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

**Summary**

SSDs were fit to predicted test results for fish exposed to Diazinon. 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 data set comprised a mixture of predicted values chosen from each of the three surrogate species according to the Web ICE selection criteria. 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 Diazinon test results

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| statistic | rainbow trout | bluegill | fathead | mixture | empirical |
| Sample size (n) | 26 | 16 | 18 | 32 | 42 |
| Best Distribution (by AICc) | gumbel | triangular | triangular | gumbel | logistic |
| Goodness of fit P-value | 1 | 1 | 1 | 1 | 0.95 |
| CV of the HC05 | 0.09 | 0.25 | 0.16 | 0.18 | 0.6 |
| HC05 | 125.4 | 109.1 | 1003.5 | 95.6 | 311.8 |
| HC10 | 139.4 | 130.0 | 1210.7 | 119.3 | 603.5 |
| HC50 | 226.0 | 273.0 | 2673.4 | 327.5 | 4208.8 |
| HC90 | 482.1 | 572.9 | 5903.3 | 1597.1 | 29353.9 |
| HC95 | 644.0 | 683.0 | 7122.2 | 2926.0 | 56822.2 |
| Mortality Thresh.1 (slope = 4.5) | 11.0 | 9.58 | 88.2 | 8.4 | 27.4 |
| Indirect Effects Threshold1 (slope = 4.5) | 65.1 | 56.62 | 520.9 | 49.6 | 161.8 |

1Slope of dose-response curve = 4.5

Predicted values from rainbow trout and bluegill produced estimates of HC05 that were comparable to the empirical data, as did predicted values generated from the mixture dataset. However, predicted values from fathead minnow produced estimates of the HC05 that were an order of magnitude greater than the empirical tested 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) show some evidence of lack-of-fit for the data set generated from a mixture of surrogates and for the empirical data, however, p-values from goodness of fit tests did not show significant lack of fit. However, variances in the SSDs for predicted values were generally much smaller than the variance in the SSD for empirical test results. The variance of the distribution fit using all predicted values was closer to that of the empirical test results.

Cross-tabulation of predicted values with empirical test results show that Web ICE predictions were positively correlated with empirically measured toxicity values (correlation coefficients on the order of 0.7 – 0.8) for bluegill and fathead minnow. The rainbow trout predicted values and the mixed dataset produced non-significant negative correlations with empirical test results. The discrepancy between predicted and tested values was positively correlated with toxicity distance for the rainbow trout and fathead minnow predicted value datasets.

**I. Data**

Data were received from Elizabeth Donovan on 12 September 2014 in the file:

“Diazinon SSD\_WebICE.xlsx”

From these files I created four working files:

1. DiazinonFWFishIcePredRainbowTrout.xlsx

2. DiazinonFWFishIcePredBluegill.xlsx

3. DiazinonFWFishIcePredFathead.xlsx

4. DiazinonFWFishIcePredAllThree.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 Diazinon

|  |  |
| --- | --- |
| Surrogate Species | Predicted Values |
| rainbow trout | 26 |
| bluegill | 16 |
| fathead minnow | 18 |
| mixture | 32 |

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 empirical dataset on freshwater fish originally provided by Kris Garber (“diazinon fish-amph data for SSD.xlsx”, 14 July 2014) and updated by Scott Glaberman (“SSD Data Diazinon 10.10.14.xlsx”, 10 October 2014, n=42) was reanalyzed after converting that dataset from mg/L to µg/L.

Five potential distributions for the Diazinon data (log-normal, log-logistic, log-triangular, log-gumbel, and Burr). 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 burr distribution (Table 4). When bluegill and fathead minnow were used as surrogates, the triangular distribution provided the best fit (Tables 5, 6). For the dataset comprised of values predicted from a mixture of the three surrogates, the gumbel distribution provided the best fit, followed closely by the burr distribution (Table 7). For the empirical data, the logistic distribution provided the best fit, followed closely by the normal and triangular distributions (Table 8). Estimates of the HC05 were quite similar between all sets of predicted values and the empirical test results, with the exception of the dataset comprised of predicted values from fathead minnow alone. In this case the HC05 estimates were about an order of magnitude higher than for the other datasets.

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| gumbel | 125.4 | 338.9 | 0.0 | 0.7 |
| burr | 125.4 | 341.5 | 2.5 | 0.2 |
| logistic | 99.3 | 343.6 | 4.7 | 0.1 |
| normal | 104.0 | 344.1 | 5.2 | 0.0 |
| triangular | 102.4 | 345.9 | 7.0 | 0.0 |

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| triangular | 109.1 | 226.4 | 0.0 | 0.5 |
| gumbel | 120.4 | 227.4 | 1.0 | 0.3 |
| logistic | 92.3 | 229.6 | 3.2 | 0.1 |
| burr | 120.3 | 230.4 | 4.0 | 0.1 |
| normal | 76.8 | 230.8 | 4.5 | 0.1 |

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| triangular | 1003.5 | 342.8 | 0.0 | 0.6 |
| normal | 1011.9 | 344.4 | 1.6 | 0.3 |
| logistic | 978.7 | 345.7 | 2.9 | 0.1 |
| gumbel | 1030.2 | 348.1 | 5.3 | 0.0 |
| burr | 1023.7 | 350.1 | 7.3 | 0.0 |

Table 7. Comparison of distributions for freshwater fish toxicity values predicted from a mixture of all three surrogate species.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| gumbel | 95.6 | 504.3 | 0.0 | 0.8 |
| burr | 95.5 | 506.7 | 2.4 | 0.2 |
| triangular | 47.5 | 516.3 | 12.1 | 0.0 |
| normal | 46.6 | 517.8 | 13.5 | 0.0 |
| logistic | 37.3 | 517.8 | 13.6 | 0.0 |

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| distribution | HC05 | AICc | ∆AICc | Weight |
| logistic | 311.8 | 489.2 | 0.0 | 0.39 |
| normal | 259.6 | 489.7 | 0.5 | 0.30 |
| triangular | 198.8 | 489.8 | 0.7 | 0.28 |
| burr | 260.7 | 494.9 | 5.7 | 0.02 |
| gumbel | 232.6 | 496.7 | 7.5 | 0.01 |

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 Diazinon, based on rainbow trout regressions.



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



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



Figure 4. Log-gumbel SSD for WebICE predicted values for freshwater fish LC50s for Diazinon, based on a mixture of three surrogate species.



Figure 5. Log-logistic SSD for Diazinon 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. Surrogate species used to generate WebICE predicted values are circled in red.



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

To test goodness-of-fit I fit all five distributions to each of the five datasets and ran bootstrap goodness-of-fit tests with 5,000 bootstrap replicates. I used three different fitting methods (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 (Table 9) fit to the empirical data. The coefficient of variation for the HC05 was always below 1.

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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 125.43 | 11.10 | 0.09 | 107.56 | 153.70 | 1.00 |
| gumbel | MO | 122.76 | 14.13 | 0.12 | 97.99 | 153.54 | 1.00 |
| gumbel | GR | 113.37 | 15.12 | 0.13 | 76.90 | 136.48 | 1.00 |
| normal | ML | 104.02 | 16.32 | 0.16 | 78.33 | 146.30 | 1.00 |
| normal | MO | 102.31 | 16.87 | 0.16 | 74.89 | 141.12 | 1.00 |
| normal | GR | 93.87 | 16.68 | 0.18 | 59.67 | 124.01 | 1.00 |
| logistic | ML | 99.33 | 16.21 | 0.16 | 72.14 | 139.46 | 1.00 |
| logistic | MO | 103.50 | 18.91 | 0.18 | 72.09 | 145.34 | 1.00 |
| logistic | GR | 90.91 | 18.14 | 0.20 | 48.60 | 119.27 | 1.00 |
| triangular | ML | 102.40 | 7.08 | 0.07 | 85.36 | 148.14 | 1.00 |
| triangular | MO | 100.68 | 15.42 | 0.15 | 76.12 | 136.63 | 1.00 |
| triangular | GR | 95.63 | 15.02 | 0.16 | 66.68 | 125.45 | 1.00 |
| burr | ML | 125.42 | 11.09 | 0.09 | 106.07 | 152.01 | 0.88 |

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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 120.36 | 16.88 | 0.14 | 95.05 | 166.48 | 1.00 |
| gumbel | MO | 124.45 | 21.61 | 0.17 | 89.43 | 174.85 | 1.00 |
| gumbel | GR | 109.69 | 21.69 | 0.20 | 60.78 | 147.04 | 1.00 |
| normal | ML | 76.78 | 26.11 | 0.34 | 44.92 | 147.39 | 1.00 |
| normal | MO | 100.58 | 24.30 | 0.24 | 63.42 | 157.37 | 1.00 |
| normal | GR | 87.26 | 22.97 | 0.26 | 41.51 | 131.43 | 1.00 |
| logistic | ML | 92.29 | 23.82 | 0.26 | 54.38 | 157.66 | 1.00 |
| logistic | MO | 101.95 | 27.96 | 0.27 | 60.14 | 167.73 | 1.00 |
| logistic | GR | 82.83 | 24.70 | 0.30 | 30.25 | 126.48 | 0.99 |
| triangular | ML | 109.08 | 27.01 | 0.25 | 88.04 | 170.05 | 1.00 |
| triangular | MO | 98.71 | 23.25 | 0.24 | 65.41 | 155.86 | 1.00 |
| triangular | GR | 90.12 | 21.68 | 0.24 | 51.77 | 137.35 | 1.00 |
| burr | ML | 120.34 | 16.90 | 0.14 | 92.30 | 167.31 | 0.19 |

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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 1030.25 | 165.91 | 0.16 | 776.40 | 1517.49 | 1.00 |
| gumbel | MO | 1228.00 | 207.71 | 0.17 | 890.00 | 1722.25 | 1.00 |
| gumbel | GR | 1086.42 | 211.95 | 0.20 | 605.85 | 1437.00 | 1.00 |
| normal | ML | 1011.93 | 227.02 | 0.22 | 682.12 | 1615.95 | 1.00 |
| normal | MO | 983.27 | 236.37 | 0.24 | 621.68 | 1550.17 | 1.00 |
| normal | GR | 857.74 | 220.94 | 0.26 | 422.04 | 1299.57 | 1.00 |
| logistic | ML | 978.71 | 260.78 | 0.27 | 592.76 | 1656.40 | 1.00 |
| logistic | MO | 997.21 | 267.60 | 0.27 | 575.59 | 1633.46 | 1.00 |
| logistic | GR | 815.59 | 238.68 | 0.29 | 303.97 | 1238.02 | 1.00 |
| triangular | ML | 1003.50 | 165.43 | 0.16 | 808.19 | 1562.38 | 1.00 |
| triangular | MO | 964.11 | 221.44 | 0.23 | 650.85 | 1509.88 | 1.00 |
| triangular | GR | 884.65 | 211.42 | 0.24 | 514.92 | 1336.81 | 1.00 |
| burr | ML | 1023.72 | 205.43 | 0.20 | 740.77 | 1593.28 | 0.16 |

Table 12. Range of HC05 values (μg/L) for Diazinon SSDs based on a mixture of all three surrogate species.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 95.62 | 17.08 | 0.18 | 72.28 | 138.10 | 1.00 |
| gumbel | MO | 71.72 | 20.35 | 0.28 | 40.67 | 121.31 | 1.00 |
| gumbel | GR | 60.05 | 16.98 | 0.28 | 24.93 | 90.25 | 0.94 |
| normal | ML | 46.65 | 16.84 | 0.36 | 24.07 | 97.98 | 0.95 |
| normal | MO | 45.07 | 18.41 | 0.41 | 22.07 | 93.95 | 0.94 |
| normal | GR | 37.31 | 14.77 | 0.40 | 13.43 | 70.96 | 0.87 |
| logistic | ML | 37.29 | 13.54 | 0.36 | 17.41 | 80.22 | 0.63 |
| logistic | MO | 46.42 | 21.22 | 0.46 | 19.95 | 100.84 | 0.70 |
| logistic | GR | 34.80 | 14.99 | 0.43 | 9.16 | 66.59 | 0.48 |
| triangular | ML | 47.47 | 24.81 | 0.52 | 32.65 | 97.06 | 1.00 |
| triangular | MO | 43.25 | 16.28 | 0.38 | 22.93 | 86.26 | 1.00 |
| triangular | GR | 38.77 | 14.25 | 0.37 | 17.50 | 70.93 | 1.00 |
| burr | ML | 95.55 | 17.09 | 0.18 | 70.29 | 135.26 | 0.00 |

Table 13. Range of HC05 values (μg/L) for Diazinon SSDs based on measured freshwater fish LC50s

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| distribution | method | HC05 | SE | CV | LCL | UCL | P |
| gumbel | ML | 232.6 | 89.6 | 0.4 | 119.7 | 582.5 | 1.00 |
| gumbel | MO | 428.7 | 180.0 | 0.4 | 197.7 | 894.7 | 1.00 |
| gumbel | GR | 329.3 | 133.6 | 0.4 | 93.3 | 603.6 | 1.00 |
| normal | ML | 259.6 | 130.9 | 0.5 | 105.4 | 745.5 | 1.00 |
| normal | MO | 245.2 | 155.1 | 0.6 | 90.1 | 674.0 | 1.00 |
| normal | GR | 183.8 | 105.7 | 0.6 | 40.6 | 438.2 | 0.98 |
| logistic | ML | 311.8 | 177.4 | 0.6 | 106.7 | 908.2 | 0.95 |
| logistic | MO | 254.1 | 175.6 | 0.7 | 76.4 | 749.7 | 0.93 |
| logistic | GR | 165.1 | 103.7 | 0.6 | 21.2 | 413.1 | 0.82 |
| triangular | ML | 198.8 | 71.3 | 0.4 | 109.8 | 622.2 | 1.00 |
| triangular | MO | 233.4 | 140.2 | 0.6 | 95.0 | 635.0 | 1.00 |
| triangular | GR | 195.8 | 111.4 | 0.6 | 61.2 | 489.3 | 1.00 |
| burr | ML | 260.7 | 133.6 | 0.5 | 106.2 | 796.4 | 0.01 |

**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 (μg/L) of the fitted SSDs for Diazinon Web ICE predicted LC50s based on rainbow trout.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 125.4 | 139.4 | 226.0 | 482.1 | 644.0 |
| gumbel | MO | 122.8 | 137.1 | 226.6 | 498.6 | 673.9 |
| gumbel | GR | 113.4 | 128.6 | 228.5 | 563.1 | 794.8 |
| normal | ML | 104.0 | 126.0 | 247.5 | 486.2 | 588.7 |
| normal | MO | 102.3 | 124.4 | 247.5 | 492.4 | 598.5 |
| normal | GR | 93.9 | 116.3 | 247.5 | 526.6 | 652.4 |
| logistic | ML | 99.3 | 123.4 | 233.9 | 443.1 | 550.6 |
| logistic | MO | 103.5 | 129.1 | 247.5 | 474.2 | 591.6 |
| logistic | GR | 90.9 | 117.2 | 247.5 | 522.4 | 673.6 |
| triangular | ML | 102.4 | 123.5 | 272.8 | 602.5 | 726.9 |
| triangular | MO | 100.7 | 119.6 | 247.5 | 512.0 | 608.2 |
| triangular | GR | 95.6 | 114.7 | 247.5 | 533.7 | 640.4 |
| burr | ML | 125.4 | 139.4 | 226.0 | 482.0 | 643.8 |

Table 15. Estimated quantiles (μg/L) of the fitted SSDs for Diazinon Web ICE predicted LC50s based on bluegill.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 120.4 | 137.6 | 253.8 | 663.2 | 957.2 |
| gumbel | MO | 124.5 | 141.6 | 254.7 | 640.2 | 910.5 |
| gumbel | GR | 109.7 | 128.0 | 258.4 | 778.7 | 1186.9 |
| normal | ML | 76.8 | 103.7 | 300.0 | 867.7 | 1172.4 |
| normal | MO | 100.6 | 126.3 | 282.4 | 631.0 | 792.6 |
| normal | GR | 87.3 | 113.1 | 282.4 | 704.9 | 913.6 |
| logistic | ML | 92.3 | 121.5 | 272.9 | 612.7 | 806.7 |
| logistic | MO | 102.0 | 132.0 | 282.4 | 603.8 | 782.0 |
| logistic | GR | 82.8 | 113.1 | 282.4 | 705.1 | 962.5 |
| triangular | ML | 109.1 | 130.0 | 273.0 | 572.9 | 683.0 |
| triangular | MO | 98.7 | 120.7 | 282.4 | 660.4 | 807.7 |
| triangular | GR | 90.1 | 112.2 | 282.4 | 710.8 | 884.6 |
| burr | ML | 120.3 | 137.6 | 253.9 | 663.1 | 956.9 |

Table 16. Estimated quantiles (μg/L) of the fitted SSDs for Diazinon Web ICE predicted LC50s based on fathead minnow.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 1030.2 | 1219.0 | 2626.3 | 8757.9 | 13875.9 |
| gumbel | MO | 1228.0 | 1404.6 | 2593.3 | 6787.0 | 9802.5 |
| gumbel | GR | 1086.4 | 1273.5 | 2629.5 | 8202.1 | 12667.9 |
| normal | ML | 1011.9 | 1275.7 | 2887.9 | 6537.5 | 8241.5 |
| normal | MO | 983.3 | 1247.4 | 2887.9 | 6685.5 | 8481.7 |
| normal | GR | 857.7 | 1121.5 | 2887.9 | 7436.2 | 9723.0 |
| logistic | ML | 978.7 | 1299.6 | 2991.8 | 6887.4 | 9145.4 |
| logistic | MO | 997.2 | 1306.1 | 2887.9 | 6385.3 | 8363.1 |
| logistic | GR | 815.6 | 1124.1 | 2887.9 | 7418.9 | 10225.5 |
| triangular | ML | 1003.5 | 1210.7 | 2673.4 | 5903.3 | 7122.2 |
| triangular | MO | 964.1 | 1189.6 | 2887.9 | 7010.6 | 8650.3 |
| triangular | GR | 884.6 | 1109.7 | 2887.9 | 7515.5 | 9427.3 |
| burr | ML | 1023.7 | 1244.2 | 2709.8 | 8071.0 | 12114.6 |

Table 17. Estimated quantiles (μg/L) of the fitted SSDs for Diazinon Web ICE predicted LC50s based on all three surrogate species.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 95.6 | 119.3 | 327.5 | 1597.1 | 2926.0 |
| gumbel | MO | 71.7 | 95.0 | 342.2 | 2556.8 | 5513.6 |
| gumbel | GR | 60.1 | 82.4 | 348.4 | 3348.2 | 7949.0 |
| normal | ML | 46.6 | 76.1 | 428.5 | 2412.1 | 3936.6 |
| normal | MO | 45.1 | 74.1 | 428.5 | 2477.6 | 4074.3 |
| normal | GR | 37.3 | 64.0 | 428.5 | 2870.4 | 4921.5 |
| logistic | ML | 37.3 | 64.9 | 330.6 | 1684.3 | 2930.4 |
| logistic | MO | 46.4 | 81.6 | 428.5 | 2250.6 | 3956.1 |
| logistic | GR | 34.8 | 65.8 | 428.5 | 2790.5 | 5277.2 |
| triangular | ML | 47.5 | 72.3 | 426.4 | 2514.6 | 3829.0 |
| triangular | MO | 43.3 | 67.1 | 428.5 | 2736.1 | 4245.4 |
| triangular | GR | 38.8 | 61.4 | 428.5 | 2989.2 | 4736.4 |
| burr | ML | 95.5 | 119.2 | 327.5 | 1597.0 | 2925.6 |

Table 18. Estimated quantiles (μg/L) of the fitted SSDs for Diazinon empirical LC50s for freshwater fish

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| dist | method | HC05 | HC10 | HC50 | HC90 | HC95 |
| gumbel | ML | 232.6 | 368.1 | 2988.8 | 79926.1 | 280558.6 |
| gumbel | MO | 428.7 | 601.0 | 2806.5 | 31505.5 | 79374.1 |
| gumbel | GR | 329.3 | 486.6 | 2887.8 | 47231.2 | 137395.6 |
| normal | ML | 259.6 | 466.2 | 3678.2 | 29016.8 | 52112.4 |
| normal | MO | 245.2 | 446.0 | 3678.2 | 30334.8 | 55170.0 |
| normal | GR | 183.8 | 356.2 | 3678.2 | 37980.1 | 73619.0 |
| logistic | ML | 311.8 | 603.5 | 4208.8 | 29353.9 | 56822.2 |
| logistic | MO | 254.1 | 500.6 | 3678.2 | 27025.8 | 53251.4 |
| logistic | GR | 165.1 | 362.9 | 3678.2 | 37278.4 | 81942.7 |
| triangular | ML | 198.8 | 344.2 | 3489.3 | 35371.1 | 61235.4 |
| triangular | MO | 233.4 | 395.8 | 3678.2 | 34180.2 | 57967.0 |
| triangular | GR | 195.8 | 343.5 | 3678.2 | 39387.5 | 69080.9 |
| burr | ML | 260.7 | 456.9 | 3348.0 | 40710.3 | 100554.6 |

**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 Diazinon 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 | 11.02 | 0.53 | 37.17 | 65.10 | 28.68 | 90.37 |
| gumbel | MO | 10.78 | 0.52 | 36.38 | 63.72 | 28.07 | 88.44 |
| gumbel | GR | 9.96 | 0.48 | 33.60 | 58.85 | 25.93 | 81.68 |
| normal | ML | 9.14 | 0.44 | 30.83 | 53.99 | 23.79 | 74.94 |
| normal | MO | 8.99 | 0.43 | 30.32 | 53.11 | 23.40 | 73.71 |
| normal | GR | 8.25 | 0.39 | 27.82 | 48.72 | 21.47 | 67.63 |
| logistic | ML | 8.73 | 0.42 | 29.44 | 51.56 | 22.71 | 71.56 |
| logistic | MO | 9.09 | 0.43 | 30.68 | 53.72 | 23.67 | 74.57 |
| logistic | GR | 7.99 | 0.38 | 26.94 | 47.19 | 20.79 | 65.50 |
| triangular | ML | 8.99 | 0.43 | 30.35 | 53.15 | 23.42 | 73.78 |
| triangular | MO | 8.84 | 0.42 | 29.84 | 52.26 | 23.02 | 72.53 |
| triangular | GR | 8.40 | 0.40 | 28.34 | 49.64 | 21.87 | 68.90 |
| burr | ML | 11.02 | 0.53 | 37.17 | 65.10 | 28.68 | 90.36 |

Table 20. Thresholds (μg/L) for determination of action area based on Web ICE predicted values of Diazinon 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 | 10.57 | 0.51 | 35.67 | 62.47 | 27.52 | 86.71 |
| gumbel | MO | 10.93 | 0.52 | 36.88 | 64.60 | 28.46 | 89.66 |
| gumbel | GR | 9.63 | 0.46 | 32.51 | 56.93 | 25.08 | 79.02 |
| normal | ML | 6.74 | 0.32 | 22.76 | 39.85 | 17.56 | 55.32 |
| normal | MO | 8.84 | 0.42 | 29.81 | 52.21 | 23.00 | 72.47 |
| normal | GR | 7.66 | 0.37 | 25.86 | 45.29 | 19.95 | 62.87 |
| logistic | ML | 8.11 | 0.39 | 27.35 | 47.90 | 21.11 | 66.49 |
| logistic | MO | 8.96 | 0.43 | 30.22 | 52.92 | 23.31 | 73.45 |
| logistic | GR | 7.28 | 0.35 | 24.55 | 42.99 | 18.94 | 59.67 |
| triangular | ML | 9.58 | 0.46 | 32.33 | 56.62 | 24.94 | 78.59 |
| triangular | MO | 8.67 | 0.41 | 29.25 | 51.23 | 22.57 | 71.11 |
| triangular | GR | 7.92 | 0.38 | 26.71 | 46.78 | 20.61 | 64.93 |
| burr | ML | 10.57 | 0.51 | 35.67 | 62.46 | 27.52 | 86.70 |

Table 21. Thresholds (μg/L) for determination of action area based on Web ICE predicted values of Diazinon 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 | 90.49 | 4.33 | 305.34 | 534.75 | 235.59 | 742.24 |
| gumbel | MO | 107.87 | 5.16 | 363.95 | 637.40 | 280.82 | 884.72 |
| gumbel | GR | 95.43 | 4.56 | 321.99 | 563.91 | 248.44 | 782.71 |
| normal | ML | 88.89 | 4.25 | 299.91 | 525.25 | 231.41 | 729.05 |
| normal | MO | 86.37 | 4.13 | 291.42 | 510.37 | 224.85 | 708.40 |
| normal | GR | 75.34 | 3.60 | 254.21 | 445.21 | 196.15 | 617.96 |
| logistic | ML | 85.97 | 4.11 | 290.06 | 508.00 | 223.81 | 705.11 |
| logistic | MO | 87.59 | 4.19 | 295.55 | 517.61 | 228.04 | 718.45 |
| logistic | GR | 71.64 | 3.43 | 241.72 | 423.33 | 186.51 | 587.59 |
| triangular | ML | 88.15 | 4.22 | 297.41 | 520.87 | 229.48 | 722.98 |
| triangular | MO | 84.69 | 4.05 | 285.74 | 500.42 | 220.47 | 694.60 |
| triangular | GR | 77.71 | 3.72 | 262.19 | 459.18 | 202.30 | 637.35 |
| burr | ML | 89.92 | 4.30 | 303.41 | 531.36 | 234.10 | 737.54 |

Table 22. Thresholds (μg/L) for determination of action area based on Web ICE predicted values of Diazinon LC50s from a mixture of three surrogate species

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 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 | 8.40 | 0.40 | 28.34 | 49.63 | 21.87 | 68.89 |
| gumbel | MO | 6.30 | 0.30 | 21.26 | 37.23 | 16.40 | 51.67 |
| gumbel | GR | 5.28 | 0.25 | 17.80 | 31.17 | 13.73 | 43.27 |
| normal | ML | 4.10 | 0.20 | 13.82 | 24.21 | 10.67 | 33.61 |
| normal | MO | 3.96 | 0.19 | 13.36 | 23.39 | 10.31 | 32.47 |
| normal | GR | 3.28 | 0.16 | 11.06 | 19.37 | 8.53 | 26.88 |
| logistic | ML | 3.28 | 0.16 | 11.05 | 19.35 | 8.53 | 26.86 |
| logistic | MO | 4.08 | 0.19 | 13.76 | 24.09 | 10.61 | 33.44 |
| logistic | GR | 3.06 | 0.15 | 10.31 | 18.06 | 7.96 | 25.07 |
| triangular | ML | 4.17 | 0.20 | 14.07 | 24.64 | 10.86 | 34.20 |
| triangular | MO | 3.80 | 0.18 | 12.82 | 22.45 | 9.89 | 31.16 |
| triangular | GR | 3.41 | 0.16 | 11.49 | 20.12 | 8.87 | 27.93 |
| burr | ML | 8.39 | 0.40 | 28.32 | 49.59 | 21.85 | 68.84 |

Table 23. Thresholds (μg/L) for determination of action area using empirical values for Diazinon 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 | 20.4 | 1.0 | 68.9 | 120.7 | 53.2 | 167.6 |
| gumbel | MO | 37.7 | 1.8 | 127.1 | 222.5 | 98.0 | 308.9 |
| gumbel | GR | 28.9 | 1.4 | 97.6 | 170.9 | 75.3 | 237.2 |
| normal | ML | 22.8 | 1.1 | 76.9 | 134.8 | 59.4 | 187.0 |
| normal | MO | 21.5 | 1.0 | 72.7 | 127.3 | 56.1 | 176.7 |
| normal | GR | 16.1 | 0.8 | 54.5 | 95.4 | 42.0 | 132.4 |
| logistic | ML | 27.4 | 1.3 | 92.4 | 161.8 | 71.3 | 224.6 |
| logistic | MO | 22.3 | 1.1 | 75.3 | 131.9 | 58.1 | 183.0 |
| logistic | GR | 14.5 | 0.7 | 48.9 | 85.7 | 37.8 | 118.9 |
| triangular | ML | 17.5 | 0.8 | 58.9 | 103.2 | 45.5 | 143.2 |
| triangular | MO | 20.5 | 1.0 | 69.2 | 121.1 | 53.4 | 168.1 |
| triangular | GR | 17.2 | 0.8 | 58.0 | 101.7 | 44.8 | 141.1 |
| burr | ML | 22.9 | 1.1 | 77.3 | 135.3 | 59.6 | 187.9 |

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

To further examine the small variances of SSDs fit to predicted values compared to test results, the taxa from each set of predicted values was cross-tabulated with corresponding taxa for which empirical test results were available (Tables 24 – 27). These tables also report the discrepancy as absolute value of the difference between predicted and tested toxicity value, scaled to the tested tox value (e.g., the discrepancy for *Lepomis macrochirus* when *Oncorhynchus mykiss* is used as a surrogate is |266.23 − 328.60|/328.60 = 0.19) 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, again scaled to the species toxicity value. For example, the distance between *Oncorhynchus mykiss* and *Lepomis macrochirus*, when *Oncorhynchus mykiss* is used as the surrogate is (|147.97−328.60|)/328.60 = 0.55.

Two correlations were examined on each of these sets of cross-tabulated 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 Table 28. In all cases, the predicted and tested values were significantly correlated. However, in two cases (predicted values from rainbow trout and bluegill) there was also a highly significant correlation between the discrepancy and distance statistics, suggesting that an estimated toxicity value would be less accurate, as the difference in sensitivity between surrogate and predicted species grows.

Table 24. Cross-tabulated toxicity values (μg/L) for Web ICE predictions based on rainbow trout regressions.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Taxon | Web ICE | Geomean | Discrepancy | Distance |
| *Oncorhynchus mykiss* | 189.74 | 147.97 | 0.28 | 0.00 |
| *Salvelinus namaycush* | 194.64 | 602.00 | 0.68 | 0.75 |
| *Oncorhynchus clarkii* | 211.04 | 2166.10 | 0.90 | 0.93 |
| *Lepomis macrochirus* | 266.23 | 328.60 | 0.19 | 0.55 |
| *Oncorhynchus tshawytscha* | 272.83 | 126797.08 | 1.00 | 1.00 |
| *Pimephales promelas* | 493.43 | 7407.26 | 0.93 | 0.98 |
| *Carassius auratus* | 739.37 | 9000.00 | 0.92 | 0.98 |
| *Poecilia reticulata* | 1035.26 | 3366.00 | 0.69 | 0.96 |

Table 25. Cross-tabulated toxicity values (μg/L) for Web ICE predictions based on bluegill regressions.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Taxon | Web ICE | Geomean | Discrepancy | Distance |
| *Salvelinus fontinalis* | 126.4 | 723.0 | 0.83 | 0.55 |
| *Salvelinus namaycush* | 216.2 | 602.0 | 0.64 | 0.45 |
| *Oncorhynchus mykiss* | 222.8 | 148.0 | 0.51 | 1.22 |
| *Lepomis macrochirus* | 263.6 | 328.6 | 0.20 | 0.00 |
| *Oncorhynchus clarkii* | 271.3 | 2166.1 | 0.87 | 0.85 |
| *Pimephales promelas* | 519.6 | 7407.3 | 0.93 | 0.96 |
| *Poecilia reticulata* | 684.2 | 3366.0 | 0.80 | 0.90 |
| *Carassius auratus* | 819.1 | 9000.0 | 0.91 | 0.96 |

Table 26. Cross-tabulated toxicity values (μg/L) for Web ICE predictions based on fathead minnow regressions.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Taxon | Web ICE | Geomean | Discrepancy | Distance |
| *Salvelinus namaycush* | 801.4 | 602.0 | 0.33 | 11.30 |
| *Oncorhynchus clarkii* | 1504.9 | 2166.1 | 0.31 | 2.42 |
| *Oncorhynchus mykiss* | 2446.7 | 148.0 | 15.53 | 49.06 |
| *Salvelinus fontinalis* | 2601.4 | 723.0 | 2.60 | 9.24 |
| *Lepomis macrochirus* | 3297.9 | 328.6 | 9.04 | 21.54 |
| *Pimephales promelas* | 5574.2 | 7407.3 | 0.25 | 0.00 |
| *Carassius auratus* | 5605.2 | 9000.0 | 0.38 | 0.18 |
| *Poecilia reticulata* | 5798.8 | 3366.0 | 0.72 | 1.20 |

Table 27. Cross-tabulated toxicity values (μg/L) for Web ICE predictions based on all three surrogate species.

|  |  |  |
| --- | --- | --- |
| Taxon | Predicted  (Web ICE) | Tested  (geomeans) |
| *Salvelinus fontinalis* | 126 | 723 |
| *Oncorhynchus mykiss* | 190 | 190 |
| *Salvelinus namaycush* | 195 | 602 |
| *Oncorhynchus clarkii* | 211 | 2166 |
| *Lepomis macrochirus* | 264 | 264 |
| *Oncorhynchus tshawytscha* | 273 | 126797 |
| *Cyprinus carpio* | 3343 | 0 |
| *Pimephales promelas* | 5574 | 6941 |
| *Carassius auratus* | 5605 | 9000 |
| *Poecilia reticulata* | 5799 | 3366 |

Table 28. Correlations between cross-tabulated toxicity values

|  |  |  |
| --- | --- | --- |
| Surrogate Species | correlation between predicted and tested | Correlation between discrepancy and distance |
| rainbow trout | ρ = −0.0.1534, p = 0.72 | ρ = 0.84, p = 0.009 |
| bluegill | ρ = 0.86, p = 0.007 | ρ = 0.59, p = 0.12 |
| fathead minnow | ρ = 0.77, p = 0.03 | ρ = 0.96, p = 1\*10-4 |
| mixture of surrogates | ρ = −0.22, p = 0.59 | n/a |