**ATTACHMENT 4-3. Supplemental Information 3.** Species Sensitivity Distributions for Chlorpyrifos Predicted Values from Web Ice

**Summary**

SSDs were fit to predicted test results for fish exposed to Chlorpyrifos. Five distributions were tested against four sets of predicted values. The first set was predicted from rainbow trout (*Onchorhynchus mykiss*) data, the second from bluegill (*Lepomis macrochirus*) data, the third from fathead minnow data (*Pimephales promelas*), and the fourth was predicted from a mixture of all three surrogates. Only data for species typically tested in freshwater were used.

Summary statistics for SSDs are presented below.

Table 1. Summary statistics for SSDs fit to Chlorpyrifos test results

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| statistic | rainbow trout | bluegill | fathead  minnow | mixture | empirical |
| Best Distribution (by AICc) | gumbel | triangular | triangular | triangular | triangular |
| Goodness of fit P-value | 0.57 | 0.81 | 1.00 | 0.43 | 0.79 |
| CV of the HC05 | 0.13 | 0.31 | 0.09 | 0.40 | 0.42 |
| HC05 | 4.7 | 1.6 | 48.3 | 3 | 5.8 |
| HC10 | 5.4 | 2.1 | 57.3 | 4.7 | 10.4 |
| HC50 | 10.3 | 6.5 | 117.2 | 30 | 118.3 |
| HC90 | 28.8 | 19.8 | 239.7 | 192.7 | 1347 |
| HC95 | 42.5 | 25.8 | 284 | 299.5 | 2397 |
| Mortality Thresh.1 (slope = 4.5) | 0.41 | 0.14 | 4.25 | 0.26 | 0.51 |
| Indirect Effects Threshold1 (slope = 4.5) | 2.42 | 0.84 | 25.10 | 1.55 | 3.03 |

1Slope of dose-response curve = 4.5

Predicted values from rainbow trout, bluegill, and the mixture of all three surrogates produced estimates of HC05 that were lower than that generated from the empirical data (Table 1). However, predicted values from fathead minnow produced estimates of the HC05 that were an order of magnitude greater than the empirical value. HC05 estimates from the predicted data appeared to be more precisely estimated (smaller coefficients of variation and smaller estimates of sampling variance in the HC05). Plotted SSDs (Figs. 1-5) do show some evidence of lack of fit, though no supporting evidence was found in goodness-of-fit tests. Predicted values generated using a single surrogate generally produced an SSD with less variance than that produced using the empirical data, with the exception of the mixed dataset using all three surrogates (Figs. 1 - 5). The use of all three surrogates simultaneously would be strongly recommended for this pesticide.

Cross-tabulation of predicted values with empirical test results show that Web ICE predictions did not find significant correlations among tested and predicted values, though this may be due to lack of power. In contrast to some results from Malathion, no relationship between toxicological distance and accuracy of the predicted values was found, though again this could be due to lack of power.

**I. Data**

Data were received from Elizabeth Donovan on 8 October 2014 in the file:

“Chlorpyrifos SSD\_WebICE.xlsx”

From this file I created three working files:

1. ChlorpyrifosFWFishIcePredRainbowTrout.xlsx

2. ChlorpyrifosFWFishIcePredBluegill.xlsx

3. ChlorpyrifosFWFishIcePredFathead.xlsx

4. ChlorpyrifosFWFishIcePredAllThree.xlsx

These working files each contain three fields (Table 2).

Table 2. Fields in working files

|  |  |  |
| --- | --- | --- |
| Field in working files | Field in received file | Column in  received file |
| 1. Genus | Scientific | C |
| 2. Species | Scientific | C |
| 3. Toxicity | Measured Toxicity (ug/L) | D |

Table 3. Distribution of predicted values available for Chlorpyrifos

|  |  |
| --- | --- |
| Surrogate Species | Predicted Values |
| rainbow trout | 23 |
| bluegill | 11 |
| fathead minnow | 24 |
| all three | 30 |

For each analysis the surrogate species empirical test value(s) were added to the dataset to allow comparison of the predicted distribution to the value of the surrogate species. For further comparison, the previous empirical dataset on freshwater fish provided by Melissa Panger (“SSD Data\_Fish and Amphibians\_(Mortality)\_Chlorpyrifos.xlsx”, 2 July 2014) was reanalyzed after converting that dataset from mg/L to µg/L.

Five potential distributions for the Chlorpyrifos data (log-normal, log-logistic, log-triangular, log-gumbel, and Burr) were considered. To fit each of the first four distributions, the toxicity values were common log (log10) transformed. The best-fit distribution was explored using Akaike’s information criterion. Finally, the direct and indirect effect thresholds were calculated and five quantiles from the fitted SSDs (HC05, HC10, HC50, HC90, HC95) were reported.

**II. Comparison of distributions using AICc**

AICc was used to compare the five distributions for both datasets. For these comparisons all SSDs were fit using maximum likelihood.

Based on AICc the datasets disagreed on which distribution best fit the predicted values. For values predicted from rainbow trout, the gumbel distribution fit best, but was followed closely by the triangular distribution (Table 4). For the bluegill data, the burr distribution received the lowest AICc score, but failed to converge (providing values of 0 for all quantiles and estimating sampling variance as infinite). These results were not considered further. The next best distribution for the bluegill data was the triangular distribution, followed closely by the normal and logistic distributions (Table 5). For the fathead minnow data, the triangular distribution provided the best fit, followed closely by the normal and gumbel distributions (Table 6). For the predicted values from a mixture of all three surrogates, the triangular distribution provided the best fit, again followed by the normal and gumbel (Table 7). Finally, for the empirical data, the triangular distribution provided the best fit, followed closely by the normal, burr, and logsitic distributions (Table 7). Estimates of the HC05 were similar for the predicted values based on rainbow trout, bluegill, the mixture set from three surrogates, and the empirical data. These were all a bit lower than the HC05 estimates from the empirical data (Table 8). The predicted values based only on fathead minnow produced the largest HC05estimates, about an order of magnitude greater than the empirical estimates of the HC05.

Table 4. Comparison of distributions for freshwater fish toxicity values predicted from rainbow trout.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| gumbel | 4.7 | 169.3 | 0.0 | 0.5 |
| triangular | 4.1 | 171.2 | 1.9 | 0.2 |
| burr | 4.7 | 172.0 | 2.6 | 0.1 |
| normal | 3.8 | 172.4 | 3.1 | 0.1 |
| logistic | 3.4 | 173.3 | 4.0 | 0.1 |

Table 5. Comparison of distributions for freshwater fish toxicity values predicted from bluegill.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| burr | 0.0 | 82.3 | 0.0 | 0.3 |
| triangular | 1.6 | 82.6 | 0.2 | 0.3 |
| normal | 1.4 | 83.2 | 0.9 | 0.2 |
| logistic | 1.3 | 84.5 | 2.2 | 0.1 |
| gumbel | 1.5 | 85.0 | 2.6 | 0.1 |

Table 6. Comparison of distributions for freshwater fish toxicity values predicted from fathead minnow.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| triangular | 48.3 | 282.5 | 0.0 | 0.5 |
| normal | 45.1 | 284.1 | 1.6 | 0.2 |
| gumbel | 50.3 | 284.5 | 2.0 | 0.2 |
| logistic | 41.6 | 285.9 | 3.4 | 0.1 |
| burr | 50.3 | 287.1 | 4.6 | 0.0 |

Table 7. Comparison of distributions for freshwater fish toxicity values predicted from all three surrogates.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| triangular | 3.0 | 321.4 | 0.0 | 0.5 |
| normal | 2.3 | 323.5 | 2.1 | 0.2 |
| gumbel | 3.1 | 323.7 | 2.2 | 0.2 |
| burr | 3.1 | 326.1 | 4.7 | 0.1 |
| logistic | 1.6 | 327.1 | 5.7 | 0.0 |

Table 8. Comparison of distributions for empirical freshwater fish toxicity data for Chlorpyrifos

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| triangular | 5.8 | 251.3 | 0.0 | 0.4 |
| normal | 5.6 | 252.5 | 1.3 | 0.2 |
| burr | 2.0 | 253.4 | 2.1 | 0.2 |
| logistic | 5.7 | 253.5 | 2.2 | 0.1 |
| gumbel | 5.5 | 256.9 | 5.6 | 0.0 |

The cumulative distribution functions for each of the above datasets are plotted below.

Figure 1. Log-gumbel SSD for WebICE predicted values for freshwater fish LC50s for Chlorpyrifos, based on rainbow trout regressions.



Figure 2. Log-triangular SSD for WebICE predicted values for freshwater fish LC50s for Chlorpyrifos, based on bluegill regressions.



Figure 3. Log-triangular SSD for WebICE predicted values for freshwater fish LC50s for Chlorpyrifos, based on fathead minnow regressions.



Figure 4. Log-triangular SSD for WebICE predicted values for freshwater fish LC50s for Chlorpyrifos, based on all three surrogates.



Figure 5. Log-triangular SSD for Chlorpyrifos LC50s for freshwater fish. Red points indicate single toxicity values. Black points indicate multiple toxicity values. Blue line indicates full range of toxicity values for a given taxon.



**IV. Goodness of fit and the importance of fitting method**

To test goodness-of-fit all five distributions were fit to each of the five datasets and bootstrap goodness-of-fit tests with 5,000 bootstrap replicates were run. Three different fitting methods were used (maximum likelihood, moment estimators, and graphical methods), though not all methods are available for all distributions. Tables 9 – 13 give results of these fitting exercises. No distribution showed significant lack-of-fit, except the Burr distribution. The coefficient of variation for the HC05 was always below 1 for predicted values, but larger than 1 for several distributions and methods for the empirical data.

Table 9. Range of HC05 values (μg/L) for Chlorpyrifos SSDs estimated from Web ICE predicted values using rainbow trout

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 4.66 | 0.59 | 0.13 | 3.75 | 6.18 | 0.57 |
| gumbel | MO | 4.66 | 0.77 | 0.17 | 3.36 | 6.42 | 0.56 |
| gumbel | GR | 4.16 | 0.76 | 0.18 | 2.41 | 5.41 | 0.23 |
| normal | ML | 3.76 | 0.81 | 0.21 | 2.58 | 5.90 | 0.43 |
| normal | MO | 3.67 | 0.88 | 0.24 | 2.37 | 5.86 | 0.37 |
| normal | GR | 3.25 | 0.78 | 0.24 | 1.76 | 4.81 | 0.16 |
| logistic | ML | 3.40 | 0.79 | 0.23 | 2.09 | 5.52 | 0.20 |
| logistic | MO | 3.73 | 0.96 | 0.26 | 2.25 | 5.96 | 0.25 |
| logistic | GR | 3.10 | 0.85 | 0.27 | 1.28 | 4.54 | 0.11 |
| triangular | ML | 4.08 | 1.01 | 0.25 | 3.26 | 6.39 | 1.00 |
| triangular | MO | 3.60 | 0.79 | 0.22 | 2.45 | 5.50 | 1.00 |
| triangular | GR | 3.34 | 0.76 | 0.23 | 2.03 | 4.94 | 0.98 |
| burr | ML | 4.66 | 0.59 | 0.13 | 3.65 | 6.11 | 0.77 |

Table 10. Range of HC05 values (μg/L) for Chlorpyrifos SSDs estimated from Web ICE predicted values using bluegill

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 1.55 | 0.44 | 0.29 | 0.96 | 3.16 | 0.70 |
| gumbel | MO | 1.86 | 0.62 | 0.33 | 1.03 | 3.48 | 0.85 |
| gumbel | GR | 1.46 | 0.54 | 0.37 | 0.44 | 2.53 | 0.49 |
| normal | ML | 1.43 | 0.59 | 0.41 | 0.67 | 3.51 | 0.61 |
| normal | MO | 1.34 | 0.69 | 0.52 | 0.57 | 3.20 | 0.56 |
| normal | GR | 1.01 | 0.53 | 0.53 | 0.24 | 2.30 | 0.33 |
| logistic | ML | 1.28 | 0.66 | 0.51 | 0.47 | 3.44 | 0.54 |
| logistic | MO | 1.37 | 0.74 | 0.54 | 0.51 | 3.39 | 0.57 |
| logistic | GR | 0.91 | 0.49 | 0.54 | 0.13 | 1.97 | 0.30 |
| triangular | ML | 1.62 | 0.50 | 0.31 | 1.10 | 3.73 | 0.81 |
| triangular | MO | 1.30 | 0.64 | 0.49 | 0.61 | 3.02 | 0.53 |
| triangular | GR | 1.07 | 0.53 | 0.49 | 0.35 | 2.34 | 0.35 |
| burr | ML | 0.00 | 0.00 | NaN | 0.00 | 5.62 | 0.36 |

Table 11. Range of HC05 values (μg/L) for Chlorpyrifos SSDs estimated from Web ICE predicted values using fathead minnow

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 50.28 | 5.61 | 0.11 | 41.77 | 64.81 | 1.00 |
| gumbel | MO | 53.78 | 7.08 | 0.13 | 41.33 | 69.37 | 1.00 |
| gumbel | GR | 49.14 | 7.32 | 0.15 | 31.92 | 61.10 | 1.00 |
| normal | ML | 45.05 | 7.84 | 0.17 | 33.21 | 64.40 | 1.00 |
| normal | MO | 44.19 | 8.15 | 0.18 | 31.02 | 63.06 | 1.00 |
| normal | GR | 40.05 | 7.91 | 0.20 | 23.73 | 54.36 | 1.00 |
| logistic | ML | 41.60 | 8.32 | 0.20 | 28.15 | 62.14 | 0.99 |
| logistic | MO | 44.75 | 9.20 | 0.21 | 29.73 | 66.49 | 0.99 |
| logistic | GR | 38.62 | 8.45 | 0.22 | 19.07 | 52.33 | 0.96 |
| triangular | ML | 48.35 | 4.34 | 0.09 | 40.93 | 67.30 | 1.00 |
| triangular | MO | 43.43 | 7.50 | 0.17 | 31.93 | 61.30 | 1.00 |
| triangular | GR | 40.93 | 7.17 | 0.18 | 27.46 | 55.35 | 1.00 |
| burr | ML | 50.28 | 5.62 | 0.11 | 40.64 | 64.75 | 0.52 |

Table 12. Range of HC05 values (μg/L) for Chlorpyrifos SSDs estimated from Web ICE predicted values using all three surrogates

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 3.15 | 0.89 | 0.28 | 1.93 | 6.03 | 0.49 |
| gumbel | MO | 3.74 | 1.37 | 0.37 | 1.86 | 7.24 | 0.69 |
| gumbel | GR | 2.99 | 1.06 | 0.35 | 0.98 | 5.09 | 0.35 |
| normal | ML | 2.26 | 1.01 | 0.45 | 1.00 | 5.81 | 0.21 |
| normal | MO | 2.16 | 1.16 | 0.54 | 0.90 | 5.29 | 0.18 |
| normal | GR | 1.70 | 0.85 | 0.50 | 0.47 | 3.59 | 0.10 |
| logistic | ML | 1.59 | 0.84 | 0.53 | 0.53 | 4.63 | 0.11 |
| logistic | MO | 2.24 | 1.36 | 0.61 | 0.81 | 6.08 | 0.20 |
| logistic | GR | 1.55 | 0.86 | 0.56 | 0.27 | 3.51 | 0.10 |
| triangular | ML | 3.00 | 1.20 | 0.40 | 1.99 | 6.69 | 0.43 |
| triangular | MO | 2.06 | 1.02 | 0.50 | 0.92 | 4.80 | 0.15 |
| triangular | GR | 1.79 | 0.86 | 0.48 | 0.67 | 3.92 | 0.10 |
| burr | ML | 3.14 | 0.89 | 0.28 | 1.81 | 5.87 | 0.00 |

Table 13. Range of HC05 values for Chlorpyrifos SSDs based on measured freshwater fish LC50s

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 5.46 | 2.76 | 0.51 | 2.28 | 19.56 | 0.75 |
| gumbel | MO | 9.86 | 6.23 | 0.63 | 3.59 | 27.58 | 0.97 |
| gumbel | GR | 6.77 | 4.02 | 0.59 | 1.11 | 16.16 | 0.82 |
| normal | ML | 5.58 | 3.81 | 0.68 | 1.63 | 23.30 | 0.66 |
| normal | MO | 5.10 | 5.41 | 1.06 | 1.28 | 19.88 | 0.60 |
| normal | GR | 3.34 | 2.94 | 0.88 | 0.40 | 11.20 | 0.42 |
| logistic | ML | 5.73 | 4.74 | 0.83 | 1.18 | 26.71 | 0.59 |
| logistic | MO | 5.32 | 5.94 | 1.12 | 1.11 | 23.19 | 0.58 |
| logistic | GR | 2.86 | 2.92 | 1.02 | 0.15 | 10.00 | 0.37 |
| triangular | ML | 5.84 | 2.48 | 0.42 | 3.01 | 24.80 | 0.79 |
| triangular | MO | 4.81 | 4.72 | 0.98 | 1.49 | 19.12 | 0.64 |
| triangular | GR | 3.68 | 3.29 | 0.89 | 0.69 | 12.47 | 0.46 |
| burr | ML | 2.04 | 3.18 | 1.56 | 0.13 | 36.23 | 0.83 |

**V. Calculation of other quantiles**

Tables 14 - 18 provide estimates of the HC05 as well as other quantiles of the fitted SSDs.

Table 14. Estimated quantiles of the fitted SSDs for Chlorpyrifos Web ICE predicted LC50s based on rainbow trout.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 4.7 | 5.4 | 10.3 | 28.8 | 42.5 |
| gumbel | MO | 4.7 | 5.4 | 10.4 | 29.1 | 43.1 |
| gumbel | GR | 4.2 | 4.9 | 10.5 | 34.5 | 54.4 |
| normal | ML | 3.8 | 4.8 | 11.6 | 28.1 | 36.0 |
| normal | MO | 3.7 | 4.7 | 11.6 | 28.6 | 36.9 |
| normal | GR | 3.2 | 4.3 | 11.6 | 31.5 | 41.7 |
| logistic | ML | 3.4 | 4.6 | 10.9 | 26.1 | 35.1 |
| logistic | MO | 3.7 | 5.0 | 11.6 | 27.2 | 36.3 |
| logistic | GR | 3.1 | 4.3 | 11.6 | 31.2 | 43.6 |
| triangular | ML | 4.1 | 5.0 | 12.4 | 30.7 | 38.0 |
| triangular | MO | 3.6 | 4.5 | 11.6 | 30.1 | 37.7 |
| triangular | GR | 3.3 | 4.2 | 11.6 | 32.0 | 40.6 |
| burr | ML | 4.7 | 5.4 | 10.3 | 28.8 | 42.5 |

Table 15. Estimated quantiles of the fitted SSDs for Chlorpyrifos Web ICE predicted LC50s based on bluegill.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 1.5 | 2.0 | 5.7 | 30.8 | 58.5 |
| gumbel | MO | 1.9 | 2.3 | 5.7 | 23.7 | 41.0 |
| gumbel | GR | 1.5 | 1.9 | 5.8 | 34.9 | 69.1 |
| normal | ML | 1.4 | 2.0 | 6.7 | 22.0 | 30.9 |
| normal | MO | 1.3 | 1.9 | 6.7 | 23.2 | 33.1 |
| normal | GR | 1.0 | 1.5 | 6.7 | 29.0 | 44.0 |
| logistic | ML | 1.3 | 2.0 | 7.0 | 25.0 | 38.5 |
| logistic | MO | 1.4 | 2.0 | 6.7 | 21.7 | 32.4 |
| logistic | GR | 0.9 | 1.5 | 6.7 | 29.4 | 48.7 |
| triangular | ML | 1.6 | 2.1 | 6.5 | 19.8 | 25.8 |
| triangular | MO | 1.3 | 1.8 | 6.7 | 24.9 | 34.0 |
| triangular | GR | 1.1 | 1.5 | 6.7 | 29.1 | 41.3 |
| burr | ML | 0.0 | 1.3 | 9.3 | 18.8 | 20.1 |

Table 16. Estimated quantiles of the fitted SSDs for Chlorpyrifos Web ICE predicted LC50s based on fathead minnow.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 50.3 | 57.3 | 104.1 | 265.8 | 380.2 |
| gumbel | MO | 53.8 | 60.6 | 104.1 | 243.5 | 336.9 |
| gumbel | GR | 49.1 | 56.3 | 105.1 | 279.6 | 406.4 |
| normal | ML | 45.1 | 55.4 | 114.5 | 236.7 | 290.8 |
| normal | MO | 44.2 | 54.5 | 114.5 | 240.3 | 296.5 |
| normal | GR | 40.1 | 50.5 | 114.5 | 259.4 | 327.1 |
| logistic | ML | 41.6 | 53.6 | 112.8 | 237.6 | 306.0 |
| logistic | MO | 44.7 | 56.8 | 114.5 | 230.7 | 292.8 |
| logistic | GR | 38.6 | 50.9 | 114.5 | 257.5 | 339.3 |
| triangular | ML | 48.3 | 57.3 | 117.2 | 239.7 | 284.0 |
| triangular | MO | 43.4 | 52.3 | 114.5 | 250.6 | 301.7 |
| triangular | GR | 40.9 | 49.8 | 114.5 | 262.9 | 320.1 |
| burr | ML | 50.3 | 57.3 | 104.1 | 265.7 | 380.1 |

Table 17. Estimated quantiles of the fitted SSDs for Chlorpyrifos Web ICE predicted LC50s based on all three surrogates.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 3.1 | 4.5 | 23.4 | 310.1 | 832.3 |
| gumbel | MO | 3.7 | 5.2 | 23.8 | 256.3 | 635.9 |
| gumbel | GR | 3.0 | 4.4 | 24.3 | 360.4 | 1009.8 |
| normal | ML | 2.3 | 4.0 | 31.0 | 238.4 | 425.2 |
| normal | MO | 2.2 | 3.9 | 31.0 | 246.9 | 444.7 |
| normal | GR | 1.7 | 3.2 | 31.0 | 297.7 | 565.3 |
| logistic | ML | 1.6 | 3.4 | 30.0 | 268.1 | 564.8 |
| logistic | MO | 2.2 | 4.4 | 31.0 | 220.4 | 429.4 |
| logistic | GR | 1.6 | 3.3 | 31.0 | 289.1 | 617.9 |
| triangular | ML | 3.0 | 4.7 | 30.0 | 192.7 | 299.5 |
| triangular | MO | 2.1 | 3.5 | 31.0 | 277.7 | 466.8 |
| triangular | GR | 1.8 | 3.1 | 31.0 | 311.2 | 537.6 |
| burr | ML | 3.1 | 4.5 | 23.4 | 310.0 | 831.6 |

Table 18. Estimated quantiles of the fitted SSDs for Chlorpyrifos empirical LC50s for freshwater fish

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 5.5 | 9.1 | 94.6 | 3711.2 | 15084.5 |
| gumbel | MO | 9.9 | 14.7 | 90.6 | 1575.0 | 4688.7 |
| gumbel | GR | 6.8 | 10.9 | 94.6 | 2822.4 | 10329.0 |
| normal | ML | 5.6 | 11.1 | 124.7 | 1404.0 | 2788.8 |
| normal | MO | 5.1 | 10.3 | 124.7 | 1506.1 | 3051.7 |
| normal | GR | 3.3 | 7.4 | 124.7 | 2092.2 | 4653.3 |
| logistic | ML | 5.7 | 13.1 | 149.2 | 1698.4 | 3883.6 |
| logistic | MO | 5.3 | 11.8 | 124.7 | 1314.1 | 2926.8 |
| logistic | GR | 2.9 | 7.5 | 124.7 | 2085.6 | 5435.0 |
| triangular | ML | 5.8 | 10.4 | 118.3 | 1347.0 | 2397.0 |
| triangular | MO | 4.8 | 9.0 | 124.7 | 1734.0 | 3235.2 |
| triangular | GR | 3.7 | 7.2 | 124.7 | 2153.3 | 4229.0 |
| burr | ML | 2.0 | 8.1 | 204.8 | 988.3 | 1433.3 |

**VI. Calculation of thresholds**

Thresholds were calculated using a probit curve with the HC05 as the mean and three different slopes (2, 4.5, and 9). Calculated thresholds are provided in Tables 19 - 23.

Table 19. Thresholds (μg/L) for determination of action area based on Web ICE predicted values of Chlorpyrifos LC50s from rainbow trout

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distrib. | method | Mortality Threshold (10-6) | | | Indirect Effects Threshold (10-1) | | |
| slope = 4.5 | slope = 2 | slope = 9 | slope = 4.5 | slope = 2 | slope = 9 |
| gumbel | ML | 0.41 | 0.02 | 1.38 | 2.42 | 1.06 | 3.35 |
| gumbel | MO | 0.41 | 0.02 | 1.38 | 2.42 | 1.07 | 3.36 |
| gumbel | GR | 0.37 | 0.02 | 1.23 | 2.16 | 0.95 | 3.00 |
| normal | ML | 0.33 | 0.02 | 1.12 | 1.95 | 0.86 | 2.71 |
| normal | MO | 0.32 | 0.02 | 1.09 | 1.91 | 0.84 | 2.65 |
| normal | GR | 0.29 | 0.01 | 0.96 | 1.69 | 0.74 | 2.34 |
| logistic | ML | 0.30 | 0.01 | 1.01 | 1.76 | 0.78 | 2.45 |
| logistic | MO | 0.33 | 0.02 | 1.11 | 1.94 | 0.85 | 2.69 |
| logistic | GR | 0.27 | 0.01 | 0.92 | 1.61 | 0.71 | 2.24 |
| triangular | ML | 0.36 | 0.02 | 1.21 | 2.12 | 0.93 | 2.94 |
| triangular | MO | 0.32 | 0.02 | 1.07 | 1.87 | 0.82 | 2.59 |
| triangular | GR | 0.29 | 0.01 | 0.99 | 1.73 | 0.76 | 2.40 |
| burr | ML | 0.41 | 0.02 | 1.38 | 2.42 | 1.06 | 3.35 |

Table 20. Thresholds (μg/L) for determination of action area based on Web ICE predicted values of Chlorpyrifos LC50s from bluegill

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distrib. | method | Mortality Threshold (10-6) | | | Indirect Effects Threshold (10-1) | | |
| slope = 4.5 | slope = 2 | slope = 9 | slope = 4.5 | slope = 2 | slope = 9 |
| gumbel | ML | 0.14 | 0.01 | 0.46 | 0.80 | 0.35 | 1.11 |
| gumbel | MO | 0.16 | 0.01 | 0.55 | 0.97 | 0.43 | 1.34 |
| gumbel | GR | 0.13 | 0.01 | 0.43 | 0.76 | 0.33 | 1.05 |
| normal | ML | 0.13 | 0.01 | 0.42 | 0.74 | 0.33 | 1.03 |
| normal | MO | 0.12 | 0.01 | 0.40 | 0.69 | 0.31 | 0.96 |
| normal | GR | 0.09 | 0.00 | 0.30 | 0.52 | 0.23 | 0.72 |
| logistic | ML | 0.11 | 0.01 | 0.38 | 0.67 | 0.29 | 0.93 |
| logistic | MO | 0.12 | 0.01 | 0.41 | 0.71 | 0.31 | 0.98 |
| logistic | GR | 0.08 | 0.00 | 0.27 | 0.47 | 0.21 | 0.65 |
| triangular | ML | 0.14 | 0.01 | 0.48 | 0.84 | 0.37 | 1.17 |
| triangular | MO | 0.11 | 0.01 | 0.39 | 0.67 | 0.30 | 0.94 |
| triangular | GR | 0.09 | 0.00 | 0.32 | 0.56 | 0.25 | 0.77 |
| burr | ML | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

Table 21. Thresholds (μg/L) for determination of action area based on Web ICE predicted values of Chlorpyrifos LC50s from fathead minnow

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distrib. | method | Mortality Threshold (10-6) | | | Indirect Effects Threshold (10-1) | | |
| slope = 4.5 | slope = 2 | slope = 9 | slope = 4.5 | slope = 2 | slope = 9 |
| gumbel | ML | 4.42 | 0.21 | 14.90 | 26.10 | 11.50 | 36.22 |
| gumbel | MO | 4.72 | 0.23 | 15.94 | 27.91 | 12.30 | 38.75 |
| gumbel | GR | 4.32 | 0.21 | 14.56 | 25.51 | 11.24 | 35.40 |
| normal | ML | 3.96 | 0.19 | 13.35 | 23.38 | 10.30 | 32.46 |
| normal | MO | 3.88 | 0.19 | 13.10 | 22.94 | 10.11 | 31.84 |
| normal | GR | 3.52 | 0.17 | 11.87 | 20.79 | 9.16 | 28.86 |
| logistic | ML | 3.65 | 0.17 | 12.33 | 21.59 | 9.51 | 29.97 |
| logistic | MO | 3.93 | 0.19 | 13.26 | 23.23 | 10.23 | 32.24 |
| logistic | GR | 3.39 | 0.16 | 11.45 | 20.04 | 8.83 | 27.82 |
| triangular | ML | 4.25 | 0.20 | 14.33 | 25.10 | 11.06 | 34.83 |
| triangular | MO | 3.82 | 0.18 | 12.87 | 22.54 | 9.93 | 31.29 |
| triangular | GR | 3.59 | 0.17 | 12.13 | 21.24 | 9.36 | 29.49 |
| burr | ML | 4.42 | 0.21 | 14.90 | 26.10 | 11.50 | 36.22 |

Table 22. Thresholds (μg/L) for determination of action area based on Web ICE predicted values of Chlorpyrifos LC50s from all three surrogates

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distrib. | method | Mortality Threshold (10-6) | | | Indirect Effects Threshold (10-1) | | |
| slope = 4.5 | slope = 2 | slope = 9 | slope = 4.5 | slope = 2 | slope = 9 |
| gumbel | ML | 0.28 | 0.01 | 0.93 | 1.63 | 0.72 | 2.27 |
| gumbel | MO | 0.33 | 0.02 | 1.11 | 1.94 | 0.86 | 2.70 |
| gumbel | GR | 0.26 | 0.01 | 0.89 | 1.55 | 0.68 | 2.16 |
| normal | ML | 0.20 | 0.01 | 0.67 | 1.17 | 0.52 | 1.63 |
| normal | MO | 0.19 | 0.01 | 0.64 | 1.12 | 0.49 | 1.56 |
| normal | GR | 0.15 | 0.01 | 0.50 | 0.88 | 0.39 | 1.22 |
| logistic | ML | 0.14 | 0.01 | 0.47 | 0.83 | 0.36 | 1.15 |
| logistic | MO | 0.20 | 0.01 | 0.66 | 1.16 | 0.51 | 1.61 |
| logistic | GR | 0.14 | 0.01 | 0.46 | 0.81 | 0.36 | 1.12 |
| triangular | ML | 0.26 | 0.01 | 0.89 | 1.55 | 0.69 | 2.16 |
| triangular | MO | 0.18 | 0.01 | 0.61 | 1.07 | 0.47 | 1.48 |
| triangular | GR | 0.16 | 0.01 | 0.53 | 0.93 | 0.41 | 1.29 |
| burr | ML | 0.28 | 0.01 | 0.93 | 1.63 | 0.72 | 2.27 |

Table 23. Thresholds (μg/L) for determination of action area using empirical values for Chlorpyrifos LC50s for freshwater fish

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distrib. | method | Mortality Threshold (10-6) | | | Indirect Effects Threshold (10-1) | | |
| slope = 4.5 | slope = 2 | slope = 9 | slope = 4.5 | slope = 2 | slope = 9 |
| gumbel | ML | 0.48 | 0.02 | 1.62 | 2.83 | 1.25 | 3.93 |
| gumbel | MO | 0.87 | 0.04 | 2.92 | 5.12 | 2.26 | 7.10 |
| gumbel | GR | 0.59 | 0.03 | 2.01 | 3.51 | 1.55 | 4.87 |
| normal | ML | 0.49 | 0.02 | 1.65 | 2.90 | 1.28 | 4.02 |
| normal | MO | 0.45 | 0.02 | 1.51 | 2.65 | 1.17 | 3.67 |
| normal | GR | 0.29 | 0.01 | 0.99 | 1.74 | 0.76 | 2.41 |
| logistic | ML | 0.50 | 0.02 | 1.70 | 2.98 | 1.31 | 4.13 |
| logistic | MO | 0.47 | 0.02 | 1.58 | 2.76 | 1.22 | 3.83 |
| logistic | GR | 0.25 | 0.01 | 0.85 | 1.49 | 0.65 | 2.06 |
| triangular | ML | 0.51 | 0.02 | 1.73 | 3.03 | 1.34 | 4.21 |
| triangular | MO | 0.42 | 0.02 | 1.43 | 2.50 | 1.10 | 3.47 |
| triangular | GR | 0.32 | 0.02 | 1.09 | 1.91 | 0.84 | 2.65 |
| burr | ML | 0.18 | 0.01 | 0.61 | 1.06 | 0.47 | 1.47 |

**VII. Comparison of Predicted and Tested Toxicity**

To further compare SSDs fit to predicted values to SSDs generated from test results, the taxa from each set of predicted values were cross tabulated with corresponding taxa for which empirical test results were available (Tables 24 – 28). These tables also report the discrepancy as absolute value of the difference between predicted and tested toxicity value, scaled to the empirical toxicity value and the toxicological distance as the absolute value of the difference between the tested toxicity value of the surrogate test species and that of every other species (see Malathion Predicted Values report for sample calculations).

Two correlations were examined for each of these sets of crosstablulated data, between the predicted and tested toxicity values and between the discrepancy statistic and the distance statistic. The latter test was done to examine whether predicted values get worse as the distance (measured as relative sensitivity to the chemical) increases between taxa.

Results of these correlations are presented in Tables 24-28. For these datasets, the predicted and empirical values were not significantly correlated. There was no correlation between toxicological distance and predictive accuracy. The former result is likely due to low power in these small cross-tabulation datasets.

Table 24. Crosstabulated toxicity values for Web ICE predictions based on rainbow trout regressions.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Taxon | Predicted  (Web ICE) | Tested  (geomeans) | Discrepancy | Distance |
| *Oncorhynchus mykiss* | 8.2 | 8.2 | 0.0 | 0.0 |
| *Oncorhynchus clarkii* | 10.4 | 18.6 | 0.4 | 10.3 |
| *Salvelinus namaycush* | 12.4 | 141.1 | 0.9 | 132.9 |
| *Lepomis macrochirus* | 13.6 | 3.0 | 3.5 | 5.2 |
| *Ictalurus punctatus* | 27.1 | 61.3 | 0.6 | 53.0 |
| *Pimephales promelas* | 30.4 | 212.3 | 0.9 | 204.1 |

Table 25. Crosstabulated toxicity values for Web ICE predictions based on bluegill regressions.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Taxon | Web ICE | Geomean | Discrepancy | Distance |
| *Lepomis macrochirus* | 3.0 | 3.0 | 0.0 | 0.0 |
| *Oncorhynchus mykiss* | 3.4 | 8.2 | 0.6 | 5.2 |
| *Oncorhynchus clarkii* | 10.0 | 18.6 | 0.5 | 15.6 |
| *Salvelinus namaycush* | 10.2 | 141.1 | 0.9 | 138.1 |
| *Pimephales promelas* | 11.8 | 212.3 | 0.9 | 209.3 |
| *Ictalurus punctatus* | 18.0 | 61.3 | 0.7 | 58.2 |

Table 26. Crosstabulated toxicity values for Web ICE predictions based on fathead minnow regressions.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Taxon | Web ICE | Geomean | Discrepancy | Distance |
| *Salvelinus namaycush* | 60.5 | 141.1 | 0.6 | 71.2 |
| *Oncorhynchus clarkii* | 86.8 | 18.6 | 3.7 | 193.7 |
| *Oncorhynchus mykiss* | 117.2 | 8.2 | 13.2 | 204.1 |
| *Lepomis macrochirus* | 156.2 | 3.0 | 50.8 | 209.3 |
| *Pimephales promelas* | 212.3 | 212.3 | 0.0 | 0.0 |
| *Ictalurus punctatus* | 214.5 | 61.3 | 2.5 | 151.1 |
| *Oreochromis mossambicus* | 340.8 | 20.2 | 15.9 | 192.1 |

Table 27. Crosstabulated toxicity values for Web ICE predictions based on all three surroates.

|  |  |  |
| --- | --- | --- |
| Taxon | Web ICE | Geomean |
| Lepomis macrochirus | 3.0 | 3.0 |
| Oncorhynchus mykiss | 8.2 | 8.2 |
| Oncorhynchus clarkii | 10.4 | 18.6 |
| Salvelinus namaycush | 12.4 | 141.1 |
| Pimephales promelas | 212.3 | 212.3 |
| Ictalurus punctatus | 214.5 | 61.3 |
| Oreochromis mossambicus | 340.8 | 20.2 |

Table 28. Correlations between crosstabulated toxicity values

|  |  |  |
| --- | --- | --- |
| Surrogate Species | correlation between predicted and tested | Correlation between discrepancy and distance |
| rainbow trout | ρ = 0.66, p = 0.16 | ρ = -0.14, p = 0.79 |
| bluegill | ρ = 0.45, p = 0.37 | ρ = 0.80, p = 0.06 |
| fathead minnow | ρ = -0.05, p = 0.92 | ρ = 0.56, p = 0.19 |
| all three | ρ = 0.10, p = 0.86 | n/a |