**APPENDIX 2-5. Simazine Species Sensitivity Distribution Analysis for Aquatic Plants**

SSDs were fit to toxicity data for vascular and nonvascular aquatic plants exposed to simazine. Five distributions were tested and a variety of methods were used to determine whether different subsets of data should be modeled independently. Aquatic vascular plant growth data were insufficient to derive a separate SSD. Ultimately, the results from the all aquatic plant SSDs were used.  **Table 1** provides a summary of the results.

**Table 1. Summary statistics for SSDs fit to simazine test results.**

|  |  |
| --- | --- |
| Statistic | AllAquatic Plants |
| Best Distribution (by AICc) | Logistic |
| Goodness of fit P-value | 0.38 |
| CV of the HC05 | 0.87 |
| HC05 | 14.68 |
| HC10 | 29.08 |
| HC50 | 217 |
| HC90 | 1620 |
| HC95 | 3210 |

1. Data

Data used in this analysis are detailed in **Table 6** (at the end of the document) and were from registrant submitted studies as well as an ECOTOX query (**APPENDIX 2-2**). **Table 2** provides the distribution of the test results for simazine including the number of species represented. Insufficient data were available to derive separate SSDs for vascular aquatic plants since only three species were tested. Therefore, one set of distributions was derived: all aquatic plants (combines vascular and nonvascular aquatic plants).

**Table 2. Distribution of test results available for simazine.**

|  |  |  |
| --- | --- | --- |
| Data Subset | Test results | Species |
| All Aquatic Plants | 33 | 19 |
| Nonvascular Aquatic Plants | 24 | 16 |
| Aquatic Plants | 9 | 3 |

**Figure 1** shows the distribution of test results among species, indicating that a few species have been repeatedly tested (two species have been tested 5 times each), but the majority of species have been tested fewer than three times, with 14 species having only one test result.

 

**Figure 1. Distribution of the number of test results per species in simazine aquatic plant data.**

Five potential distributions for the simazine data were considered, including log-normal, log-logistic, log-triangular, log-gumbel, and Burr. To fit each of the first four distributions, the toxicity values were first common log (log10) transformed. Finally, effect thresholds and five quantiles from the fitted SSDs (HC05, HC10, HC50, HC90, HC95) were calculated and reported.

1. Comparison of distributions using AICc

Akaike’s Information Criterion corrected for sample size (AICc) was used to compare the five distributions for the aquatic plant dataset. For these comparisons all SSDs were fit using maximum likelihood. The AICc suggested that the logistic distribution provided the best fit (**Tables 3**).

**Table 3. Comparison of distributions for all aquatic aquatic plant toxicity data for simazine.**

| distribution | AICc | ∆AICc | Weight | HC05 |
| --- | --- | --- | --- | --- |
| logistic | 288.2030 | 0 | 0.3563 | 14.6830 |
| gumbel | 288.9047 | 0.7017 | 0.2509 | 20.9207 |
| normal | 289.5804 | 1.3774 | 0.1790 | 14.4400 |
| burr | 290.1695 | 1.9665 | 0.1333 | 21.8067 |
| triangular | 291.1774 | 2.9744 | 0.0805 | 12.4762 |

1. Goodness of fit

The plot of the cumulative distribution functions for the best-fit distributions (as determined by AICc) suggest little evidence of lack-of-fit (**Figure 2**). Similarly, bootstrap goodness-of-fit tests did not show evidence for lack-of-fit (P-values > 0.05, **Table 4**), with the exception of the Triangular distribution. In general, the coefficient of variation for the HC05 was below 1 for the competitive distributions.



**Figure 3. Log-logistic SSD for simazine toxicity values for all aquatic aquatic plants pooled.** Black points indicate single toxicity values. Red points indicate average of multiple toxicity values for a single species. Blue line indicates full range of toxicity values for a given taxon.

**Table 4. Range of HC05 values for simazine SSDs for all aquatic plants.**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Distribution** | **Method** | **HC05** | **SE** | **CV** | **Lower CI** | **Upper CI** | **P** |
| Normal | ML | 14.44 | 12.8956 | 0.893 | 4.5125 | 52.6894 | 0.1858 |
| Normal | MO | 13.3533 | 11.605 | 0.8691 | 3.6084 | 45.8786 | 0.1409 |
| Normal | GR | 10.9285 | 7.3966 | 0.6768 | 2.1903 | 29.826 | 0.0869 |
| Logistic | ML | 14.683 | 11.9104 | 0.8112 | 4.4967 | 48.7862 | 0.3397 |
| Logistic | MO | 13.8752 | 13.5293 | 0.9751 | 3.148 | 54.9421 | 0.2847 |
| Logistic | GR | 9.3423 | 7.7781 | 0.8326 | 0.9798 | 31.5578 | 0.1828 |
| Triangular | ML | 12.4762 | 13.4608 | 1.0789 | 6.0055 | 58.9276 | 0.035 |
| Triangular | MO | 12.6568 | 11.6211 | 0.9182 | 4.5658 | 46.5052 | 0.0759 |
| Triangular | GR | 12.0298 | 8.9221 | 0.7417 | 3.462 | 38.4711 | 0.0609 |
| Gumbel | ML | 20.9207 | 11.0373 | 0.5276 | 10.3851 | 52.3048 | 0.3936 |
| Gumbel | MO | 24.4567 | 13.2108 | 0.5402 | 10.2819 | 61.8633 | 0.5674 |
| Gumbel | GR | 18.9381 | 10.2503 | 0.5413 | 4.8947 | 43.3259 | 0.2587 |
| Burr | ML | 21.8067 | 15.8364 | 0.7262 | 6.0534 | 67.5482 | 0.4106 |

ML=maximum likelihood, MO= moment estimators, and GR=graphical methods

LCp and UCp=projections of the confidence limits of the HC05 (LCx and UCx) onto the cumulative distribution function of the fitted distribution.

1. Calculation of other quantiles

**Table 5** provides estimates of the HC05 as well as other quantiles of the fitted SSDs.

**Table 5. Estimated quantiles of the fitted SSDs for simazine EC50s for all aquatic plants.**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Distribution** | **Method** | **HC05** | **HC10** | **HC50** | **HC90** | **HC95** |
| Normal | ML | 14.44 | 27.1294 | 250.9195 | 2.32E+03 | 4.36E+03 |
| Normal | MO | 13.3533 | 25.5251 | 250.9195 | 2.47E+03 | 4.72E+03 |
| Normal | GR | 10.9285 | 21.8354 | 250.9195 | 2.88E+03 | 5.76E+03 |
| Logistic | ML | 14.683 | 29.0831 | 217.0086 | 1.62E+03 | 3.21E+03 |
| Logistic | MO | 13.8752 | 28.9271 | 250.9195 | 2.18E+03 | 4.54E+03 |
| Logistic | GR | 9.3423 | 21.5334 | 250.9195 | 2.92E+03 | 6.74E+03 |
| Triangular | ML | 12.4762 | 23.5184 | 341.4509 | 4.96E+03 | 9.34E+03 |
| Triangular | MO | 12.6568 | 22.4296 | 250.9195 | 2.81E+03 | 4.97E+03 |
| Triangular | GR | 12.0298 | 21.527 | 250.9195 | 2.92E+03 | 5.23E+03 |
| Gumbel | ML | 20.9207 | 31.2769 | 195.8769 | 3.49E+03 | 1.05E+04 |
| Gumbel | MO | 24.4567 | 35.2624 | 187.1956 | 2.57E+03 | 6.99E+03 |
| Gumbel | GR | 18.9381 | 28.8237 | 195.8527 | 3.96E+03 | 1.25E+04 |
| Burr | ML | 21.8067 | 35.9317 | 212.2496 | 1.98E+03 | 4.44E+03 |

**Table 6** provides all of the available EC50 values for aquatic plants (within the 96-hour to 14-day timeframe-unless otherwise noted). These data sets are the same as reported in the effects characterization and provide additional data for the formulated products. Values that were included in the SSD (*i.e.,* TGAI) are marked with an \*.

**Table 6. Available effective lethal concentration (EC50) data for aquatic plants exposed to simazine as TGAI or formulation.**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Family** | **Genus** | **Species** | **Common Name** | **EPA Group** | **Comparable Adjusted Mean Concentrations** | **Preferred Units** | **Ref #** | **Classification** |
| Chlorococcaceae | Chlorococcum | sp. | Green Algae | Nonvascular | 8 | ug/L | 17259 | Supplemental |
|  | Anabaena | flos-aquae | Nonvascular | 36 | ug/L |  | Acceptable |
| Scenedesmaceae | Selenastrum | sp. | Green Algae | Nonvascular | 48.6 | ug/L | 84045 |  |
| Scenedesmaceae | Selenastrum | sp. | Green Algae | Nonvascular | 57.3 | ug/L | 84045 |  |
| Scenedesmaceae | Scenedesmus | quadricauCX | Green Algae | Nonvascular | 65 | ug/L | 17259 | Supplemental |
| Scenedesmaceae | Selenastrum | sp. | Green Algae | Nonvascular | 73.6 | ug/L | 84045 |  |
| Oocystaceae | Chlorella | pyrenoidosa | Green Algae | Nonvascular | 82 | ug/L | 158793 |  |
| Oocystaceae | Chlorella | pyrenoidosa | Green Algae | Nonvascular | 82 | ug/L | 61983 |  |
| Oocystaceae | Ankistrodesmus | sp. | Green Algae | Nonvascular | 87 | ug/L | 17259 | Supplemental |
| Prasiolaceae | Hormidium | flaccidum | Algae | Nonvascular | 90 | ug/L | 17259 | Supplemental |
|  | Navicula | pelliculosa | Nonvascular | 90 | ug/L |  | Acceptable |
| Scenedesmaceae | Pseudokirchneriella | subcapitata | Green Algae | Nonvascular | 100 | ug/L | 17639 |  |
| Oocystaceae | Chlorella | pyrenoidosa | Green Algae | Nonvascular | 100 | ug/L | 17259 | Supplemental |
|  | Selenastrum | capricornutum | Nonvascular | 100 | ug/L |  | Acceptable |
|  | Lemna | gibba |  | Vascular | 140 | ug/L |  | Acceptable |
| Scenedesmaceae | Scenedesmus | quadricauCX | Green Algae | Nonvascular | 150 | ug/L | 71458 |  |
| Scenedesmaceae | Scenedesmus | quadricauCX | Green Algae | Nonvascular | 150 | ug/L | 71458 |  |
| Lemnaceae | Lemna | gibba | Inflated Duckweed | Vascular | 156 | ug/L | 174511 |  |
| Lemnaceae | Lemna | aequinoctialis | Lesser Duckweed | Vascular | 162.8 | ug/L | 174511 |  |
| Scenedesmaceae | Pseudokirchneriella | subcapitata | Green Algae | Nonvascular | 200 | ug/L | 69584 |  |
| Prasiolaceae | Stichococcus | sp. | Green Algae | Nonvascular | 200 | ug/L | 17259 | Supplemental |
| Lemnaceae | Lemna | aequinoctialis | Lesser Duckweed | Vascular | 209.8 | ug/L | 174511 |  |
| Scenedesmaceae | Pseudokirchneriella | subcapitata | Green Algae | Nonvascular | 220 | ug/L | 69584 |  |
| Scenedesmaceae | Pseudokirchneriella | subcapitata | Green Algae | Nonvascular | 220 | ug/L | 69584 |  |
| Lemnaceae | Lemna | minor | Duckweed | Vascular | 226.6 | ug/L | 174511 |  |
| Lemnaceae | Lemna | minor | Duckweed | Vascular | 229.1 | ug/L | 174511 |  |
| Scenedesmaceae | Pseudokirchneriella | subcapitata | Green Algae | Nonvascular | 252 | ug/L | 165277 |  |
| Scenedesmaceae | Scenedesmus | acutus var. acutus | Green Algae | Nonvascular | 257 | ug/L | 65945 |  |
| Lemnaceae | Lemna | gibba | Inflated Duckweed | Vascular | 276.1 | ug/L | 174511 |  |
| Scenedesmaceae | Pseudokirchneriella | subcapitata | Green Algae | Nonvascular | 297 | ug/L | 98204 |  |
| Lemnaceae | Lemna | gibba | Inflated Duckweed | Vascular | 300 | ug/L | 60827 |  |
| Lemnaceae | Lemna | gibba | Inflated Duckweed | Vascular | 400 | ug/L | 60827 |  |
| Scenedesmaceae | Scenedesmus | acutus | Green Algae | Nonvascular | 400 | ug/L | 17259 | Supplemental |
| Lemnaceae | Lemna | gibba | Inflated Duckweed | Vascular | 420 | ug/L | 60827 |  |
| Lemnaceae | Lemna | sp. | Duckweed | Vascular | 422 | ug/L | 174699 |  |
| Lemnaceae | Lemna | sp. | Duckweed | Vascular | 564 | ug/L | 174699 |  |
| Lemnaceae | Lemna | gibba | Inflated Duckweed | Vascular | 570 | ug/L | 60827 |  |
| Lemnaceae | Lemna | gibba | Inflated Duckweed | Vascular | 600 | ug/L | 60827 |  |
|  | Skeletonema | costatum |  | Nonvascular | 600 | ug/L |  | Acceptable |
| Lemnaceae | Lemna | sp. | Duckweed | Vascular | 636 | ug/L | 174699 |  |
| Scenedesmaceae | Pseudokirchneriella | subcapitata | Green Algae | Nonvascular | 748.5 | ug/L | 83543 |  |
| Oocystaceae | Chlorella | vulgaris | Green Algae | Nonvascular | 2173.8 | ug/L | 65938 |  |
| Oocystaceae | Chlorella | sp. | Green Algae | Nonvascular | 3300 | ug/L | 17259 | Supplemental |
| Dictyosphaeriaceae | Dictyosphaerium | pulchellum | Green Algae | Nonvascular | 28000 | ug/L | 17259 | Supplemental |

\* Indicates study was conducted with TGAI and value used to derive SSD.

 NA = Studies are acceptable for ECOTOX but have not been formally reviewed by EFED scientists.

1If a species was not represented with a 96 hour study, and other values were available from shorter/longer duration studies (up to 10 days) then the data were included and the duration was listed next to the LC50 value as an indicator. If there were multiple other durations, the value from the study closer to a 96h duration was selected and if there were multiple values for the same duration, the range is indicated.