Chapter 3 – Final Simazine Exposure Characterization

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Environmental Transport and Fate Characterization

The main routes of dissipation for simazine are microbial degradation under aerobic conditions, runoff, and leaching. Because of its persistence and mobility, simazine can move into surface and ground water. Simazine has a low vapor pressure and Henry’s Law Constant (**Table 3-1**), suggesting low potential for volatilization.

Table 3-1. Physical and Chemical Properties of Simazine.

|  |  |
| --- | --- |
| **Property** | **Value** |
| Melting Point (°C) | 225 |
| Molecular Weight (g/mol) | 201.66 |
| Water Solubility@20°C (mg/L) | 5.3 |
| Vapor Pressure@ 20°C (Torr) | 6.1x10-9 |
| Henrys Law Constant (calculated@25°C) (atm-m3 mole-1) | 3.2x10-10 |
| Kow | 122 |

Although the submitted guideline studies for simazine, atrazine, and propazine would indicate that triazines do not degrade by abiotic hydrolysis at pH 5, 7, and 9 (MRID 00027856), open-literature studies show variable acid-catalyzed hydrolysis half-lives for triazines in different matrices including soils, clay suspensions, organic matter, and groundwater (Mabey and Mill, 1978; Hance, 1967; Armstrong et al., 1967; Burkhard and Guth, 1981; Khan, 1978; Widmer et al., 1993; Gamble et al., 1983; Plust et al., 1981; Navarro et al., 2004). A hydrolysis half-life for simazine specifically was observed to be 310 d in non-sterile groundwater at 20 °C and pH of 6.66 (Navarro et al., 2004). The hydrolysis of triazines leads to formation of hydroxytriazine compounds.

Simazine is resistant to direct photodegradation in water (t1/2 > 386 d; MRID 42503708) and to photodegradation on soil (t1/2=132 d; MRID 42739101).

Simazine is moderately persistent to persistent in aerobic loam soils (t1/2 ranges from 80 to 650 days) based on the Goring et al. (1975) classification. Simazine has a half-life of 74 d in aerobic aquatic environments (MRID 43004501, 46561301, 43004502). Simazine is also persistent in anaerobic aquatic environments (t1/2 > 1,766 d) and potentially persistent in anaerobic soil environments as no degradation occurred within a 51-day study duration (MRID 40614411, 00027857).

Soil sorption coefficients for simazine (KF) range from 0.5 to 4.3 mL/g (1/n = 0.79-1.4) (MRID 41442903). Simazine KF values are significantly correlated with soil organic carbon content (r2 = 0.99, p-value = 0.003), indicating that soil organic carbon content is a primary determinant of simazine’s mobility in soil. The average KFOC of 123.25 mL/gOC­ (n = 4; MRID 41442903) indicates a UN Food and Agriculture Organization (FAO) mobility classification of moderately mobile in soil (FAO, 2000).

Field dissipation studies show that simazine dissipation is driven by microbially mediated degradation and by leaching. The half-life of simazine in one terrestrial field study was 36 d in the top 8 inches of soil in bare ground plots in Florida (MRID 40634202). Another study detected simazine 480 d after application in 18 to 24 inches of soil in Nebraska (half-life could not be calculated; MRID 00027863). The half-life in four aquatic field dissipation studies in multiple states ranged from 10 d to stable (MRIDs 00027829, 40614420, 40614421, 40614422). Microbially mediated degradation is an important route of dissipation in the cited aquatic field studies. The half-lives in the terrestrial and aquatic field dissipation studies were often shorter than the half-lives in the laboratory studies, which may be attributed to the availability of multiple routes of dissipation and degradation in the field dissipation studies.

For more details, refer to the Preliminary Ecological Risk Assessment for Simazine (USEPA, 2016a). For a summary of all half-lives used in this assessment, refer to the **Aquatic Modeling Input Parameters Section**.

Identification of Transformation Products of Concern

There are two major types of transformation products for simazine. **Table 3-2** gives the chemical names and structures for simazine transformation products found in laboratory studies. The chlorotriazine transformation products (i.e., DIA, DACT/DDA) are formed through dealkylation of the amino groups. The hydroxytriazine products (i.e., OEET) are formed through substitution of a chlorine by a hydroxy group. Dealkylation is a microbially mediated process, while hydroxylation is both abiotic and microbially mediated. DIA and DDA are also transformation products of atrazine and propazine. Other minor products (<10% of applied a.i.) aside from DDA include deisopropylhydroxyatrazine (DIHA), ammeline, 2-amino-4-ethylamino-6-methoxy-s-triazine (MAET), o-methyl Hydroxysimazine, and 2-chloro-4-ethylamino-6-hydroxyethylamino-s-triazine.

An analysis of the residues of concern is provided in **APPENDIX 1-8**. Based on the analysis of formation and toxicity data on the known transformation products, aquatic modeling of the parent compound alone for each of the triazines is considered adequate for determining potential exposure concentrations to aquatic organisms.

**Table 3-2.** **Chemical Names and Structures for Simazine and Transformation Products.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Name** | **Chemical Name** | **Chemical Formula** | **CAS Reg No.** | **Structure** |
| Simazine (parent) | 6-chloro-N,N’-diethyl-1,3,5-triazine-2,4-diamine | C7H12ClN5 | 122-34-9 |  |
| Deisopropylatrazine (CEAT/DIA/G-28279) | 2-chloro-6-ethylamino-4-amino-s-triazine | C5H8ClN5 | 1007-28-9 |  |
| Hydroxysimazine (OEET/HS/G-30414) | bis(ethylamino)-1,3,5-triazin-2-ol | C7H13N5O | 2599-11-3 |  |
| Diadealkylatrazine (CAAT/DACT/DDA/  GS-28273) | chlordiamino-s-triazine | C3H4ClN5 | 3397-62-4 |  |
| Deisopropylhydroxyatrazine (OIAT/DIHA/GS-17792) | 2-hydroxy-6-ethylamino-4-amino-s-triazine | C5H9N5O | 7313-54-4 |  |
| Ammeline (OAAT/GS-17791) | 4,6-diamino-2,5-dihydro-1,3,5-triazin-2-one | C3H5N5O | 645-92-1 |  |
| G-28516 | 2-chloro-4-ethylamino-6-hydroxyethylamino-s-triazine | C3H9ClN5O | – |  |
| MAET (G-31709) | 2-amino-4-ethylamino-6-methoxy-s-triazine | C6H11N5O | 30360-56-6 |  |
| o-methyl hydroxysimazine (G-30044) | N2,N4-diethyl-6-methoxy-1,3,5-triazine-2,4-diamine | C8H15N5O | 673-04-1 |  |

Measures of Aquatic Exposure

In general, maximum application rates and minimum application retreatment intervals are modeled to estimate the exposure to simazine based on the use summary table (**APPENDIX 1-3**) developed for simazine, unless otherwise noted.

Simazine-specific modeling scenarios are used for modeling each use. This includes the selection of scenarios and agronomic practices (e.g., applications methods, dates). Table 3-6 includes model input parameters as well as the justification for selecting these parameters; however, the general approaches used are described below.

Aquatic Exposure Models

Aquatic exposures (surface water and benthic sediment pore water) are quantitatively estimated for representative simazine uses included on the use summary table (**APPENDIX 1-3**) by HUC 2 Regions (**Figure 3-1**) and by aquatic bin (2-7) using the Pesticide Root Zone Model (PRZM5) coupled to the Variable Volume Water Model (VVWM)[[1]](#footnote-2) in the Pesticides in Water Calculator (PWC). As mentioned elsewhere, the flowing aquatic bins include bin 2 (low flow), bin 3 (moderate flow), and bin 4 (high flow). The static aquatic bins include bin 5 (low volume), bin 6 (moderate volume), and bin 7 (high volume). Additional information on aquatic bins is available in **ATTACHMENT 1-2**. Aquatic bin 1 represents aquatic habitats associated with terrestrial habitats (e.g., riparian zones, seasonal wetlands) and is simulated using the PRZM5/VVWM and the Plant Assessment Tool (**Section 3.5**). Aquatic bins 8 and 9 are intertidal and subtidal near shore habitats, respectively, and aquatic bin 10 is the offshore marine habitat. EFED does not currently have standard conceptual models designed to estimate EECs for these estuarine/marine systems. EFED and the Services have assigned surrogate freshwater flowing or static systems to evaluate exposure for these estuary and marine bins. Aquatic bin 5 will be used as surrogate for pesticide exposure to species in tidal pools; aquatic bins 2 and 3 will be used for exposure to species at low and high tide, and aquatic bins 4 and 7 will be used to assess exposure to marine species that occasionally inhabit offshore areas.

EFED modeled these flowing and static bins in previous Biological Evaluations (BEs) by using watershed drainage areas developed from flowing waterbody relationships and static bin runoff estimates (USEPA, 2016b; USEPA, 2016c; USEPA, 2016d). However, the results have not been as expected. In short, one would expect daily concentrations in flowing bins to be lower than those in static bins, given that water, and any pesticide, is flowing out of the system. However, in most of the modeling runs, the EECs for the flowing bins were higher, and in many cases an order of magnitude higher, than the static bins. In large part, the higher EECs were the result of modeling a large watershed using assumptions that were designed to simulate a smaller watershed. For example, it was assumed that the watershed was entirely treated on the same day. For a large watershed, it is not expected that this assumption is appropriate. For the static waterbodies, the watershed-to-waterbody ratio was not really known but was derived by determining the watershed size needed to generate runoff sufficient to fill the waterbody. This relationship relied on modeling conducted using topography, surface soil characteristics, and precipitation specific to the PWC model and scenarios considered highly vulnerable to surface water runoff. As a result, there was much uncertainty with the EECs that were being generated from the modeling in the previously completed BEs.

For simazine, EFED has relied on two standard waterbodies which have been traditionally used in EFED to estimate EECs for the various bins. The standard farm pond was used to develop EECs for the medium and large static bins (e.g., bins 6 and 7) and the index reservoir for the medium and large flowing bins (e.g., bins 3 and 4). For the smallest flowing and static bins (bin 2 and 5), EFED derived edge of field estimates from the PRZM daily runoff file (e.g., ZTS file). **Table 3-3** provides a crosswalk of the bins and how they were modeled. While the standard farm pond is bigger than bin 6, the EECs estimated for bin 6 in previous BEs were similar to those generated for bin 7, and so an economy of modeling was deemed appropriate. While the index reservoir has a much lower effluent flowrate than bins 3 and 4, it has been used as a vetted flow-through waterbody for EFED for years, with an accepted watershed-to-waterbody ratio developed for an actual vulnerable watershed (Shipman Reservoir, Shipman, IL) and has been reviewed by a previous Federal Insecticide Fungicide Rodenticide Act (FIFRA) Scientific Advisory Panel (SAP) (Jones et al, 1998). EFED expects the EECs that are generated using the index reservoir to be a conservative surrogate for those observed in bins 3 and 4. The watershed area associated with the index reservoir is roughly an order of magnitude smaller than the average area for a HUC 12 (the smallest areal delineation for an aquatic species range), but within the range of minimum and maximum values (9.54x107 m2, 2.08x103 – 9.24x109 m2). Lastly, bins 2 and 5 are very small waterbodies and the EECs in them would be reflective of concentrations in a headwater stream or a standing puddle that received runoff at the edge of a treated field. As such, edge-of-field concentrations were estimated and used as a surrogate for EECs in these waterbodies.

For bin 1, a wetland the size of the standard farm pond (1 ha) is modeled receiving runoff from a 10-ha field. The depth of the wetland varies from 0.5 to 15 cm, simulating the potential for the wetland to fill up and dry down, and is simulated in PRZM/VVWM using the varying volume and flow through model. The sediment layer is increased from the standard 5 cm to 15 cm to represent the typical active root zone for wetland species of forbs and woody plants. The wetland is simulated in PRZM/VVWM using the variable volume. The results of the wetland modeling are then processed in the Plant Assessment Tool (**Section 3.5**)

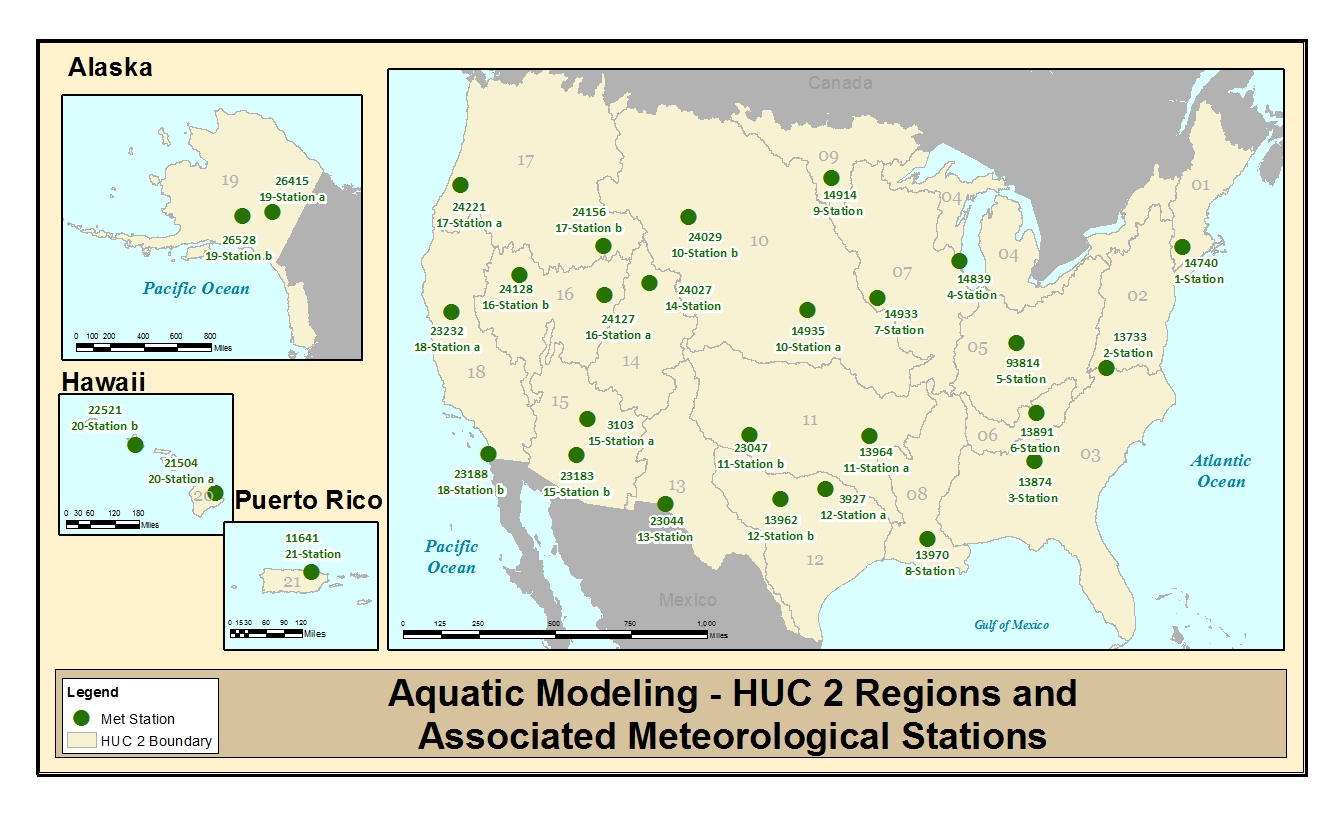
Table 3-. Aquatic Bin, Modeled Waterbody Crosswalk.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Aquatic Bin** | **Description** | **Width (m)** | **Length (m)** | **Depth (m)** | **Flow (m3/s)** | **Waterbody Used for Modeling** |
| 1 | Wetland | 64 | 157 | 0.15 | Variable1 | Custom |
| 2 | Low-flowing waterbody | 2 | Field2 | 0.1 | 0.001 | Edge-of-field |
| 3 | Medium-flowing waterbody | 8 | Field2 | 1 | 1 | Index reservoir |
| 4 | High-flowing waterbody | 40 | Field2 | 2 | 100 | Index reservoir |
| 5 | Low-volume, static waterbody | 1 | 1 | 0.1 | N/A | Edge-of-field |
| 6 | Medium-volume, static waterbody | 10 | 10 | 1 | N/A | Farm pond |
| 7 | High-volume, static waterbody | 100 | 100 | 2 | N/A | Farm pond |

1 The depth and flow rate in this waterbody is variable, depending on rainfall.

2 The habitat being evaluated is the reach or segment that abuts or is immediately adjacent to the treated field. This habitat is assumed to run the entire length of the treated area.

More detailed information can be found in **ATTACHMENT 3-1. Background Document Aquatic Exposure Estimation for Endangered Species**.

Figure 3-1. Hydrologic Unit Code (HUC) 2-Digit Regions and Associated Metrological Data.

HUC and Use Site Crosswalk

The National Agricultural Statistics Census of Agriculture 2012 (NASS) data along with the Cropland Data Layer (CDL) were used to determine which crops would be modeled within each represented HUC 2. Additionally, specific geographic limitations on how a product may be applied to particular crops were considered when determining what rates would be simulated for different HUC 2 regions. If the NASS data indicated any acreage of a crop was grown in a specific HUC 2, it was assumed that the crop was grown in that HUC 2, and aquatic EECs were generated for these HUC 2 regions for that crop. If there were no reported NASS cropped acres grown within a particular HUC 2, aquatic EECs for that HUC 2 region and use pattern were not determined. A crop use layer-HUC 2 region matrix for simazine is provided in **APPENDIX 3-1**.

Scenario Selection

A PWC scenario was developed for each landcover class and HUC 2 where crops in that landcover were grown based on the NASS 2012 census data. A PWC-scenario was not developed for cranberry because it was simulated using PFAM. **APPENDIX 3-1** provides a crosswalk between the use site and the landcover used to represent the use site as well as which HUC 2 regions were evaluated for each use pattern. An explanation of how the PWC scenario matrix was developed is provided in **ATTACHMENT 3-1**.

Application Practices

Application Method

During application of pesticides, methods of application as well as product formulation used by an applicator can impact the magnitude of off-site transport of the active ingredient. Label directions (such as spray drift buffers, application equipment, and droplet size restrictions) as well as product formulation are considered as part of the development of the use scenario modeled.

There are several different types of simazine applications included in the use summary table (**APPENDIX 1-3**) including those that occur in both agricultural and non-agricultural settings. Simazine applications may occur at different times throughout the year including multiple applications to the same crop. When multiple types of applications are allowed on a crop within one calendar year, all applications are simulated considering the appropriate application timing (*e.g.*, dormant, foliar, and post-harvest applications to a crop) and label directions. Simazine can be applied as a liquid for all crops.

Spray Drift

Current labels for simazine include spray drift language that specifies a 66 ft buffer on the point of runoff to streams and a 200 ft buffer on lakes, reservoirs, or other impounded natural waterbodies. The registrant has committed to additional 15 ft ground buffers on streams, rivers, estuarine/marine environments, and endangered species habitats. This results in 81 ft stream buffers, 200 ft buffers on ponds, and 15 ft ground buffers for the wetland (assuming endangered species habitat for this assessment). Aerial applications are not allowed for simazine. For a tabulated summary of the buffers, see **Table 3-4**.

Table 3-. Label and Committed Spray Drift Buffers.

|  |  |
| --- | --- |
| **Buffer Description** | **Ground Application**  **Buffer Distance (ft)** |
| Streams (existing) | 66 |
| Lakes/Reservoirs (existing) | 200 |
| Streams, Rivers, and E/M1 (committed) | 15 ft |
| Endangered species | 15 ft |
| Total stream | 81 ft |
| Total pond | 200 ft |
| Total wetland | 15 ft |

1 E/M = estuarine and marine

The registrants also committed to requiring coarse to ultra-coarse droplet sizes, which was modeled in AgDRIFT using “fine to medium/coarse” for ground applications. See **Table 3-5** for a summary of spray drift fractions in each bin. For applications that would not be expected to result in spray drift (e.g., microsprinkler), no drift was modeled (i.e., drift fraction is zero).

Table 3-. Estimated Spray Drift Fractions for Different Aquatic Bins and Application Methods.

|  |  |  |  |
| --- | --- | --- | --- |
| **Aquatic Bin** | **Depth (m)** | **Width (m)** | **Ground App. Spray Drift Fraction**  **(unitless)** |
| 1 | 0.15 | 64 | 0.0082 |
| 41 | 2.74 | 82 | 0.0051 |
| 7 | 2 | 64 | 0.0028 |

1 Drift fraction for this waterbody also takes into account spray drift entering a 4 m wide stream which enters the waterbody.

The use of handheld application equipment is not expected to result in substantial drift. All crops permit the use of ground boom equipment and such higher-drift (and presumably higher-exposure) application methods were chosen as conservative proxies for all alternate application methods for the relevant crops, for purposes of quantitative exposure estimation.

Application Timing

In selecting application dates for aquatic modeling, EPA considers a number of factors including label directions, timing of pest pressure, meteorological conditions, and pre-harvest restriction intervals. Agronomic information was consulted to determine the timing of crop emergence, pest pressure and seasons for different crops. General sources of information include crop profiles (<https://ipmdata.ipmcenters.org/#cropprofiles>), agricultural extension bulletins, and/or available state-specific use information.

Simazine may be applied during different seasons and the directions for use indicate the timing of application*.* For most uses, PWC model inputs for the application dates were chosen based on these timings, the crop emergence and/or harvest timings, and precipitation data for the associated meteorological station. Application dates were selected to represent conservative and reasonable estimates. When choosing an application date within a time window, the 15th of the month with the highest amount of precipitation (for the meteorological station for the PWC scenario) for that time window was chosen as pesticide loading to surface water is directly affected by precipitation events. Once the first day of application was selected, minimum retreatment intervals were assumed to determine when subsequent applications would occur. If multiple types of applications were allowed on one crop within one year, such as pre-plant along with a foliar application(s), the retreatment interval was selected to reflect the specified timings. Pre-harvest intervals (the minimum time between an application and harvest) were also considered when appropriate. For details on application date selection, see **APPENDIX 1-3** and **APPENDIX 3-1**.

Special Agricultural Considerations

Multiple Crop-cycles Per Year

Some state-specific labels permit applications on crops that may be planted in rotation (e.g., various vegetables), or that may be grown in multiple crop seasons per year. This phenomenon could result in more simazine applied to a given field per year, than would necessarily be expected based upon label instructions. While crop rotations are possible for some uses, rotations were not modeled.

PFAM

To determine EECs for cranberry uses, EFED used the Pesticides in Flooded Applications Model (PFAM, version 2.0). PFAM was developed specifically to estimate exposure to pesticides used in flooded agriculture, such as cranberry bogs. The model simulates two linked compartments when the field is flooded: a water column and a sediment zone (benthos). Each compartment is completely mixed and at internal equilibrium with respect to sorption of the chemical (Young, 2013). Pesticide moves between the compartments via a time-limited, first-order mass-transfer process. The model accounts for hydrolysis, photolysis, and metabolism in water, sediment, and soil (when no water is present), sorption, and volatilization. The model considers the environmental fate properties of pesticides and allows for the specification of common management practices associated with flooded agriculture, such as scheduled flooding and water releases. Water, sediment, and pesticide may flow out of the flooded field, particularly upon deliberate water release. Changes in water body conditions (temperature, water levels, wind speed, etc.) and resulting changes in degradation rates are simulated on a daily time step. Pesticide application and flooding sequences are mapped onto the time series in 1-year cycles for the duration of a 30-year simulation.

Cranberries may be grown in bogs that are temporarily, deliberately flooded to control pests, prevent freezing, and/or to facilitate harvest. After flooding, water may be held on site, recirculated to other cranberry growing areas, or released to adjacent waterbodies (rivers, streams, lakes, etc.). For cranberries, a 12-inch flood was modeled on October 15, followed by draining of the bog on October 18. The modeled flood date was selected as a plausible date of harvest. A winter flood from December 15 to March 15 was also simulated.

Modeling results from PFAM relate to a very specific use pattern for applications to cranberry in MA, OR, and WA only. Cranberry bogs could serve as a habitat for amphibians or may serve as a food source for listed birds and mammals that rely on aquatic organisms. However, EECs modeled with aquatic and wetland bins using PWC for other berries with simazine use encompass the EECs from use on cranberries. Additionally, species that are anticipated to utilize cranberry bogs would be captured in the wetland bin, which generates higher EECs than cranberries. Therefore, output from PFAM is not included in the effects determination exposure values but included for characterization.

Plant Assessment Tool (PAT)

The Plant Assessment Tool (PAT) employs mechanistic representations of fate (e.g., degradation) and transport (e.g., runoff), using data that are typically available for pesticides, to model runoff and spray drift exposure to terrestrial and wetland environments. For terrestrial plants, runoff and erosion are modeled using PRZM and spray drift is modeled using AgDRIFT deposition values. The model uses a mixing cell approach to represent water within the active root zone area of soil, and accounts for flow through the terrestrial plant exposure zone (T-PEZ) caused by both treated field runoff and direct precipitation onto the T-PEZ. Pesticide losses from the T-PEZ occur from transport (i.e., washout and infiltration below the active root zone) and degradation. Wetlands are modeled using PRZM/VVWM and are then processed in PAT to estimate aquatic (mass per volume of water) and terrestrial (mass per area) concentrations. Aquatic plants exposure is modeled using the PRZM/VVWM models and the standard farm pond.

Non-Agricultural Uses and Considerations

The only non-agricultural use of simazine is turf for fairways, lawns, and similar areas. Simazine can be applied by ground equipment only. Exposure from the residential turf use is modeled using the urban conceptual model used in previous assessments, including the pyrethroids registration review assessment (USEPA, 2016e, DP Barcode 429641) and is outlined in the following section.

* + 1. Exposure from Residential Turf Use

The EPA residential conceptual model is based on a house on a fenced quarter acre lot with a driveway leading to the street (**Figure 3-2**). Different parts of the lot are modeled using impervious, residential, or right-of-way PWC scenarios. The results of each scenario are weighted according to the ratio expected for a given use profile. Residential simazine use is only on turf. The lot is 10,816 ft2 (104 ft x 104 ft), with a 1000 ft2 (31.6 ft x 31.6 ft) house, 1200 ft2 garden, 375 ft2 (25 ft x 15 ft) driveway, and 1000 ft2 other untreated areas (patio, garbage cans, etc.). Subtracting these features from the lot results in 7,241 ft2 that is assumed to be treated turf and modeled with the residential PWC scenario. Additionally, 2 ft of overapplication is assumed at the turf application rate onto the length of the driveway (25 ft) on each side and modeled as 100 ft2 of the lot using the impervious PWC scenario. It is assumed that no overspray to the street occurs due to the fence line. In total, this results in the residential turf scenario covering 66.9% of the lot and impervious scenario covering 0.9% of the lot. The remaining 32.2% of the lot are untreated and there are no right-of-way exposure pathways (e.g., fence over pervious surfaces).

An estimate of the number of residential lots in a 10-ha watershed has been previously evaluated for California Red-legged Frog (CRLF) and other endangered species assessments (i.e., Appendix G of USEPA 2009a). The assumption previously made was 58 lots arranged in 10 lot blocks, resulting in an additional adjustment factor of 0.587. This additional adjustment factor was not incorporated in this assessment, resulting in a conservative estimate of exposure from residential use.

A screenshot of a cell phone

Description automatically generated

Figure 3-2. Residential Exposure Conceptual Model.

Aquatic Modeling Input Parameters

The following sections discuss methods used for aquatic modeling. Summaries of the environmental fate model input parameters used in the PWC for aquatic modeling is presented inTable 3-6. Input parameters are selected in accordance with the following EPA guidance documents:

* Guidance for *Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides*, Version 2.1[[2]](#footnote-3) (USEPA, 2009),
* *Guidance for Evaluating and Calculating Degradation Kinetics in Environmental Media[[3]](#footnote-4)* (NAFTA, 2012; USEPA, 2012b), and
* *Guidance on Modeling Offsite Deposition of Pesticides Via Spray Drift for Ecological and Drinking Water Assessmen*t[[4]](#footnote-5) (USEPA, 2013)

Table 3-. Input Values Used for Tier II Surface Water Modeling with PWC.

| **Parameter** | **Estimated Values** | **EFED Modeling**  **Value** | **Source/Comment** |
| --- | --- | --- | --- |
| Soil sorption coefficient (Koc) (mL/goc) | 123 | 123 | MRID 41257905 |
| Aerobic aquatic metabolism half-life, 25 °C (days) | 74.4 | 223 | MRID 43004502  **Value is 3x the half-life of a single system** |
| Anaerobic aquatic metabolism half-life, 25 °C (days) | 666 | 1999 | MRID 40614411  **Value is 3x the half-life of a single system** |
| Aqueous photolysis half-life, 40 °N (days) | Stable | Stable (0) | MRID 42503708 |
| Hydrolysis half-life, 20 °C (days) | Stable | Stable (0) | MRID 00027856 |
| Aerobic soil metabolism half-life, 25 °C (days) | 126, 991, 88.9 | 119 | MRID 00158638  MRID 43004501  MRID 46561301  **90th percentile confidence bound on the mean2**  (SD=13.6, t90,n-1= 1.886, n=3) |
| Molecular weight (g/mol) | 201.7 | 201.7 | Simazine RED |
| Vapor pressure, 20 °C (torr) | 6.1 x 10-9 | 6.1 x 10-9 | MRID 00023955 |
| Water solubility, 25 °C (mg/L) | 3.5 | 3.5 | MRID 00023955 |
| Foliar degradation half-life (days) | n/a | Stable (0) | Input parameter guidance (USEPA, 2009) |
| Application efficiency | n/a | Aerial: 0.95  Ground: 0.99  Granular: 1.0 | Input parameter guidance (USEPA, 2009) |
| Drift fraction | n/a | See 3.4.2 |  |
| n/a = estimated values from study data are not applicable  1 Temperature corrected from 20 °C to 25 °C  2 tinput = average t1/2 + [t90,n-1 \* SD/sqrt(n)] | | | |

Aquatic Modeling Results

The estimated environmental concentrations (EECs) derived from the PWC modeling based on maximum labeled rates included in the master use summary document, by HUC 2, are summarized for the various aquatic bins in **Table 3-7** and **Table 3-8**, for water column and pore water, respectively. The complete set of modeling inputs and results are available in **APPENDIX 3-1**. PWC runs and post-processed results are provided in **APPENDIX 3-2**. The range of EECs reflects the various application rates and timings for the various crops and scenarios modeled in the HUC 2 regions.

Table 3-. The Range of PWC Daily Average Water Column EECs for Simazine.

| **HUC 2** | **Range of 1-in-15 year Daily Average EECs (µg/L)** | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Bin 1** | **Bin 2** | **Bin 3** | **Bin 4** | **Bin 5** | **Bin 6** | **Bin7** |
| HUC 1 | 52 - 307 | 115 - 1140 | 28 - 113 | 28 - 113 | 115 - 1140 | 30 - 140 | 30 - 140 |
| HUC 2 | 59 - 366 | 108 - 1146 | 27 - 116 | 27 - 116 | 108 - 1146 | 19 - 78 | 19 - 78 |
| HUC 3 | 70 - 670 | 110 - 1674 | 42 - 253 | 42 - 253 | 110 - 1674 | 41 - 257 | 41 - 257 |
| HUC 4 | 53 - 478 | 111 - 1598 | 26 - 111 | 26 - 111 | 111 - 1598 | 21 - 129 | 21 - 129 |
| HUC 5 | 47 - 429 | 114 - 1196 | 26 - 177 | 26 - 177 | 114 - 1196 | 16 - 153 | 16 - 153 |
| HUC 6 | 59 - 440 | 110 - 1837 | 24 - 209 | 24 - 209 | 110 - 1837 | 18 - 222 | 18 - 222 |
| HUC 7 | 55 - 709 | 109 - 1251 | 17 - 141 | 17 - 141 | 109 - 1251 | 10 - 135 | 10 - 135 |
| HUC 8 | 61 - 646 | 116 - 2004 | 34 - 221 | 34 - 221 | 116 - 2004 | 25 - 195 | 25 - 195 |
| HUC 9 | 116 - 760 | 130 - 856 | 31 - 128 | 31 - 128 | 130 - 856 | 27 - 113 | 27 - 113 |
| HUC 10a | 70 - 862 | 115 - 883 | 18 - 137 | 18 - 137 | 115 - 883 | 10 - 137 | 10 - 137 |
| HUC 10b | 140 - 701 | 99 - 882 | 20 - 104 | 20 - 104 | 99 - 882 | 11 - 88 | 11 - 88 |
| HUC 11a | 67 - 590 | 104 - 1351 | 39 - 251 | 39 - 251 | 104 - 1351 | 26 - 207 | 26 - 207 |
| HUC 11b | 115 - 1280 | 113 - 1416 | 24 - 240 | 24 - 240 | 113 - 1416 | 15 - 160 | 15 - 160 |
| HUC 12a | 66 - 829 | 112 - 1347 | 24 - 156 | 24 - 156 | 112 - 1347 | 17 - 138 | 17 - 138 |
| HUC 12b | 76 - 1130 | 104 - 1294 | 24 - 212 | 24 - 212 | 104 - 1294 | 18 - 168 | 18 - 168 |
| HUC 13 | 168 - 670 | 90 - 1205 | 10 - 111 | 10 - 111 | 90 - 1205 | 5.2 - 86 | 5.2 - 86 |
| HUC 14 | 272 - 1300 | 105 - 1309 | 18 - 130 | 18 - 130 | 105 - 1309 | 8.5 - 94 | 8.5 - 94 |
| HUC 15a | 73 - 655 | 111 - 1769 | 14 - 134 | 14 - 134 | 111 - 1769 | 12 - 135 | 12 - 135 |
| HUC 15b | 117 - 945 | 112 - 1893 | 13 - 213 | 13 - 213 | 112 - 1893 | 6.4 - 121 | 6.4 - 121 |
| HUC 16a | 148 - 1230 | 112 - 1958 | 16 - 147 | 16 - 147 | 112 - 1958 | 10 - 83 | 10 - 83 |
| HUC 16b | 125 - 502 | 113 - 1634 | 7.8 - 59 | 7.8 - 59 | 113 - 1634 | 4.6 - 30 | 4.6 - 30 |
| HUC 17a | 56 - 526 | 111 - 1037 | 28 - 249 | 28 - 249 | 111 - 1037 | 38 - 389 | 38 - 389 |
| HUC 17b | 137 - 1070 | 100 - 913 | 7.1 - 128 | 7.1 - 128 | 100 - 913 | 3.7 - 72 | 3.7 - 72 |
| HUC 18a | 62 - 579 | 114 - 1754 | 29 - 170 | 29 - 170 | 114 - 1754 | 23 - 107 | 23 - 107 |
| HUC 18b | 146 - 488 | 111 - 1783 | 15 - 146 | 15 - 146 | 111 - 1783 | 7.8 - 93 | 7.8 - 93 |

Table 3-. The Range of PWC Pore Water EECs for Simazine.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **HUC 2** | **Range of 1-in-15 year Pore Water EECs (µg/L)** | | | | | |
| **Bin 21** | **Bin 3** | **Bin 4** | **Bin 51** | **Bin 6** | **Bin7** |
| HUC 1 | 116 - 1162 | 18 - 738 | 18 - 738 | 116 - 1162 | 24 - 281 | 24 - 281 |
| HUC 2 | 108 - 1346 | 19 - 263 | 19 - 263 | 108 - 1346 | 16 - 135 | 16 - 135 |
| HUC 3 | 110 - 1678 | 21 - 1143 | 21 - 1143 | 110 - 1678 | 29 - 278 | 29 - 278 |
| HUC 4 | 111 - 1599 | 15 - 430 | 15 - 430 | 111 - 1599 | 17 - 141 | 17 - 141 |
| HUC 5 | 115 - 1219 | 16 - 348 | 16 - 348 | 115 - 1219 | 14 - 162 | 14 - 162 |
| HUC 6 | 111 - 1844 | 17 - 397 | 17 - 397 | 111 - 1844 | 16 - 246 | 16 - 246 |
| HUC 7 | 110 - 1368 | 16 - 349 | 16 - 349 | 110 - 1368 | 8.9 - 166 | 8.9 - 166 |
| HUC 8 | 116 - 2012 | 18 - 910 | 18 - 910 | 116 - 2012 | 18 - 362 | 18 - 362 |
| HUC 9 | 133 - 1051 | 19 - 185 | 19 - 185 | 133 - 1051 | 22 - 95 | 22 - 95 |
| HUC 10a | 115 - 906 | 15 - 257 | 15 - 257 | 115 - 906 | 8.6 - 119 | 8.6 - 119 |
| HUC 10b | 100 - 890 | 17 - 130 | 17 - 130 | 100 - 890 | 9.1 - 72 | 9.1 - 72 |
| HUC 11a | 104 - 1366 | 22 - 842 | 22 - 842 | 104 - 1366 | 21 - 291 | 21 - 291 |
| HUC 11b | 113 - 1430 | 19 - 192 | 19 - 192 | 113 - 1430 | 14 - 124 | 14 - 124 |
| HUC 12a | 112 - 1361 | 17 - 556 | 17 - 556 | 112 - 1361 | 14 - 212 | 14 - 212 |
| HUC 12b | 104 - 1303 | 19 – 343 | 19 - 343 | 104 - 1303 | 14 - 160 | 14 - 160 |
| HUC 13 | 90 - 1214 | 7.3 - 106 | 7.3 - 106 | 90 - 1214 | 3.7 - 79 | 3.7 - 79 |
| HUC 14 | 105 - 1323 | 15 – 117 | 15 - 117 | 105 - 1323 | 7.7 - 77 | 7.7 - 77 |
| HUC 15a | 111 - 1772 | 10 – 112 | 10 - 112 | 111 - 1772 | 11 - 122 | 11 - 122 |
| HUC 15b | 113 - 1917 | 10 – 151 | 10 - 151 | 113 - 1917 | 5.2 - 90 | 5.2 - 90 |
| HUC 16a | 112 - 1961 | 12 – 106 | 12 - 106 | 112 - 1961 | 7.9 - 64 | 7.9 - 64 |
| HUC 16b | 113 - 1636 | 6.1 – 51 | 6.1 - 51 | 113 - 1636 | 3.8 - 26 | 3.8 - 26 |
| HUC 17a | 113 - 1058 | 16 – 131 | 16 - 131 | 113 - 1058 | 33 - 321 | 33 - 321 |
| HUC 17b | 100 - 936 | 5.4 – 94 | 5.4 - 94 | 100 - 936 | 3.0 - 57 | 3.0 - 57 |
| HUC 18a | 114 - 1757 | 17 – 105 | 17 - 105 | 114 - 1757 | 18 - 90 | 18 - 90 |
| HUC 18b | 111 - 1786 | 10 – 108 | 10 - 108 | 111 - 1786 | 6.1 - 72 | 6.1 - 72 |
| 1 Pore water concentrations for bins 2 and 5 have been estimated using edge-of-field runoff from the dissolved and eroded soil amounts from the ZTS file. | | | | | | |

Currently EFED models flowing waterbodies in its FIFRA assessments using the index reservoir, a waterbody with a surface area of 5.26x105 m2 and a depth of 2.74 m, with a watershed area of 1.728x106 m2. This conceptual model is based upon the Shipman Reservoir in Illinois and has been reviewed by EPA’s FIFRA SAP. Although the dimensions are smaller than those of a bin 3 or 4 and the flowrate is much lower, EFED has confidence in the estimated concentrations developed using the index reservoir and believes these EECs can be used as a conservative surrogate for bins 3 and 4 until EFED can validate a conceptual model for bins 3 and 4.

Simulations for wet-harvested cranberry growing areas resulted in similar EECs. PFAM results included 1-in-10 year daily average EECs of 13.8 to 809 µg/L for concentrations of simazine in cranberry bogs. These EECs are within the range of EECs generated using PWC for various HUC 2 regions and aquatic bins.

Available Monitoring Data

Examination of the EPA 303(d) list of impaired waters[[5]](#footnote-6) on August 5, 2020, indicates 4 waterbody impairments caused by simazine in California rivers and streams.

Water monitoring data were obtained from the National Water Quality Monitoring Council’s Water Quality Data Portal (USEPA and USGS, 2013), which is supplied by the USGS NWIS and EPA STORET databases of monitoring data collected across the United States by numerous federal, state, tribal and local agencies. Prominent contributors to this database include the USGS National Water-Quality Assessment Program (NAWQA) and various state and local agencies.

In general, the surface water monitoring data include sampling sites that represent a range of aquatic environments including small and large water bodies, rivers, reservoirs, and urban and agricultural locations, but are limited for some areas of the United States where simazine use occurs. Also, the sampling sites, as well as the number of samples, vary by year. The vulnerability of the sampling site to simazine contamination varies substantially due to use, soil characteristics, weather and agronomic practices. It is unlikely that the monitoring programs in the Water Quality Portal were specifically designed to target simazine use. Therefore, peak concentrations of simazine likely went undetected in these programs. Overall, the extent to which historical values represent current agronomic or labeled use instructions is uncertain.

While there are many individual samples collected and analyzed for simazine across the United States, it would not be appropriate to combine these data sources to generate exposure estimates or to use these datasets to represent exposure on a national or even regional basis. While these data demonstrate potential exposure, using the measured concentrations as an upper bound exposure estimate would not be a reasonable approach for the reasons given above, including limited sample frequency, limited use information, and sampling site variability, on a national or even a regional basis. Therefore, model estimated concentrations should be considered a suitable upper bound concentration for simazine.

Water Quality Portal

Comprehensive surface and ground water simazine data were obtained in June 2020 in a download of data from the Water Quality Data Portal (<http://www.waterqualitydata.us/>). **Table 3-9** provides a summary of the results by HUC 2 region, with sampling occurring from 1975 to 2020 at almost 14,400 sites in every HUC 2 region. As this summary includes historical data, detections in HUCs 19-22 are not unexpected despite recent updates to the labels.

Table 3-. Water Quality Portal Monitoring Data Summarized by HUC-2 for Simazine.

| **HUC-21** | **Years** | **Number of Sites** | **Number of Samples** | **Number of Samples Labeled Non Detections** | **Measured Detection Range (µg/L)** |
| --- | --- | --- | --- | --- | --- |
| 1 | 1976 - 2019 | 144 | 1348 | 1155 | 0 - 0.69 |
| 2 | 1976 - 2020 | 1409 | 8725 | 4779 | 0 - 1080 |
| 3 | 1976 - 2020 | 1867 | 12891 | 7587 | 0 - 145.3 |
| 4 | 1976 - 2020 | 744 | 5118 | 2723 | 0 - 13.3 |
| 5 | 1976 - 2020 | 693 | 7864 | 3136 | 0 - 25 |
| 6 | 1976 - 2019 | 93 | 1145 | 497 | 0 - 0.7 |
| 7 | 1976 - 2020 | 2245 | 32534 | 29154 | 0 - 119 |
| 8 | 1975 - 2020 | 495 | 5801 | 2646 | 0 - 20.6 |
| 9 | 1976 - 2019 | 341 | 1612 | 1558 | 0 - 0.24 |
| 10 | 1976 - 2020 | 1949 | 26405 | 23427 | 0 - 623 |
| 11 | 1976 - 2020 | 922 | 11097 | 9698 | 0 - 22 |
| 12 | 1976 - 2020 | 371 | 3768 | 1648 | 0 - 11.2 |
| 13 | 1976 - 2019 | 253 | 1598 | 1435 | 0 - 0.67 |
| 14 | 1976 - 2020 | 194 | 1053 | 1023 | 0 - 0.065 |
| 15 | 1976 - 2019 | 113 | 1107 | 779 | 0 - 10 |
| 16 | 1976 - 2020 | 231 | 1388 | 1271 | 0 - 0.13 |
| 17 | 1976 - 2020 | 1281 | 14687 | 10550 | 0 - 13 |
| 18 | 1976 - 2020 | 971 | 6305 | 3005 | 0 - 290 |
| 19 | 1976 - 2019 | 9 | 82 | 82 | — |
| 20 | 1976 - 2017 | 60 | 139 | 125 | 0 - 3.3 |
| 21 | 1976 - 2013 | 5 | 37 | 37 | — |
| 22 | 2011 - 2012 | 3 | 4 | 4 | — |

1 Note that historical monitoring data does not reflect updates to labels or commitment letters (for example, data in HUCs 19-22)

Aquatic Exposure Summary

Model-derived EECs represent an upper bound on potential exposure as a result of the use of simazine. Comparing the concentrations in the medium and high flowing and static bins (3, 4, 6, and 7) to the highest measured concentrations, the modeled values are roughly the same order of magnitude as the measured concentrations. The medium and high flowing and static bins were used for comparison purposes as these would seem to represent typical waterbodies considered for ambient water monitoring, as they typically have flow and water present all year. EPA believes monitoring data can be used as part of the weight-of-evidence evaluation to evaluate potential exposure.

Uncertainties in Aquatic Modeling and Monitoring Estimates

Exposure to aquatic organisms from pesticide applications is estimated using PWC EECs. Regional differences in exposure are assessed using regionally-specific PWC scenarios (e.g., information on crop growth and soil conditions) and meteorological conditions at the HUC 2 level (**Section 3.3. Scenario Selection**). The information used in these scenarios is designed to reflect conditions conducive to runoff. In instances where PWC scenarios do not exist in a HUC 2, surrogate scenarios from other HUCs are used. For fields where agricultural practices that result in less conservative scenario parameters are employed (i.e., conditions less conducive to runoff and pesticide loading of waterbodies), the potential for lower EECs would be expected.

The static waterbodies modeled with PWC are fixed volume systems with no outlet, resulting in the potential for accumulation of pesticide over time. Effects due to the increase and/or decrease of the water level in the waterbody and thus the concentration of pesticide in the waterbody are not modeled.

Flowing waterbodies are modeled in the PWC using the constant volume and flow through custom waterbody option. Effects due to the increase and/or decrease of the water level and flowrate in the waterbody and thus the concentration of pesticide in the waterbody are not modeled.

The assessment relies on maximum use patterns (**APPENDIX 1-3**). In situations where use patterns are less than the labeled maximums, environmental exposures will be lower.

The aquatic modeling conservatively assumes that the waterbody abuts the treated area. As such, any reduction in loading from runoff that could occur as the result of managed vegetative filter strips or unmanaged naturally-occurring interfaces between treated areas and waterbodies are not taken into account.

The aquatic modeling assumes a constant wind of 10 mph blowing directly toward the waterbody (**Section 3.4.2. Spray Drift**). These assumptions are conducive to drift transport and result in maximum potential loading to the waterbody. However, in many situations the wind will not be blowing constantly and directly toward the water body at this speed; therefore, aquatic deposition will likely be less than predicted. Additionally, many labels and applicator best management practices encourage not applying pesticides when the wind is blowing in the direction of sensitive areas (*i.e.*, listed species habitat). Lastly, reductions in spray drift deposition due to air turbulence, interception of spray drift on nearby plant canopy, and applications during low wind speeds are not taken into account in the spray drift estimates; therefore, loading due to spray drift may be over-estimated.

There is uncertainty associated with the selection of PWC input parameters. In this regard, one of the important parameters that can impact concentration estimates is the selection of application dates (**Section 3.4.3. Application Timing**); runoff and potential pesticide loading are greatest when applications immediately precede major precipitation events. Although the pesticide application dates are selected to be appropriate and protective (*i.e.*, selected with consideration for label restrictions and simulated cropping dates, pest pressures, and high precipitation meteorological conditions), uncertainty nevertheless results because the application window (the time span during a season that a pesticide may likely be applied) for a pesticide may be wide and actual application dates may vary over the landscape. While data sources exist that allow for determination of historical application dates (*e.g.*, California’s Pesticide Use Report and pesticide use surveys), it is uncertain how these dates reflect future application events. Additionally, the PWC model uses the same application dates for the 30-year simulation. While it is unlikely that an application would occur on the same dates every year for 30 years, this modeling process allows for a distribution of EECs to be developed that captures the peak loading events.

The PWC is a field-scale model. Flowing water bodies such as streams and rivers with physical parameters consistent with aquatic bins 3 and 4 have watershed areas well beyond those of typical agricultural fields. Initial modeling efforts in previous BEs, applying the field-scale model to these large watersheds and using the same scenario parameters as those used for the other bins, resulted in extremely high EECs which have not been observed in the environment, nor would be expected to occur due to fluid dynamic processes such as advective dispersion (**Figure 3-3**), where the peak concentration is dampened as it moves from a low flowing stream (bin 2) to a higher flowing river (bins 3 and 4). It is acknowledged that a watershed/basin-scale model capable of evaluating the impact of pesticide and water transport at the field-scale and aggregating these loadings to waterbodies at the larger watershed-scale is needed to evaluate these flowing aquatic systems.

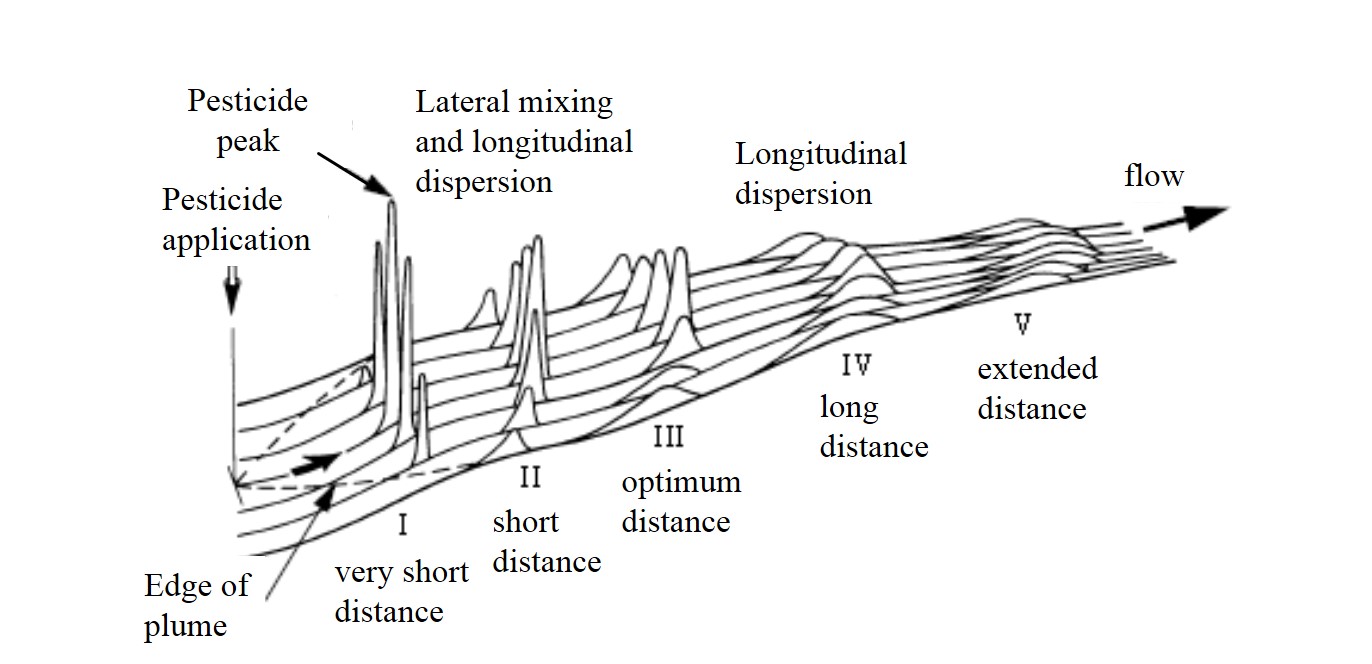


Figure 3-3. Effect of Pesticide Concentration via Advective Dispersion

Uncertainties with the Plant Assessment Tool (PAT)

The PAT model does not account for site specific field management and hydrology (e.g, terracing, contour farming, runoff and erosion controls, irrigation/drainage ditches, rills and creeks) which may result in less opportunity for runoff into the T-PEZ. Many different factors (e.g., slope; surface roughness; flow path length; etc.) can influence the occurrence, distance of, and prevalence of runoff onto the T-PEZ. These factors may vary greatly between different application sites (e.g., corn; wheat; potato; grape; bare field; turf).

The PAT model assumes that the water leaving the field as surface runoff is driven primarily by the amount of rainfall and the curve number, which is a function of the land use (i.e. row crops, pasture, fallow), management (i.e., straight row cropping, conservation tillage, etc.), and hydrologic soil conditions (i.e., high runoff potential with very slow infiltration rates; Young and Fry, 2016). Runoff leaving the field is assumed to enter the T-PEZ along the downslope field edge and coverage of the T-PEZ area conceptually happens instantaneously as the calculations are on a daily timestep rather than shorter timestep (e.g., hourly). As a result, the T-PEZ does not account for differences in the runoff loading (e.g., point entry and fan shaped sheet flow vs. uniform sheet flow entry), gradients in concentration due to interception and infiltration (e.g., buffering capacity of the T-PEZ), rain intensity and infiltration capacity relationships (e.g., pulsed rain events vs. one intense rain event). These natural features of the landscape may result in higher concentrations from runoff at the edge of the T-PEZ nearer the treated field than estimated in the model.

There are many different types of wetlands (e.g., depressional, groundwater fed, flow through, permanently flooded, and ephemeral) that may be present in landscapes receiving runoff from pesticide use sites. The default WPEZ model was selected to be representative and conservative (in terms of final pesticide concentrations) and acts as a surrogate for other types of wetlands. This assumption may result in overestimation of pesticide loading and fate than would be observed in some wetland systems.

Measures of Terrestrial Exposure

Terrestrial animals may be exposed to simazine through multiple routes of exposure, including diet, drinking water, dermal and inhalation exposure. Terrestrial dietary items may consist of plants, invertebrates or vertebrates (amphibians, reptiles, birds or mammals) that inhabit terrestrial areas or aquatic dietary items (fish, invertebrates or plants). However, due to simazine’s low log kOW value (2.09), significant bioaccumulation in aquatic food items is not expected and potential risk from this route of exposure is considered low. Therefore, estimates of exposure through consumption of aquatic food items using KABAM or BCF values are not calculated. A detailed discussion of the conceptual framework for estimating terrestrial exposure concentrations is provided in **ATTACHMENT 1-1**.

Two major parameters are used in terrestrial exposure modeling to characterize a species: body weight and diet. Estimates of body weights are necessary to estimate dose-based exposures through diet, drinking water, inhalation and dermal exposure routes. Information on the dietary requirements of listed species are necessary to determine relevant exposures through consumption of contaminated prey. Species-specific assumptions related to diet and body weight are provided within the model. The foliar dissipation half-life of the chemical can also impact the duration of exposure to predicted terrestrial EECs. A default foliar dissipation half-life of 35 days is used for simazine for terrestrial exposure modeling, based on data reported by Willis and McDowell (1987).

To improve efficiency and expand EFED’s modeling capabilities to other, non-dietary routes of exposure for terrestrial organisms, models have been developed to integrate the relevant exposure pathways and allow for batch processing of multiple analyses. For use in the pilot BEs (USEPA, 2016f), the Terrestrial Effects Determination (TED) tool was developed, which integrated T-REX, T-HERPS, the earthworm fugacity model, components of KABAM and AgDRIFT into one model platform. As part of the development of the draft biological opinion for chlorpyrifos, diazinon and malathion, the TED tool was converted to the terrestrial MAGtool, which further expanded the TED tool to predict the magnitude of effect at a population scale and incorporate the degree of overlap of a species range with potential use sites for a chemical (and associated off site transport areas) into the effects determination. The MAGtool has replaced the TED tool for modeling terrestrial exposure in the biological evaluations. A complete description of the MAGtool can be found in **ATTACHMENT 4-1**.

When the MAGtool is run for each species, terrestrial exposure concentrations are uniquely calculated for each species depending on relevant use overlap with the species range, available usage data, application rates associated with these relevant uses and the dietary items, habitat and obligate relationships for that species. As EECs will vary for each species, they are reported with the individual species in the individual effects determinations (**APPENDIX 4-1**).

To provide a bounding of potential terrestrial EECs used in the effects determinations, EECS were calculated for the range of application rates for simazine (a lower bound application rate of 1 lb a.i./A with 1 application per year and an upper bound application rate of 4 a.i./A with 1 application per year) and are provided below in **Table 3-12**. How the EECs will be applied will vary with each step of the analysis (*e.g.,* use of upper bound EECs in Step 1 vs. distribution of EECs in Step 2) and could be slightly higher with mid-range application rates applied multiple times. Additionally, other information considered in Step 2 (*e.g.,* typical use rates, use rates based on maximum usage in a species range, distribution of EECs, etc.), could alter the EECs used to assess a species exposure. All uses for simazine and associated application rates are provided in **APPENDIX 1-3**.  **summarizes** the mean and upper bound dietary-based EECs and the associated base model that is used in the MAGtool to predict the EECs.

Table 3-10summarizes the mean and upper bound dietary-based EECs and the associated base model that is used in the MAGtool to predict the EECs.

Table 3-. Mean and Upper Bound Dietary Based EECs Calculated for Food Items Consumed by Listed Mammals, Birds, Terrestrial-phase Amphibians or Reptiles Based on Foliar Applications.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Food Item** | **Model** | **Lower bound application rate**  **(1 lb a.i./A x 1 application/year)** | | **Upper bound application rate**  **(4 a.i./A x 1 applications/year)** | |
| **Upper Bound** | **Mean** | **Upper Bound** | **Mean** |
| Short Grass | T-REX | 240 | 85 | 960 | 340 |
| Tall Grass, nectar and pollen | T-REX | 110 | 36 | 440 | 144 |
| Broadleaf plants | T-REX | 135 | 45 | 540 | 180 |
| Seeds, fruit and pods | T-REX | 15 | 7 | 60 | 28 |
| Arthropods (above ground) | T-REX | 94 | 65 | 376 | 260 |
| Soil-dwelling invertebrates (earthworms) | Earthworm fugacity | 16 | NA**1** | 63 | NA**1** |
| Small mammals (15 g, short grass diet) | T-HERPS | 229 | 81 | 915 | 324 |
| Large mammals (1000 g, short grass diet)2 | T-HERPS | 37 | 13 | 147 | 52 |
| Small birds (20 g, insect diet) | T-HERPS | 107 | 74 | 482 | 296 |
| Small terrestrial phase amphibians or reptiles (2 g; insect diet) | T-HERPS | 5.2 | 3.6 | 21 | 14.4 |
| Fish, aquatic invertebrates and aquatic plants | NA3 |  | | | |

1 NA as upper bound and mean residues only applicable to items dependent on residues on foliage

2 Also represent residues in carrion.

3 NA due to lack of bioaccumulation of atrazine in aquatic dietary items

Values represent potential exposures for animals feeding on the treated field or in adjacent habitat directly adjacent to the field.

Literature Cited

For Master Record Identification (MRID) Number citations refer to **APPENDIX 2-4** OPPIN bibliography.

Armstrong, D.E., G. Chesters, and R.F. Harris. 1967. Atrazine hydrolysis in soil. *Soil Science Soc. Amer. Proc.* 31:61-66.

Burkhard, N. and J.A. Guth. 1981. Chemical hydrolysis of 2-chloro-4,6-bis (alkylamino)-1,3,5-triazine herbicides and their breakdown in soil under the influence of adsorption. *Pesticide Sci.* 12:45-52.

FAO. 2000. Appendix 2. Parameters of pesticides that influence processes in the soil. In FAO Information Division Editorial Group (Ed.), Pesticide Disposal Series 8. Assessing Soil Contamination. A Reference Manual. Rome: Food & Agriculture Organization of the United Nations (FAO). Available at <http://www.fao.org/DOCREP/003/X2570E/X2570E06.htm>

Gamble, D.S., S.U. Khan, and O.S. Tee. 1983. Atrazine hydrolysis: Proton Catalysis at 25 °C. *Pesticide Science*. 14:537-545

Goring, C. A. I., Laskowski, D. A., Hamaker, J. H., & Meikle, R. W. 1975. Principles of pesticide degradation in soil. In R. Haque & V. H. Freed (Eds.), Environmental dynamics of pesticides. NY: Plenum Press. Available at <https://link.springer.com/chapter/10.1007%2F978-1-4684-2862-9_9>

Hance, R.J. 1967. Decomposition of herbicides in the soil by non‐biological chemical processes. *Journal of the Science of Food and Agriculture.* 18:11, 544-547.

Jones, R.D., Abel, S., Effland, W., Matzner, R., Parker, R. 1998. An Index Reservoir for Use in Assessing Drinking Water Exposure. [https://archive.epa.gov/scipoly/sap/meetings/web/html/](https://archive.epa.gov/scipoly/sap/meetings/web/html/072998_mtg.html)

[072998\_mtg.html](https://archive.epa.gov/scipoly/sap/meetings/web/html/072998_mtg.html)

Khan, S.U. 1978. Kinetic of hydrolysis of atrazine in aqueous fulvic acid solution. *Pesticide Sci.* 9:39-43.

Mabey, W.R. and T. Mill. 1978. Critical Review of Hydrolysis of Organic Compounds in Water under Environmental Conditions. *Journal of Physical and Chemical Reference Data* 7(2):383-415.

Majewski, M. S., & Capel, P. D. 1995. Pesticides in the Atmosphere: Distribution, Trends, and Governing Factors. Chelsea, MI: Ann Arbor Press.

NAFTA. 2012. Guidance for Evaluating and Calculating Degradation Kinetics in Environmental Media. December 2012. NAFTA Technical Working Group on Pesticides. Available at <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/guidance-calculate-representative-half-life-values>

Navarro, S., N. Vela, M.J. Gimenez, and G. Navarro. 2004. Persistence of four s-triazine herbicides in river, sea, groundwater samples exposed to sunlight and darkness under laboratory conditions. *Sci. Total Environ.* 329:87-97.

Plust, S.J., J.R. Loehe, F.J. Feher, J.H. Benedict, and H.F. Herbrandson. 1981. Kinetics and Mechanism of Hydrolysis of Chloro-1,3,5-triazines. Atrazine. *J. Org. Chem.* 46, 3661-3665.

USEPA. 2009a. *Potential Risks of Alachlor Use to Federally Threatened California Red-legged Frog (Rana aurora draytonii) and Delta Smelt (Hypomesus transpacificus).* June 16, 2009. Environmental Fate and Effects Division. Office of Pesticide Programs. U. S. Environmental Protection Agency.

USEPA. 2009b. Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides, Version 2.1. Environmental Fate and Effects Division. Office of Pesticide Programs. U.S. Environmental Protection Agency. Available at <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/guidance-selecting-input-parameters-modeling>

USEPA. 2012. Standard Operating Procedure for Using the NAFTA Guidance to Calculate Representative Half-life Values and Characterizing Pesticide Degradation. November 30, 2012. Environmental Fate and Effects Division. Office of Pesticide Programs. U.S. Environmental Protection Agency. Available at <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/guidance-calculate-representative-half-life-values>.

USEPA. 2013. Guidance on Modeling Offsite Deposition of Pesticides Via Spray Drift for Ecological and Drinking Water Assessment. Environmental Fate and Effects Division. Office of Pesticide Programs. Office of Chemical Safety and Pollution Prevention. U.S. Environmental Protection Agency. Available at <http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2013-0676>

USEPA. 2016a. *Preliminary Ecological Risk Assessment for Simazine*. April 13, 2016. Environmental Fate and Effects Division. Office of Pesticide Programs. U. S. Environmental Protection Agency.

USEPA. 2016b. *Biological Evaluation for Chlorpyrifos Endangered Species Assessment*. March 31, 2016. Environmental Fate and Effects Division. Office of Pesticide Programs. U. S. Environmental Protection Agency. Available at <https://www.epa.gov/endangered-species/biological-evaluation-chapters-chlorpyrifos-esa-assessment>.

USEPA. 2016c. *Biological Evaluation for Diazinon Endangered Specis Assessment*. March 31, 2016. Environmental Fate and Effects Division. Office of Pesticide Programs. U.S. Environmental Protection Agency. Available at <https://www.epa.gov/endangered-species/biological-evaluation-chapters-diazinon-esa-assessment>.

USEPA. 2016d. *Biological Evaluation for Malathion Endandered Species Assessment*. March 31, 2016. Environmental Fate and Effects Division. Office of Pesticide Programs. U. S. Environmental Protection Agency. Available at <https://www.epa.gov/endangered-species/biological-evaluation-chapters-malathion-esa-assessment>.

USEPA. 2016e. *Preliminary Comparative Environmental Fate and Ecological Risk Assessment for the Registration Review of Eight Synthetic Pyrethroids and the Pyrethrins*. September 30, 2016. Environmental Fate and Effects Division. Office of Pesticide Programs. U. S. Environmental Protection Agency.

USEPA. 2016f. *Provisional Models for Endangered Species Pesticide Assessments*. Environmental Fate and Effects Division. Office of Pesticide Programs. U.S. Environmental Protection Agency. Available at <https://www.epa.gov/endangered-species/provisional-models-endangered-species-pesticide-assessments#Terrestrial>.

Widmer, S.K., J.M. Olsen, W.C. Koskinen. 1993. Kinetics of atrazine hydrolysis in water. *J Environ. Sci. and Health. Part B: Pesticides, Food Contaminants and Agricultural Wastes.* 28:19-28.

Willis, G.H. and McDowell, L.L. 1987. Pesticide persistence on foliage. Environ. Contam. Toxicol, 100:23 73.

Young, D. 2013. *Pesticides in Flooded Applications Model (PFAM): Conceptualization, Development, Evaluation, and User Guide*. EPA-734-R-13-001. July 18, 2013. Environmental Fate and Effects Division. Office of Pesticide Programs. U.S. Environmental Protection Agency. Available at <http://nepis.epa.gov/Exe/ZyPDF.cgi?Dockey=P100LE7H.txt>

Young, D., Fry, M. 2016. PRZM5 A Model for Predicting Pesticides in Runoff, Erosion, and Leachate, Revision A. USEPA/OPP734S16001. May 12, 2016.

1. The exposure models can be found at: <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment> [↑](#footnote-ref-2)
2. <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/guidance-selecting-input-parameters-modeling> (accessed October 2020) [↑](#footnote-ref-3)
3. <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/guidance-calculate-representative-half-life-values> (accessed October 2020) [↑](#footnote-ref-4)
4. The draft guidance is available at www.regulations.gov docket number: EPA-HQ-OPP-2013-0676 [↑](#footnote-ref-5)
5. <https://iaspub.epa.gov/waters10/attains_nation_cy.control?p_report_type=T> [↑](#footnote-ref-6)