be used for FRE for reptiles and terrestrial-phase amphibians.

* + 1. Vapor inhalation dose

The on-field dose of volatilized pesticide inhaled by an animal is estimated using **Equation 23.** This equation accounts for the pesticide concentration in air as a result of volatilization from plant leaves (Cair(t)(vol)) and the volume of air respired (Vinhalation), multiplied by 24 to estimate the dose over a 24 hour period. These factors considered together result in a mass of pesticide (mg) respired by the animal over the course of a day. This number is converted to a dose basis by dividing by the BW of the assessed species.

**Equation 23**.

Air concentrations in treated agricultural fields are calculated using a two-compartment model (**Equation 24**). These compartments include the crop foliage and the air that is between the crop canopy and the soil of the treated field. In this equation, t is time in hours and r is the foliar dissipation rate constant of the chemical of interest. The mass of the plant (mplant) per hectare is assumed to be 25,000 kg. The total pesticide mass applied to a 1-ha treated field (Mpesticide; **Equation 25**) combined with dissipation between the time of application and time t are used to estimate the total mass of pesticide available for partitioning between crop leaf and canopy air. The density of the crop tissue (ρplant) assumed to be fresh leaf is 0.77 kg/L, based on the Hazardous Waste Identification Rule (HWIR) Farm Food chain Model (USEPA 1999[[16]](#footnote-17)). The air compartment volume (Vair) is represented by a 1-ha area, with a height set at the top of the canopy at time of application (**Equation 26**). The available pesticide residue is then partitioned between the two compartments (air and leaf mass) through the application of the volume-based biotransfer factor (Bvol) developed for the HWIR model (**Equation 27**). It is assumed that the air temperature (T) is a constant value of 298.1 K (equivalent to 25oC, 77oF). A temperature of 25oC was chosen because Henry’s law constant and octanol-water partition coefficient (Kow) values for pesticides are frequently available at this temperature; however, the relevance to the actual environment at the time of pesticide application is an uncertainty. The total available residues establish an upper limit of available pesticide concentration in the air as a result of volatilization from (treated) leaf surfaces.

**Equation 24**.

**Equation 25.**

**Equation 26.**

**Equation 27.** 

1. Dissipation

After the initial application, the simulated chemical is dissipated from the media of interest. The concentration of a pesticide on that media represents the sum of residues based on the following application and remaining residues from previous applications. The foliar dissipation half-life is used to model dissipation from grass, leaves, seeds, fruit and arthropods. This also impacts pesticide concentrations in vertebrate prey and dermal contact doses. For the earthworm model and puddles, dissipation is based on the aerobic soil metabolism half-life.

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