APPENDIX D

Species-Specific Results of the Analysis of Extrapolation Error

Table D-1. *Predicted geometric mean maximum allowable toxicant concentrations (PGMATCs) for each RAU and each species of fish.*

	RAU	PGMATC[a] (mg/L)									
		Carp	Buffalo	Channel catfish	White bass	Green sunfish	Bluegill sunfish	Largemouth bass	Black crappie	Rainbow trout	Brook trout
1	Carbon monoxide										
2	Sulfur oxides										
3	Nitrogen oxides										
4	Acid gases	8.8	8.8	11.6	3.3	6.7	3.1	2.5	1.6	2.6	2.6
5	Alkaline gases	43.5	43.5	32.9	18.0	18.0	18.0	18.0	18.0	15.3	14.9
6	Hydrocarbon gases	1,565,162	1,565,162	11,313	29,185	29,185	29,185	29,185	29,185	19,705	19,705
7	Formaldehyde	b	b	b	b	b	b	b	b	b	b
8	Volatile organochlorines	533	1245	600	135	705	814	744	110	566	566
9	Volatile carboxylic acids	941	933	518	213	213	213	213	213	252	252
10	Volatile O & S heterocyclics	b	b	b	b	b	b	b	b	b	b
11	Volatile N heterocyclics	b	b	b	b	b	b	b	b	b	b
12	Benzene	421	252	144	116	116	116	116	116	125	86
13	Aliphatic/alicyclic hydrocarbons	218	255	166	66	66	66	66	66	68	68
14	Mono- or diaromatic hydrocarbons	120	146	91	65	65	65	65	65	65	50
15	Polycyclic aromatic hydrocarbons	190	190	134	79	121	98	86	22	74	74
16	Aliphatic amines	b	b	b	b	b	b	b	b	b	b
17	Aromatic amines	b	b	b	b	b	b	b	b	b	b
18	Alkaline N heterocyclics	562	590	590	347	141	141	141	141	159	159
19	Neutral N, O, S heterocyclics	b	b	b	b	b	b	b	b	b	b
20	Carboxylic acids	48,548	48,548	1435	2001	2001	2001	2001	2001	1317	1317
21	Phenols	462	387	207	182	308	302	271	52	208	131
22	Aldehydes and ketones	12.7	12.7	11.7	4.9	10.7	5.4	8.1	2.4	4.0	4.4
23	Nonheterocylic organo S	b	b	b	b	b	b	b	b	b	b
24	Alcohols	b	b	b	b	b	b	b	b	b	b
25	Nitroaromatics	b	b	b	b	b	b	b	b	b	b
26	Esters	33.0	287.4	160.9	133.0	40.5	26.6	22.8	8.1	145.9	97.6
27	Amides	b	b	b	b	b	b	b	b	b	b
28	Nitriles	215	389	237	65	236	220	196	41	160	160
29	Tars	b	b	b	b	b	b	b	b	b	b
30	Respirable particles	b	b	b	b	b	b	b	b	b	b
31	Arsenic	238	479	247	229	409	424	383	67	257	281
32	Mercury (inorganic)	34.2	34.2	26.9	14.0	14.0	14.0	14.0	14.0	11.9	12.0
32A	Mercury (methyl)	11.7	11.7	10.9	4.5	4.5	4.5	4.5	4.5	2.3	4.4
33	Nickel	94	876	410	433	147	124	110	26	552	296
34	Cadmium	11.1	1.5	2.0	0.5	76.7	57.0	51.3	14.8	0.2	0.3
35	Lead	54	171	104	77	393	404	364	65	61	102

Table D-2. Probabilities of chronic toxic effects on fish populations due to RAC 4 at annual median ambient concentrations for the Lurgi/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	1.0017	0.5003	Class
Bigmouth buffalo	1.0017	0.5003	Class
Smallmouth buffalo	1.0017	0.5003	Class
Channel catfish	0.7580	0.4529	Class
White bass	2.6564	0.6942	a
Green sunfish	1.3084	0.5578	Genus
Bluegill sunfish	2.8465	0.7244	Species
Largemouth bass	3.4440	0.7399	Family
Black crappie	5.6337	0.7859	Family

[a]Bluegill - Perciformes

Table D-3. Probabilities of chronic toxic effects on fish populations due to RAC 5 at annual median ambient concentrations for the Lurgi/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	2.7565	0.6832	Class
Bigmouth buffalo	2.7565	0.6832	Class
Smallmouth buffalo	2.7565	0.6832	Class
Channel catfish	3.6404	0.7149	Class
White bass	6.6493	0.8330	Class
Green sunfish	6.6493	0.8330	Class
Bluegill sunfish	6.6493	0.8330	Class
Largemouth bass	6.6493	0.8330	Class
Black crappie	6.6493	0.8330	Class

Table D-4. Probabilities of chronic toxic effects on fish populations due to RAC 9 at annual median ambient concentrations for the Lurgi/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0756	0.0950	Family
Bigmouth buffalo	0.0763	0.0943	a
Smallmouth buffalo	0.0763	0.0943	a
Channel catfish	0.1372	0.1730	Class
White bass	0.3336	0.3098	Class
Green sunfish	0.3336	0.3098	Class
Bluegill sunfish	0.3336	0.3098	Class
Largemouth bass	0.3336	0.3098	Class
Black crappie	0.3336	0.3098	Class

[a]Fathead minnow - Cypriniformes

Table D-5. Probabilities of chronic toxic effects on fish populations due to RAC 31 at annual median ambient concentrations for the Lurgi/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0326	0.0369	Family
Bigmouth buffalo	0.0162	0.0282	Class
Smallmouth buffalo	0.0162	0.0282	Class
Channel catfish	0.0315	0.0662	Class
White bass	0.0340	0.0441	Class
Green sunfish	0.0190	0.0181	Genus
Bluegill sunfish	0.0184	0.0123	Species
Largemouth bass	0.0203	0.0227	Family
Black crappie	0.1161	0.1721	Family

Table D-6. Probabilities of chronic toxic effects on fish populations due to RAC 32A at annual median ambient concentrations for the Lurgi/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0072	0.0101	Class
Bigmouth buffalo	0.0072	0.0101	Class
Smallmouth buffalo	0.0072	0.0101	Class
Channel catfish	0.0077	0.0162	Class
White bass	0.0187	0.0216	Class
Green sunfish	0.0187	0.0216	Class
Bluegill sunfish	0.0187	0.0216	Class
Largemouth bass	0.0187	0.0216	Class
Black crappie	0.0187	0.0216	Class

Table D-7. Probabilities of chronic toxic effects on fish populations due to RAC 33 at annual median ambient concentrations for the Lurgi/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0099	0.0073	Family
Bigmouth buffalo	0.0011	0.0008	Class
Smallmouth buffalo	0.0011	0.0008	Class
Channel catfish	0.0023	0.0042	Class
White bass	0.0022	0.0010	Class
Green sunfish	0.0063	0.0033	Genus
Bluegill sunfish	0.0075	0.0027	Species
Largemouth bass	0.0085	0.0066	Family
Black crappie	0.0355	0.0670	Family

Table D-8. Probabilities of chronic toxic effects on fish populations due to RAC 34 at annual median ambient concentrations for the Lurgi/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0076	0.0026	Species
Bigmouth buffalo	0.0551	0.0884	Class
Smallmouth buffalo	0.0551	0.0884	Class
Channel catfish	0.0427	0.0845	Class
White bass	0.1617	0.1816	Class
Green sunfish	0.0011	0.0001	Genus
Bluegill sunfish	0.0015	0.0001	Species
Largemouth bass	0.0017	0.0004	Family
Black crappie	0.0057	0.0097	Family

Table D-9. Probabilities of chronic toxic effects on fish populations due to RAC 35 at annual median ambient concentrations for the Lurgi/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0183	0.0168	Family
Bigmouth buffalo	0.0057	0.0080	Class
Smallmouth buffalo	0.0057	0.0080	Class
Channel catfish	0.0094	0.0207	Class
White bass	0.0123	0.0134	Class
Green sunfish	0.0025	0.0008	Genus
Bluegill sunfish	0.0024	0.0004	Species
Largemouth bass	0.0027	0.0012	Family
Black crappie	0.0152	0.0329	Family

Table D-10. Probabilities of chronic toxic effects on fish populations due to RAC 4 at annual median ambient concentrations for the Koppers-Totzek/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.8924	0.4796	Class
Bigmouth buffalo	0.8924	0.4796	Class
Smallmouth buffalo	0.8924	0.4796	Class
Channel catfish	0.6753	0.4334	Class
White bass	2.3665	0.6728	a
Green sunfish	1.1657	0.5330	Genus
Bluegill sunfish	2.5357	0.7020	Species
Largemouth bass	3.0682	0.7201	Family
Black crappie	5.0189	0.7701	Family

[a]Bluegill-Perciformes

Table D-11. Probabilities of chronic toxic effects on fish populations due to RAC 5 at annual median ambient concentrations for the Koppers-Totzek/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.8527	0.4701	Class
Bigmouth buffalo	0.8527	0.4701	Class
Smallmouth buffalo	0.8527	0.4701	Class
Channel catfish	1.1262	0.5208	Class
White bass	2.0569	0.6435	Class
Green sunfish	2.0569	0.6435	Class
Bluegill sunfish	2.0569	0.6435	Class
Largemouth bass	2.0569	0.6435	Class
Black crappie	2.0569	0.6435	Class

Table D-12. Probabilities of chronic toxic effects on fish populations due to RAC 9 at annual median ambient concentrations for the Koppers-Totzek/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.6911	0.4256	Family
Bigmouth buffalo	0.6972	0.4269	a
Smallmouth buffalo	0.6972	0.4269	a
Channel catfish	1.2547	0.5429	Class
White bass	3.0498	0.6930	Class
Green sunfish	3.0498	0.6930	Class
Bluegill sunfish	3.0498	0.6930	Class
Largemouth bass	3.0498	0.6930	Class
Black crappie	3.0498	0.6930	Class

[a]Fathead minnow - Cypriniformes

Table D-13. Probabilities of chronic toxic effects on fish populations due to RAC 31 at annual median ambient concentrations for the Koppers-Totzek/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0113	0.0096	Family
Bigmouth buffalo	0.0056	0.0082	Class
Smallmouth buffalo	0.0056	0.0082	Class
Channel catfish	0.0109	0.0247	Class
White bass	0.0118	0.0126	Class
Green sunfish	0.0066	0.0040	Genus
Bluegill sunfish	0.0064	0.0022	Species
Largemouth bass	0.0071	0.0055	Family
Black crappie	0.0403	0.0792	Family

Table D-14. Probabilities of chronic toxic effects on fish populations due to RAC 33 at annual median ambient concentrations for the Koppers-Totzek/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0048	0.0024	Family
Bigmouth buffalo	0.0005	0.0003	Class
Smallmouth buffalo	0.0005	0.0003	Class
Channel catfish	0.0011	0.0016	Class
White bass	0.0010	0.0003	Class
Green sunfish	0.0031	0.0010	Genus
Bluegill sunfish	0.0036	0.0007	Species
Largemouth bass	0.0041	0.0022	Family
Black crappie	0.0173	0.0343	Family

Table D-15. Probabilities of chronic toxic effects on fish populations due to RAC 34 at annual median ambient concentrations for the Koppers-Totzek/Fischer-Tropsch process

Species	Ratio of ambient concentration to to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Carp	0.0047	0.0011	Species
Bigmouth buffalo	0.0339	0.0573	Class
Smallmouth buffalo	0.0339	0.0573	Class
Channel catfish	0.0262	0.0562	Class
White bass	0.0993	0.1246	Class
Green sunfish	0.0007	0.0000	Genus
Bluegill sunfish	0.0009	0.0000	Species
Largemouth bass	0.0010	0.0002	Family
Black crappie	0.0035	0.0052	Family

APPENDIX E

Detailed Methods and Assumptions for Ecosystem Uncertainty Analysis

APPENDIX E

DETAILED METHODS AND ASSUMPTIONS FOR ECOSYSTEM UNCERTAINTY ANALYSIS

E.1 ORGANIZING TOXICITY DATA

The first step in Ecosystem Uncertainty Analysis (EUA) is selection of appropriate toxicity data and association of the data with components of SWACOM.

Toxicity data on phytoplankton are sparse. It is possible to find values for green algae, such as Selenastrum capricornutum, and these data are used for all 10 algal populations if no other information is available. If data are available on diatoms and blue-greens, then a further division is possible based on physiological parameters in the model and past experience with SWACOM. Like diatoms, species 1-3 appear early in the spring and are associated with low temperatures and high nutrient concentrations. Species 4 to 7 dominate the spring bloom and are associated with intermediate temperatures and light. Species 8 to 10 appear in the summer and are tolerant of high temperatures and low nutrient concentrations.

The identification of the zooplankton is more tenuous. Based on model behavior and physiological parameters, species 12 and 13 are identified with Cladocerans. The ubiquitous data for Daphnia magna are used for species 12. When data are available for Daphnia pulex, they are used for species 13. The remaining zooplankters (species 11, 14 and 15, and species 13 when no data was available for D. pulex) are simply identified as crustaceans. Of the available data, the smallest concentration is assigned to 15 and the largest to 11. Species 14 (and 13 when necessary) is assigned an intermediate value between these extremes. Assuming species 15 to be the most sensitive is conservative. Since blue-green algae increase is one of our endpoints, we assign the greatest sensitivity to the consumer (i.e., 15) which is most abundant during the summer of the simulated year.

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LC_{50} data for fathead minnow (Pimephales sp.), bluegill (Lepomis macrochirus), and guppy (Poecilia reticulata) are assigned to forage fish (species 16, 17 and 18). When data on these species are not available, others are substituted, such as goldfish or mosquitofish. The game fish (species 19) was identified as rainbow trout.

E.2 TRANSFORMING TOXICITY DATA

A critical step in applying EUA involves changing parameter values in SWACOM. This requires three important assumptions which are outlined below.

E.2.1 The General Stress Syndrome (GSS)

Toxicity tests provide information on mortality (or similar endpoint) but provide little insight on the mode of action of the chemicals. Thus, some assumption must be made about how the toxicant affects physiological processes in SWACOM. In an application that focuses on a single chemical it may be possible to obtain detailed information on modes of action. However, the present effort must cover a number of Risk Assessment Units, and it was necessary to make a single overall assumption.

We assumed that organisms respond to all toxicants according to a General Stress Syndrome (GSS). For phytoplankton, this involved decreased maximum photosynthetic rate, increased Michaelis-Menten constant, increased susceptibility to grazing, decreased light saturation, and decreased nutrient assimilation. For zooplankton and fish, the syndrome involves increased respiration, decreased grazing rates, increased susceptibility to predation, and decreased nutrient assimilation. For all organisms, the optimum temperature was assumed to be unchanged. The GSS represents how organisms respond to most toxicants. Where observations were recorded for the chemicals used in this assessment, the researchers noted hyperactivity, increased operculation and other symptoms consistent with the assumption of the GSS. However, some organics might have a "narcotic" effect which would be opposite to the reaction assumed here.

The General Stress Syndrome defines the direction of change of each parameter in SWACOM. It is also necessary to make an assumption about the relative change in each parameter. We have assumed that all parameters of SWACOM change by the same percentage. This assumption can be removed only if considerable information is available on modes of action of each chemical.

E.2.2 The MICROCOSM Simulations

The key to arriving at new parameters is simulation of the experiments which generated the toxicity data. This involves simulating each species in isolation with light, temperature, food supply, and nutrients set at constant levels that would maintain the population indefinitely. Then the parameters are altered together in the direction indicated by the GSS until we duplicate the original experiment. Thus, for an LC_{50} (96 hours), we find the percentage change which halves the population in 4 d.

At the conclusion of the MICROCOSM simulations, we have the percentage change in the parameters which matches the experiment. We must now make an additional assumption to arrive at the expected response for concentrations below the LC_{50} or EC_{50}. We assume a linear dose response. Thus, an environmental concentration 1/5 of the LC_{50} would cause a 10% reduction in the population. The MICROCOSM simulations are then repeated with this new endpoint to arrive at a new percentage change in the parameters. Since most response curves are concave, our assumption should be conservative.

E.2.3 Choosing Uncertainties

To implement the analysis, it is necessary to associate uncertainties with the parameter changes. We assume that all parameter changes have an associated uncertainty of plus or minus 100%. This assumption seems sufficiently conservative. One might wish to adopt a more complex strategy which would combine information on modes of action with a Delphi survey of experienced researchers to arrive at more specific estimates of uncertainty.

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