**Chapter 1 – Final Simazine Problem Formulation**

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Introduction

This problem formulation provides the foundation for the simazine Biological Evaluation (BE) for all federally listed endangered and threatened species, as well as those that are proposed and candidates for listing and experimental populations (in sum referred to as “listed species”). This BE also includes an analysis of designated critical habitats. The methods employed in this BE follow the Revised Method for National Level Listed Species Biological Evaluations of Conventional Pesticides (referred to as the “Revised Method”)[[1]](#footnote-2). The assessment for simazine represents EPA’s Biological Evaluation (BE) for all listed species and designated critical habitats.

Included in this chapter is a description of the federal action; the mode and mechanism of action of simazine; summaries of its uses (based on registered product labels and commitment letters from all technical registrants), usage, and fate; definition of the residue of concern and an analysis plan for how the BE will be conducted. As part of the FIFRA registration review process, a detailed Problem Formulation for the FIFRA ecological risk assessment of simazine was finalized in May 2013[[2]](#footnote-3) (USEPA, 2013, DP Barcode D407490). The problem formulation considered data needs for both a FIFRA ecological risk assessment and an assessment for potential impacts on listed species.

Description of the Federal Action

In 2006, the U.S. Environmental Protection Agency (EPA) initiated Registration Review to reevaluate all registered pesticide active ingredients on a regular cycle. EPA is required to review each pesticide active ingredient at least every 15 years to make sure that it has the ability to assess risks to human health and the environment as science evolves and policies and practices may change, all pesticide products in the marketplace continue to meet the standard of registration. Registration Review includes labels registered under Sections 3, 24(c), and 18 of FIFRA. The federal action relevant to this BE is the Registration Review for simazine, which encompasses the review of all the registered uses and the approved product labels for all pesticide products containing simazine.

Mode and Mechanism of Action

Three chlorotriazine herbicides have current registrations in the United States: simazine (6-chloro-N,N′-diethyl-1,3,5-triazine-2,4-diamine; PC code 080807); atrazine (6-chloro-N-ethyl-N′-(1-methylethyl)-1,3,5-triazine-2,4-diamine; PC code 080803); and propazine (6-chloro-N,N′-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine; PC code 080808). These three chemicals differ only in number and/or position of methyl groups on moieties branched in identical positions off the triazine ring, thus are structurally nearly identical.  Based upon the available guideline and non-guideline toxicity studies, these chlorotriazines result in similar herbicidal effects to terrestrial and aquatic plants.

In plants, simazine binds with a protein complex of the photosystem II in chloroplast photosynthetic membranes (Schulz et al., 1990). The result is an inhibition in the transfer of electrons through the light reactions of photosynthesis that in turn inhibits the formation and release of oxygen, production of adenosine triphosphate, and the fixation of carbon dioxide into sugars. Plant death results from starvation and oxidative damage caused by the breakdown in photosynthesis.

While this pathway is not found in animals, simazine and the 3 chlorinated degradates all exhibit neuroendocrine effects seen across mammals and can alter hormone levels in rats that may result in developmental and reproductive consequences. In addition to this primary effect in mammals, acute and chronic exposure of animals has shown significant reduction in body weight and organ weights across multiple mammal and bird species.

Use and Usage Characterization

Use data are based on registered product labels and include pesticide application information relevant to a treatment site (*e.g.*, an orchard). EPA determines the uses based on registered labels, including any agreed upon changes to these labels from the technical registrants, and defines crop or non-crop sites to which a pesticide may be applied. Use data also describe the maximum application rates, method (*e.g.,* aerial or ground spray), re-treatment intervals and number of applications that may occur according to registered product labels.

Usage data describe how the pesticide has been applied to multiple use sites within a state, region or the US. EPA also reviews actual usage data that documents the actual applications of a pesticide, including information such as actual application rates and timing, and spatial distribution of applications across multiple sites (usually based on survey data). The key difference between use and usage is potential applications vs. actual applications.

## Use Data (as Defined on Registered Product Labels)

The label on a pesticide package or container is legally enforceable. The label provides information about how to handle and safely use the pesticide product and avoid harm to human health and the environment. Using a pesticide in a manner that is inconsistent with the use directions on the label is a violation of FIFRA and can result in enforcement actions to correct the violations. Simazine is currently registered on a variety of agricultural and non-agricultural use sites (**APPENDIX 1-1**). This BE assesses all currently registered labels and any agreed upon changes to these labels from the technical registrants (for implementation on all formulated product labels). While the current labels may not reflect all the agreed upon changes, the technical registrants have agreed in the form of commitment letters (see **APPENDIX 1-2**) to update the simazine formulated product labels to be reflective of these changes (uses summarized in **APPENDIX 1-3**). Major changes in the commitment letters include restriction of applications to the contiguous United States (ConUS) only, removal of certain use patterns, and implementation of new buffers and mandatory spray drift language (see **APPENDI**X **1-2** for specific details). EPA plans to formalize these changes through the appropriate processes prior to finalizing the BEs.

Simazine is one of the most widely used herbicides in North America. It is a chlorotriazine herbicide registered in the U.S. to control annual broadleaf and grass weeds in alfalfa, almond, apple, avocado, blueberry, broccoli, Brussels sprouts, cabbage, caneberries, cherry, citrus, corn (field, sweet), cranberry, filbert (hazelnut), grapefruit, grapes, kale, kohlrabi, lemon, macadamia nut (bushnut), nectarine, olive, orange, peach, pear, pecan, plum, strawberry, and walnut (English/black). Simazine is also registered for use on nursery stock, christmas tree plantations, ornamental ponds and aquaria, turfgrass for fairways, lawns, and similar areas (includes farm buildings, non-agricultural areas, and uncultivated agricultural areas; warm season grasses). Simazine may be applied by ground broadcast, band application, chemigation, or spot treatment. Simazine has many preemergence uses in corn.

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 technical registrant has committed to additional 15 ft ground buffers on streams, rivers, estuarine/marine environments, and listed species habitats. This results in 81 ft stream buffers, 200 ft buffers on ponds, and 15 ft ground buffers for wetlands (assuming listed species habitat for this assessment). Aerial applications are not allowed for simazine. In general, the single maximum simazine application rates do not exceed 4 lb a.i./A nationwide for flowable formulations.

## Usage Data

Based on usage data compiled by EPA’s Office of Pesticide Program’s Biological and Economic Analysis Division (BEAD), approximately 3 million pounds are applied each year to crops, and 670,000 pounds are applied to non-agricultural sites.

Between 2013 and 2017, the annual total agricultural usage averaged approximately 2.9 million pounds of simazine active ingredient (a.i.), whereas the average total treated acreage was 2.5 million. During this time frame, the crops with the most usage in terms of annual average total pounds of active ingredient applied were corn (2,300,000 lbs), oranges (200,000 lbs), and wine grapes (80,000 lbs). The crop with the most usage in terms of total treated acreage was also corn (2,200,000 A). On average, the states with the most agricultural usage in terms of pounds a.i. applied per year were Illinois with 902,000 lbs, California ~748,784 lbs and Indiana 500,000 lbs. Over the 5-year period the agricultural usage decreased from ~3.5 million pounds in 2013 to ~2 million pounds in 2017 **(APPENDIX 1-4**).

Most recent non-agricultural usage data from 2013 – 2017 shows that the largest use in terms of average annual pounds applied is for Christmas tree plantings (400,000 lbs.) and golf courses (200,000 lbs) **(APPENDIX 1-4).**

# Overview of Environmental Fate

The major transport routes off the treated area for simazine include runoff and spray drift. The main routes of dissipation for simazine are microbial degradation under aerobic conditions in water and soil, 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, suggesting low potential for volatilization. Simazine is moderately soluble in water with reported aqueous solubility values ranging from 3.5 to 11 mg/L at 20-25oC. Bioaccumulation of simazine is expected to be low due to a low octanol water partitioning coefficient (Kow = 122) and low bioconcentration factors (BCF). Soil sorption coefficients for simazine (KF) range from 0.5 to 4.3 ml/g (1/n=0.79-1.40) (MRID 41442903). Information on leaching and adsorption/desorption indicate that simazine is considered moderately mobile according to the Food and Agricultural Organization (FAO) mobility classification system[[3]](#footnote-4). Additional details on the fate of simazine are provided in **Chapter 3** of the Biological Evaluation.

# Residue of Concern

Environmental fate data indicate that deisopropylatrazine (DIA) and hydroxysimazine (HS) are the major transformation products of simazine (>10% applied a.i.) and that diadealkylatrazine (DDA) is a minor chlorotriazine degradation product (<10% applied a.i.). The degradate diadealkylatrazine is often commonly referred to as DACT. DIA and DDA are formed through dealkylation of the amino groups on the simazine molecule, while HS is formed through substitution of a chlorine by a hydroxy group. Dealkylation is a microbial-mediated process, while hydroxylation is both abiotic and microbial-mediated process. Formation of transformation products is further discussed in **Chapter 3**. DIA and DDA are also degradation products of atrazine and propazine.

An analysis of the residues of concern is provided in **APPENDIX 1-8**. Based on the analysis of formation and toxicity data of 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. In the terrestrial environment, consideration is given to formation of transformation products, through the consideration of toxicity data and foliar dissipation half-lives (**Chapters 2 and 3**).

# Analysis Plan

Listed species and designated critical habitats that were listed as of Jan 30, 2019 are considered in this BE (see **APPENDIX 4-1** for complete species lists). Effects determinations were made for 1795 listed species and 792 designated critical habitats.

As described in the Revised Method, listed species risk assessments for pesticides include three steps. Steps 1 and 2 are represented by the BE, which evaluates whether an individual of a listed species is reasonably expected to be exposed to a pesticide, and, if so, distinguishes effects that are likely to adversely affect an individual of a species from those that are not likely to adversely affect an individual. This process is also applied to the designated critical habitat of listed species (when available). In Step 1, for every listed species and designated critical habitat, EPA determines whether simazine will have No Effect (NE) or May Affect (MA) (separate determinations made for each species and critical habitat). For those species and critical habitats with MA determinations in Step 1, EPA will determine if simazine is Not Likely to Adversely Affect (NLAA) or Likely to Adversely Affect (LAA) each individual species or critical habitat.

Details on the method, models and tools used for making NE, NLAA and LAA determinations are provided in the Revised Method. This analysis plan identifies simazine specific information that is used in the Revised Method to complete this BE.

Step 1 begins with an analysis of the potential overlap of the action area and individual species ranges or critical habitat. For species or critical habitats with no overlap (*i.e.,* species found outside of the action area), NE determinations are made. The simazine overlap analysis is conducted using ArcGIS version 10.7. The action area is derived using potential use sites and the off-site transport zone. The currently registered uses, incorporating changes based on commitment letters (summarized in **Section 3** and **APPENDIX 1-3**) include agricultural, and non-agricultural uses. For simazine’s ornamental ponds and aquaria use pattern, reliable data are not available to map the locations of the potential use sites. The spatial extent of these uses are limited and overlap with other simazine uses; therefore, these uses are assumed to be covered by other uses and are not incorporated in the action area as an individual layer, but are captured in the total spatial footprint for simazine. For simazine, agricultural and non-agricultural use sites are used to derive the action area (along with the associated off-site transport zone).

A number of spatial data sources were used to generate Use Data Layers (UDLs), which map the potential use sites for simazine. In ConUS, agricultural use patterns UDLs are represented by using the US Department of Agriculture’s (USDA) Crop Data Layer (CDL)[[4]](#footnote-5). This analysis utilizes data from 2013-2017. As the commitment letters restrict the use of simazine to the contiguous United States, areas outside of ConUS (*e.g.,* Hawaii, Puerto Rico, etc.) were not included in the analysis. **APPENDIX 1-6** includes a crosswalk between simazine’s registered agricultural crops and the CDL. **APPENDIX 1-6** also defines how individual CDL layers are grouped into UDL categories[[5]](#footnote-6) and temporally combined to account for the accuracy of the data. USDA’s 2012 Census of Agriculture (CoA) is also used to improve accuracy by expanding the agricultural UDLs to meet or exceed the reported acres in the CoA (**ATTACHMENT 1-3**). For non-agricultural use patterns in ConUS additional UDLs were created to represent simazine’s registered uses. The data sources used for these UDLs included but are not limited to the NLCD 2011, GAP Protected Areas Database, LandFire and NAVTEQ; for additional details see **APPENDIX 1-6** which summarizes all spatial data used to generate the agricultural and non-agricultural UDLs used for simazine’s potential use site footprints.

The Step 2 overlap analysis incorporates simazine usage data, which are provided in the SUUM (SIAB Use and Usage Matrix), combining it with information from the CoA (**APPENDIX 1-4****, ATTACHMENT 1-4**). **APPENDIX 1-7** describe how the usage data for simazine, the CoA, and the potential use sites are combined to estimate the number of treated acres relevant to a given species located in ConUS. These appendices also explain how the off-site transport zone (specifically spray drift) is adjusted based on available usage data.

The Revised Method document stated “Over time, EPA expects to update the MAGtool and other models and tools described in this document. When a pesticide BE is conducted, it will incorporate the most current versions of models and tools intended for use in the BEs.” This BE is consistent with the Revised Method and includes two method updates that are intended to improve the methods for assessing exposure and effects to plants. First, this BE utilizes a refined exposure model for plants inhabiting terrestrial, wetland and aquatic habitats. Second, this BE incorporates surrogate endpoints for plants when No Observed Adverse Effects Concentrations (NOAEC) values are not available. These approaches are discussed below.

To estimate exposures to plants in aquatic, wetland, and terrestrial habitats, this BE uses the Plant Assessment Tool (PAT), a new tool designed to refine screening-level exposure estimates to plants typically generated using TerrPlant. 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 the Pesticide Root Zone Model (PRZM; which is part of PWC) and spray drift is modeled using AgDRIFT deposition values (also incorporated into the MAGtool).  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 and the Variable Volume Water Model (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 pond. The results from PAT are summarized for use in the MAGtool in the same way as the results from PWC.

For listed terrestrial and wetland plant species, NOAECs from seedling emergence and vegetative vigor studies are used to represent toxicity endpoints. There are often cases where NOAECs are not available (*e.g*., statistically significant effects occurred at all test concentrations) or are considered unreliable. Consistent with OPP’s longstanding practice, in cases where NOAECs are not available or reliable, an ICx value is used as a surrogate. Based on an analysis of the variability in the dry weight and height data of the controls of commonly tested species in vegetative vigor and seedling emergence studies, x values were assigned based on test type and endpoint (**Table 1-1**; supporting details in **ATTACHMENT 1-5**). This analysis does not consider the biological significance of the percent effect but rather identifies an ICx value at which we have confidence the measured effect is discernible. **Table 1-1** Presents the ICx values that will be used as the Step 1 and 2 thresholds when a reliable NOAEC value is not available.

**Table 1-1.** Alternate Step 1 and 2 thresholds.

|  |  |  |
| --- | --- | --- |
| **Test Type** | **Dry Weight** | **Shoot Height** |
| Vegetative Vigor | IC15 | IC10 |
| Seedling Emergence | IC20 | IC10 |

**Chapter 2** of this BE includes simazine’s toxicity endpoints and **Chapter 3** includes the exposure analysis. These toxicity endpoints and exposure estimates are used in Steps 1 and 2. **Chapter 2** also summarizes incident reports that are associated with applications of simazine (incident reports associated with illegal uses or misuses are not included in the assessment). **Chapter 3** summarizes available monitoring data. **Chapter 4** includes the species and critical habitat-specific determinations for simazine. For exposure in terrestrial habitats, the MAGtool[[6]](#footnote-7) (version 2.2) is used (additional details in **ATTACHMENT 1-1** and tool documentation). For aquatic habitats, exposure is estimated using the Pesticide in Water Calculator (PWC; version 1.52[[7]](#footnote-8)) and, where appropriate, the Pesticide in Flooded Applications Model (PFAM, version 2[[8]](#footnote-9)). Aquatic scenarios (referred to as “bins”) used to estimate exposures for each listed species with aquatic habitats are provided in **ATTACHMENT 1-2**. For plants, exposure is estimated using PAT. The MAGtool is used to integrate exposure, effects, and listed species life history information in order to make NE, NLAA and LAA determinations.

1. Available at: <https://www.epa.gov/endangered-species/revised-method-national-level-listed-species-biological-evaluations-conventional> [↑](#footnote-ref-2)
2. Simazine Registration Review Docket Folder. <https://www.regulations.gov/docket?D=EPA-HQ-OPP-2013-0251-0002> [↑](#footnote-ref-3)
3. [↑](#footnote-ref-4)
4. USDA National Agricultural Statistics Service Cropland Data Layer. 2013-2017. Published crop-specific data layer [Online]. Available at <https://www.nass.usda.gov/Research_and_Science/Cropland/SARS1a.php> (accessed 3/2018; verified 2/2020). USDA-NASS, Washington, DC. [↑](#footnote-ref-5)
5. Categories include: corn, cotton, rice, soybeans, wheat, vegetables and ground fruit, other grains, other row crops, other crops, pasture/hay, citrus, vineyards and other orchards. [↑](#footnote-ref-6)
6. Information on the models and tools used to support this biological evaluation are available at: <https://www.epa.gov/endangered-species/models-and-tools-endangered-species-pesticide-assessments> (Accessed September 2020). [↑](#footnote-ref-7)
7. Available online at: [https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment#aquatic](https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment%23aquatic) (Accessed September 2020). [↑](#footnote-ref-8)
8. Ibid. [↑](#footnote-ref-9)