Atrazine MOA Ecological Subgroup:

Recommendations for aquatic community Level of Concern (LOC) and method to apply LOC(s) to monitoring data.

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Recommendations

Based on the reported results from available micro- and mesocosm studies for which atrazine was tested, aquatic plant community structural change is recommended as the endpoint of concern. The following ‘screening’ trigger values (µg/L atrazine) for monitoring atrazine in 2^{nd} or 3^{rd} order Midwestern streams are recommended:

- 14-day average = 38
- 30-day average = 27
- 60-day average = 18
- 90-day average = 12

Atrazine monitoring data that exceed any of these values indicate that the changes in the aquatic plant community structure could be affected. We recommend that if monitoring data exceed any of these triggers, the CASM model should be run using the refined chemograph from the monitoring site that exceeds the trigger. If the results from this model run (Average Primary Producer Steinhaus Similarity deviations) are greater than 5% (the index delineating no to slight effect in micro- and mesocosm studies from those with significant effects), then the mitigation process begins.

Introduction

This document presents the goals, endpoints, methods and supporting rationale developed and agreed to by the subgroup to arrive at the above recommendations. In summary, threshold concentrations were determined from realistic and complex time variable atrazine exposure profiles (chemographs) for modeled aquatic community structure changes. Methods were developed to estimate ecological community responses for monitoring data sets of interest based on their relationship to micro- and mesocosm study results, and thus to determine whether a certain exposure profile at a site may have exceeded a level-of-concern.

Goal for Ecological Sub-Group

The subgroup was charged to reach agreement on the ecological level of concern (LOC), i.e., magnitude and duration of exposure of aquatic plants to atrazine that potentially adversely affect aquatic communities and/or ecosystems. This required a two step process: (1) Determine the magnitude and duration of exposure of aquatic plants to atrazine that constitute LOC(s) for aquatic communities and/or ecosystems, and (2) Determine the best available method(s) to interpret monitoring data relative to these LOC(s).

Endpoints

The initial assessment endpoint was chosen based on the reported results from 77 micro- and mesocosm studies for which atrazine was tested: change in aquatic community structure and function of primary producers. This endpoint appeared to be the most sensitive of the effect endpoints affecting aquatic plants. Further, the effect of atrazine on aquatic plants, whether direct or indirect, appeared to be more sensitive than effects on other organisms in the aquatic ecosystem, e.g., aquatic invertebrates, fish. Thus, by focusing on aquatic plant community structural changes, we would be in effect, protecting against adverse effects on the rest of the aquatic community. The measurement endpoints reported in available studies which tested atrazine were: laboratory – growth (rate) and biomass; microcosms, mesocosms and models - reduction in primary production and changes in structure of primary producer communities.

Community Level Studies

Ecological responses of aquatic communities to atrazine exposures can be assessed using community level studies, such as micro- and mesocosms. The subgroup reviewed 25 different studies with 77 reported effects/no effects on aquatic plants (See Appendix 1). Twenty-four results were from tests on ponds or lakes; 20 on artificial streams; and, 33 were microcosm tests. Eight results were on macrophytes, 29 on periphyton, and 40 on phytoplankton. However, only a limited number of exposure profiles could be tested in these studies. Typically, one to three concentrations of atrazine were tested in these studies each with a single application to the test system at initiation. Atrazine concentrations were often kept constant for a variable duration period before the concentrations slowly decrease with time. Unfortunately, the variable quality of these studies and the many different study designs did not always allow a reliable association of exposure magnitude and duration to a certain community level effect, and in many cases the duration of the studies was too short to document community recovery.

The subgroup was convinced that the LOC for aquatic communities and/or ecosystems should be based on effects on aquatic plant communities demonstrated in atrazine micro- and mesocosm studies. To better understand the impact of exposure duration and magnitude on aquatic communities, the subgroup had to relate the effects reported in these studies to specific exposure durations and magnitudes. First, the 77 study results had to be quantified as to severity of effects of atrazine on the aquatic plant community. Brock et al 2000 analyzed a majority of the study results and quantified them as follows:

<u>Effect Scores (Brock et al 2000):</u>
1 = no effect
2 = slight effect
3 = significant effect followed by return to control levels within 56 d
4 = significant effect without return to control levels during an observation period of less than 56 d
5 = significant effect without return to control levels for more than 56 d

Studies not analyzed by Brock but considered in this analysis were scored with the same methods. The distribution of the scores for the 77 study results were as follows (also see Appendix 1):

<u>Distribution of Effect Scores:</u>
15 - #1;
12 - #2;
12 - #3;
23 - #4;
15 - #5

Next, the 77 effect scores representing the results from the 25 micro- and mesocosm studies for atrazine were plotted against the study specific test concentrations and exposure durations in Figure 1.

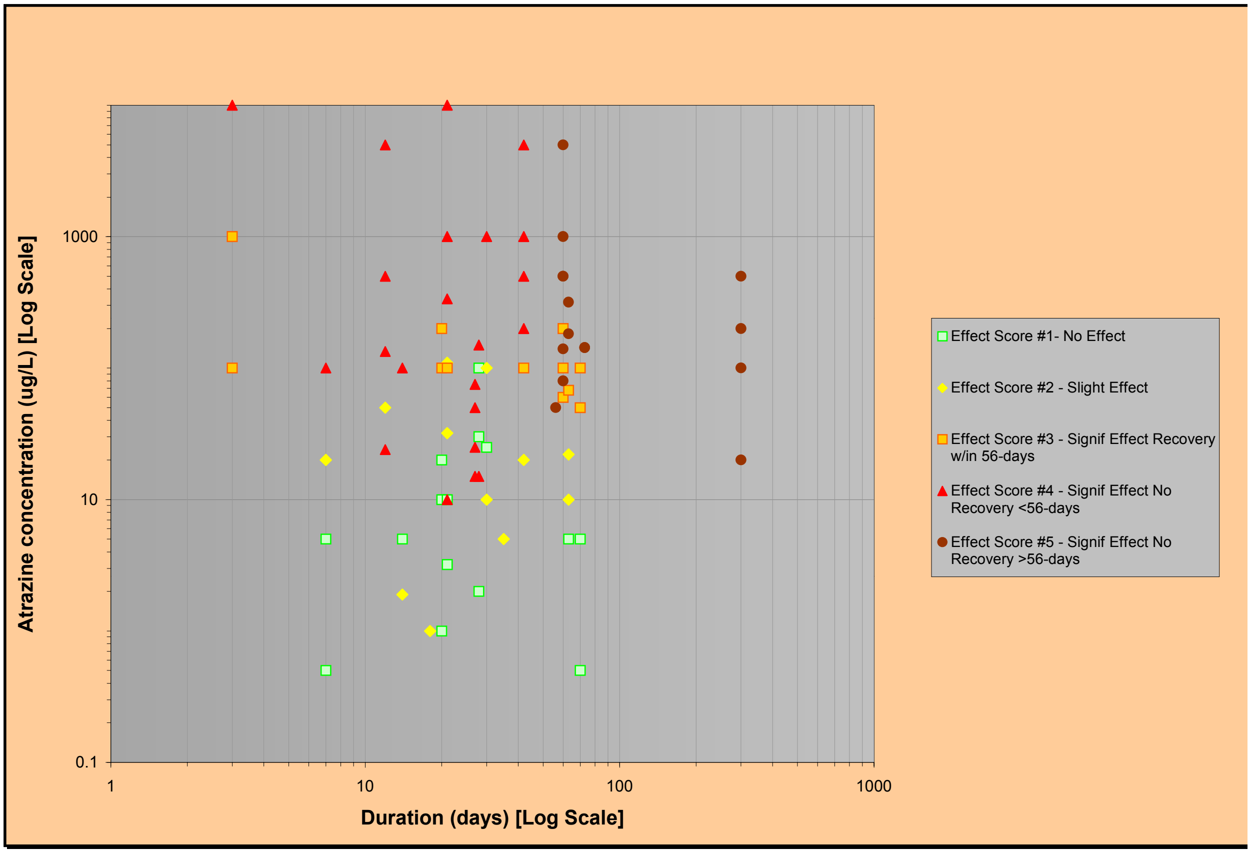

Figure 1: Micro- and mesocosm study effect concentrations scored according to Brock et al 2000 and plotted against the study specific exposure duration

As expected, based on the mode of action of atrazine that inhibits primary production by reversibly blocking photosynthesis, the effects observed in micro- and mesocosm studies generally become more severe with increasing exposure time and magnitude.

The challenge for step two was to define an appropriate exposure concentration and duration relationship that properly defines duration specific levels of concern. For that purpose, the group decided to use ecological modeling to simulate a large number of exposure durations and magnitudes for the ecological response in a generic Midwestern 2^{nd} to 3^{rd} order stream. Two ecological models were initially considered: (1) the Comprehensive Aquatic Systems Model (CASM) (Bartell et al. 2000, Bartell et al 1999, DeAngelis et al 1989), and (2) AQUATOX[1]. The decision to use CASM was made after a preliminary comparison revealed that CASM could include a larger number of species in the community structure, which appeared to better support our assessment endpoint. In addition, CASM had a relatively uncomplicated exposure profile for a chemical such as atrazine. Further, Syngenta, which agreed to fund the CASM modeling runs, had easy access to the CASM contractor (Steve Bartell with The Cadmus Group, Inc.). Currently, EPA

[1] See http://www.epa.gov/waterscience/models/aquatox/about.html and http://www.myweb.cableone.net/dickpark/AQTXFacts.htm

is funding AQUATOX model runs using similar exposure and duration scenarios. A comparative analysis between the CASM and AQUATOX model results will be performed following the completion of the AQUATOX modeling runs.

Model Parameterization

A large number of single-species laboratory toxicity test results on atrazine toxicity to aquatic organisms (See Giddings et al 2000), including aquatic plants (macrophytes, periphyton, and phytoplankton) were available (Figure 2). A subset of these data (CASM EC50 geometric means) was selected and used to drive the toxicity of atrazine to aquatic organisms in the CASM simulation model (See Appendix 2). The modeled toxicity profile included twenty-six producer species (10 plankton, 10 periphyton, 6 macrophytes), and 17 consumer species. Three toxicity scenarios were modeled: 10^{th} centile, geometric mean, and 90th centile for species with more than one toxicity study. The geometric mean scenario (toxicity scenario 1) was chosen for the reported model results.

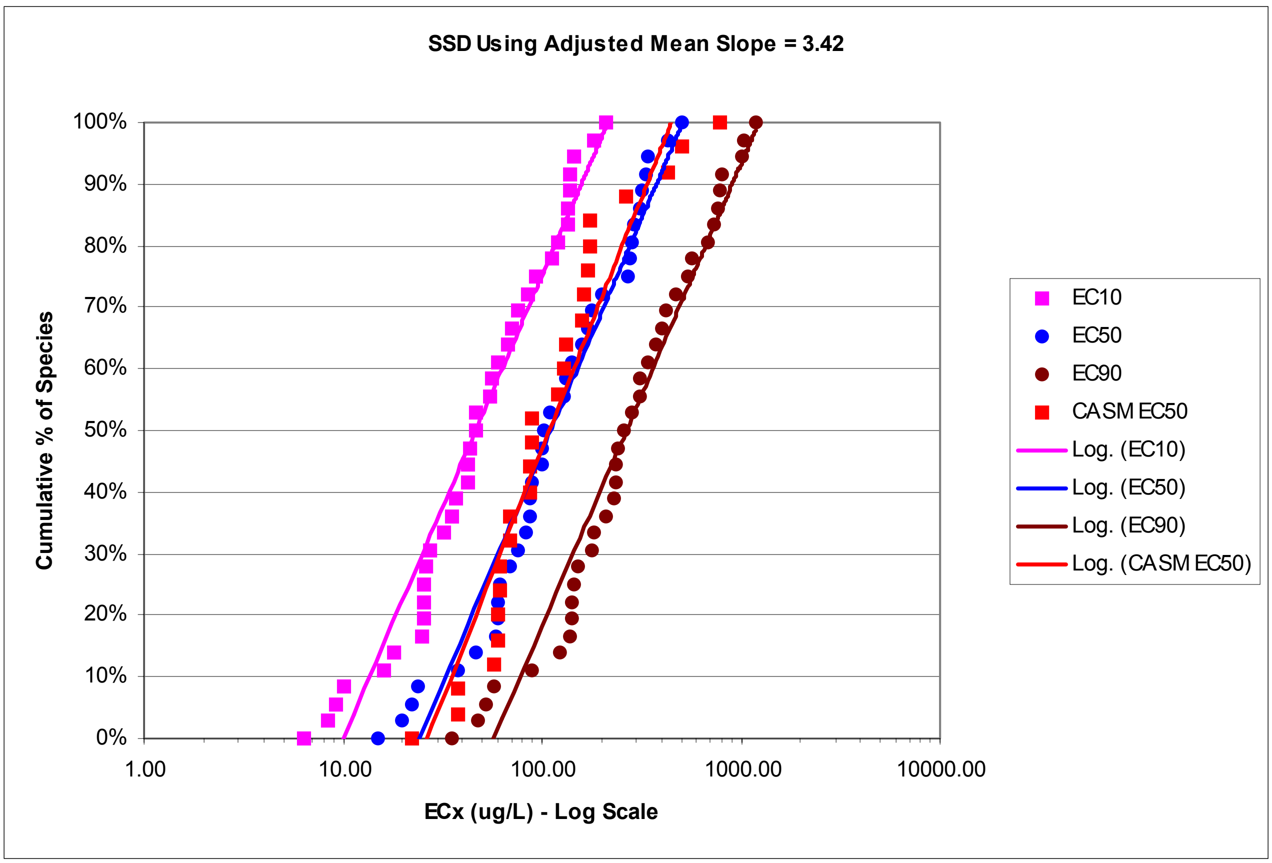

Figure 2: Plant Species Sensitivity Distribution for EC10, EC50, and EC90 values overlaid with the Plant Species Sensitivity Distribution (EC50 geometric mean) used to parameterize CASM.

CASM Model Simulations

CASM is an ecological food chain model. It was set-up to run simulations for exposure durations from 1 to 260 days, and concentrations from 20 to 220 µg/L atrazine. The scenarios were designed to simulate a generic 2^{nd} or 3^{rd} order Midwestern stream, typical for the majority of atrazine use on corn and sorghum. The CASM model provides the following results: production – modeled as biomass production (g Carbon m^{-2}) for 1 m^2 surface area) (Appendix 3a), and community structure (similarity) – species population size derived from species daily biomass (Appendix 3b). Thus, the model integrates direct and indirect effects to indicate changes in community structure. The endpoint selected for the model results was percent (%) change in aquatic community structure (as determined by Steinhaus Similarity coefficient) of primary producers (phytoplankton, periphyton, macrophytes).

CASM Steinhaus similarity analysis

Coefficients of similarity are used to determine whether the composition of two communities is similar. The Steinhaus coefficient or similarity index is based on the species abundances (in this case indicated by the species specific daily biomass) common to two communities. The index is described in the following equation:

$$S = \frac{2 * \sum_{k=1}^{n} Min(a_{1,k}, a_{2,k})}{\sum_{k=1}^{n} a_{1,k} + \sum_{k=1}^{n} a_{2,k}}$$

Where $a_{i,k}$: abundances of species k in sample I

The similarity indices for each possible pair of samples per day are calculated and this results in a matrix of between (different treatments) similarities as in Figure 3.

	1d1	1d2	1d3	etc.	Xd260
1d1		B	B	B	B
1d2			B	B	B
1d3				B	B
etc.				B	B
Xd260					B

Figure 3. Example of a matrix of similarities resulting from Similarity Index calculations.

Similarity indices were calculated for primary producers, consumers, and fish over exposure periods from 1 to 20 days (See Appendix 3b). The results show that the changes in percent (%) change in aquatic community structure of primary producers is a more sensitive (conservative) measurement endpoint than the same for consumers or fish.

Determining the LOC - CASM Steinhaus similarity vs. the effects of Atrazine exposure in micro- and mesocosm studies

A wide range of single pulses of different duration and magnitude were simulated and used to calculate community structure changes. Community structure changes were expressed as percent (%) change in the Steinhaus similarity index that was calculated based on the simulated daily biomass for each individual species and plotted over time.

Table 1: A) Maximum daily percent change[a] in community structure (Steinhaus similarity) of primary producers for a modeled generic 2nd-3rd order Midwestern stream.

Atrazine conc. [µg/L]	Pulse duration [d][b]							
	1	3	5	10	20	60	130	260
20	0.1[c]	0.2	0.7	0.9	1	1.2	1.2	2.3
25	0.8	1.9	2.9	5	7.8	11.7	13	15.5
30	0.8	1.9	2.9	5	7.8	11.7	13	15.8
40	1.1	2.3	3.2	5.2	8	11.7	13.1	16.6
50	1.1	2.3	3.1	5.2	7.9	11.6	13.1	17.5
70	3.7	8	10.7	13.8	16.1	17.3	18.1	22.5
90	4.4	9.4	12.6	15.9	18.2	18.2	18.3	23.5
130	4.5	9.6	12.7	15.8	17.8	17.8	17.8	20.1
170	5.6	13.1	18.1	24.1	29.7	56.3	67.1	72.4
220	5.7	13.2	18.2	24	29.7	56.3	67.1	72.3

B) Year end percent change[a] in community structure (Steinhaus similarity) of primary producers for a modeled generic 2nd-3rd order Midwestern stream.

Atrazine conc. [µg/L]	Pulse duration [d][b]							
	1	3	5	10	20	60	130	260
20	0[c]	0	0	0.2	0.2	0.2	0.2	2.3
25	0.7	1.7	2.7	4.7	7.3	10.9	12.1	15.5
30	0.7	1.7	2.7	4.6	7.2	10.8	12.1	15.8
40	0.7	1.9	3	4.9	7.5	11	12.4	16.6
50	0.7	1.9	2.9	4.9	7.5	10.9	12.9	17.5
70	1.5	3.7	5.2	7.9	10.9	14.6	17.6	22.5
90	1.7	4.1	5.7	8.5	11.6	15.5	18.3	23.5
130	1.7	4	5.7	8.4	11.5	15.3	16.4	20.1
170	2	5.4	8.1	15.5	27.9	51.7	61.2	71.5
220	2	5.3	8.1	15.4	27.8	51.6	61.1	71.1

C) Average percent change[a] in community structure (Steinhaus similarity) of primary producers for a modeled generic 2nd-3rd order Midwestern stream.

Atrazine conc. [µg/L]	Pulse duration [d][b]							
	1	3	5	10	20	60	130	260
20	0[c]	0	0.1	0.4	0.4	0.5	0.5	0.7
25	0.5	1.2	1.9	3.4	5.1	7.4	8.2	8.5
30	0.4	1.2	2	3.5	5.2	7.6	8.4	8.7
40	0.8	1.8	2.6	4.1	5.8	8.3	9.3	9.7
50	0.8	1.8	2.6	4.2	6	8.9	10.1	10.7
70	2.2	4.8	6.4	9.1	11.6	14.9	16.9	17.5
90	2.6	5.6	7.4	10.2	12.8	15.8	17.5	18
130	2.6	5.6	7.4	10.2	12.7	15.4	16.3	16.4
170	2.9	6.8	9.8	16.3	25.5	40.6	46.3	48.4
220	2.9	6.8	9.8	16.4	25.5	40.6	46.3	48.4

[a]Based on the mean values of 100 Monte Carlo simulations using the Comprehensive Aquatic Systems Model (CASM)
[b]Consecutive days of constant exposure beginning on model day 105 (April 15)
[c]Results using the geometric mean values of EC_{50} assigned to modeled populations (Toxicity Scenario 1)

For further evaluation, the maximum daily percent (Table1 A), year-end percent, i.e. at day 260 post application (Table 1 B), and the average percent change in community structure in the primary producer community (Table 1 C) were calculated. Maximum daily deviations indicate the short-term (temporary) maximum change in community structure. The average community structure change integrates short-term changes and long-term recovery of the communities. A comparison of short-and long-term %-impact shows that for concentrations >20 µg/L, short-term changes are always between 1- to 2-fold the average response. For example, an average 5% community structure change may cause a less than or equal to 10% short-term (temporary) change in primary producer community structure. The average percent change in community structure was chosen for the reported results since it captures the short-term changes as well as recovery.

The modeling results in Table 1C were used to help define duration-specific levels of concern. Two approaches were used. First, the simulated response (or effect) had to be set in context to the micro- and mesocosm data. A similarity index value was estimated for each micro- and mesocosm test result by finding the average model similarity deviations (%) of a simulated exposure profile closest to the conditions used in each study (test concentration and exposure duration) (See Appendix 1 for assigned index values for each of the 77 test results). Next, the index values were plotted against the Brock et al effect scores for each micro- and mesocosm test results for comparison (See Figure 4). There is a lot of scatter that is reflective of the diversity of this data; however, there is a clear, strong correlation of the scores with the index. An index value of 5 (vertical red line on the figure) conservatively separates the 3/4/5 from the 1-2 scores. That means that a 5% change in community structure (Steinhaus similarity) of the CASM simulations compares to a large majority of the micro- and mesocosm studies with no to slight effects (leaving only 8% potential false negatives and false positives, i.e., false negatives - 6 out of 77 studies above the effects score 3 line and to the left of the 5% line; false positives - 6 out of 77 studies blow the effects score 3 line and to the right of the 5% line).

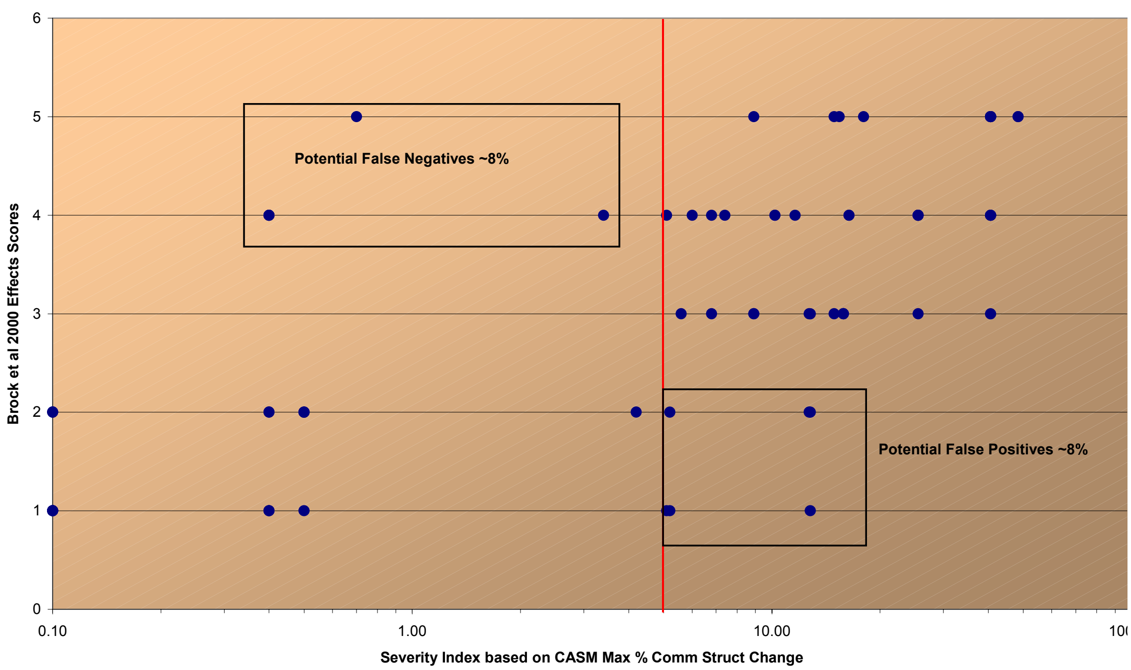

Figure 4. Correlation between the Similarity Index [CASM AVG % change in community structure for 77 atrazine micro- and mesocosm studies] and the Brock et al 2000 effect scores.

For the second approach, the CASM simulation results in Table 1C were interpolated to develop a set of concentration / duration pairs equivalent to 5% effect from CASM. The interpolated results follow:

Time (days)	Concentration (µg/L)
2.1	220
2.6	130
3	75
5	63
10	53
20	24.8
60	23.3
130	22.9
260	22.7

For times greater than 3 days, a linear interpolation was performed across the different concentrations at each time. For times from 60 to 260 days, the abrupt shift in response between 20 and 25 :g/L made interpolation tenuous, but the best estimate would seem to be in the mid-part of the range and this did not involve much uncertainty given the narrow range. For times less than 3 days, the response did not reach 5%, but the additional points seem to be points needed at high concentrations. Thus, interpolations were performed across times at a fixed concentration instead of across concentrations at a fixed time.

Next, these concentration-duration pairs, representing the 5% index points based on interpolation, were plotted with lines connecting each point on Figure 1 (See Figure 5 below).

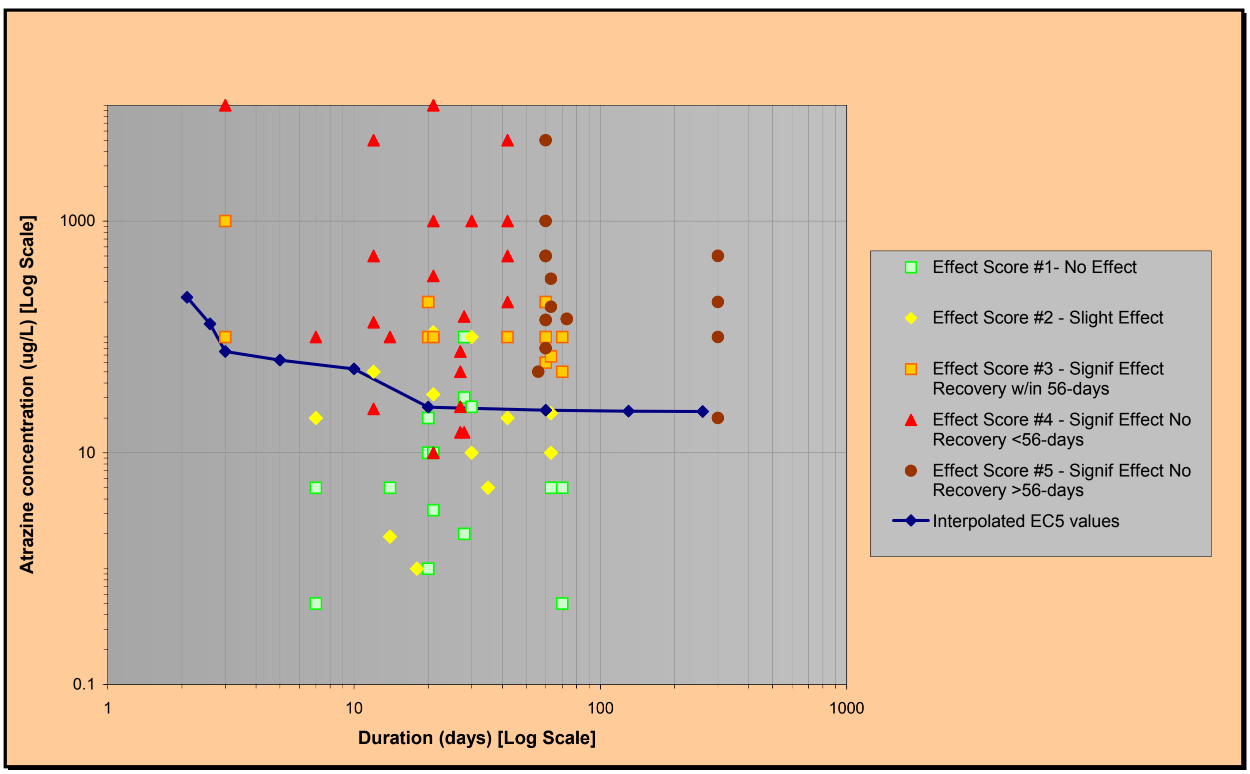

Figure 5. Micro- and mesocosm study effect concentrations scored according to Brock et al 2000 and plotted against the study specific exposure duration. Interpolated 5% CASM Similarity Index points plotted.

The plot of the interpolated 5% Similarity index points, like Figure 4, conservatively separates the 3/4/5 from the 1-2 scores. Based on both approaches, the subgroup agreed that an index of 5%, meaning a 5% change in community structure of primary producers, is a reasonable LOC for atrazine exposures in freshwater environments.

Applying the LOC to Monitoring Data - CASM simulations with time-variable exposure scenarios

CASM simulations can be used to test whether the LOC of concern was exceeded for any exposure time-series (e.g. in a monitoring program). To avoid repeated CASM simulations for exposure profiles that are of no concern, an easy to apply screening method to predict if an exposure profile causes a CASM result above the trigger is needed. An easy screening method would define a time integrated exposure dose that correlates with the CASM simulation results for a series of original atrazine monitoring chemographs. CASM simulations were conducted for a total of 128-atrazine original and amplified monitoring datasets for a range of rivers and streams from different watershed size in agricultural areas in Ohio (Heidelberg data set). The amplification was necessary because most of the simulations with original atrazine monitoring data resulted in effects below the 5% similarity trigger. Even with amplification between 2- to 5-fold, the maximum community similarity change was slightly about 10%, the consequence being that ca. 80% of the CASM simulations resulted in effects below 5%. For the same chemographs, time integrated exposure concentrations were calculated for averaging periods of 14, 30, 60, and 90 days.

The time-weighted concentrations were then correlated to the CASM results of the corresponding chemographs by seeking the concentrations that would trigger CASM simulations with plant community structure changes > 5% (See Appendix 4). Assuming an acceptable prediction error of 5% for the 128 data sets (i.e. at the 95th centile), the estimated time weighted trigger values are 49, 32, 21, and 15 µg/L for the 14-, 30-, 60-, and 90-day average, respectively. Assuming an acceptable prediction error of only 2% (i.e. at the 98th centile), the estimated time weighted trigger values are 44, 27, 18, and 13 µg/L for the 14-, 30-, 60-, and 90-day average, respectively. Assuming an acceptable prediction error of only 1% (i.e. at the 99th centile), the estimated time weighted trigger values are 38, 27, 18, and 12 µg/L for 14-, 30-, 60-, and 90-day average, respectively (see Table 2 below).

***Trigger* [µg/L Atrazine in 2nd or 3rd Order Streams] w/ Decreasing Error Predictions [5%, 2%, 1%]**			
14day Ave = 49.2	30day Ave = 31.9	60day Ave = 21.0	90day Ave = 15.0
14day Ave = 44.1	30day Ave = 27.1	60day Ave = 18.2	90day Ave = 13.0
14day Ave = 37.7	30day Ave = 26.8	60day Ave = 17.5	90day Ave = 11.8

Table 2. Triggers in terms of four different rolling average concentrations of atrazine in 2nd and 3rd order midwestern streams along with error predictions. Since these are recommended as screening triggers, the triggers with the lowest error prediction (1%) are recommended.

The 30-day and 60-day triggers appear to be less variable across error predictions than the 14-day and 90-day triggers, and thus may be better choices if just two triggers were selected. However, any of the four can be used. A step-wise data evaluation scheme incorporating the methods described above is provided in Figure 6.

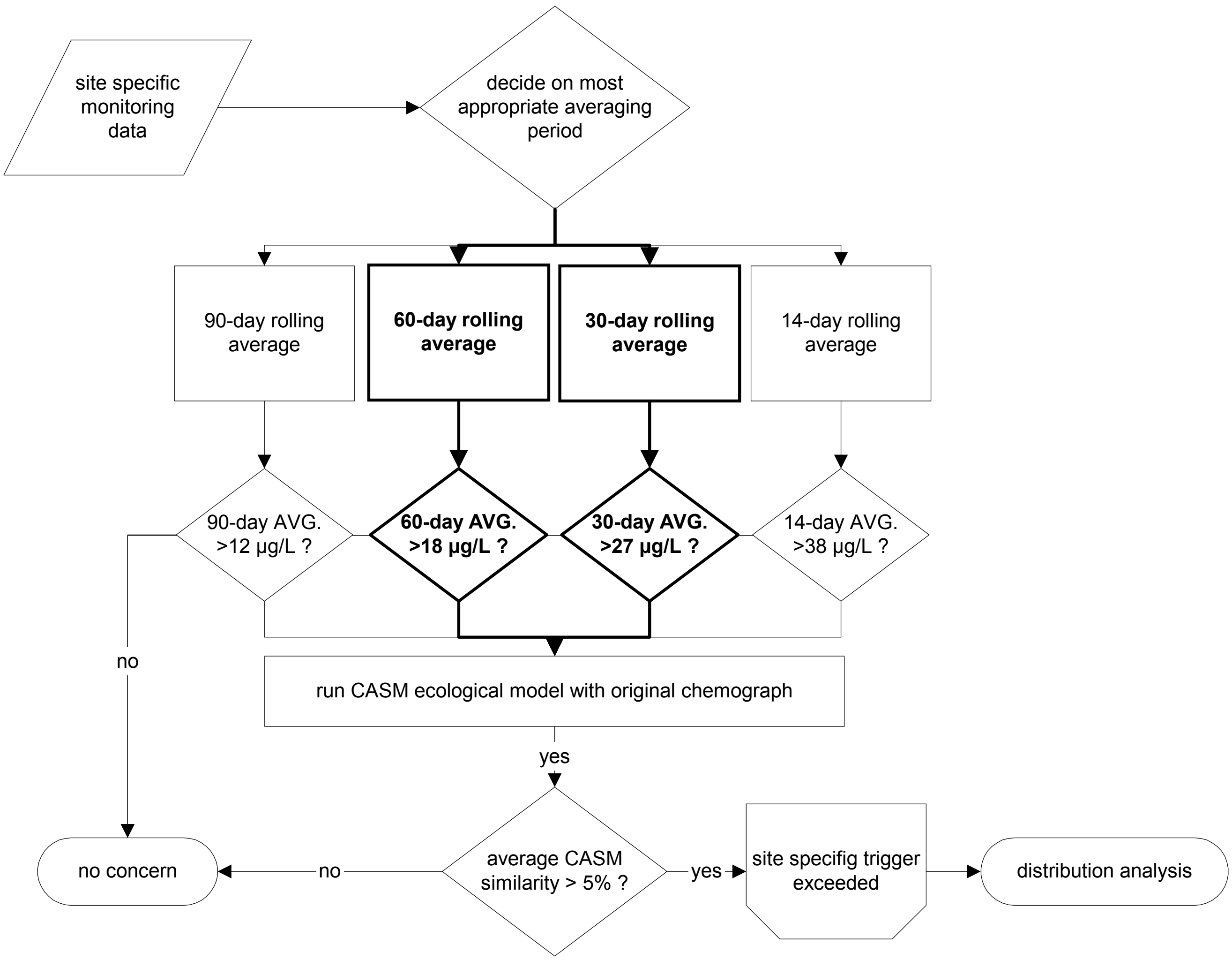

Figure 6: Proposed steps to analyze the potential ecological impact of atrazine based on monitoring data.

Discussion of Uncertainty in Selection of Data, Methods, and Decisions Critical to Defining the LOC

Reference Data for LOC(s)

Since the potential risk of atrazine to aquatic communities will be based on a set of micro- and mesocosm tests, the critical decision is which tests to include or exclude. The large set of available studies for atrazine included in this analysis (Appendix 1) have various strengths and weaknesses and use many different testing designs and methods. The key point here is that there are a large number of such studies and the subgroup decided to be relatively inclusive, rather than excluding data for various limited uncertainties or ambiguities. This approach provides a better data set for weight-of-evidence and allows for addressing "false-negatives" and "false-positives" in light of the overall frequency/magnitude of the wide range of possible exposure situations. It would not be prudent to rely on any one or two of these studies to guide the LOC decisions.

Quantification of Results of Micro- and Mesocosm Tests

The subgroup decided to use the effect scores in Brock et al 2000 to quantify the results of the micro- and mesocosm tests. The subgroup reached general agreement that the scores assigned to the 77 results were reasonable, and that scores of 2 ('slight' effect) do not constitute a level-of-concern, while scores of 3 (a pronounced 'slight effect') do. Brock et al further characterized a score of 2 as *"effects reported in terms of 'slight'; 'transient', and short-term and/or quantitatively restricted response of sensitive endpoints, and effects only observed at individual samplings."* Scores of 3 were characterized as a *"clear response of sensitive endpoints, but total recovery within 8 weeks after the last application, and effects reported as 'temporary effects on several sensitive species'; 'temporary elimination of sensitive species'; 'temporary effects on less sensitive species / endpoints', and effects observed at some subsequent samplings."* This last decision is perhaps the most critical risk decision here, because these scores define the actual level of protection being sought. Therefore, Appendix 1 is arranged by decreasing effects score and shows the range and nature of effects represented by the different scores.

Another aspect of quantification is the exposure duration that any score and concentration relate to. This might not seem to be an issue because the exposure duration is fixed and specified in any test, but for long exposures in which severe effects occur early, might not these effects be better related to a shorter duration? For example, the significant effects (scored as a 5 and described as a decrease in macrophyte coverage in the pond by 95%) in the Kettle et al. 1987 study were related to a full year's exposure (actually 300 days). However, the study also reported that there was ~60% decrease in coverage after 60 days. The subgroup decided to stay with the 300 day test duration because (1) the exposures in the study were constant over the whole time period, (2) Brock et al as well as other authors reported the test duration as ~1 year, and (3) the most dramatic effect without testing for recovery did occur after the ~year long exposure duration. Yet, some could argue that 60% decrease in macrophyte coverage is significant and should also be scored as a 5 and included. However, the uncertainty resulting from this observation for the calculation of the time specific LOC(s) in this document is very small because, as shown in Figure 5, the concentrations causing community structure changes do not further decrease for constant exposure periods longer than 20 to 30 days, i.e. longer exposure periods do not significantly change the effect threshold. The Kettle et al study was conducted at the borderline of this threshold concentration (ca. 20 µg/L). In the weight-of-evidence approach applied here, it constitutes only one of the large numbers of such studies that also measured less severe impact at the comparable concentrations and exposure durations.

Extrapolation of Micro- and Mesocosm Tests to Different Exposure Time Series

Another critical decision for the subgroup was to use an aquatic ecological community model as the extrapolation tool. It is important to emphasize that this does not mean that the subgroup believes that the model accurately predicts the effects in any particular community, but rather that it is a useful means for integrating the kinetics of various processes (toxic effects on photosynthesis, plant growth dynamics, interactions among plant species across a growing season) and describing the RELATIVE effects of different exposure time series on the overall response.

It is important to point out that more developmental work needs to be done regarding the formulation and efficacy of the model to be used. The use of CASM for these initial efforts can be justified based both on logistical grounds and on the large set of species used in it. In addition, another aquatic ecological community model is currently being tested – AQUATOX, in order to provide comparative results either to establish the robustness of model applications or as an alternative model to actually use. The response simulated by these models must always be set in relation to the micro- and mesocosm data identified as the most relevant measure for setting the aquatic community LOC(s).

Another development area is the formulation of CASM with regard to toxic effects (i.e., the general stress syndrome). It was encouraging that a comparison was done contrasting the GSS to simply reducing photosynthesis, and that the latter produced smaller effects that made applying results less practical. However, some members of the subgroup thought that we should still be concerned about model results that rely on a toxic response that differs from what we think is correct. This does not necessarily mean changing the GSS, but instead could involve justifying it better based on looking more closely at available data, or by comparing how the overall assessment (not just the immediate model results) would differ using the GSS versus an alternative formulation.

Parameterization of Model

The critical data here are the plant laboratory toxicity data assigned to each species in CASM. These data are the key factor determining the concentration at which CASM predicts significant effects (slightly above 20 µg/L) and describing the "step-wise" nature of the effects versus concentration. Because the subgroup was concerned with effect levels that reflect the more sensitive organisms, Figure 2 and Appendix 2 show that the decision to use the geometric mean toxicity values (EC50s) for CASM appears to adequately represent plant species sensitivity distribution. However, one consequence of the limited number of possible species in the model is that only a few species represent sensitivities below the 10^{th} centile and above the 90^{th} centile. Additional analyses using the 10^{th} and the 90^{th} centile of the EC50 instead of geometric means was conducted to test for the potential impact of the species sensitivity on the CASM results (Appendix 5). For the majority of the simulations, the lower toxicity profiles (scenario 2) did not cause significantly higher responses than the geometric mean scenario. It was also observed that the higher and lower toxicity scenarios did not necessarily bracket the geometric mean scenario. This can partly be explained by the complex nature of the food-chain interactions in the ecological model. The impact of slightly different species sensitivity distributions used to parameterize the model is therefore probably low, when compared to relative importance of the species composition in the food-chain model.

The subgroup recognizes that different species have different relative importance in CASM results and this varies seasonally. Even if each CASM species is linked to the most relevant laboratory species, the original selection of CASM species and the assignment of the laboratory data represent a major uncertainty and further evaluation using model parameterizations representing different generic aquatic communities are recommended.

Selection of Model Variable to Relate to Micro- and Mesocosm Results

The selection of this endpoint is a critical decision, even if model results are calibrated to the micro- and mesocosm data, because different endpoints have different time-dependencies. These differences will affect the relative level of concern for different exposure series. While the subgroup believes that the average similarity index is a reasonable choice, we also recognize that its meaning is somewhat uncertain. The critical point is the time trajectory of the index when the effect on the average community structure is less than that at the end of the year. The subgroup recognizes that the recommended average index combines direct toxic effects and consequent shifts in later seasonal plant succession. However, it is important to note that this index can have different time dependence than an endpoint such as overall primary productivity, and thus is a key decision. The subgroup believes that future efforts should include taking a few different endpoints through the whole process and documenting how much the end results are affected.

Setting the LOC for Model Variable Relative to Micro- and Mesocosm Results

The subgroup agreed that plotting the Brock index against a similarity index effect based on direct interpolation of the dense matrix of model results provides a good way of selecting the LOC for the model index. The critical decision here is the accepted frequency and nature of false positives and negatives. This decision as well as the decision to use Brock et al 2000 for scoring the reported results of the micro- and mesocosm tests, are key management decision points. The LOC values for the different time-averaging periods given in Figure 6 are based on the most conservative calculations made at a 99th centile prediction accuracy.

Applying Model-Based LOC(s) to Monitoring Results

The development of a rolling average screening test based on CASM results using realistic hydrographs is simple and rigorous. Since it is a screening step, the subgroup decided to minimize the false negatives and also include all four averaging periods for a more reliable check. Even with this conservative screen, there would be only several false positives. The data set on which CASM was run is loaded with amplified hydrographs, so that the actual incidence of false negatives from running CASM would be much less. An important point to reiterate here is that this screening step is NOT a risk decision point. The subgroup agreed that if these triggers were exceeded, then further evaluation of appropriate values would be needed before entering the mitigation process.

There are two key points to be considered regarding the application of the model based LOC(s) to the monitoring results. First, although this hydrograph set is very rich, it does have some limitations that make the general applicability of the averaging periods uncertain. Second, the averaging period recommendations are based on daily and 4-day observations, and do not address the uncertainties that might occur with applying more sparse data to the calculation of averages. While the monitoring program will produce additional hydrographs for refining the recommended averages, it would also be prudent to consider that future development needs to address the issue of averages from sparse data.

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Appendix 1

Micro- and mesocosm studies table with Brock scores and estimated average % change in community structure (Steinhaus similarity) of primary producers

Appendix 2

Ecotoxicity profiles for CASM

Appendix 3a

CASM results – change in annual production

Appendix 3b

CASM Steinhaus similarity index graphs for producers, consumers and fish

Appendix 4

Comparison of annual average CASM Steinhaus similarity for a series of chemographs calculated with the Logistic regression vs. actual CASM simulations.

Appendix 5

Comparison of simulated change in annual production for phytoplankton, periphyton, macrophytes, zooplankton, benthic invertebrates, and fish for CASM parameterizations using the geometric mean values of EC_{50} (toxicity scenario 1), the 90th centile (toxicity scenario 2) and the 10th centile (toxicity scenario 3) of the EC_{50} values.