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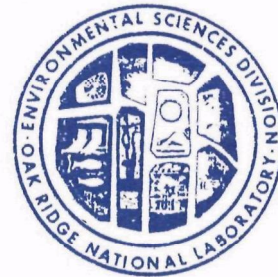
Unit Release Risk Analysis for Environmental Contaminants of Potential Concern in Synthetic Fuels Technologies

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ENVIRONMENTAL SCIENCES DIVISION
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ENVIRONMENTAL SCIENCES DIVISION
UNIT RELEASE RISK ANALYSIS FOR ENVIRONMENTAL CONTAMINANTS OF
POTENTIAL CONCERN IN SYNTHETIC FUELS TECHNOLOGIES

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SUMMARY

The Environmental Sciences Division, Oak Ridge National Laboratory, is analyzing the potential environmental risks associated with commercial-scale synthetic liquid fuels (synfuels) technologies. The overall objective of this environmental risk analysis project, which is funded by the Office of Research and Development, U.S. Environmental Protection Agency, is to guide research on environmental aspects of synfuel technologies by identifying the most hazardous synfuel-derived contaminants and the most important sources of scientific uncertainty concerning the fate and effects of these contaminants.

The general strategy adopted for the project involves (1) grouping the contaminants present in effluents and products of commercial-scale processes into 38 categories termed Risk Analysis Units (RACs), (2) defining generalized reference environments with characteristics representative of regions in which synfuels plants may be sited, and (3) assessing risks of five distinct, adverse ecological effects: reductions in fish populations, development of algal blooms that detract from water use, reductions in timber yield or undesirable changes in forest composition, reductions in agricultural production, and reductions in wildlife populations.

This report presents results of a unit release risk analysis, i.e., an analysis that assumes identical release rates for all RACs. The primary purpose of this analysis is to compare the relative hazards of the 38 RACs, based purely on their environmental toxicology and chemistry, and to quantify and compare the major sources of uncertainty concerning their fate and effects.

Two reference environments were employed: an eastern environment resembling eastern Kentucky or West Virginia and a western environment resembling the western slope of the Rocky Mountains in northern Colorado or southern Wyoming. Estimates of concentrations of released contaminants in the air, soil, and surface water of the two reference environments were obtained, using a simple Gaussian-plume atmospheric dispersion and deposition model and a steady-state surface water fate model.

Risk to the five ecological endpoints were estimated using one or more of three techniques: the quotient method, analysis of extrapolation error, and ecosystem uncertainty analysis. In the quotient method, estimated environmental concentrations were simply compared to toxicological benchmarks such as LC₅₀'s* available for standard test organisms. In analysis of extrapolation error, statistical relationships between the sensitivities to contaminants of the various taxa of fish and between acute- and chronic-effects concentrations were used to estimate, with appropriate error bounds, chronic-effects thresholds for reference fish species characteristic of the two reference environments. In ecosystem uncertainty analysis, an aquatic ecosystem model was used to compute risk estimates that explicitly incorporate biological phenomena such as competition and predation that can magnify or offset the direct effects of contaminants on organisms.

With only environmental transport and toxicity of the 38 classes of contaminants accounted for, acid gases (primarily hydrogen sulfide), esters, mercury, and cadmium were found to have the greatest potential effects on fish populations. Based on the ecosystem uncertainty analysis, it appears that contaminants that are highly toxic to fish are the most likely to produce increases in algal biomass. Existing data were insufficient for performing separate risk analyses for forests and crops. For terrestrial plants in general, hydrogen sulfide was found to be the most toxic gaseous pollutant. Of contaminants likely to be deposited on soil, arsenic, cadmium, and nickel appear most likely to accumulate to toxic levels. The most serious threats to wildlife, considering only inhalation exposures, are aldehydes and ketones, cadmium, arsenic, and respirable particles.

Between-site comparisons were performed for aqueous releases. Because of differences in important hydrological parameters, especially sediment loading, estimated half-lives of many contaminants differ significantly between sites. Sedimentation rates of hydrophobic contaminants are higher in the western river. Photolysis rates of

*LC₅₀ = concentration lethal to 50% of population exposed.

photodegradable compounds are higher in the eastern river. The salmonid fishes found in western rivers are more sensitive to many contaminants (most notably cadmium) than are the fish typically found in eastern rivers.

A number of significant uncertainties were identified. Toxicological data suitable for use in risk analysis are sparse for most organisms other than fish. The data that do exist are frequently of limited utility because of the diversity and lack of comparability of the test systems employed. Magnitudes of uncertainty concerning (1) the expected environmental concentrations of contaminants in the vicinity of synfuels plants and (2) predicted effects thresholds for fish were compared. This comparison shows that, at least for the contaminants occurring in synfuels products and effluents, uncertainty concerning the toxicological effects of contaminants is much greater than is uncertainty concerning environmental transport.

ABSTRACT

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This report contains results of a risk analysis study of 38 categories of chemical contaminants [Risk Analysis Units (RACs)] that may be released to the environment by synthetic fuels production facilities. The analysis includes modeling of the environmental transport and fate of contaminants in the atmosphere and in surface water, and quantification of risks for five ecological endpoints. Two generic "reference environments" with meteorological, hydrological, and biological characteristics representative of (1) the central appalachian coal basin and (2) the western slope of the Rocky Mountains were used. A uniform release rate was assumed for all RACs. Consequently, the primary objectives of the risk analysis were to (1) estimate the relative risks of the RACs as functions of their environmental chemistry and toxicology, and (2) to quantify and compare the major sources of uncertainty concerning the fate and effects of the contaminants.

1. INTRODUCTION

Environmental risk analysis is defined as the process of identifying and quantifying probabilities of adverse changes in the environment resulting from human activities. This includes explicit incorporation and, to the extent possible, quantification of scientific uncertainties regarding the adverse effects being considered. The Environmental Sciences Division, Oak Ridge National Laboratory, has been developing and demonstrating methods for environmental risk analysis for the Office of Research and Development, U.S. Environmental Protection Agency (USEPA). The methods being employed in this project were described by Barnthouse et al. (1982). Although the concept of risk is applicable to many types of environmental problems, this project is focusing on risks associated with toxic environmental contaminants derived from synthetic liquid fuels technologies. The overall objective of the project is to guide research on environmental aspects of synfuel technologies by identifying the most hazardous contaminants (or classes of contaminants) and the most important sources of scientific uncertainty concerning the fate and effects of contaminants. The analyses, results, and conclusions of this research are intended to be generic and are not estimates of actual impacts of specific plants at specific sites.

For purposes of risk analysis, the thousands of potentially significant contaminants present in waste streams and products of synthetic liquid fuels technologies have been grouped into the 38 categories, termed Risk Analysis Units (RACs), listed in Table 1.1. Five ecological endpoints are addressed: (1) reductions in fish populations, (2) development of algal populations that detract from water use, (3) reductions in timber yield or undesirable changes in forest composition, (4) reductions in agricultural production, and (5) reductions in wildlife populations. Rather than descriptions of specific sites, the risk analyses employ generalized reference environments, with characteristics representative of regions in which synfuels plants may be sited. Two reference environments are being employed in research for the USEPA: an eastern environment resembling

Table 1-1. Risk Analysis Categories (RACs)

RAC Number	Name	Description
1	Carbon monoxide	CO
2	Sulfur oxides	SO _x
3	Nitrogen oxides	NO _x
4	Acid gases	H ₂ S, HCN
5	Alkaline gases	NH ₃
6	Hydrocarbon gases	Methane through butanes, acetylene, ethene through butenes; C ₁ -C ₄ alkanes, alkynes and cyclocompounds; bp < ~20°C
7	Formaldehyde	HCHO
8	Volatile organochlorines	To bp ~120°C; CH ₂ Cl ₂ , CHCl ₃ , OCl ₄
9	Volatile carboxylic acids	To bp ~120°C; formic and acetic acids only
10	Volatile O & S heterocyclics	To bp ~120°C; furan, THF, thiophene
11	Volatile N heterocyclics	To bp ~120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines
12	Benzene	Benzene
13	Aliphatic/alicyclic hydrocarbons	C ₅ (bp ~40°C) and greater; paraffins, olefins, cyclocompounds, terpenoids, waxes, hydroaromatics
14	Mono- or diaromatic hydrocarbons (excluding benzene)	Toluene, xylenes, naphthalenes, biphenyls, alkyl derivatives
15	Polycyclic aromatic hydrocarbons	Three rings and greater; anthracene, BaA, BaP, alkyl derivatives
16	Aliphatic amines (excluding N heterocyclics)	Primary, secondary, and tertiary nonheterocyclic nitrogen, MeNH ₂ , diMeNH, triMeN
17	Aromatic amines (excluding N heterocyclics)	Anilines, naphthylamines, amino pyrenes; nonheterocyclic nitrogen
18	Alkaline N heterocyclics ("azaarenes") (excluding "volatiles")	Quinolines, acridines, benzacridines (excluding pyridines)
19	Neutral N, O, S heterocyclics (excluding "volatiles")	Indoles, carbazoles, benzofurans, dibenzothiophenes
20	Carboxylic acids (excluding "volatiles")	Butyric, benzoic, phthalic, stearic
21	Phenols	Phenol, cresols, catechol, resorcinol
22	Aldehydes and ketones ("carbonyls") (excluding formaldehyde)	Acetaldehyde, acrolein, acetone, benzaldehyde
23	Nonheterocyclic organo-sulfur	Mercaptans, sulfides, disulfides, thiophenols, CS ₂
24	Alcohols	Methanol, ethanol
25	Nitroaromatics	Nitrobenzenes, nitropyrenes
26	Esters	Acetates, phthalates, formates
27	Amides	Acetamide, formamide, benzamides
28	Nitriles	Acrylonitrile, acetonitrile
29	Tars	
30	Respirable particles	
31	Arsenic	As, all forms
32	Mercury	Hg, all forms
33	Nickel	Ni, all forms
34	Cadmium	Cd, all forms
35	Lead	Pb, all forms
36	Other trace elements	
37	Radioactive materials	²²⁶ Ra
38	Other remaining materials	

eastern Kentucky or West Virginia, and a western environment resembling the western slope of the Rocky Mountains in northern Colorado or southern Wyoming. Descriptions of the meteorology, hydrology, demography, land-use patterns, and biota of these two reference environments have been developed by Travis et al. (1983).

This report presents results of a unit release risk analysis, i.e., an analysis that assumes identical release rates for all of the RACs listed in Table 1.1. The unit release risk analysis is intended to compare the relative hazards of the various RACs, based purely on their environmental chemistry and toxicology, and to quantify and compare the major sources of uncertainty concerning their fate and effects. In addition, the unit release risk analysis provides initial information on the relative risks of the RACs to eastern and western ecosystems. Finally, this analysis identifies significant gaps in the chemical and toxicological data bases that are used for synfuels risk analysis.

2. EXPOSURE ASSESSMENT

The exposure assessments presented in this section used the atmospheric transport and deposition and surface water transport and transformation models described in Travis et al. (1983). Exposure assessments were performed for both the eastern and the western sites described by Travis et al. (1983).

2.1 SURFACE WATER

Estimates of the concentrations of 30 RACs in the surface waters of the eastern and western reference sites were calculated. The only RACs for which analyses were not performed were gases (e.g., CO₂, SO₂, NO_x) that could not reasonably be expected to occur in aqueous effluents. A unit release rate of 4.12×10^{-2} g/s was assumed for all RACs in both reference environments. This number was the median of 17 release rates employed in a preliminary risk analysis for indirect coal liquefaction and therefore was felt to be a reasonable value.

2.1.1 Stream Characteristics

The environmental parameters used in determining stream characteristics were stream flow (m³/s), stream width (m), reach length (m), sediment load (mg/L), sediment density (g/m³), the depth of the biologically active sediment (cm), the fraction of organic carbon in the sediment (unitless), stream temperature (K), current velocity (m/s), wind velocity (m/s), and the radius of sediment particles (cm). Estimates of stream flow, temperature, and suspended solids for the eastern site were set within ranges observed by the U.S. Geological Survey (USGS) for the Big Sandy River at Louisa, Kentucky, and the Monongahela river at Braddock, Pennsylvania (USGS 1977, 1979). For the western site, these estimates were obtained from USGS data for the Colorado River at De Beque, Colorado (USGS 1980). Values for the other stream parameters were taken from Southworth (1979). Irradiance values [photons/(cm²·s)] for estimating photolysis rates were obtained from Zepp and Cline (1977).

The effects of environmental variability on contaminant transport and fate were quantified, using the probabilistic version of the surface water transport model. Probability distributions for flow, temperature, and suspended solids were generated based on the means, minima, and maxima of these parameters observed at the USGS stations. Normal distributions for particle radius, organic carbon fraction, current velocity, and wind velocity were derived from ranges used by Southworth (1979). Because current velocity and sediment load are influenced by stream flow, a correlation coefficient of 0.7 was specified between flow and velocity and between flow and suspended solids. All environmental parameters used in the exposure assessments are presented in Tables 2.1-1 and 2.1-2.

2.1.2 Contaminant Characteristics

For determining the characteristics of organic contaminants, (Table 2.1-3), the chemical properties used were molecular weight (g/mol), aqueous solubility (g/L), octanol-water partition coefficient (unitless), quantum yield of direct photolysis (unitless), molar extinction coefficient [(cm·L)/mol], and vapor pressure (mmHg). Although microbial degradation rates can be accommodated in the model, none was used for the unit release assessment. Molecular weights of organic compounds were obtained from Weast (1980); aqueous solubility data were obtained from Verschueren (1977); octanol-water partition coefficients were obtained from Leo et al. (1971) and Briggs (1981). Equations relating vapor pressure to ambient temperature were generated from data points reported in Verschueren (1977). These equations are linear approximations that should provide adequate accuracy over the small temperature range (280 - to 310 K) involved.

Derived characteristics of organic contaminants were calculated using functional relationships obtained from the literature. Henry's Law coefficients were approximated using the method of Dilling (1977). Mass transfer rates and dissolved fractions were calculated using the method of Southworth (1979). Particulate settling velocities were calculated from Stoke's Law (Weast 1980). Direct photolysis rate constants for anthracene and quinoline were calculated using the method

Table 2.1-1. Stream characteristics for the eastern reference site

Environmental parameter	Units	Mean value	Standard deviation	Minimum value	Maximum value
Stream flow	m ³ /s	120	75	50	600
Reach length	m	1000	0	1000	1000
Stream width	m	40	0	40	40
Suspended solids	mg/L	25	20	1	250
Sediment depth	cm	1	0	1	1
Solids density	g/cm ³	1.02	0	1.02	1.02
Fraction organic carbon		0.1	0.1	0.05	0.25
Particle radius	cm	0.005	0.0025	0.001	0.01
Temperature	K	298	3	283	310
Current velocity	m/s	0.25	0.1	0.1	1.0
Wind velocity	m/s	1.5	0.1	0.25	4.0

Table 2.1-2. Stream characteristics for the western reference site

Environmental parameter	Units	Mean value	Standard deviation	Minimum value	Maximum value
Stream flow	m ³ /s	175	100	40	600
Reach length	m	1000	0	1000	1000
Stream width	m	20	0	20	20
Suspended solids	mg/L	260	200	50	1000
Sediment depth	cm	1	0	1	1
Solids density	g/cm ³	1.02	0	1.02	1.02
Fraction organic Carbon		0.1	0.1	0.05	0.25
Particle radius	cm	0.005	0.0025	0.001	0.01
Temperature	K	292	3	280	305
Current velocity	m/s	0.5	0.2	0.2	2.0
Wind velocity	m/s	1.5	0.1	0.25	4.0

Table 2.1-3. Contaminant characteristics

RAC	Representative contaminant	Molecular or atomic weight ^a (g/mol)	Aqueous solubility ^b (g/L)	Octanol-water partition coefficient (log P)	Quantum yield of photolysis (unitless)
4	Hydrogen sulfide	34.06			
5	Ammonia	17.03			
6	Butane	58.12	6.1 E-02		
7	Formaldehyde	30.03			
8	Methylene chloride	84.93	1.67 E+01		
9	Acetic acid	60.05	3.80 E-02	-0.17 ^c	
10	Thiophene	84.14	4.43 E-01	1.81 ^c	
11	Pyridine	79.10	3.00 E-02	0.650 ^c	
12	Benzene	78.12	1.78 E+00	2.13 ^c	
13	Cyclohexane	84.16	5.5 E-02	4.0 ^c	
14	Toluene	92.15	5.15 E-01	2.69 ^c	
15	Anthracene	178.24	7.50 E-05	4.45 ^c	0.003 ^d
17	Aniline	93.13	3.40 E+01	0.90 ^c	
19	Dibenzofuran	168.21	3.00 E-03	4.12 ^c	
20	Butanoic acid	88.1	5.62 E+01	0.79 ^c	
21	Phenol	94.11	8.20 E+01	1.46 ^c	
22	Acrolein	56.07	9.74 E-01	0.90 ^e	
23	Methanethiol	48.11	4.00 E-05	-0.660 ^c	
24	Methanol	32.04	2.7 E-01	-0.74 ^c	
25	Nitrobenzene	123.11	1.9 E+00	2.31 ^e	
26	Methyl phthalate	194.19	5.0 E+00		
28	Acrylonitrile	53.06	3.83 E-01	-0.92 ^c	
31	Arsenic	74.92			
32	Mercury	200.59			
33	Nickel	58.71			
34	Cadmium	112.40			
35	Lead	207.19			
36	Fluorine	19.00			

^aWeast (1980).

^bVerschuieren (1977).

^cLeo et al. (1971).

^dZepp and Schlotzhauer (1979).

^eBriggs (1981).

of Zepp and Cline (1977). Adsorption/desorption coefficients were approximated using the method of Karickhoff et al. (1979).

Because of their complex environmental chemistry, removal processes for trace elements were not directly modeled. Rates of removal due to sedimentation were estimated using an adsorption-desorption coefficient of 200. The results of Schell and Sibley's (1982) study of distribution coefficient for radionuclides suggest that this is a conservative estimate for most trace elements under most environmental conditions.

2.1.3 Results

Comparisons were performed for both reference streams, using a source rate of 4.12×10^{-2} g/s for all contaminants. The means, medians, and upper 95% concentrations (i.e., the concentrations equaled or exceeded in 5% of the Monte Carlo simulations) in 1-km stream reaches immediately adjacent to the release sites are presented in Table 2.1-4. For all practical purposes, the concentrations computed using contaminant-specific removal rates are identical to concentrations computed from pure dilution. Thus, at least in the immediate vicinity of contaminant sources located on rivers such as the eastern and western reference streams, the environmental removal processes modeled have very little influence on steady-state contaminant concentrations. It is possible, however, that some of the processes not modeled, e.g., hydrolysis, complexation, or microbial degradation, may occur more rapidly than do photolysis, sedimentation, and volatilization.

Estimates of the half-lives of 23 reference contaminants for which removal rates were calculated are presented in Table 2.1-5. These values can be interpreted as estimates of the time required to reduce the total mass of contaminant in the water column by one-half after cessation of contaminant release. The half-lives range from 100 to 5000 h accounting for the negligible influence of removal processes on the steady-state contaminant concentrations. For many contaminants, the half-lives differ markedly between sites, principally because of the tenfold difference in sediment loads between the eastern and western rivers. For contaminants for which sedimentation is the

Table 2.1-4. Near-field contaminant concentrations (g/L) in the eastern and western reference streams^a

Reference environment	Contaminant	Mean	Median	95% ^b
Eastern	Anthracene	3.4 E-07	3.0 E-07	6.4 E-07
Eastern	All others	3.4 E-07	3.0 E-07	6.7 E-07
Eastern	Dilution only	3.4 E-07	3.0 E-07	6.7 E-07
Western	All	2.8 E-07	2.2 E-07	6.4 E-07
Western	Dilution only	2.8 E-07	2.2 E-07	6.4 E-07

^aRelease rate = 4.12 E-02 g/s for all contaminants.

^bConcentration expected to be equaled or exceeded on 5% of days.

Table 2.1-5. Median half-lives and dominant removal processes of contaminants in eastern and western reference stream reaches

RAC	Reference contaminant	Eastern site		Western site	
		Median half-life (h)	Dominant removal process ^a	Median half-life (h)	Dominant removal process ^a
9	Acetic Acid	1.1 E+03	V	9.0 E+02	V
10	Thiophene	1.3 E+03	V	1.1 E+03	V
11	Pyridine	1.3 E+03	V	1.0 E+03	V
12	Benzene	1.2 E+03	V	8.9 E+02	V
13	Cyclohexane	6.9 E+02	V	2.2 E+02	S
14	Toluene	1.3 E+03	V	7.2 E+02	V
15	Anthracene	8.6 E+01	P	7.6 E+01	S
16	Methylamine	8.0 E+02	V	6.5 E+02	V
17	Aniline	1.4 E+03	V	1.2 E+03	V
18	Quinoline	2.8 E+03	P	5.0 E+03	V
19	Dibenzofuran	5.6 E+02	S	1.3 E+02	S
20	Butanoic acid	1.4 E+03	V	1.1 E+03	V
21	Phenol	1.4 E+03	V	1.2 E+03	V
22	Acrolein	1.1 E+03	V	1.2 E+03	V
23	Methanethiol	1.0 E+03	V	8.1 E+02	V
24	Methanol	8.1 E+02	V	6.6 E+02	V
25	Nitrobenzene	1.6 E+03	V	1.0 E+03	V
28	Acrylonitrile	1.0 E+03	V	8.5 E+02	V
31	Arsenic	4.8 E+03	S	5.7 E+02	S
32	Mercury	4.8 E+03	S	5.7 E+02	S
33	Nickel	4.8 E+03	S	5.7 E+02	S
34	Cadmium	4.8 E+03	S	5.7 E+02	S
35	Lead	4.8 E+03	S	5.7 E+02	S

^aV = volatilization.

S = sedimentation.

P = photolysis.

dominant removal process, half-lives are 5 to 10 times longer in the eastern river than in the western river. Conversely, photolysis, which is the dominant removal process for anthracene and quinoline in the eastern river, is greatly reduced in the western river. For anthracene, this decrease is more than offset by an increase in sedimentation rate; for the highly soluble quinoline, the decrease in photolysis results in an approximate doubling of the half-life.

2.2 ATMOSPHERIC DISPERSION AND DEPOSITION

The terrestrial assessment was based on an atmospheric release rate for all RACs of 10^9 g/year (a reasonable release rate for major gaseous pollutants from a synfuels plant). The emissions were partitioned among five sources based on their distribution among sources at an indirect coal liquefaction plant. The sources were a 150-m stack, a 6.5-m lock-hopper vent, a 25-m cooling tower, and area emissions from a tank farm and fugitive sources.

The short-range atmospheric dispersion code AIRDOS-EPA (Moore et al. 1979) was used in the environmental risk analysis to calculate ground-level atmospheric concentrations and deposition. This code is summarized in Travis et al. (1983), who also describe the method for calculating accumulation in soil. Soil concentrations are calculated for a 35-year accumulation period, using site-specific parameters for soil bulk density, precipitation, evapotranspiration, and irrigation, and taking into account removal by leaching, biological degradation, and chemical degradation.

Because most phytotoxicity studies are conducted in solution culture, we have added a calculated concentration in soil solution that is not described in previous documents. For calculation of the soil solution concentration, the total accumulation in the soil compartment is first calculated as above: that is, the depositing material is summed over the lifetime of the facility and corrected for leaching, degradation, and other removal processes. The retained material is then partitioned between the solid and solution phases of the soil compartment assuming the relationship,

$$C_{iss} = \frac{C_{is}}{K_d} , \quad (1)$$

where

C_{iss} = the concentration of compound i in root zone soil solution ($\mu\text{g/L}$),

C_{is} = the concentration of compound i in root zone soil ($\mu\text{g/kg}$),

K_d = the distribution coefficient (L/kg).

Because K_d is in the denominator of Eq. (1), the soil solution concentration C_{iss} could take on extremely high values with small values of K_d . In order to bound the maximum value of C_{iss} , it is assumed that the upper-bound concentration is represented by the total deposited and retained material divided by the quantity of water in the root zone defined by d or

$$C_{iss}^{\max} = \frac{D_i [1 - \exp(-\lambda_{si} t_b)]}{10 \rho \theta d \lambda_{si}} , \quad (2)$$

where

D_i = the ground-level deposition rate of compound i [$\mu\text{g}/(\text{m}^2 \cdot \text{s})$],

λ_{si} = the sum of all soil removal rate constants (L/s),

t_b = the period of long-term buildup in soil, equal to the length of time that the source term is in operation (s),

10 = a conversion factor from g/cm^2 to kg/m^2 [$(10,000 \text{ cm}^2/1 \text{ m}^2)$ ($1 \text{ kg}/1000 \text{ g}$)],

ρ = soil bulk density (g/cm^3),

θ = volumetric water content (cm^3/cm^3),

d = the depth of the root zone (cm),

r = soil volumetric water content (mL/cm^3).

If C_{iss} calculated via Eq. (1) exceeds C^{\max} calculated via Eq. (2), then C_{iss} is set equal to C^{\max} . The value of θ used in Eq. (2) is very important in providing a reasonable estimate of C^{\max} . Since

Table 2.2-1. Maximum ambient atmospheric and soil concentrations of RACs at the eastern and western reference sites

RAC	Annual average concentration in air ($\mu\text{g}/\text{m}^3$)		Concentration in soil ^a ($\mu\text{g}/\text{kg}$)		Concentration in soil solution ^a ($\mu\text{g}/\text{L}$)	
	Eastern	Western	Eastern	Western	Eastern	Western
	1 Carbon monoxide	65.7	93.3	a	a	a
2 Sulfur oxides	0.134	0.331	a	a	a	a
3 Nitrogen oxides	0.112	0.263	a	a	a	a
4 Acid gases	65.2	92.4	a	a	a	a
5 Alkaline gases	9.82	15.4	a	a	a	a
6 Hydrocarbon gases	63.4	88.2	25.5	35.2	26.4	36.4
7 Formaldehyde	43.7	61.9	2240	2810	4610	5780
8 Volatile organochlorines	65.4	92.7	4.93	6.93	4.63	6.51
9 Volatile carboxylic acids	4.46	7.51	829	1080	1710	2220
10 Volatile O & S heterocyclics	66.7	94.9	2.74	3.87	2.28	3.23
11 Volatile N-heterocyclics	4.45	7.49	243	335	501	691
12 Benzene	67.5	96.4	28.1	38.7	21.6	29.8
13 Aliphatic/alicyclic hydrocarbons	26.2	29.5	623	699	44.5	49.9
14 Mono- or diaromatic hydrocarbons	59.0	82.8	34.3	47.8	6.85	9.55
15 Polycyclic aromatic hydrocarbons	70.5	99.8	6330	8760	97.4	135
16 Aliphatic amines	56.6	80.3	639	863	1320	1780
17 Aromatic amines	50.8	63.8	257	304	531	626
18 Alkaline N heterocyclics	4.45	7.50	445	627	171	241
19 Neutral N, O, S heterocyclics	4.76	8.04	0.181	0.305	0.0475	0.0802
20 Carboxylic acids	27.9	40.7	804	1120	670	931
21 Phenols	43.3	59.5	13100	11200	19300	16500
22 Aldehydes and ketones	55.6	78.6	89.4	126	184	260
23 Nonheterocyclic organosulfur	50.4	65.9	60.3	78.3	27.4	35.6
24 Alcohols	62.3	88.6	614	815	1270	1680
25 Nitroaromatics	56.7	80.4	1350	1850	792	1090
26 Esters	56.7	80.4	2050	2530	4230	5220
27 Amides	64.0	91.0	73.4	101	151	207
28 Nitriles	64.1	91.1	103	137	213	283
29 Tars	65.9	93.7	a	a	a	a
30 Respirable particles	65.9	93.7	a	a	a	a
31 Arsenic	4.35	7.33	1.57 E+06	1.81 E+06	7860	9050
32 Mercury	0.336	0.584	53.6	40.5	5.36	4.05
33 Nickel	47.9	68.1	1.58 E+06	1.71 E+06	10500	11400
34 Cadmium	4.19	7.06	2.36 E+05	1.45 E+05	36200	22300
35 Lead	4.30	7.12	5.51 E+05	7.48 E+05	612	831

^aNo accumulation in soil.

measured values of K_d are usually under saturated conditions, θ in Eq. (2) represents total soil porosity.

These calculations generate sector-average ground-level concentrations in air, soil, and soil solution in 16 directions at 500-m intervals from 1,500 to 50,000 m from the source. The highest annual average concentrations are presented in Table 2.2-1. These results are based on a release rate for all RACs of 10^9 g/year.

3. AQUATIC ENDPOINTS

3.1 QUOTIENT METHOD

Also known as the "ratio method," this approach to assessing the relative hazard of several constituents has been used in such fields as environmental health and epidemiology. The quotient is calculated from the ratio of the known or estimated concentration of a chemical in the environment to a concentration of that chemical proven or calculated (by extrapolation from experimental data) to be toxic to certain organisms at a particular test endpoint. The endpoint, known as a toxicological benchmark, may be one of several, among them the USEPA water quality criteria (USEPA 1980a-p), the effective concentration causing a designated effect on 20% of the test organisms (EC_{20}), the mean toxic concentration (MTC), the threshold bioaccumulation concentration (TBC), the lowest observed toxic concentration (LOTC), the median tolerance limit (TL_m), and the concentration required to kill 50% of the test organisms (LC_{50}). The benchmarks used in this risk analysis are presented in Appendix A.

Since this report compares potential toxic differences between groups of chemicals (RACs), benchmarks common to as many of the RACs as possible were preferred. LC_{50} and TL_m , the two benchmarks most frequently found in aquatic toxicological literature, were selected to represent acute toxicity (Table A-1). Chronic effects are presented as the geometric mean maximum allowable toxicant concentration (GMATC), which is the geometric mean of the highest no-observed-effect concentration and the lowest observed effect concentration (Table A-2). In contrast, benchmarks used in algal tests can vary between studies, and therefore, different test endpoints were selected for this report (Table A-3).

Appendix A does not include all extant data on the responses of freshwater organisms to the test chemicals. For example, for the extensively tested heavy metals, several representative values are included for the sake of brevity.

As in the selection of benchmarks, the test species chosen for tabulation were those that appear most frequently in the literature. Invertebrates were usually represented by cladocerans (Daphnia species), with insect data presented when available. The fish species selected are those usually used in toxicity testing, namely, fathead minnows (Pimephales promelas), bluegills (Lepomis macrochirus), and rainbow trout (Salmo gairdneri). Data for algal assays are sparse, so all species appearing in the literature, to our knowledge, were included in Table A-3.

Table 3.1-1 presents the highest quotients for each RAC and category of effect for both the eastern and western sites. The acute toxicity quotients were calculated using the upper 95th percentile concentration (Sect. 2), an estimate of the worst acute exposure, assuming stable plant operation. The chronic quotients were calculated using the annual median concentration, and algal quotients were calculated for both concentrations, since the distinction between acute and chronic effects is not clear for algae. The higher the value of these quotients, the greater the risk of acute effects on organisms inhabiting the reference stream.

Quotients are interpreted according to the best judgment of the analyst (Barntouse et al. 1982). A value of 0.01 (1.0 E-02) or less indicates little apparent environmental significance; 0.1 to 10 (1.0 E+01) suggests possible or potential adverse effects; and greater than 10 describes a chemical of probable environmental concern. While these interpretations are consistent with current practice in hazard assessment, their utility in screening chemicals for risk analysis must be confirmed by experimental research and environmental monitoring.

To facilitate evaluation of the data in Table 3.1-1, the range of quotients for each RAC (for which data were available) is plotted for fish acute toxicity and for algal toxicity (Figs. 3.1-1 and 3.1-2). Thus, the relative toxicities of most of the chemicals is readily apparent. Although 18 of the 24 RACs in Fig. 3.1-1 overlap between the limits of 0.01 (E-02) and 0.00001 (E-05), only five of them (RACs 4, 15, 22, 32, and 34) extend beyond the limit of 0.01 (E-02) and one

Table 3.1-1. Toxicity quotients for toxicity to fish and algae (ambient contaminant concentration/toxic benchmark concentration) for unit release

RAC	RAC Name	Highest quotient - eastern site ^a				Highest quotient - western site ^a			
		Fish, acute		Fish, chronic	Algae	Fish, acute		Fish, chronic	Algae
		95%	Median	Median	95%	95%	Median	Median	95%
1	Carbon monoxide	b	b	b	b	b	b	b	b
2	Sulfur oxides	c	c	c	c	c	c	c	c
3	Nitrogen oxides	c	c	c	c	c	c	c	c
4	Acid gases	7.47 E-02				7.11 E-02			
5	Alkaline gases	9.88 E-03				9.41 E-03			
6	Hydrocarbon gases	1.36 E-07				1.30 E-07			
7	Formaldehyde	1.34 E-05				1.28 E-05			
8	Volatile organochlorines	2.46 E-05	2.52 E-04			2.34 E-05	1.84 E-04		
9	Volatile carboxylic acids	7.64 E-06				7.27 E-06			
10	Volatile O & S heterocyclics	b	b	b	b	b	b	b	b
11	Volatile N heterocyclics	b	b	b	b	b	b	b	b
12	Benzene	1.27 E-04		5.75 E-07	1.28 E-06	1.21 E-04		4.21 E-07	1.22 E-06
13	Aliphatic/alicyclic hydrocarbons	4.80 E-05				4.57 E-05			
14	Mono- or diaromatic hydrocarbons	2.92 E-04	4.87 E-04	9.15 E-06	2.04 E-05	2.78 E-04	3.56 E-04	6.70 E-06	1.94 E-05
15	Polycyclic aromatic hydrocarbons	1.59 E-02		5.50 E-06	1.17 E-05	1.60 E-02		4.06 E-06	1.18 E-05
16	Aliphatic amines	b	b	b	b	b	b	b	b
17	Aromatic amines			3.02 E-02	6.72 E-02			2.21 E-02	6.40 E-02
18	Alkaline N heterocyclics	4.48 E-04				4.27 E-04			
19	Neutral N, O, S heterocyclics	b	b	b	b	b	b	b	b
20	Carboxylic acids	3.73 E-06				3.56 E-06			
21	Phenols	8.67 E-05	1.38 E-04	1.51 E-05	3.36 E-05	8.26 E-05	1.09 E-04	1.11 E-05	3.20 E-05
22	Aldehydes and ketones	1.46 E-02	1.44 E-02			1.39 E-02	1.05 E-02		
23	Nonheterocyclic organosulfur	b	b	b	b	b	b	b	b
24	Alcohols	b	b	b	b	b	b	b	b
25	Nitroaromatics	b	b	b	b	b	b	b	b
26	Esters	9.21 E-04	3.78 E-02	2.75 E-03	6.11 E-03	8.77 E-04	2.76 E-02	2.01 E-03	5.82 E-03
27	Amides	b	b	b	b	b	b	b	b
28	Nitriles	6.65 E-05	1.16 E-04			6.34 E-05	8.50 E-05		
29	Tars	d	d	d	d	d	d	d	d
30	Respirable particles	No aquatic emissions							
31	Arsenic	5.04 E-05	6.04 E-05	1.30 E-04	2.90 E-04	4.80 E-05	4.42 E-05	9.53 E-05	2.76 E-04
32	Mercury	2.80 E-02	1.31 E-00	3.78 E-03	8.40 E-03	2.67 E-02	9.61 E-01	2.76 E-03	8.00 E-03
33	Nickel	1.46 E-04	2.77 E-03	3.02 E-03	6.72 E-03	1.39 E-04	2.03 E-03	2.21 E-03	6.40 E-03
34	Cadmium	6.72 E-01	1.78 E-01	6.04 E-02	1.34 E-01	6.40 E-01	1.30 E-01	4.42 E-02	1.28 E-01
35	Lead	1.12 E-03	1.59 E-02	6.04 E-04	1.34 E-03	1.07 E-03	1.16 E-02	4.42 E-04	1.28 E-03
36	Other trace elements	2.92 E-04	2.67 E-06			2.78 E-04	1.96 E-06		

^aThe quotients are calculated using the lowest acute LC₅₀ or TL_m for fish in each RAC (Table A-1), the lowest chronic response by a fish (Table A-2), and the lowest algal response (Table A-3) with either the median or upper 95th percentile of the predicted ambient contaminant concentration at the eastern and western sites (Table 2.1-4).

^bNo toxicity data.

^cAquatic problems associated with pH, not direct toxicity.

^dNo aquatic emissions.

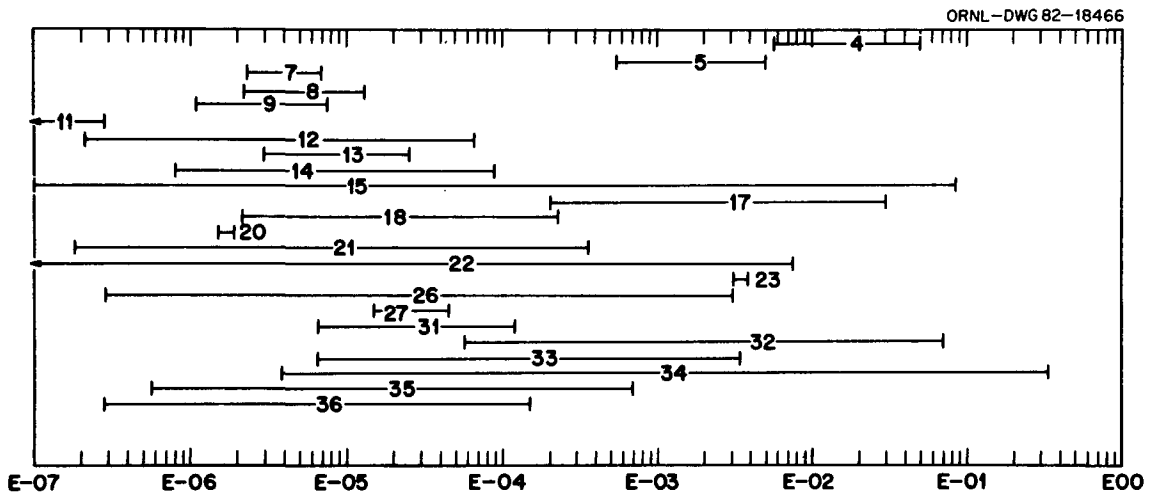


Fig. 3.1-1. RACs (Table 1.1) arranged according to their acute toxicities to fish, as determined by the quotient method using the unit release concentrations from the eastern site. The scale ranges from 1.0×10^{-7} (E-07) to 1.0 (E+00). The farther to the right an RAC appears in the figure, the greater its potential for adverse environmental effects.

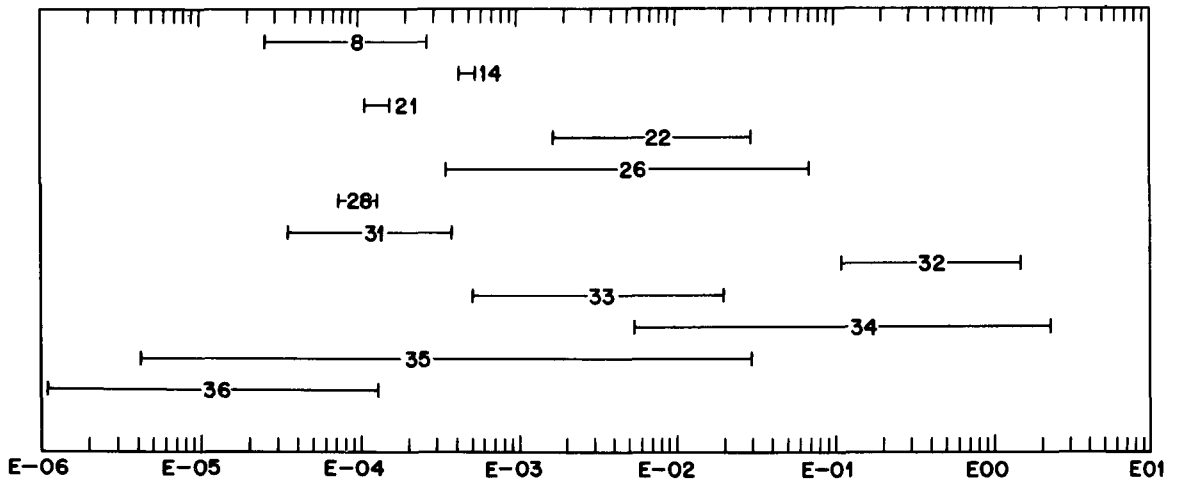


Fig. 3.1-2. RACs (Table 1.1) arranged according to their toxicities to freshwater algae, as determined by the quotient method using the annual median unit release concentrations from the eastern site. The scale ranges from 1.0×10^{-7} (E-07) to 1.0 (E+00). The farther to the right an RAC appears in the figure, the greater its potential for adverse environmental effects.

(RAC 34) exceeds 0.1 (E-01). These six (acid gases, polycyclic aromatic hydrocarbons, aldehydes and ketones, mercury, and cadmium), then, can be considered as most likely to harm fish and merit further risk analyses and research on their ecological effects. Conversely, RACs 7, 8, 9, 12-14, 18, 20, 21, 26, 31, 35, and 36 (Table 1.1) appear to represent the least threat to the freshwater fish. Only two RACs, aromatic amines (17) and cadmium (34), appear to pose a significant threat of algal toxicity.

The high ranking of RAC 15 may be due to the inclusion of data obtained using the trout embryo-larval acute assay, which appears to be considerably more sensitive than more commonly used tests for acute toxicity. If the other contaminants had been tested using this assay, their estimated toxicities would likely have been substantially higher.

Barnthouse et al. (1982) discussed the uncertainties involved in applying the quotient method to environmental data. One of the major inherent problems is that of comparing results from dissimilar tests. Although an attempt was made in this analysis to avoid such pitfalls by comparing, when possible, the same test species and benchmarks, uncontrolled variables inevitably remain. For example, in tests with certain metals (nickel, cadmium, and lead), water hardness is important in determining the concentrations of these metals that are required to elicit a toxic response (Table 3.1-1), a fact reflected in the USEPA criteria for each. Usually, the data are insufficient to compare quotients from tests using the same organisms in both soft and hard water. Also, in some instances, the analyst must compare quotients derived from tests using water of unspecified or inconsistent quality.

This exercise with the quotient method, in addition to suggesting which of the assigned RACs pose the greatest potential environmental threat, emphasizes the lack of toxicological research on algae as important components of the ecosystem and on synfuels-related organic compounds in general. Despite obvious weaknesses, the method does provide a useful means of screening data from a variety of sources.

3.2 ANALYSIS OF EXTRAPOLATION ERROR

This method of risk analysis is based on the fact that application of the results of laboratory toxicity tests to the field requires a series of extrapolations, each of which is made with some error (Barntouse et al. 1982). The products of the extrapolation are estimates of the centroid and distribution of the ambient concentration of a chemical at which a particular response will occur. The risk of occurrence of the prescribed response is equal to the probability that the response concentration is less than the ambient concentration given the probability distribution of each. In this section, we extrapolate from acute toxic concentrations for test species of fish to chronic responses of the reference commercial and game species characteristic of the eastern and western reference sites (Travis et al. 1983). The acute toxicity criterion is the 96-h LC_{50} . The chronic toxicity criterion is the life-cycle maximum allowable toxicant concentration (MATC), an interval bounded by the highest no-observed-effects concentration and the lowest concentration causing a statistically significant effect on growth, survival, or reproduction in a life-cycle toxicity test (Mount and Stephan 1969). The geometric mean of the bounds (GMATC) is used as a point estimate of the MATC as was done in calculating the national water quality criteria (USEPA 1980a-p).

3.2.1 Methods

A detailed description of the computational methods used for the analysis of extrapolation error (AEE) is contained in Suter and Vaughan (1954). Acute toxicity data from the Columbia National Fisheries Research Laboratory (Johnson and Finley 1980) were used for the extrapolation between species. Life-cycle toxicity data (Suter et al. 1983) were used to develop a regression relationship between acute toxicity data and chronic toxicity data. Variances associated with extrapolating acute toxicity between taxa and acute to chronic toxicity were accumulated to provide an estimate of the variability associated with the estimate of chronic toxicity, and used in obtaining estimates of risk when given estimates of the distribution of the ambient contaminant concentrations.

Twenty-one RACs have been analyzed by the extrapolation error method (Table 3.2-1). These are all of the RACs for which 96-h LC_{50} 's could be found. The ratio of the ambient concentration of an RAC to its predicted GMATC (PGMATC) is presented as an estimate of the hazard with respect to chronic toxicity. Risk, which is defined as the probability that the ambient contaminant concentration exceeds the GMATC, is also presented. Both the hazard and risk estimates are based on the annual average ambient concentrations (Table 2.1-4).

In general, the extrapolation between species was performed using the regression relationship between the tested and assessed fish at the same taxonomic level and having in common the next higher level. For example, if the fish are in the same family but different genera, the extrapolation would be made between genera. There were three instances when our hierarchical approach failed because of the limitation in the acute toxicity data for the contaminant. The only acute toxicity data available for hydrogen sulfide (RAC 4) and for fluoranthene (RAC 15) were for bluegill sunfish (Lepomis macrochirus); and the only acute toxicity data available for indan (RAC 13) and for quinoline (RAC 18) were for fathead minnow (Pimephales promelas). Difficulties arose with RACs 4 and 15 in estimating the acute toxicity of white bass (Morone chrysops) and with RACs 13 and 18 in estimating the acute toxicity of bigmouth and smallmouth buffalo (Ictiobus cyprinellus and I. bulbalus). The problem arose because no fish in the family Percichthyidae or in the genus Ictiobus were tested at the Columbia National Fisheries Research Laboratory. The genus Ictiobus falls within the family Catostomidae, which was tested at the Columbia National Fisheries Research Laboratory, but the Cyprinidae-Catostomidae relationship had insufficient sample size ($n = 1$). Hence, further statistical relationships were developed comparing bluegill sunfish to all Perciformes other than bluegills ($R^2 = 0.91$) and fathead minnow to all Cypriniformes other than fathead minnow ($R^2 = 0.92$).

Table 3.2-1. Ranges of ratios of ambient concentrations to PGMATC and probabilities of exceeding the PGMATC for unit release, eastern and western sites

RAC	Ratio of ambient concentration to PGMATC ^a		Probability of exceeding the PGMATC ^a	
	Eastern	Western	Eastern	Western
1	b	b	b	b
2	b	b	b	b
3	b	b	b	b
4	0.0261-0.1940	0.0839-0.0839	0.0468-0.2261	0.1117-0.1117
5	0.0069-0.0168	0.0144-0.0149	0.0097-0.0196	0.0090-0.0149
6	0.0000-0.0000	0.0000-0.0000	0.0000-0.0214	0.0002-0.0002
7	b	b	b	b
8	0.0002-0.0027	0.0004-0.0004	0.0000-0.0053	0.0001-0.0001
9	0.0003-0.0014	0.0009-0.0009	0.0000-0.0015	0.0008-0.0008
10	b	b	b	b
11	b	b	b	b
12	0.0007-0.0026	0.0018-0.0026	0.0001-0.0035	0.0002-0.0011
13	0.0011-0.0046	0.0032-0.0032	0.0002-0.0071	0.0046-0.0046
14	0.0021-0.0046	0.0034-0.0044	0.0008-0.0062	0.0008-0.0026
15	0.0016-0.0136	0.0030-0.0030	0.0004-0.0262	0.0021-0.0021
16	b	b	b	b
17	b	b	b	b
18	0.0005-0.0021	0.0014-0.0014	0.0000-0.0027	0.0015-0.0015
19	b	b	b	b
20	0.0000-0.0002	0.0002-0.0002	0.0000-0.0267	0.0016-0.0016
21	0.0007-0.0058	0.0011-0.0017	0.0000-0.0115	0.0001-0.0005
22	0.0238-0.1263	0.0507-0.0550	0.0266-0.1711	0.0538-0.0628
23	b	b	b	b
24	b	b	b	b
25	b	b	b	b
26	0.0011-0.0374	0.0015-0.0374	0.0007-0.0667	0.0002-0.0009
27	b	b	b	b
28	0.0008-0.0075	0.0014-0.0014	0.0001-0.0146	0.0006-0.0006
29	b	b	b	b
30	b	b	b	b
31	0.0006-0.0045	0.0008-0.0009	0.0000-0.0088	0.0000-0.0001
32	0.0088-0.0216	0.0184-0.0186	0.0130-0.0252	0.0132-0.0197
32A	0.0259-0.0675	0.0498-0.0948	0.0428-0.0853	0.0478-0.0964
33	0.0003-0.0115	0.0004-0.0008	0.0001-0.0225	0.0000-0.0001
34	0.0039-0.5739	0.7237-1.1682	0.0008-0.3908	0.4308-0.5332
35	0.0007-0.0056	0.0022-0.0036	0.0000-0.0091	0.0003-0.0009

^aSpecies-specific values are presented in Appendix D.

^bNo toxicity data.

3.2.2 Results

The species-specific values of the PGMATCs, quotients, and the risks of exceeding the GMATC for the annual median ambient contaminant concentrations are presented in Appendix D. The species-specific hazard and risk values are presented only for those RACs with a hazard greater than or equal to 0.01. They are summarized in Table 3.2-1. The RACs for which any of the nine eastern species had a nonzero hazard or risk are (in decreasing rank order): acid gases, mercury (methyl), aldehydes and ketones, cadmium, mercury (inorganic), alkaline gases, esters, polycyclic aromatic hydrocarbons, and nickel. The RACs for which either of the western species had a nonzero risk are (in decreasing rank order): cadmium, acid gases, mercury (methyl), aldehydes and ketones, mercury (inorganic), alkaline gases, polycyclic aromatic hydrocarbons, esters, and nickel. These rankings are based on the geometric mean across the nine eastern species or two western species of either the hazard quotients or the risk probabilities (the results were the same for hazard and risk). Cadmium, acid gases, and mercury (methyl) were each the most toxic RAC for at least one of the fish species.

The differences in the relative rankings between species is attributable to variation in three factors: (1) the magnitudes of the LC_{50} 's of different species that have been tested for a particular chemical, (2) differences in sensitivity that are expressed as biases in the extrapolation between the test species and site species, and (3) the variance associated with the extrapolation.

3.3 ECOSYSTEM UNCERTAINTY ANALYSIS

3.3.1 Explanation of Method

Ecosystem uncertainty analysis (EUA) estimates the risk associated with both direct and indirect effects of toxicants. It considers data on a variety of test organisms rather than emphasizing a single taxonomic group. By integrating effects across trophic levels, EUA considers components of environmental risk that are not included in other methods.

The method uses the Standard Water Column Model, (SWACOM) (O'Neill and Giddings 1979; O'Neill et al. 1982). SWACOM is an adaptation of an earlier model, CLEAN (Park et al. 1974), and considers ten phytoplankton, five zooplankton, three forage fish, and a game fish population. The model simulates the annual cycle of a lake and incorporates temperature, light, and nutrient responses. Changes can be made to tailor SWACOM for toxicological assessments in a variety of aquatic ecosystems. The model is designed to simulate a generalized water column and sacrifices site specificity to emphasize complex interactions and indirect effects.

Available toxicity data primarily concern mortality. Therefore, assumptions about the mode of action of the toxicant are required to determine appropriate changes in model parameters. We have assumed that organisms respond to all chemicals according to a general stress syndrome. For example, they increase respiration rates, decrease photosynthetic and grazing rates, and become more susceptible to predation. This assumption permits us to define percent changes in model parameters which result in the same mortality as measured in the laboratory. This extrapolation of laboratory data involves considerable uncertainty. In our analysis, the uncertainties are preserved by associating each parameter change with a probability distribution. In calculating risk, parameter values are selected from the distributions, and a simulation is performed with SWACOM. The process is repeated 500 times. The risk associated with an undesirable effect, such as a significant reduction in game fish, is estimated by the frequency of simulations that showed this effect. Further details of the method are given in Appendix E and in O'Neill et al. (1982).

The data used to implement the EUA are shown in Table 3.3-1. Estimates of risk can be made for nine RACs. These RACs were the only chemical groups for which adequate data seem to exist.

3.3.2 Results of Ecosystem Uncertainty Analysis

Results of the EUA are given in Table 3.3-2. Two endpoints were considered: a quadrupling of the peak biomass of noxious blue-green algae and a 25% decrease in game fish biomass. These endpoints were

Table 3.3-1. Values of LC₅₀/EC₅₀ (mg•L⁻¹) used to calculate E matrix for SWACOM (Appendix E)

Trophic level	Model Species	Benzene ^a	Naphthalene ^b	Quinoline ^c	Phenol ^d	Arsenic ^e	Nickel ^f	Cadmium ^g	Lead ^h	Mercury ⁱ
Algae	1-3	525.0	33.0	25.0	258.0	2.32	0.50	0.16	0.50	0.01
	4-7	525.0	33.0	25.0	20.0	2.32	0.50	0.06	0.50	0.01
	8-10	525.0	33.0	117.0	95.0	2.32	0.50	0.06	0.50	0.01
Zooplankton	11	450.0	8.6	57.2	300.0	4.47	9.67	0.5	40.8	0.78
	12	380.0	8.6	28.5	36.4	5.28	0.85	0.0099	0.45	0.005
	13	300.0	6.5	48.2	58.1	1.35	1.93	0.14	27.4	0.53
	14	233.8	4.5	39.3	157.0	2.49	4.91	0.25	14.0	0.27
	15	17.6	2.5	30.3	14.0	0.51	0.15	0.0035	0.67	0.01
Forage fish	16	33.0	6.6	1.5	36.0	15.6	4.87	0.63	4.61	0.15
	17	22.0	78.3	1.5	16.4	41.8	5.27	1.94	23.8	0.24
	18	34.0	150.0	1.5	34.9	26.0	4.45	1.63	31.5	0.50
Game fish	19	5.3	2.3	11.0	9.0	13.3	0.05	0.002	1.17	0.25

Values taken from the following water quality criteria documents:

^aEPA 440/5-80-018 (USEPA 1980c).

^bEPA 440/5-80-059 (USEPA 1980e).

^cO'Neill et al. (1982).

^dEPA 440/5-80-066 (USEPA 1980g).

^eEPA 440/5-80-021 (USEPA 1980i).

^fEPA 440/5-80-060 (USEPA 1980n).

^gEPA 440/5-80-025 (USEPA 1980o).

^hEPA 440/5-80-057 (USEPA 1980p).

ⁱEPA 440/5-80-058 (USEPA 1980m).

Table 3.3-2. Risks associated with nine risk assessment units, as estimated by ecosystem uncertainty analysis [Values based on the 95th percentile concentration for the eastern site ($6.72 \times 10^{-4} \text{ mg}\cdot\text{L}^{-1}$)]

RAC number	Chemical	Fourfold increase in Blue-green algae bloom	25% reduction in Game fish biomass
12	Benzene	0.088	0.038
14	Naphthalene	0.092	0.040
17	Quinoline	0.086	0.040
21	Phenol	0.086	0.038
31	Arsenic	0.088	0.040
32	Mercury	0.424	0.350
33	Nickel	0.178	0.054
34	Cadmium	0.544	0.972
35	Lead	0.110	0.042

chosen as indicative of minimal effects that could be detected in the field. Results are shown for the upper 95th percentile concentration for the eastern site, that is, the highest concentration of interest in the study. Because the estimated contaminant concentrations in the western river were similar to those in the eastern river, a separate analysis using the western scenario was not necessary.

None of the risk values is exactly zero, because there is a minimal risk of an increase in algae (0.086) or a decrease in fish (0.038) even though the environmental concentration of the toxicants is zero. This reflects residual uncertainty in simulating ecosystem behavior. For example, there is always some probability of a small decrease in fish due to environmental variability.

Considering this residual uncertainty, the risks calculated by EUA are very small for most of the chemicals. A unit release of phenol represents no risk over and above the uncertainty from environmental variability. The additional risks involved in a unit release of benzene, naphthalene, quinoline, and arsenic are also minimal.

The EUA does forecast significant risks for both endpoints associated with two of the RACs: cadmium and mercury. It also projects small risks associated with lead and nickel. The risk values associated with cadmium and mercury are high even at the minimal concentrations involved in the unit release calculations.

3.3.3 Patterns of Sensitivity Across Populations

No two species show identical sensitivities, and the way the sensitivities (i.e., LC_{50} 's) are distributed can influence the response of the ecosystem. For illustrative purposes, we concentrated on six of the chemicals in table 3.3-1, excluding nickel, benzene, and quinoline. The distribution of sensitivities in the table will be referred to as the "population" pattern. To remove differences among populations in the same trophic level, the standard approach would be to take the geometric mean of the LC_{50} 's. However, the data were not measured for the same period of time, and some of the values were EC_{50} 's and EC_{20} 's. We assumed a simple mortality process described by $x(t) = x(0) \exp(-d t)$, where $x(0)$ is the initial population size,

$x(t)$ is the size at time t , and d is the mortality rate. We assume that mortality is a function of concentration, $d = aC$. We know the fraction, $F_1 = x(t)/x(0)$, that survive at one concentration, C_1 , measured over one time period, t_1 . Since $(\ln F_1)/(C_1 t_1) = -a = (\ln F_2)/(C_2 t_2)$, we can then estimate the concentration, C_2 , that would result in a different fraction, F_2 , measured over a different time period, t_2 . By simple rearrangement we find

$$C_2 = (C_1 t_1 \ln F_2)/(t_2 \ln F_1) \quad (3)$$

Using Eq. (3), and taking geometric means, we arrive at an LC_{50} for each trophic level (Table 3.3-3). This distribution will be referred to as the "trophic" pattern. We apply this approach once again to arrive at a single LC_{50} value that removes even the trophic pattern. This value is shown in the last line of Table 3.3-3 and will be referred to as "no pattern."

The upper half of Table 3.3-4 shows the percent difference in annual biomass for each trophic level, comparing the trophic pattern to the no-pattern case. For phenol, the game fish is more sensitive than the no-pattern LC_{50} . The other trophic levels are relatively insensitive. Therefore, the toxicant reduces game fish and has little direct effect on the other organisms. However, because game fish are reduced, the forage fish experience less predation and show a slight increase. Because there are more forage fish, there are fewer zooplankton. Because there is less grazing, phytoplankton increases. As a result of trophic interactions, the zooplankton, which have the lowest sensitivity, have as great a decrease as the game fish. The same type of pattern is seen with cadmium; however, the game fish is now ten times more sensitive and the effect is magnified.

With naphthalene and mercury, the LC_{50} of the zooplankton is close to the no-pattern concentration. As a result, there are direct effects on both game fish and zooplankton. The forage fish, relatively insensitive to the toxicant, are also decreased because of reductions in their food supply.

Table 3.3-3. Trophic patterns in sensitivity. Values are geometric means of the values in Table 3.3-1, after those values were modified by means of Eq. (3) in the text. The last line in the table gives the geometric mean across trophic levels, once again modified by Eq. (3).

	Phenol	Naphthalene	Cadmium	Mercury	Arsenic	Lead
Phytoplankton	26	33	0.050	0.0084	2.3	0.5
Zooplankton	67	5.6	0.057	0.089	2.1	5.4
Forage fish	27	43	1.2	0.36	26.0	15.0
Game fish	9	2	0.002	0.25	13.0	1.2
No-pattern	18	4.7	0.025	0.054	2.6	1.0

Table 3.3-4. Comparison of responses to different patterns of sensitivity. The upper portion gives percent differences in average annual biomass, comparing the trophic pattern to the no-pattern case (Table 3.3-3). The lower portion compares the trophic pattern (Table 3.3-3) to the full population pattern (Table 3.3-1).

	Phenol	Naphthalene	Cadmium	Mercury	Arsenic	Lead
Trophic vs no pattern						
Phytoplankton	0.14	9.0	19.0	2.0	-0.02	0.36
Zooplankton	-1.0	-7.0	-19.0	-4.0	-1.0	-0.49
Forage fish	1.0	-2.0	25.0	-4.0	2.0	3.0
Game fish	-1.0	-6.0	-33.0	-0.47	5.0	6.0
Population vs trophic pattern						
Phytoplankton	6.0	6.0	1.0	11.0	1.0	10.0
Zooplankton	-6.0	-5.0	-6.0	-6.0	-1.0	-10.0
Forage fish	-8.0	-6.0	-4.0	-5.0	-4.0	-10.0
Game fish	-6.0	-5.0	-4.0	-3.0	-3.0	-10.0

The phytoplankton and zooplankton both show LC_{50} 's that are close to the no-pattern concentration for arsenic. Therefore, they are directly affected and their populations decrease. However, the reductions occur during the spring blooms. Because nutrients are not exhausted during this period, as they usually are, plankton survive during the remainder of the year. The result is a lower average size for the plankton, but higher plankton concentrations during the period of maximum growth of the fish populations. Therefore, fish show a slight increase in response to arsenic.

A similar phenomenon occurs with lead. Here the phytoplankton populations are the most sensitive. Therefore, their spring peak is decreased, cutting off the food supply to the zooplankton. The resulting decrease in the zooplankton permits the phytoplankton to increase slightly during the remainder of the year. The counter-intuitive result is that the most sensitive trophic level, phytoplankton, actually shows a slight increase in its annual average population size.

It is clear from Table 3.3-4 that the pattern of sensitivities across the trophic levels alters the response of the ecosystem. Our use of geometric means and Eq. (3) guarantees that all chemicals have exactly the same effect in the absence of pattern. Therefore, the percent differences truly reflect the effect of trophic pattern. In some cases (e.g., phenol), the effect of pattern is small, causing deviations from the no-pattern case of 1% or less. In other cases, (e.g., cadmium) the effects are large, causing differences as large as 33%. What is very clear is that ignoring the effect of trophic patterns can lead to significant errors.

The next step is to compare the trophic and population patterns (Table 3.3-4). The percent differences are shown in the lower portion of Table 3.3-4. The results show that a consistent bias is introduced by ignoring population patterns. For all chemicals, the average phytoplankton biomass is larger and the consumer trophic levels are always smaller.

One of the purposes of the unit release calculations was to rank the relative risk associated with the RACs. The rankings for the nine chemical groups according to EUA are given in Table 3.3-6. The table compares this ranking with the ranking resulting from normalized LC_{50} 's. These normalized values are calculated by adjusting all LC_{50} values used in SWACOM to the same endpoint (50% mortality in 7 d) and taking a geometric mean across populations and trophic levels. The method is explained in more detail in Appendix E. The normalized LC_{50} seems to be a reasonable estimator. This indicates that such a normalized value might be of use in determining the relative risks of different chemicals, especially when the toxicological data are insufficient to permit application of EUA.

3.3.4 Population Sensitivity Patterns and Risk

In a final set of studies, we examined the effect of population patterns on risk. We performed the analysis for phenol at a reasonable environmental concentration of 0.178 mg/L (Barntouse et al. 1982). The first three rows of Table 3.3-5 compare the three patterns. There are only small differences between the no-pattern and trophic cases. However, the bias in ignoring population patterns has a large effect: the risk of a blue-green algal bloom has doubled, and the risk of 25% reduction in game fish has almost tripled. The indications are that it is important to include the variability in sensitivity to a chemical within a trophic level. Ignoring this pattern would underestimate risk by a factor of ~ 2 .

Rows 4 and 5 in Table 3.3-5 compare the risk when all populations in a trophic level are set to the sensitivity of the most sensitive or least sensitive species. Setting all populations to the least sensitive species produces risks that are only slightly below the no-pattern case. Setting all populations to the most sensitive produces results only slightly higher than the population pattern. Synergistic effects can influence production as though all populations were as sensitive as the most sensitive species.

Table 3.3-5. Risk associated with a fourfold increase in noxious blue-green algae blooms and 25% reduction in average annual biomass of game fish. The table compares the risks, expressed as percentages, resulting from different simulation experiments described in the text.

	Fourfold increase in blue-green algae	25% reduction in game fish
No pattern	14.4	7.2
Trophic pattern	15.0	7.6
Standard pattern	34.8	20.6
All populations set at:		
Most sensitive	36.8	30.6
Least sensitive	10.2	6.4
Population sensitivities rearranged to:		
Least sensitive in spring	35.8	22.6
Most sensitive in spring	10.0	6.2

Table 3.3-6. Ranking of nine chemicals according to their calculated risk effect (Table 3.3-2) and their LC₅₀'s (EC₅₀'s) normalized across population and trophic levels

	Normalized LC ₅₀	Ranking of risk
Cadmium	0.025	1
Mercury	0.054	2
Lead	1.041	4
Nickel	1.250	3
Arsenic	2.616	6
Naphthalene	4.683	5
Quinoline	7.019	7
Phenol	17.800	9
Benzene	31.080	8

The final two cases use the population pattern, but within each trophic level, the sensitivities are temporally reassigned. In the first case, the most sensitive species occurs in the spring and the least sensitive in the summer. In the second case, the order is reversed. Rearranging the sensitivities causes approximately the same range of results as assigning all species to the lowest or highest sensitivities. The seasonal arrangement of sensitivities is about equal in importance to the actual magnitude of the sensitivities. This indicates once again the importance of population patterns of sensitivity.

3.3.5 Importance of Patterns of Sensitivity

The results indicate that synergistic effects are important. Toxic stress will interact with other constraints in the ecosystem, causing the greatest effect when natural environmental stress is greatest. Different responses during the year are likely to be related to those components of the system that are undergoing their greatest growth. It is particularly important to recognize that ignoring differences in sensitivities among populations can cause a significant bias.

Because the real benefit in applying EUA lies in its ability to detect higher-order effects, it is clear that EUA is most usefully applied when sufficient data exist to quantify the population type of pattern; i.e., multiple toxicity values should be available for each (or most) of the trophic levels. Without this information, many of the synergistic mechanisms in the ecosystem will not be represented, and higher-order effects predicted by the model may be strongly biased.

4. TERRESTRIAL ENDPOINTS

The quotient method, as discussed in Barnthouse et al. (1982), consists of deriving the quotients of ambient concentrations of toxicants divided by toxicological benchmark concentrations. It is used in this section to provide an indication of the inherent toxicities of the RACs. The other risk analysis methods are not readily applicable to terrestrial organisms because of the much smaller toxicological data base for effects of most RACs on forests, crops, and wildlife, the lack of standard tests and toxicological benchmarks in the existing data base, and even the lack of agreed-upon standard responses for terrestrial biota. Because meteorological differences between the sites do not change the ranking of the RACs, only results for the eastern site will be presented.

4.1 VEGETATION

The phytotoxicity data for the gaseous and volatile RACs are presented in Table B-1, the concentrations in ambient ground-level air are in Table 2.2-1, and the quotients of the ratios of these values are in Table 4.1-1. The ambient concentrations are the increment of the entire RAC to the background concentration at the point of maximum ground-level concentration (Sect. 2.2). It is assumed that the RAC is composed entirely of the representative chemical, and that the background concentration is zero. Quotients are calculated from two classes of data: (1) the lowest toxic concentration found in the literature for any flowering plant species as an indication of maximum toxic potential of the RAC, and (2) the range across studies of the lowest concentrations causing effects on growth or yield of the whole plant or some plant part. The latter set of responses is relatively consistent and closely related to crop and forest yields.

Of the 15 RACs for which data on toxicity in air were found, the worst atmospheric toxicant in the unit release is RAC 6 (hydrocarbon gases). This rank is biased, since the worst-case representative chemical (ethylene) is a plant hormone, whereas most members of this RAC are essentially inert (National Research Council 1976). However,

Table 4.1-1. Toxicity quotients for terrestrial plants. Ambient concentrations of RACs in air (annual, median, ground-level) and in soil (soil solution or whole dry soil) are divided by concentrations causing reductions in growth, yield, or other toxic responses^a

RAC	RAC Name	Phytotoxicity in air				Phytotoxicity in soil or soil solution			
		Ambient concentration/ lowest toxic concentration		Range of ambient concentration/ growth-effects concentration		Soil concentration/ lowest toxic concentration		Range of soil concentration/ growth-effects concentration	
		Eastern	Western	Eastern	Western	Eastern	Western	Eastern	Western
1	Carbon monoxide	3.65 E-02	5.18 E-02	5.97 E-06	8.48 E-06	b	b	b	b
2	Sulfur oxides	2.06 E-03	5.09 E-03	3.44 E-04-	8.49 E-04-	b	b	b	b
				1.03 E-03	2.55 E-03				
3	Nitrogen oxides	5.33 E-04	1.25 E-03	2.80 E-05-	6.58 E-05-	t	b	b	t
				5.33 E-04	1.25 E-03				
4	Acid gases	2.33 E-01	3.3 E-01	2.33 E-01	3.3 E-01	b	b	b	b
5	Alkaline gases	4.68 E-03	7.33 E-03			b	b	b	b
6	Hydrocarbon gases	5.51 E-01	7.67 E-01	2.65 E-02-	3.69 E-02-				
				9.26 E-02	1.29 E-01				
7	Formaldehyde	1.77 E-01	2.51 E-01						
8	Volatile organochlorines	2.52 E-04	3.57 E-04						
9	Volatile carboxylic acids					2.85 E-03	3.7 E-03	2.85 E-03	3.7 E-03
10	Volatile O & S heterocyclics	c	c	c	c	c	c	c	c
11	Volatile N-heterocyclics					5.38 E-03	7.42 E-03	5.38 E-03	7.42 E-03
12	Benzene	2.25 E-03	3.21 E-03						
13	Aliphatic/alicyclic hydrocarbons	2.34 E-11	2.63 E-11			1.77 E-03	1.98 E-03		
14	Mono/diaromatic hydrocarbons	3.14 E-04	4.40 E-04			6.85 E-05	9.55 E-05	6.85 E-05	9.55 E-05
15	Polycyclic aromatic hydrocarbons					6.33 E+02 ^d	8.76 E+02 ^d	1.95 E+02-	2.7 E+02-
								6.33 E+02 ^d	8.76 E+02 ^d
16	Aliphatic amines					1.89 E-01	2.54 E-01		
17	Aromatic amines	1.88 E-01	2.36 E-01						
18	Alkaline nitrogen heterocyclics	c	c	c	c	c	c	c	c
19	Neutral N, O, S heterocyclics					4.75 E-06	8.02 E-06	4.75 E-07-	8.02 E-07-
								4.75 E-06	8.02 E-06
20	Carboxylic acids					5.03 E-01 ^d	7.0 E-01 ^d	2.68 E-02-	3.72 E-02-
								5.03 E-01 ^d	7.0 E-01 ^d
21	Phenols					9.65 E-03	8.25 E-03		
22	Aldehydes and ketones	2.22 E-01	3.14 E-01			1.84 E-03	2.6 E-03	1.84 E-03	2.6 E-03
23	Nonheterocyclic organosulfur	1.87 E-02	2.44 E-02	1.03 E-01	1.34 E-01	1.44 E-04 ^d	1.86 E-04 ^d		
24	Alcohols					1.27 E-06	1.68 E-06		
25	Nitroaromatics	c	c	c	c	c	c	c	c
26	Esters	c	c	c	c	c	c	c	c
27	Amides					3.34 E-07 ^d	4.59 E-07 ^d	3.34 E-07 ^d	4.59 E-07 ^d
28	Nitriles	c	c	c	c	c	c	c	c
29	Tars	c	c	c	c	c	c	c	c
30	Respirable particles	c	c	c	c	c	c	c	c
31	Arsenic					5.23 E+02 ^d	6.03 E+02 ^d	2.45 E+01-	2.83 E+01-
								5.23 E+02 ^d	6.03 E+02 ^d
32	Mercury	3.36 E-02	5.84 E-02			5.36 E-03	4.05 E-03	4.92 E-05-	3.72 E-05-
								5.36 E-03	4.05 E-03
33	Nickel					3.16 E+01 ^d	3.42 E+01 ^d	3.74 E-02-	4.06 E-02-
								3.16 E+01 ^d	3.42 E+01 ^d
34	Cadmium					1.81 E+02	1.12 E+02	4.02 E+00-	2.48 E+00-
								1.81 E+02	1.12 E+02
35	Lead					1.1 E+00 ^d	1.5 E+02 ^d	9.87 E-03-	1.34 E-02-
								1.1 E+00 ^d	1.5 E+00 ^d

^aAmbient air concentrations, soil and soil solution concentrations are presented in Table 2.2-1. Toxic concentrations are presented in Appendix B.

^bNo accumulation in soil.

^cNo phytotoxicity data.

^dQuotients calculated from concentrations in soil and results of tests performed in soil. Quotients without superscript d were calculated from concentrations in soil solution and results of tests performed in nutrient solution.

since atmospheric ethylene has caused significant damage to crops near urban areas and in the vicinity of petrochemical plants (National Research Council 1976), the emission rate of this gas should be specifically considered in the future. The five most phytotoxic RACs in air (ignoring ethylene) are mercury (32), acid gases (4), aldehydes and ketones (22), aromatic amines (17), and formaldehyde (7). Although some phytotoxicity data were found for 15 RACs, data on growth-related effects are available for only 6 RACs. Of these six, acid gases and nonheterocyclic organosulfur were the highest ranking. These ranks result from differential dispersion as well as differential toxicity. In particular, the relatively low ranking of sulfur oxides and nitrogen oxides (RACs 2 and 3) is primarily due to their emission from the tall boiler stack rather than from the short stack, from cooling towers, or from area sources.

The phytotoxicity of materials deposited on the landscape is a more complex phenomenon than that of gases and vapors. Deposited nongaseous RACs were assumed to accumulate in the soil over the 35-year life of the liquefaction plant. Loss due to decomposition and leaching from this soil horizon was calculated by the terrestrial food chain model (Sect. 2.2).

The toxicity data (Table B-3) were primarily derived from exposure of plants or plant parts to solutions of the chemicals rather than contaminated soil because few data are available on toxicity in soil. While the results of tests conducted in soil can be directly compared to concentrations in whole soil, results of tests conducted in solution must be compared to a calculated concentration in soil solution. Because the concentration in soil solution is more difficult to model than concentration in whole soil and requires more simplifying assumptions, these numbers are less reliable. In addition, as with the gases and vapors, the toxicity data come from a wide variety of tests and measured responses that are not equivalent. Finally, for most of the RACs, only one or two chemicals have been tested. We cannot determine whether the chemicals used are representative of the entire RAC.

No data were found for the phytotoxicity in root exposures of RACs 6, 7, 8, 10, 12, 17, 18, 25, 26, and 28. Because the atmospheric transport model AIRDOS-EPA has a deposition velocity of zero for inorganic gases and does not model the formation of aerosols, it is assumed that RACs 1 through 5 do not accumulate in the soil. This assumption is likely to be acceptable except in the case of SO_4 deposition in forests with acid soils. The effects of SO_4 deposition in forests result from regional-scale emissions and atmospheric processes and are therefore well beyond the scope of this report. The most phytotoxic RACs deposited in soil are polycyclic aromatic hydrocarbons (RAC 15), cadmium (34), arsenic (31), nickel (33), and lead (35). The high rank of RAC 15 is suspect because benzo(a)pyrene and other polycyclic aromatic hydrocarbons (PAHs) appear to act as plant hormones, stimulating growth at low concentrations. Although PAHs can modify plant growth at concentrations as low as 0.5 ng/g soil, it does not appear likely that their presence in synfuel emissions would reduce plant yields. Thus, heavy metals appear to be the most serious phytotoxicants in soil, and methods for predicting their effects require attention.

4.2 WILDLIFE

Table 4.2-1 presents the lowest toxicity quotients for the two sites for terrestrial animals. The quotients were calculated from the lowest lethal concentration for any species and from the lowest concentration producing any toxic effect (Table B-3) divided by the highest annual median ground-level concentration in air derived from unit releases of all RACs (Sect. 2.2). Carcinogenesis and other genotoxic effects are not included. Data from all species are lumped because there were not enough data on the nonmammalian taxa for separate treatment. Data on the avian toxicity of industrial chemicals are virtually nonexistent. Yet the responses of birds are likely to be considerably different from those of mammals for the following reasons: (1) the complex respiratory systems of birds with both lungs and air sacs must modify the rate and pattern of deposition, (2) birds possess lower levels of mixed-function oxidases, epoxide hydrolases,

Table 4.2-1. Toxicity quotients for terrestrial animals. Annual median ground-level concentrations in air are divided by lethal concentrations and the lowest toxic concentrations.^a

RAC	RAC name	Lowest lethal concentration		Lowest toxic concentration	
		Eastern	Western	Eastern	Western
1	Carbon monoxide	7.14 E-08	1.01 E-07	1.53 E-03	2.17 E-03
2	Sulfur oxides	7.44 E-06	1.84 E-05	1.34 E-03	3.31 E-03
3	Nitrogen oxides	4.87 E-06	1.14 E-05	1.19 E-04	2.80 E-04
4	Acid gases	3.10 E-04	4.40 E-04	9.31 E-04	1.32 E-03
5	Alkaline gases	1.40 E-05	2.2 E-05	7.55 E-04	1.18 E-03
6	Hydrocarbon gases			1.71 E-07	2.38 E-07
7	Formaldehyde	7.67 E-05	1.09 E-04	1.21 E-02	1.72 E-01
8	Volatile organochlorines	4.67 E-04	6.62 E-04	1.33 E-03	1.89 E-03
9	Volatile carboxylic acids	3.19 E-07	5.36 E-07	2.97 E-05	5.01 E-05
10	Volatile O & S heterocyclics	2.22 E-06	3.16 E-06	2.22 E-06	3.16 E-06
11	Volatile N-heterocyclics	3.42 E-07	5.76 E-07	3.42 E-07	5.76 E-07
12	Benzene	3.55 E-04	5.07 E-04	3.55 E-04	5.07 E-04
13	Aliphatic/alicyclic hydrocarbons	2.85 E-07	3.21 E-07	1.87 E-05	2.11 E-05
14	Mono- or diaromatic hydrocarbons	3.93 E-05	5.52 E-05	7.47 E-04	1.05 E-03
15	Polycyclic aromatic hydrocarbons	b	b	b	b
16	Aliphatic amines	1.03 E-05	1.46 E-05	3.14 E-04	4.46 E-04
17	Aromatic amines	6.86 E-05	8.62 E-05	6.86 E-05	8.62 E-05
18	Alkaline N heterocyclics	b	b	b	b
19	Neutral N, O, S heterocyclics	b	b	b	b
20	Carboxylic acids	b	b	b	b
21	Phenols	b	b	b	b
22	Aldehydes and ketones	3.09 E-03	4.37 E-03	1.09 E-01	1.54 E-01
23	Nonheterocyclic organosulfur	3.36 E-04	4.39 E-04	5.04 E-03	6.59 E-03
24	Alcohols	4.79 E-05	6.82 E-05	8.31 E-04	1.18 E-03
25	Nitroaromatics	b	b	b	b
26	Esters	3.78 E-06	5.36 E-06	5.91 E-05	8.38 E-05
27	Amides	b	b	b	b
28	Nitriles	5.83 E-05	8.28 E-05	2.37 E-04	3.37 E-04
29	Tars	b	b	b	b
30	Respirable particles			1.43 E-01	2.04 E-01
31	Arsenic			1.74 E-01	2.93 E-01
32	Mercury			1.98 E-03	3.44 E-03
33	Nickel	2.0 E-04	2.84 E-04	2.0 E-04	2.84 E-04
34	Cadmium	8.38 E-04	1.41 E-03	4.19 E-01	7.06 E-01
35	Lead			8.16 E-03	1.42 E-02

^aAmbient air concentrations are presented in Table 2.2-1. Toxic concentrations are presented in Appendix B.

^bNo data on respiratory toxicity.

and glucuronyl transferases (detoxification enzymes) than mammals (Walker 1980); (3) birds are generally less protected by deposition of chemicals in air on vegetation and other surfaces; (4) both primary and secondary predation are more common among birds; and (5) oviparous reproduction by birds makes data on mammalian reproductive effects largely irrelevant. The data base is even smaller for reptiles, amphibians, and terrestrial invertebrates.

Lethality was considered because it is a consistent and frequently determined response that has clear population implications. The most lethal RACs in a unit release are (in decreasing rank order) aldehydes and ketones (RAC 22), cadmium (34), volatile organochlorines (8), lead (35), nonheterocyclic organosulfur (23), acid gases (4), nickel (33), and formaldehyde (7). Most of the lethality data is derived from laboratory rodents. The lowest toxic concentrations include a diversity of endpoints, most of which cannot be readily related to effects on wildlife populations but which occur at concentrations as low as a ten-thousandth of lethal concentrations. These responses range from increased airway resistance in 1-h exposures of guinea pigs to impaired lung and liver functions in human occupational exposures. The most toxic RACs by this sublethal criterion are cadmium (RAC 34), arsenic (31), respirable particles (30), formaldehyde (7), and aldehydes and ketones (22).

5. EVALUATION OF RISKS

5.1 EVALUATION OF RISKS TO FISH

Because the toxicological data base is larger for fish than for any other aquatic biota, a variety of comparisons were possible for this endpoint. The relative risks of the RACs were compared, using the quotient method, analysis of extrapolation error, and ecosystem uncertainty analysis. In addition, differences in sensitivity among fish species and differences in vulnerability of the fish communities in the eastern and western reference rivers were considered.

5.1.1 Differences Among RACs

Table 5.1-1 shows the ranking of 21 RACs for which risks could be estimated using both the quotient method (QM) and analysis of extrapolation error (AEE) for the eastern reference site. For QM, the RACs were ranked from highest to lowest based on either acute or chronic toxicity, whichever was highest (Table 3.1-1). To obtain rankings for AEE, geometric means of the risk estimates in Table 3.2-1 were calculated across species for each RAC. Although not identical, the two rankings are highly correlated. Three of the top five RACs are the same on both lists: acid gases (RAC 4), mercury (32), and cadmium (34). Esters (RAC 26) also ranked relatively high: fourth according to QM and sixth according to AEE.

Table 5.1-2 presents rankings according to QM, AEE, and ecosystem uncertainty analysis (EUA) for the nine RACs to which EUA could be applied. Again, the rankings are similar, especially for the highest RACs. Although the top four RACs according to EUA are heavy metals, many of the most toxic RACs could not be considered because of insufficient toxicological data. Given the good correlations among the three methods for those RACs that could be examined using EUA, it is conceivable that, had sufficient data been available for acid gases and esters, significant risks of reductions in fish populations would have been obtained from EUA.

Table 5.1-1. Rankings of Risk Analysis Categories (RACs), according to the quotient method (QM) and analysis of extrapolation error (AEE), in order of decreasing risk to fish

Rank	RAU (representative compound)	
	QM	AEE ^a
1	32 (mercury)	4 (acid gases)
2	34 (cadmium)	34 (cadmium)
3	4 (acid gases)	22 (aldehydes and ketones)
4	26 (esters)	32 (mercury)
5	35 (lead)	5 (alkaline gases)
6	15 (polycyclic aromatic hydrocarbons)	26 (esters)
7	22 (aldehydes and ketones)	14 (mono- or diaromatics)
8	5 (alkaline gases)	15 (polycyclic aromatic hydrocarbons)
9	33 (nickel)	13 (aliphatic/alicyclic hydrocarbons)
10	14 (mono- or diaromatics)	35 (lead)
11	18 (alkaline N-heterocyclics)	12 (benzene)
12	8 (volatile organochlorines)	28 (nitriles)
13	21 (phenols)	18 (alkaline N-heterocyclics) ^b
14	12 (benzene)	21 (phenols) ^b
15	28 (nitriles)	33 (nickel)
16	21 (arsenic)	31 (arsenic)
17	13 (aliphatic/alicyclic hydrocarbons)	9 (volatile carboxylic acids)
18	7 (formaldehyde)	8 (volatile organochlorines)
19	9 (volatile carboxylic acids)	20 (carboxylic acids)
20	20 (carboxylic acids)	6 (hydrocarbon gases)
21	6 (hydrocarbon gases)	

^aFormaldehyde (RAC 7) could not be evaluated by AEE, since only 24-h LC₅₀'s were available.

^bTied RACs.

Table 5.1-2. Rankings of nine Risk Analysis Categories (RACs), according to the quotient method (QM), analysis of extrapolation error (AEE), and ecosystem uncertainty analysis (EUA), in order of decreasing risk to fish

Rank	RAU (representative compound)		
	QM	AEE	EUA
1	32 (mercury)	34 (cadmium)	34 (cadmium)
2	34 (cadmium)	32 (mercury)	32 (mercury)
3	35 (lead)	14 (mono- or diaromatics)	33 (nickel)
4	33 (nickel)	35 (lead)	35 (lead)
5	14 (mono- or diaromatics)	12 (benzene)	14 (mono- or diaromatics) ^a
6	18 (alkaline N heterocyclics)	18 (alkaline N heterocyclics) ^a	31 (arsenic) ^a
7	21 (phenols)	21 (phenols)	18 (alkaline N heterocyclics) ^a
8	12 (benzene)	33 (nickel)	12 (benzene) ^b
9	31 (arsenic)	31 (arsenic)	21 (phenols) ^b

^aTied observations.

^bTied observations.

5.1.2 Differences in Sensitivity Among Fish Species

Table D-1 shows that there are substantial differences among fish species with respect to sensitivity to the various RACs. Several species, notably the black crappie, rainbow trout, and brook trout, appear to be unusually sensitive to a wide range of toxic chemicals, based on current information. The carp and buffalo appear unusually insensitive. For most contaminants, PGMATCs for different fish species range over two orders of magnitude. Table 3.2-1 demonstrates the importance of considering the uncertainty associated with estimates of PGMATCs or other toxicological benchmarks. Estimated PGMATCs for nearly all species-RAC combinations are 10 or more times higher than the estimated ambient contaminant concentrations. Nonetheless, there are five RACs for which there is a 5% or greater risk that the ambient concentration in the eastern river may exceed the PGMATC for one or more species. For the western river, four RACs have a 5% or greater risk of exceeding one or more PGMATCs.

The model experiments described in Sects. 3.3.3 and 3.3.4 show that differences in sensitivity among ecologically similar populations can markedly increase or decrease the ultimate effects of a given contaminant concentration. It was found, for the particular parameterization of the Standard Water Column Model used in this analysis, that the responses of the model ecosystem assuming a range of sensitivities to contaminants for the populations within each trophic level were similar to the responses obtained when all populations were assumed to be as sensitive as the most sensitive species (Table 3.3-5). Although different model parameters might produce different results, it is clear that uncertainty about the relative sensitivities of different populations introduces substantial uncertainties into estimates of risks of higher-order ecological effects.

5.1.3 Differences in Risk Between Sites

Under the scenarios used in the unit release analysis, there are few differences in the ecological risks of the various RACs between the eastern and western sites. There are significant between-site differences in half-life for many of the RACs (Table 2.1-5) due to

differences in sediment load, depth, and current velocity. However, in the near field, dilution is the primary determinant of contaminant concentration, and stream flows in the two rivers are similar.

AEE shows, however, that there are differences in potential ecological risks to fish, due to differences in the sensitivities of the fish species in the two rivers. The two trout species in the western river are relatively sensitive to cadmium compared to the species in the eastern river. In addition, they are among the most sensitive species to several other highly toxic contaminants, notably methylmercury and hydrogen sulfide (Table 3.2-1).

5.2 EVALUATION OF RISKS OF ALGAL BLOOMS

Fewer conclusions are possible for algae than for fish, in part because of the relative scarcity of data on the effects of synfuels-derived contaminants on algae. Equally important, however, is the lack of standardization of test systems for algae. The test results summarized in Table 3.1-3 reflect more than a dozen combinations of toxicological responses and test durations. Consequently, QM could not be used to develop a meaningful ranking of the RACs. For the same reasons, interspecies differences in sensitivity and intersite differences in vulnerability could not be considered.

Although the use of EUA analysis to determine effects on phytoplankton was also limited because of insufficient data, the problem of test incomparability was partly remedied through use of the microcosm simulations (Appendix E) and normalization procedures (Sect. 3.3.3). These procedures made possible approximate comparisons between results of tests performed using different toxicological endpoints.

Estimates of the risks of fourfold increases in algal biomass resulting from unit releases of nine RACs are presented in Table 3.3-2. The results for algae are similar to those obtained for fish in that the same four RACs produced the greatest risks to both fish and algae. This similarity cannot be explained on the basis of the relative toxicity of the nine RACs to algae. The RACs most toxic to algae (viz., cadmium, mercury, lead, and nickel) produced the greatest

increases in algal biomass. The explanation for this observed counterintuitive response is that these highly toxic chemicals produce reductions in grazing intensity (due to decreased zooplankton abundance) that more than offset the toxic effects of the contaminants on algae.

5.2.1 Comparison of Uncertainties Concerning Exposure Concentrations and Effects Concentrations

A revealing comparison is possible between the magnitudes of uncertainty concerning (1) the expected environmental concentrations of contaminants in the vicinity of a synfuels plant and (2) the predicted-effects thresholds for fish. The distributions of estimated contaminant concentration in Table 2.1-4 are approximately lognormal. The variances of the corresponding log-transformed normal distributions range from 0.21 (anthracene, eastern site) to 0.42 (all contaminants, western site). These variances are 10 to 100 times lower than the error variances associated with the log-transformed PGMATCs described in Sect. 3.2.

Because the exposure analyses included only uncertainty about the values of environmental parameters, the results undoubtedly underestimate the true uncertainty for contaminant concentrations. Although we cannot directly estimate the effects on contaminant concentrations of uncertainties for volatilization, biological degradation, complexation, hydrolysis, or other removal processes, we can indirectly estimate the magnitude of uncertainty for the total removal rate that would be necessary to produce an uncertainty concerning steady-state contaminant concentrations equivalent to the calculated uncertainty of PGMATCs.

The total removal rate cannot be smaller than zero. Therefore, the 95% concentrations for the "dilution only" cases in Table 2.1-4 can be reasonably assumed to be upper bounds on contaminant concentrations no matter how high or low the contaminant removal rates are. Using the eastern reference river as an example, the upper 95% limit on contaminant concentrations for a release rate of $4.12 \text{ E-}02 \text{ g/s}$ is $6.7 \text{ E-}07 \text{ g/L}$. A lognormal distribution of concentrations with a

log-transformed variance of 3.7 (the median value of variances of log-transformed PGMATCs for the 120 taxon-RAC combinations used in this report) and an upper bound fixed by dilution would have a median of 2.7 E-08 g/L and a lower 5% concentration of 1.2 E-09 g/L. The removal rate needed to produce a steady-state concentration this low can be calculated by rearranging Eq. (2-17) of Travis et al. (1983) to obtain

$$k_t = \frac{I - QC}{VC}, \quad (4)$$

where

- k_t = combined first-order rate for all removal processes (L/s),
- I = contaminant release rate (kg/s),
- Q = stream flow rate (m³/s),
- V = reach volume (m³),
- C = contaminant concentration (kg/m³).

The lowest contaminant concentrations are expected to occur when stream flows, and consequently reach volume are high; therefore, for this example, we use the upper 95% values of Q (251 m³/s) and V (9.2 E+05 m³). Substituting these values, the contaminant release rate (4.12 E -05 kg/s), and the above contaminant concentration into Eq. (4), we calculate that a total removal rate constant of 3.7 E -02/s is required to produce a steady-state concentration of 1.2 E -09 g/L. This rate constant corresponds to a contaminant half-life of 18.7 s.

Thus, a range of uncertainty for contaminant half-lives of from ~20 s to infinity would result in near-field exposure concentrations for the eastern reference river that are as uncertain as the PGMATCs estimated in Sect. 3.2. Note that the shortest half-lives calculated for the unit release risk analysis (Table 2.1-5) are ~100 h. Uncertainty of the required magnitude would be possible only in the case of extremely reactive contaminants whose environmental chemistry is essentially unknown. It seems safe to conclude that, for the majority of contaminants of interest in synfuels risk analyses, uncertainty concerning toxicological effects is far greater than is uncertainty concerning near-field environmental concentrations.

5.3 EVALUATION OF RISKS TO VEGETATION AND WILDLIFE

The primary purpose of this analysis is to examine the availability of information on the toxicity of the full set of RACs to terrestrial plants and animals. Not surprisingly, more information was found on respiratory toxicity to animals than on phytotoxicity. Respiratory toxicity data was found for all but eight RACs in existing published data compilations (Table B-3). The untested RACs are high-molecular-weight organics to which livestock and wildlife are unlikely to be exposed in significant quantities. The animal toxicity data set, however, is complete only for mammals. In addition, dietary toxicity was not considered for lack of appropriate toxicity data and exposure models for that route of exposure. Recognizing these limitations, the most serious threat to wildlife from unit releases would be posed by aldehydes and ketones (RAC 22), cadmium (34), arsenic (31), and respirable particles (30) (Table 4.2-1).

Information concerning phytotoxicity of gaseous RACs is relatively abundant for crop species (Table B-1). Data on effects on plant growth are available for all of the gaseous RACs except ammonia, which is more likely to act as a fertilizer than as a toxicant. Of the gaseous RACs, acid gases (primarily H_2S) are the greatest threat to plant production in the unit release analysis. The low quotients for SO_x and NO_x are due to emission from a tall stack, so these RACs would contribute an increment to regional problems with combustion gases. The lack of data on responses of plants to atmospheric concentrations of most heavy metals and organic chemicals is a reflection of their low concentrations in air, even in heavily polluted areas.

All but nine of the nongaseous RACs have been tested for their effects on plants exposed in soil or in hydroponic solution. Because of the extreme variability of the physical, biological, and chemical properties of soils, the uncertainties in modeling the availability of chemicals in soil to plant roots, and the dependence of the soil model on deposition rates from the atmospheric dispersion model, the exposure assessment for plant roots is undoubtedly the most uncertain in this ecological risk analysis. In addition, the validity of tests conducted in solution culture as predictors of responses in field soils is

uncertain. Our analysis indicates that the worst soil phytotoxicants are arsenic (RAC 31), cadmium (34), and nickel (33). The actual toxicities will be highly dependent on soil chemistry including the background concentration of metals.

5.4 VALIDATION NEEDS

There are no uniquely correct methods of quantifying ecological risks. There are several plausible ways to combine uncertainties for differential sensitivities of fish taxa and acute-chronic relationships. There are also many aquatic ecosystem models. Different models produce different estimates of uncertainty and risk. Validation studies of the methods used in these risk analyses would greatly increase the credibility of the results.

There are two ways in which these synfuels risk analyses can be validated. A specific validation would involve building a synfuels industry and monitoring the resulting environmental effects. A generic validation would involve checking the assumptions and models used in the risk analyses against the results of field and laboratory studies. Given the current state of the synfuels industry, a generic validation seems more practical.

Generic validation of the environmental risk analysis methods would begin with an examination of the ability of existing published evidence to support or refute the models or their component assumptions. To a certain extent, this has been done by us as a part of our methods development (e.g., Suter et al. 1983; Suter and Vaughan, in press) and by others for generally used models such as the Gaussian-plume atmospheric dispersion model. However, there has been no systematic consideration of such major assumptions as the validity of hydroponic phytotoxicity studies nor of the risk analysis methodology as a whole. The results of validation studies would not only indicate the level of confidence that can be placed in environmental risk analyses, but also would indicate what research is necessary for further development and validation of risk analysis methods.

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APPENDIX A
Aquatic Toxicity Data

Table A-1. Acute toxicity of synfuels chemicals to aquatic animals

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^c	Reference
1	Carbon monoxide					No toxicity data	
2	Sulfur oxides					Aquatic problems associated with pH, not direct toxicity	
3	Nitrogen oxides					Aquatic problems associated with pH, not direct toxicity	
4	H ₂ S	Scud (<u>Gammarus pseudotimmaeus</u>)	LC ₅₀	96	0.022		Oseid and Smith 1974
		Bluegill (adults)	TL _m	96	0.0448	Flow-through test	Smith et al. 1976
		(juveniles)	TL _m	96	0.0478	Flow-through test	Smith et al. 1976
		(fry, 35-d-old)	TL _m	96	0.0131	Flow-through test	Smith et al. 1976
		(eggs)	TL _m	72	0.0190	Flow-through test	Smith et al. 1976
		Northern pike (eggs)	TL _m	96	0.034-0.037	DO = 2-6 ppm	Adelman and Smith 1970
		(fry)	TL _m	96	0.009-0.026	DO = 2-6 ppm	Adelman and Smith 1970
5	Ammonia	Rainbow trout (fry, 85-d-old)	TL _m	24	0.068		Rice and Stokes 1975
		(adults)	TL _m	24	0.097		Rice and Stokes 1975
		Rainbow trout	LC ₅₀	24	0.50		Herbert and Shurben 1963
		Rainbow trout	LC ₅₀	24	0.47		Lloyd and Orr 1969
		Rainbow trout (fry)	LC ₅₀	24	0.2		EIFAC 1970
		(fingerlings)	LC ₅₀	24	0.2		EIFAC 1970
6	Heptane	Mosquitofish	TL _m	96	4924		Wallen et al. 1957
7	Formaldehyde	Several fish species	LC ₅₀	24	50-120		National Research Council 1981

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^c	Reference
8	Carbon tetrachloride	<i>Daphnia magna</i>	LC ₅₀	48	35.2	Flow-through test	US EPA 1980a
		Fathead minnow	LC ₅₀	96	43.1		US EPA 1980a
		Bluegill	LC ₅₀	96	27.3		US EPA 1980a
		Bluegill	LC ₅₀	96	125.0		US EPA 1980a
	Chloroform	<i>D. magna</i>	LC ₅₀	48	28.9	US EPA 1980b	
		Bluegill	LC ₅₀	96	100.0	US EPA 1980b	
		Bluegill	LC ₅₀	96	115.0	US EPA 1980b	
		Rainbow trout	LC ₅₀	96	43.8	US EPA 1980b	
9	Acetic acid	Fathead minnow	LC ₅₀	96	88.0		Mattson et al. 1976
		Mosquitofish	TL _m	96	251.0		Wallam et al. 1957
10	Volatile O- and S-heterocyclics					No toxicity data	
11	Pyridine	Ciliate (<i>Tetrahymena pyriformis</i>)	LC ₅₀	72	1211.8	50% growth inhibition	Schultz et al. 1980
		<i>D. magna</i>	LC ₅₀	48	1165		Canton and Adema 1978
		<i>D. magna</i>	LC ₅₀	48	1755		Canton and Adema 1978
12	Benzene	<i>D. magna</i>	LC ₅₀	48	203.0-620.0	Flow-through test	US EPA 1980c
		<i>D. magna</i>	LC ₅₀	48	426.0		Canton and Adema 1978
		Fathead minnow	LC ₅₀	96	32.0		US EPA 1980c
		Fathead minnow	LC ₃₀	96	15.1		DeGraeve et al. 1982
		Mosquitofish	LC ₅₀	96	1300.0		Wallam et al. 1957
		Rainbow trout	LC ₅₀	96	5.3		US EPA 1980c
13	Cyclohexane	Fathead minnow	LC ₅₀	96	93.0	Flow-through test	Mattson et al. 1976
		Fathead minnow	TL _m	96	30.0		Pickering and Henderson 1966a
		Fathead minnow	TL _m	96	32.0		Pickering and Henderson 1966a
		Bluegill	TL _m	96	31.0		Pickering and Henderson 1966a
	Indan	Fathead minnow	LC ₅₀	96	14.0	Mattson et al. 1976	

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^c	Reference
14	Toluene	<u>D. magna</u>	LC ₅₀	48	39.22	2 tests	Millemann, et al. 1984 Pickering and Henderson 1966a Pickering and Henderson 1966a Pickering and Henderson, 1966a US EPA 1980d
		Fathead minnow	TL _m	96	44.0		
		Fathead minnow	TL _m	96	45.0		
		Bluegill	TL _m	96	24.0		
	Naphthalene	Bluegill	LC ₅₀	96	12.7		
		<u>D. magna</u>	LC ₅₀	48	2.16		
		<u>D. magna</u>	LC ₅₀	48	8.57		
		Fathead minnow	LC ₅₀	48	3.14		
		Fathead minnow	LC ₅₀	96	4.90-8.90		
	Xylene	Rainbow trout	LC ₅₀	96	2.30		
Fathead minnow		TL _m	96	42.0	Mattson et al. 1976		
	Goldfish	TL _m	96	17.0	Brenniman et al. 1976		
	Anthracene					Not toxic to fish, even in super-saturated solutions	McKee and Wolf 1963
15	Phenanthrene	<u>D. magna</u>	LC ₅₀	48	0.75	Milleman et al. 1984 Parkhurst 1981 Birge and Black 1981	
		<u>D. magna</u>	LC ₅₀	48	1.10		
		Rainbow trout (embryo-larva)	LC ₅₀	96	0.04		
	Fluoranthene	<u>D. magna</u>	LC ₅₀	48	325.0		US EPA 1980f
Bluegill		LC ₅₀	96	3.9	US EPA 1980f		
16	Aliphatic amines					No toxicity data	
17	Aniline	<u>D. magna</u>	LC ₅₀	48	0.65	Canton and Adema 1978 Canton and Adema 1978 Millemann et al. 1984 Millemann et al. 1984	
		<u>Daphnia cucullata</u>	LC ₅₀	48	0.68		
	3,5-Dimethylaniline	<u>D. magna</u>	LC ₅₀	48	0.58		
		<u>D. magna</u>	LC ₅₀	48	1.29		

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^c	Reference
18	Quinoline	Ciliate (<u><i>T. pyriforma</i></u>)	LC ₅₀	72	125.7	50% growth inhibition	Schultz et al. 1980
		<u><i>D. magna</i></u>	LC ₅₀	48	30.28		Millemann et al. 1984
		Fathead minnow	LC ₅₀	48	1.50		Millemann et al. 1984
		Fathead minnow	LC ₅₀	96	46.0		Mattson et al. 1976
	2-Methylquinoline	Ciliate (<u><i>T. pyriforma</i></u>)	EC ₅₀	72	48.7	50% growth inhibition	Schultz et al. 1980
	2,6-Dimethylquinoline	Ciliate (<u><i>T. pyriforma</i></u>)	EC ₅₀	72	33.0	50% growth inhibition	Schultz et al. 1980
19	Neutral N-,O-,S-heterocyclics					No toxicity data	
20	Benzoic acid	Mosquitofish	TL _m	96	180		Wallam et al. 1957
21	Phenol	<u><i>D. magna</i></u>	LC ₅₀	48	19.79	4 tests	Millemann et al. 1984
		<u><i>D. magna</i></u>	LC ₅₀		9.6		US EPA 1980g
		<u><i>D. magna</i></u> (Young)	TL _m	50	7.0		Dowden and Bennett 1965
		Copepod (<u><i>Mesocyclops leukarti</i></u>)	LC ₅₀		108.0		US EPA 1980g
		Fathead minnow	LC ₅₀	48	25.6		Millemann et al. 1984
		Fathead minnow	LC ₅₀	96	24.0-67.5		US EPA 1980g
		Bluegill	LC ₅₀		11.5-23.9	6 tests	US EPA 1980g
		Rainbow trout	LC ₅₀		8.9-11.6	2 flow-through tests	US EPA 1980g
	2-Methylphenol	<u><i>D. magna</i></u>	LC ₅₀	48	9.2	Soft water	US EPA 1980g
		<u><i>D. magna</i></u>	LC ₅₀	48	23.5		US EPA 1980g
Fathead minnow		TL _m	96	12.55	Pickering and Henderson 1966a		
Fathead minnow		TL _m	96	13.42	Hard water		Pickering and Henderson 1966a
	Bluegill	TL _m	96	20.78	Soft water	Pickering and Henderson 1966a	
4-Methylphenol	Fathead minnow	TL _m	96	19.0		Mattson et al. 1976	

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^c	Reference
	Mixed cresol isomers	Aquatic life	TL _m	96	1.0-10.0		Kingsbury et al. 1979
	2,4-Dimethylphenol	<u>D. magna</u>	LC ₅₀	48	2.12		US EPA 1980h
		Fathead minnow (juvenile)	LC ₅₀	96	16.75	Flow-through test	US EPA 1980h
		Bluegill	LC ₅₀	96	7.75		US EPA 1980h
	3,4-Dimethylphenol	Fathead minnow	LC ₅₀	96	14.0		Mattson et al. 1976
	2,5-Dimethylphenol	<u>D. magna</u>	LC ₅₀	48	0.96		Millemann et al. 1984
22	Acrolein	<u>D. magna</u>	LC ₅₀	48	0.057		US EPA 1980i
		<u>D. magna</u>	LC ₅₀	48	0.080		US EPA 1980i
		Mosquitofish	LC ₅₀	48	0.061		National Research Council 1981
		Bluegill	LC ₅₀	96	0.100		US EPA 1980i
		Bluegill	LC ₅₀	96	0.090		US EPA 1980i
		Brown trout	LC ₅₀	24	0.046		National Research Council 1981
		Rainbow trout	LC ₅₀	24	0.065		National Research Council 1981
		Largemouth bass	LC ₅₀	96	0.160		US EPA 1980i
		Bluegill	LC ₅₀	96	53.0		National Research Council 1981
		Acetaldehyde					
	Acetone	<u>D. magna</u>	LC ₅₀	48	12,600		
23	Nonheterocyclic organosulfur					No toxicity data	
24	Alcohols					No toxicity data	
25	Nitroaromatics					No toxicity data	
26	Di-2-ethylhexyl phthalate	<u>D. magna</u>	LC ₅₀		11.1		US EPA 1980j

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^c	Reference
	Diethyl phthalate	<i>D. magna</i>	LC ₅₀		52.1		US EPA 1980j
		Bluegill	LC ₅₀		98.2		US EPA 1980j
	Butylbenzyl phthalate	<i>D. magna</i>	LC ₅₀		92.3		US EPA 1980j
		<i>D. magna</i>	LC ₅₀	48	3.7		Gledhill et al. 1980
		Fathead minnow	LC ₅₀	96	5.3	Hardness: 160	Gledhill et al. 1980
		Fathead minnow	LC ₅₀	96	2.1	Hardness: 40	Gledhill et al. 1980
		Bluegill	LC ₅₀		43.3		US EPA 1980j
		Bluegill	LC ₅₀	96	1.7		Gledhill et al. 1980
		Rainbow trout	LC ₅₀	96	3.3		Gledhill et al. 1980
	Di-n-butyl phthalate	Scud (<i>G. pseudo-limnaeus</i>)	LC ₅₀	96	2.1		Mayer and Sanders 1973
		Fathead minnow	LC ₅₀	96	1.3		Mayer and Sanders 1973
		Bluegill	LC ₅₀	96	0.73		Mayer and Sanders 1973
		Rainbow trout	LC ₅₀	96	6.47		Mayer and Sanders 1973
27	Amides					No toxicity data	
28	Acrylonitrile	<i>D. magna</i>	LC ₅₀		7.55		US EPA 1980k
		Fathead minnow	LC ₅₀	96	14.3		US EPA 1980k
		Fathead minnow	LC ₅₀	96	18.1		US EPA 1980k
		Fathead minnow	LC ₅₀	96	10.1	Flow-through test	US EPA 1980k
		Bluegill	LC ₅₀	96	11.8		US EPA 1980k
		Bluegill	LC ₅₀		10.1		US EPA 1980k
29	Tars					No aquatic emissions	
30	Respirable particles					No aquatic emissions	
31	Arsenic	<i>D. magna</i>	TL _m	48	7.4		Hohreiter 1980
		<i>D. magna</i>	EC ₅₀	48	5.28	Immobilization	Anderson 1946
		<i>Daphnia pulex</i>	EC ₅₀	48	1.04	Immobilization	Sanders and Cope 1966
		Stonefly (<i>Pteronarcys californica</i>)	LC ₅₀	96	22.04		Sanders and Cope 1968
		Fathead minnow (juvenile)	LC ₅₀	96	15.66	Flow-through test	Cardwell et al. 1976
		Bluegill (juvenile)	LC ₅₀	96	41.76	Flow-through test	Cardwell et al. 1976
		Bluegill	LC ₅₀		15.37		US EPA 1980l
		Rainbow trout	LC ₅₀		13.34		US EPA 1980l
		Brook trout	LC ₅₀	93	14.96	Flow-through test	Cardwell et al. 1976

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^c	Reference
32	Mercury (inorganic)	<u>D. magna</u>	LC ₅₀	48	0.005		Biesinger and Christensen 1972
		<u>Stonefly (Acroneuria lycorius)</u>	TL _m	96	2.0		Warnick and Bell 1969
		Fathead minnow	LC ₅₀		0.19		US EPA 1980m
		Rainbow trout	LC ₅₀		0.31		Hohreiter 1980
		Coho salmon	LC ₅₀		0.24		US EPA 1980m
		Rainbow trout (juvenile)	LC ₅₀		0.155-0.4	4 tests	US EPA 1980m
	Methylmercury	Rainbow trout	LC ₅₀		0.03		Hohreiter 1980
		Rainbow trout (sac fry)	LC ₅₀	96	0.024		Hohreiter 1980
		(fingerling)	LC ₅₀	96	0.042		Hohreiter 1980
		(Juvenile)	LC ₅₀		0.025		US EPA 1980m
		Brook trout (juvenile)	LC ₅₀	96	0.084	Flow-through test	McKim et al. 1976
		(yearling)	LC ₅₀	96	0.065	Flow-through test	McKim et al. 1976
33	Nickel	<u>D. magna</u>	LC ₅₀		1.81	Hardness: 51	US EPA 1980n
		<u>D. magna</u>	LC ₅₀		2.34	Hardness: 100	US EPA 1980n
		<u>Mayfly (Ephemerella subvaria)</u>	TL _m	96	4.0	Hardness: 42	Warnick and Bell 1969
		<u>Stonefly (A. lycorius)</u>	TL _m	96	33.5	Hardness: 40	Warnick and Bell 1969
		Damselfly (unidentified)	TL _m	96	21.2	Hardness: 50	Rehwooldt et al. 1973
		Midge (Chironomus sp.)	TL _m	96	8.6	Hardness: 50	Rehwooldt et al. 1973
		Caddisfly (unidentified)	TL _m	96	30.2	Hardness: 50	Rehwooldt et al. 1973
		Fathead minnow	LC ₅₀		4.58-5.18	Hardness: 20 2 flow-through tests	US EPA 1980n
		Fathead minnow	TL _m	96	25.0	Hardness: 210 flow-through test	Pickering 1974
		Bluegill	TL _m	96	5.18-5.36	Hardness: 20 2 tests	Pickering and Henderson 1966b
		Bluegill	TL _m	96	39.6	Hardness: 360	Pickering and

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ⁱ	Duration (h)	Concentration (mg/L)	Notes ^j	Reference
		Rainbow trout	LC ₅₀	96	35.5	Flow-through test	Henderson 1966b
		Fish sp., general	LC ₅₀	96	4.6-9.8	Soft water	Hale 1977
		Fish sp., general	LC ₅₀	96	39.2-42.4	Hard water	Hohreiter 1980
34	Cadmium	<i>D. magna</i>	LC ₅₀		0.0099	Hardness: 51	US EPA 1980o
		<i>D. magna</i>	LC ₅₀		0.033	Hardness: 104	US EPA 1980o
		<i>D. magna</i>	LC ₅₀		0.049	Hardness: 209	US EPA 1980o
		Mayfly (<i>Ephemereilla grandis grandis</i>)	TL _m	96	28.0		Clubb et al. 1975
		Mayfly (<i>E. subvaria</i>)	TL _m	96	2.0	Hardness: 54	Warnick and Bell 1969
		Stonefly (<i>Pteronarcella badia</i>)	TL _m	96	18.0		Clubb et al. 1975
		Damselfly (unidentified)	TL _m	96	8.1	Hardness: 50	Rehwooldt et al. 1973
		Midge (unidentified)	TL _m	96	1.2	Hardness: 50	Rehwooldt et al. 1973
		(Chironomus) Caddisfly (unidentified)	TL _m	96	3.4	Hardness: 50	Rehwooldt et al. 1973
		Fathead minnow	TL _m	96	0.630	Hardness: 20	Pickering and Henderson 1966b
		Fathead minnow	TL _m	96	72.6	Hardness: 360	Pickering and Henderson 1966b
		Bluegill	TL _m	96	1.94	Hardness: 20	Pickering and Henderson 1966b
		Bluegill	LC ₅₀		21.1	Hardness: 207	US EPA 1980o
		Rainbow trout (swim-up and parr)	LC ₅₀	96	0.001-0.00175	Hardness: 23	US EPA 1980o
		Rainbow trout	LC ₅₀	96	0.00175	2 flow-through tests	
						Hardness: 31; flow-through test	US EPA 1980o
		Carp	LC ₅₀		0.24	Hardness: 55	US EPA 1980o
		Chinook salmon (Parr)	LC ₅₀		0.0035	Hardness: 23	US EPA 1980o
		Brook trout	LC ₅₀		0.0024	Hardness: 44 (sodium sulfate)	US EPA 1980o
		Green sunfish	LC ₅₀		2.84	Hardness: 20	US EPA 1980o
		Pumpkinseed	LC ₅₀		1.5	Hardness: 55	US EPA 1980o

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ^f	Duration (h)	Concentration (mg/L)	Notes ^g	Reference
35	Lead	<u>D. magna</u>	LC ₅₀		0.612	Hardness: 54	US EPA 1980p
		<u>D. magna</u>	LC ₅₀		0.952	Hardness: 110	US EPA 1980p
		Fathead minnow	LC ₅₀	96	2.4	Hardness: 20	US EPA 1980p
		Fathead minnow	TL _m	96	482.0	Hardness: 360	Pickering and Henderson 1966b
		Bluegill	TL _m	96	23.8	Hardness: 20	Pickering and Henderson 1966b
		Bluegill	TL _m	96	442.0	Hardness: 360	Pickering and Henderson 1966b
		Rainbow trout (fry)	LC ₅₀	96	0.6		Hohreiter 1980
		Rainbow trout	LC ₅₀	96	1.17	Hardness: 32; flow-through test	Davies et al. 1976
		Rainbow trout	LC ₅₀	96	1.0		Hohreiter 1980
		Rainbow trout	LC ₅₀	96	8.0		US EPA 1980p
	Brook trout	LC ₅₀	96	4.1	Hardness: 44	US EPA 1980p	
36	Fluorine	<u>D. magna</u>		48	270.0	"Toxic threshold"	Hohreiter 1980
		<u>Goldfish</u>		96	120.0	100% kill	Hohreiter 1980
		Goldfish		12-29	1000.0	100% kill in soft water	Hohreiter 1980
		Goldfish		60-102	1000.0	100% kill in hard water	Hohreiter 1980
		Rainbow trout	TL _m	240	2.3-7.5	TL _m varies with temperature	Angelovic et al. 1961

^aLatin binomials are listed in Appendix C.

^bLC₅₀ = concentration required to kill 50% of test organisms.

TL_m = median tolerance limit.

EC₂₀ = effective concentration causing a designated effect on 20% of test organisms.

^cHardness values are given in milligrams per liter as CaCO₃. DO = dissolved oxygen.

Table A-2. Chronic toxicity of synfuels chemicals to aquatic animals

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (d)	Concentration (mg/L)	Notes ^c	Reference
8	Carbon tetrachloride Chloroform	Fathead minnow	Embryo-larval		3.4		US EPA 1980a
		Rainbow trout	Embryo-larval	27	1.2	Hardness: 200	US EPA 1980b
		Rainbow trout	Embryo-larval	27	2.0	Hardness: 50	US EPA 1980b
		Rainbow trout	Embryo	23	10.6	40% teratogenesis	US EPA 1980b
12	Benzene	<u>Daphnia magna</u>	Life cycle		98.0		US EPA 1980c
14	Naphthalene	Fathead minnow	Embryo-larval		0.62		US EPA 1980e
		Fathead minnow	Embryo-larval		2.56		US EPA 1980g
		Fathead minnow	Embryo-larval		2.191		US EPA 1980h
21	Phenol 2,4-Dimethylphenol	Fathead minnow	Embryo-larval		2.56		US EPA 1980g
		Fathead minnow	Embryo-larval		2.191		US EPA 1980h
		Fathead minnow	Embryo-larval		2.475		US EPA 1980h
22	Acrolein	<u>D. magna</u>	Life cycle		0.024		US EPA 1980i
		<u>D. magna</u>	Life cycle		0.034	Survival reduced after 64 days	National Research Council 1981
		Fathead minnow	Life cycle		0.021		US EPA 1980i
26	Di-2-ethylhexyl phthalate Butylbenzyl phthalate	<u>D. magna</u>	Life cycle		0.003		US EPA 1980j
		Rainbow trout	Embryo-larval		0.008		US EPA 1980j
		<u>D. magna</u>	Life cycle		0.44		US EPA 1980j
		Fathead minnow	Embryo-larval		0.22		US EPA 1980j
28	Acrylonitrile	<u>D. magna</u>	Life cycle		3.6		US EPA 1980k
		Fathead minnow	LC ₅₀	30	2.6		US EPA 1980k
31	Arsenic	<u>D. magna</u>	Life cycle		0.912		US EPA 1980l
		<u>D. magna</u>	TL _m	21	2.85		Hohreiter 1980
		Bass sp., general		10	7.60	Toxic	Hohreiter 1980
		Pink salmon		10	5.00	Lethal	Hohreiter 1980
32	Mercuric chloride Methylmercuric chloride	<u>D. magna</u>	Life cycle		0.001 - 0.0025	4 tests	US EPA 1980m
		<u>D. magna</u>	Life cycle		0.001		US EPA 1980m
		Fathead minnow Brook trout	Life cycle		0.00023 0.00052	92% dead, 3 months	Hohreiter 1980 US EPA 1980m

Table A-2. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (d)	Concentration (mg/L)	Notes ^c	Reference
33	Nickel	<u>D. magna</u>	Life cycle		0.015	Hardness: 51	US EPA 1980n
		<u>D. magna</u>	Life cycle		0.123	Hardness: 105	US EPA 1980n
		Caddisfly (<u>Clistoronia magnifica</u>)	Life cycle		0.465	Hardness: 50	US EPA 1980n
		Fathead minnow	Embryo-larval		0.109	Hardness: 44	US EPA 1980n
		Fathead minnow	Life cycle		0.527	Hardness: 210	US EPA 1980n
		Rainbow trout	Embryo-larval		0.350	Hardness: 50	US EPA 1980n
34	Cadmium	<u>D. magna</u>	Life cycle		0.00015	Hardness: 53	US EPA 1980o
		<u>D. magna</u>	Life cycle		0.00021	Hardness: 103	US EPA 1980o
		<u>D. magna</u>	Life cycle		0.00044	Hardness: 209	US EPA 1980o
		Midge (<u>Tanytarsus dissimilis</u>)			0.0031		US EPA 1980o
		Fathead minnow	Life cycle		0.046	Hardness: 201	US EPA 1980o
		Bluegill	Life cycle		0.050	Hardness: 207	US EPA 1980o
		Brook trout	Embryo-larval		0.0017	Hardness: 36	US EPA 1980o
		Brook trout	Embryo-larval		0.0092	Hardness: 187	US EPA 1980o
		35	Lead	<u>D. magna</u>	Life cycle		0.012
<u>D. magna</u>	Life cycle				0.128	Hardness: 151	US EPA 1980p
Stonefly (<u>Acroneuria lycorias</u>)	LC50			14	64.0		Hohreiter 1980
Mayfly (<u>Ephemera subvaria</u>)	LC50			7	16.0		Hohreiter 1980
Caddisfly (<u>Hydropsyche betteri</u>)	LC50			7	32.0		Hohreiter 1980
Bluegill	Embryo-larval				0.092	Hardness: 41	US EPA 1980p
Rainbow trout	Embryo-larval				0.019	Hardness: 28	US EPA 1980p
Rainbow trout	Embryo-larval				0.102	Hardness: 35	US EPA 1980p
36	Fluorine			Rainbow trout		21	113.0
		Rainbow trout		21	250.0	100% kill, Hardness: 320, yearling trout	Hohreiter 1980

^aLatin binomials are listed in Appendix C.

^bLC₅₀ = concentration required to kill 50% of test organisms.
TL_m = median tolerance limit.

^cHardness values are given in milligrams per liter as CaCO₃.

Table A-3. Toxicity of synfuels chemicals to algae

RAC	Representative chemical(s)	Test organism	Test type ^a	Duration (h)	Concentration (mg/L)	Notes	Reference
12	Benzene	<u>Chlorella vulgaris</u>	EC ₅₀	48	525.0	Reduction in cell numbers	US EPA 1980c
14	Toluene	<u>C. vulgaris</u>	EC ₅₀	24	245.0	Reduction in cell numbers	US EPA 1980d
		<u>Selenastrum capricornutum</u>	EC ₅₀	96	433.0	Reduction in cell numbers and chlorophyll a production	US EPA 1980d
	Naphthalene	<u>C. vulgaris</u>	EC ₅₀	48	33.0	Reduction in extrapolated cell numbers	US EPA 1980e
		<u>Chlamydomonas angulosa</u>	EC ₆₁	24	34.4	61% mortality of cells	US EPA 1980e
15	Fluoranthene	<u>S. capricornutum</u>	EC ₅₀	96	54.4	Reduction in cell numbers	US EPA 1980f
		<u>S. capricornutum</u>	EC ₅₀	96	54.6	Reduction in chlorophyll a production	US EPA 1980f
17	Aniline	<u>Agmenellum quadruplicatum</u>			0.010	Diffusion from disk onto algal lawn inhibited growth for 3-7 d	Batterton et al. 1978
	P-Toluidene	<u>A. quadruplicatum</u> <u>Coccochloris elabens</u> <u>Eucapsis sp.</u> <u>Oscillatoria williamsii</u>			0.010 0.010 0.010	Diffusion from disk onto algal lawn inhibited growth for 3-7 d	Batterton et al. 1978
21	Phenol	<u>S. capricornutum</u>			20.0	Growth inhibition of 12-66% depending on time (2-3 d) and temperature (20, 24, 28°C)	US EPA 1980g
		<u>S. capricornutum</u>	EC ₅₀	24	40.0	Reduction in cell numbers	US EPA 1980g
		<u>Nitzschia linearis</u>	EC ₅₀	120	258.0	Reduction in cell numbers	US EPA 1980g
		<u>Chlorella pyrenoidosa</u>	EC ₁₀₀	48	1500.0	Complete destruction of chlorophyll	US EPA 1980g
		<u>C. vulgaris</u> <u>C. pyrenoidosa</u>	EC ₂₀ EC ₁₀₀	80 48	470.0 500.0	Growth inhibition Complete destruction of chlorophyll	US EPA 1980g US EPA 1980g
	2,4-Dimethylphenol						

Table A-3. (continued)

RAC	Representative chemical(s)	Test organism	Test type ^a	Duration (h)	Concentration (mg/L)	Notes	Reference
26	Butylbenzyl phthalate	<u>S. capricornutum</u>	EC50	96	0.11	Reduction in chlorophyll a	US EPA 1980j
		<u>S. capricornutum</u>	EC50	96	0.13	Reduction in cell numbers	US EPA 1980j
		<u>Microcystis aeruginosa</u>	EC50	96	1000.0	Reduction in cell numbers	US EPA 1980j
		<u>Navicula pelliculosa</u>	EC50	96	0.60	Reduction in cell numbers	US EPA 1980j
	Dimethyl phthalate	<u>S. capricornutum</u>	EC50	96	42.7	Reduction in chlorophyll a	US EPA 1980j
		<u>S. capricornutum</u>	EC50	96	39.8	Reduction in cell numbers	US EPA 1980j
	Diethyl phthalate	<u>S. capricornutum</u>	EC50	96	90.3	Reduction in chlorophyll a	US EPA 1980j
		<u>S. capricornutum</u>	EC50	96	85.6	Reduction in cell numbers	US EPA 1980j
31	Arsenic	<u>Cladophora</u> , <u>Spirogyra</u> ,	EC100	336	2.32	100% kill	US EPA 1980i
		<u>Zygnema sp.</u>					
		<u>Scenedesmus sp.</u>		96	20.0	Threshold effects	Cushman et al. 1977
32	Mercuric chloride	<u>C. vulgaris</u>	EC50	768	1.03	Cell division inhibition	US EPA 1980m
		Spring diatom assemblages	EC50	2	0.08	Reduction in photosynthetic activity	US EPA 1980m
	Methylmercuric chloride	<u>Coelastrum microporum</u>	EC50		2.4-4.8	Growth inhibition	US EPA 1980m
33	Nickel	<u>Chlamydomonas</u> ,			0.1-0.7	Growth reduced in all cultures in water with 50 mg/L CaCO ₃	US EPA 1980n
		<u>Chlorella</u> ,					
		<u>Haematococcus</u> ,					
	<u>Scenedesmus sp.</u>	EC16	336	0.5-10.0	Growth inhibition	Cushman et al. 1977	
	<u>Phormidium ambiguum</u>			1.5	Threshold effects	Cushman et al. 1977	
34	Cadmium	<u>Scenedesmus sp.</u>			0.0061	Reduction in cell numbers	US EPA 1980o
		<u>Scenedesmus sp.</u>			0.05-0.5	Growth inhibition	Cushman et al. 1977
		<u>C. pyrenoidosa</u>			0.25	Growth inhibition	US EPA 1980o
		<u>C. vulgaris</u>	EC50		0.06	Growth reduction	US EPA 1980o
		<u>S. capricornutum</u>			0.05	Growth reduction	US EPA 1980o
		Mixed species			0.005	Population reduction	US EPA 1980o

Table A-3. (continued)

RAC	Representative chemical(s)	Test organism	Test type ^a	Duration (h)	Concentration (mg/L)	Notes	Reference
35	Lead	<u>Ankistrodesmus</u> sp.	EC ₂₄		1.00	Growth inhibition	US EPA 1980p
		<u>Chlorella</u> sp.	EC ₅₃		0.50	Growth inhibition	US EPA 1980p
		<u>Scenedesmus</u> sp.	EC ₃₅		0.50	Growth inhibition	US EPA 1980p
		<u>Selenastrum</u> sp.	EC ₅₂		0.50	Growth inhibition	US EPA 1980p
		<u>Anabaena</u> sp.	EC ₅₀	24	15.0-26.0	Reduction in CO ₂ fixation	US EPA 1980p
		<u>Chlamydomonas</u> sp.	EC ₅₀	24	17.0	Reduction in CO ₂ fixation	US EPA 1980p
		<u>Cosmarium</u> sp.	EC ₅₀	24	5.0	Reduction in CO ₂ fixation	US EPA 1980p
		<u>Navicula</u> sp.	EC ₅₀	24	17.0-28.0	Reduction in CO ₂ fixation	US EPA 1980p
		<u>Scenedesmus</u> sp.			2.5	Threshold effects	Cushman et al. 1977

^aEC_n = concentration causing a designated effect on a given percentage of test organisms.

APPENDIX B
Terrestrial Toxicity Data

Table B-1. Toxicity of chemicals in air to vascular plants.

RAC	Representative chemical	Test organism ^a	Response ^b	Exposure		Notes ^{b,c}	Reference	
				Duration (h)	Concentration ($\mu\text{g}/\text{m}^3$)			
1	Carbon monoxide	Grapefruit	-CO ₂ uptake		1.8 E+03	Detached leaves	National Research Council 1977a	
		Red clover	-20% N fixation		1.1 E+05			National Research Council 1977a
		Several species	-Growth	552	1.1 E+07			National Research Council 1977a
		Popinac	Defoliation	24	2.3 E+07			National Research Council 1977a
2	Sulfur dioxide	Barley	-44% yield	72/week	3.9 E+02	Field, growing season	US EPA 1982	
		Durum wheat	-42% yield	72/week	3.9 E+02	Field, growing season	US EPA 1982	
		Alfalfa	-26% foliage	100	1.3 E+02	5 h/d, 5 d/weeks, 4 weeks	US EPA 1982	
		Tobacco, Bel W3	-22% foliage	100	1.3 E+02	5 h/d, 5 d/weeks, 4 weeks	US EPA 1982	
		Cocksfoot	-40% total weight	2070	1.78 E+02	103.5 h/weeks,	US EPA 1982	
		Broadbean	Reduced net photosynthesis	8	9.2 E+01	20 weeks	US EPA 1982	
		White pine	Needle damage threshold	6	6.5 E+01	Sensitive clone	US EPA 1982	
		Norway spruce	-25% volume growth	1680	1.3 E+02		US EPA 1982	
3	Nitrogen dioxide	Wheat	-12% straw yield	334	2 E+03		Zahn 1975	
		Bush bean	-27% yield	639	2 E+03		Zahn 1975	
		Spruce	-7% linear growth	1900	2-3 E+03	-17% linear growth in following year	Zahn 1975	
		Endive	-37% yield	620	2 E+03		Zahn 1975	
		Carrot	-30% yield	357	4 E+03		Zahn 1975	
		Tobacco, bean, tomato, radish, oat, soybean	Visible foliar injury	4	3.8 E+03		Heck and Tingey 1979	
		Cocksfoot and meadow grass	-Yield	2070	2.1 E+02	103.5 h/week, 20 week	Ashenden and Mansfield 1978	
4	Hydrogen sulfide	Green bean	-20% photosynthesis	3	7.0 E+02		Taylor in press	
		Green bean	-25% yield	64	2.8 E+02	4 h/d, 4 d/week for 4 week	Taylor in press	
		Alfalfa	-39% yield	672-840	4.2 E+02	Continuous fumigation	Thompson and Kats 1978	
		Lettuce	-66% yield	2112	4.2 E+02	Continuous fumigation	Thompson and Kats 1978	
		Douglas fir	-weight and linear growth	5904	4.2 E+02	Continuous fumigation	Thompson and Kats 1978	
		Sugar beets	-38% sugar +43% sugar	3216 3216	4.2 E+02 4.2 E+01	Continuous fumigation	Thompson and Kats 1978 Thompson and Kats 1978	

Table B-1. (continued)

RAC	Representative chemical	Test organism ^a	Response ^b	Exposure		Notes ^{b,c}	Reference
				Duration (h)	Concentration ($\mu\text{g}/\text{m}^3$)		
5	Ammonia	Mustard	Injury	4	2.1 E+03		National Research Council 1979b
6	Ethylene	African marigold	Epinasty	20	1.15 E+00		National Air Pollution Control Administration 1970
		Carnation	Flowers do not open	72	1.15 E+02		National Air Pollution Control Administration 1970
		Cotton	Growth inhibition	720	6.85 E+02		National Air Pollution Control Administration 1970
		Lily family	Growth inhibition	168	8.60 E+02		National Air Pollution Control Administration 1970
		Various plants	Growth inhibition	240	2.39 E+03		National Air Pollution Control Administration 1970
7	Formaldehyde	Alfalfa	Injury	5	4.9 E+02		National Research Council, 1981
		Petunia	Necrosis and leaf symptoms	48	2.47 E+02		Kingsbury et al. 1979
8	Vinyl chloride	Cowpea, cotton, squash	Injury	168	2.6 E+05		Heck and Pires 1962
12	Benzene	Pinto bean	Red-bordered spots	0.6	3.0 E+04		Kingsbury et al. 1979
13	Cyclohexene	Runner bean	LD ₅₀ , toxicity to leaves	1	1.12 E+12		Ivens, 1952
14	Toluene	Pinto bean	Bronze color	0.6	1.88 E+05		Kingsbury et al. 1979
17	Aniline	Loblolly pine	Damage	3	2.7 E+02		Cheeseman and Perry 1977
22	Acrolein	Alfalfa	Oxidant-type damage	9	2.5 E+02		Kingsbury et al. 1979
23	Carbonyl sulfide	Runner bean	LD ₅₀ , toxicity to leaves	1	2.7 E+03		Ivens 1952
		Green bean	-13% growth	64	4.9 E+02	4 h/d, 4 d/week for 4 weeks	Taylor, in press

Table B-1. (continued)

RAC	Representative chemical	Test organism ^a	Response ^b	Exposure		Notes ^{b,c}	Reference
				Duration (h)	Concentration ($\mu\text{g}/\text{m}^3$)		
32	Mercury (metallic)	Rose	Severe damage		1.0 E+01		Stahl 1969
		Sugar beet	Damage	5	2.8 E+02		Waldron and Terry 1975
		English ivy	Damage	12	1.5 E+04		Waldron and Terry 1975
	Mercuric chloride	Coleus, Thevetia and Ricinus	Abscission	168	1.0 E+01		Siegel and Siegel 1979
		Thevetia and Ricinus	Necrosis	168	1.0 E+01		Siegel and Siegel 1979
Dimethylmercury	Coleus, Thevetia and Ricinus	Abscission	36	1.0 E+01		Siegel and Siegel 1979	

^aLatin binomials are listed in Appendix C.

^bMinus sign designates a reduction in the measured response.

^cUnless "field" is noted, results are for laboratory studies.

Table B-2. Toxicity of chemicals in soil or solution to vascular plants.

RAC	Representative chemical	Test organism ^a and life stage	Test medium	Response	Duration	Concentration (µg/g)	Reference
9	Acetic acid	Barley (seedling)	Solution in sand	Root growth inhibition	5 d	600	Lynch 1977
11	Methyl pyridine	Alfalfa (sprout)	Solution	Root growth inhibition	4 d	93.1	Naik et al. 1972
13	Hexene	Oat (seedling)	Solution	Mortality		25.2	Chen and Eloffson 1978
14	Xylene	Sugar beet (seedling)	Solution	Root growth inhibition	2 d	100	Allen et al. 1961
15	Benzo(a)pyrene	Corn (sprout)	Solution	Root growth stimulation	6 h	0.0005	Deubert et al. 1979
	3,4-benzopyrene	Tobacco (seedling)	Soil	78% growth stimulation	60 d	0.01	Gräf and Nowak 1966
	1,2-benzanthracene	Tobacco (seedling)	Soil	80% growth stimulation	60 d	0.02	Gräf and Nowak 1966
	1,2,5,6-di-benzanthracene	Tobacco (seedling)	Soil	130% growth stimulation	60 d	0.02	Gräf and Nowak 1966
16	Dimethylalkylamine	Gram, rice	Solution	Mortality		7.0	Dutta et al. 1972
19	Benzothiophene	Cucumber (sprout)	Solution	9% root growth inhibition	4 d	10	Schlesinger and Mowry 1951
	Indole, 3-ethyl-1H	Oat, cress, mustard (sprout)	Solution	Growth inhibition		100	Davies et al. 1937
	Indole-3-acetic acid-1H	Oat, cress, mustard (sprout)	Solution	Growth inhibition		100	Davies et al. 1937
		Cucumber	Solution	Mortality	11 d	35	Hilton and Nomura 1964
		Pea (sprout)	Solution	Germination reduced by 50%	8 h	10	Shukla 1972

Table B-2. (continued)

RAC	Representative chemical	Test organisms and life stage	Test medium	Response	Duration	Concentration (µg/g)	Reference
20	Benzoic acid	Lettuce (seedling)	Solution on filter paper	23% growth inhibition		25	Chou and Patrick 1976
	2-hydroxy-benzoic acid	Rice (seedling)	Soil	Seedling growth inhibition	5 d	1.6	Gaur and Pareek 1976
		Lettuce (seedling)	Solution on filter paper	61% growth inhibition		25	Chou and Patrick 1976
21	Phenol	Durum wheat (seed)	Solution	Germination inhibition	4 d	2000	Badilescu et al. 1967
22	4-hydroxy-benzaldehyde	Lettuce (seedling)	Solution on filter paper	26% growth inhibition		100	Chou and Patrick 1976
23	Carbon disulfide	Apple	Soil	Root injury		420	Underhill and Cox 1940
24	Ethanol	Lettuce (seed)	Solution	Germination inhibition	44 h	1,000,000	Meyer and Mayer 1971
27	<u>N,N</u> -dimethyl-Formamide	Lettuce (seed)	Solution	Nearly total suppression of germination	24 h	1,000,000	Meyer and Mayer 1971
	2-methyl-benzamide	Poppy, chickweed, carrot, ryegrass corn, lucerne (mature)	Soil	13-87% reduction in yield	3-5 w	220,000	Pizey and Wain 1959
31	Arsenic ^b	Corn (seedling)	Soil	10% growth reduction (wet tissue weight)	4 w	64	Woolson, et al. 1971
		Cotton (mature)	Soil (fine sandy loam)	Approx. 55% reduction in yield	6 w	8°C	Deuel and Swoboda 1972
		Cotton (mature)	Soil (clay)	Approx. 40% reduction in yield	6 w	28°C	Deuel and Swoboda 1972

Table B-2. (continued)

RAC	Representative chemical	Test organism ^a and life stage	Test medium	Response	Duration	Concentration (µg/g)	Reference	
32	Mercury	Soybean (mature)	Soil (fine sandy loam)	Approx. 45% reduction in yield	6 w	3 ^C	Deuel and Swoboda 1972	
		Soybean (mature)	Soil (clay)	Approx. 40% reduction in yield	6 w	12 ^C	Deuel and Swoboda 1972	
		Cowpea		Retarded growth	-	1 ^C	Albert and Arndt 1932	
		Barley (seed-sprout)	Solution	12% growth reduction (fresh weight)	7 d post-germination	5	(as Hg ⁺⁺)	Mukhiya et al. 1983
		Barley (seed-sprout)	Solution	12% growth reduction (fresh weight)	7d post-germination	1	(as PMA) ^d	Mukhiya et al. 1983
		Lettuce (seed-sprout)	Solution	68% reduction in elongation of lettuce hypocotyl	5 d post-germination	109	(as HgCl ₂)	Nag et al. 1980
33	Nickel	Corn (mature)	Solution	10% decrease in net photosynthesis	7 d	5	Carlson et al. 1975	
		Sunflower (mature)	Solution	10% decrease in net photosynthesis	7 d	0.8	Carlson et al. 1975	
		Oats (seeds-seedlings)	Solution in coarse sand	Stunted growth	22 d post-germination	10		Vergnano and Hunter 1953
		Oats (mature)	Soil	Decreased grain yield	Whole life	50		Halstead et al. 1969
		Barley (seedling)	Solution in sand	Over 50% reduction in whole-plant fresh weight	3 weeks	281	(NiSO ₄ ·7H ₂ O)	Agarwala et al. 1977
		34	Cadmium	Corn (mature)	Solution	10% decrease in net photosynthesis	7 d	0.9
Sunflower (mature)	Solution			10% decrease in net photosynthesis	7 d	0.45	Carlson et al. 1975	

Table B-2. (continued)

RAC	Representative chemical	Test organism ^a and life stage	Test medium	Response	Duration	Concentration (µg/g)	Reference
		Soybeans (mature)	Solution in sand and vermiculite	35% decrease in fresh weight of pods	90 d	2	Huang et al. 1974
		Bean (5 weeks old)	Solution	50% growth reduction	3 weeks	0.2	Page et al. 1972
		Beet (5 weeks old)	Solution	50% growth reduction	3 weeks	0.2	Page et al. 1972
		Turnip (5 weeks old)	Solution	50% growth reduction	3 weeks	0.2	Page et al. 1972
		Corn (5 weeks old)	Solution	50% growth reduction	3 weeks	1.2	Page et al. 1972
		Lettuce (5 weeks old)	Solution	50% growth reduction	3 weeks	0.9	Page et al. 1972
		Tomato (5 weeks old)	Solution	50% growth reduction	3 weeks	4.8	Page et al. 1972
		Barley (5 weeks old)	Solution	50% growth reduction	3 weeks	5.6	Page et al. 1972
		Pepper (5 weeks old)	Solution	50% growth reduction	3 weeks	2.0	Page et al. 1972
		Cabbage (5 weeks old)	Solution	50% growth reduction	3 weeks	9.0	Page et al. 1972
		Soybean (seedling)	Soil (silty clay loam)	15% reduction in yield (dry weight)	5 weeks	2.5	Haghiri 1973
		Wheat (seedling)	Soil (silty clay loam)	20% reduction in yield (dry weight)	5 weeks	2.5	Haghiri 1973
		Lettuce (mature)	Soil (silty clay loam)	40% reduction in yield (fresh weight)	Whole life	2.5	Haghiri 1973
34	Cadmium	Sycamore (sapling)	Soil (6:1 silty clay loam and perlite)	25% reduction in new stem growth	90 d	39	Carlson and Bazzaz 1977
35	Lead	Soybeans (mature)	Solution in sand and vermiculite	35% decrease in fresh weight of pods	90 d	62	Huang et al. 1974

Table B-2. (continued)

RAC	Representative chemical	Test organism ^a and life stage	Test medium	Response	Duration	Concentration (µg/g)	Reference
		Lettuce (44 d old)	Soil (silty clay loam)	25% reduction in yield	30 d	1000 Pb(NO ₃) ₂	John and VanLaerhoven 1972
		Corn (25-d seedling)	Vermiculite and solution	20% decrease in photosynthesis	11-21 d	1000	Bazzaz et al. 1974
		Soybean (25-d seedling)	Vermiculite and solution	20% decrease in photosynthesis	11-21 d	2000	Bazzaz et al. 1974
		Sycamore (sapling)	Soil (6:1 silty clay loam and perlite)	25% reduction in new stem growth	90 d	500	Carlson and Bazzaz 1977

^aLatin binomials are listed in Appendix C.

^bArsenic shows a stimulatory effect on plants when present at low concentrations (40-50 µg/g total As or 5 µg/g extractable As in soil) (Woolson et al. 1971).

^cConcentration of water extractable contaminant.

^dPMA = phenyl mercuric acetate.

Table B-3. Toxicity of chemicals in air to animals

RAC	Representative chemical	Test organism ^a	Response ^b	Exposure		Notes	Reference
				Duration (h)	Concentration ($\mu\text{g}/\text{m}^3$)		
1	Carbon monoxide	Rabbit	Aortic lesions	4	1.51 E+05		National Research Council 1977a
		Dog	Heart damage	1,008	4.3 E+04		National Research Council 1977a
		Chicken	75% egg hatch	432	4.9 E+05	Egg exposed	National Research Council 1977a
		Rabbit	90% neonate survival	720	1.0 E+05	Mother exposed	National Research Council 1977a
		Human	Lethality		9.2 E+08		Cleland and Kingsbury 1977
2	Sulfur dioxide	Guinea pig	Increased airway resistance	1	4.2 E+02		US EPA 1982
		Guinea pig	LT ₅₀	1.1	5.8 E+06		US EPA 1982
		Dog	Increased airway resistance	5,400	1.3 E+04		US EPA 1982
	Sulfuric acid	Chicken	Modified nasal clearance		3.7 E+03	Intermittent exposure, 7 d	Wakabayashi et al. 1977
		Guinea pig	Respiratory function	1	1.0 E+02		Wakabayashi et al. 1977
		Guinea pig	Lethality	8	1.8 E+04		Wakabayashi et al. 1977
3	Nitrogen dioxide	Dog	Respiratory function	4,725	8.9 E+02		Wakabayashi et al. 1977
		Guinea pig	LC ₅₀	1	1.5 E+05		National Research Council 1977b
		Rat	11% lethality	5,120	2.3 E+04		National Research Council 1977b
		Rat	Bronchial damage	24	2.8 E+04		National Research Council 1977b
		Mouse	Defects in pulmonary microbial defense	24	3.8 E+03		National Research Council 1977b
		Rat and mouse	Pulmonary pathologies	Chronic	9.4 E+02	Also decreased resistance to infection	National Research Council 1977b
4	Hydrogen sulfide	Canaries, rats, and dogs	Pulmonary irritation	Subacute	7.0 E+04	No established chronic effects	National Research Council 1979a
		Dogs	Lethality	10-18	2.1 E+05		National Research Council 1979a

Table B-3. (continued)

RAC	Representative chemical	Test organism ^a	Response ^b	Exposure		Notes	Reference
				Duration (h)	Concentration ($\mu\text{g}/\text{m}^3$)		
5	Ammonia	Chicken	Increased disease susceptibility	72	1.3 E+04	Newcastle virus	National Research Council 1979b
		Pig	Respiratory irritation	840	4.3 E+04		National Research Council 1979b
		Rabbit	LT ₅₀	33	7.0 E+06		National Research Council 1979b
		Mouse	Lethal threshold	16	7.0 E+05		National Research Council 1979b
		Human	Throat irritation	Immediate	2.8 E+05		National Research Council 1979b
6	Acetylene	Human	Unconsciousness	0.08	3.7 E+08		National Research Council 1976
7	Formaldehyde	Rat	LC ₅₀	4	5.7 E+05		National Research Council 1981
		Guinea pigs	Increased airway resistance	1	3.6 E+02		National Research Council 1981
		Rat	Respiratory and eye irritation and liver weight loss	1,400	1.0 E+03		National Research Council 1981
8	Chloroform	Mouse	LC ₅₀		1.4 E+05		Kingsbury et al. 1979
		Human	Enlarged liver	Chronic	4.9 E+04	In workplace air	Kingsbury et al. 1979
9	Acetic acid	Mouse	LC ₅₀	1	1.4 E+07		Kingsbury et al. 1979
		Human	Irritation	0.05	2.0 E+06		Kingsbury et al. 1979
		Human	Respiratory, stomach and skin irritation	Chronic	1.5 E+05	7-12 years, workplace exposure	National Research Council 1976
10	Furan Thiophene	Rat	Lethal threshold	8-48	2.4 E+08		Kingsbury et al. 1979
		Mouse	Lethal threshold	8-48	3.0 E+07		Kingsbury et al. 1979
11	Pyridine 2-Ethylpyridine	Rat	LC ₅₀	4	1.3 E+07		Kingsbury et al. 1979
		Rat	LC ₁₀₀	3	2.4 E+07		Kingsbury et al. 1979
12	Benzene	Human	Lethal threshold	Chronic	1.9 E+05	Workplace exposure	National Research Council 1976

Table B-3. (continued)

RAC	Representative chemical	Test organism ^a	Response ^b	Exposure		Notes	Reference
				Duration (h)	Concentration ($\mu\text{g}/\text{m}^3$)		
13	Pentane	Mouse	Lethality		3.8 E+08		Kingsbury et al. 1979
	Cyclopentane	Mouse	Lethality		1.1 E+08		Kingsbury et al. 1979
	Hexane	Mouse	Lethality		1.2 E+08		Kingsbury et al. 1979
		Human	Dizziness	0.17	1.8 E+07		Kingsbury et al. 1979
	Cyclohexane	Rabbit	Lethality	1	9.2 E+07		Kingsbury et al. 1979
		Rabbit	Narcosis and convulsions	1	4.5 E+07		Kingsbury et al. 1979
	Heptane	Human	Dizziness	0.10	4.1 E+06		Kingsbury et al. 1979
	Butadiene	Human	Respiratory and eye irritation	8	1.8 E+07		Kingsbury et al. 1979
	Cyclopentadine	Rat	Liver and kidney damage	245	1.4 E+06	Exposure = 7 h/d for 35 d	Kingsbury et al. 1979
14	Toluene	Rat	Lethal threshold	4	1.5 E+07		Kingsbury et al. 1979
		Human	Psychological effects		3.8 E+05		Kingsbury et al. 1979
	Ethyl benzene	Rat	Lethal threshold	4	1.7 E+07		Kingsbury et al. 1979
		Human	Eye irritation	0.08	8.8 E+05		Kingsbury et al. 1979
	p-Xylene	Mouse	Lethal threshold	4	1.5 E+07		Kingsbury et al. 1979
	Tetrahydro-naphthalene	Guinea pig	Lethal threshold	136	1.5 E+06	8 h/d for 17 d	Kingsbury et al. 1979
Naphthalene	Human	Eye irritation and damage		7.9 E+04		Kingsbury et al. 1979	
15	(No data on respiratory toxicity, but several members of this RAC are carcinogens.)						Kingsbury et al. 1979
16	Ethylamine	Rat	Lethal threshold	4	5.5 E+06		Kingsbury et al. 1979
		"Animals"	Lung, liver, and kidney damage	1,008	1.8 E+05		Kingsbury et al. 1979
	1-Aminopropane	Rat	LC ₅₀	4	5.6 E+06		Kingsbury et al. 1979
17	Aniline	Rat	LC ₅₀	4	9.5 E+05		Kingsbury et al. 1979
	Dimethylaniline	Mouse	LC ₅₀	7	7.4 E+05	Mixed isomers	Kingsbury et al. 1979
18	(No data on respiratory toxicity)						
19	(No data on respiratory toxicity)						
20	(No data on respiratory toxicity)						
21	(No data on respiratory toxicity)						

Table B-3. (continued)

RAC	Representative chemical	Test organism ^a	Response ^b	Exposure		Notes	Reference
				Duration (h)	Concentration ($\mu\text{g}/\text{m}^3$)		
22	Acrolein	Rat	LC50	4	1.8 E04		National Research Council 1981
		Monkey	Respiratory system damage	2,160	5.1 E02		National Research Council 1981
	Acetaldehyde	Mice, rabbits, and guinea pigs	LC50	4	2.0 E06		National Research Council 1981
			LC50	0.5	6.2 E07		National Research Council 1981
	Propionaldehyde	Rat	Reduced weight gain	36	3.1 E06	6 h/d for 6 d	National Research Council 1981
	Butyraldehyde	Rat	LC50	0.5	1.7 E08		National Research Council 1981
	Butanone	Mouse	LC50	0.75	6.1 E08		National Research Council 1981
23	Methyl mercaptan	Rat	Lethal threshold		2.0 E07		Kingsbury et al. 1979
	Ethyl mercaptan	Rat	LC50		1.1 E07		Kingsbury et al. 1979
		Human	Central nervous system effects		1.0 E04		Kingsbury et al. 1979
	N-Butyl mercaptan	Rat	LC50	4	1.5 E07		Kingsbury et al. 1979
		Human	"Toxic effect"	3	1.0 E04		Kingsbury et al. 1979
	Thiophenol	Rat	LC50	4	1.5 E05		Kingsbury et al. 1979
Carbon disulfide	Human	Central nervous system effects		5.0 E04	7-year exposure	Cleland and Kingsbury 1977	
24	Methanol	Monkey	LC50		1.3 E06		Kingsbury et al. 1979
		Human	Central nervous system effects		7.5 E04		Kingsbury et al. 1979
	Ethanol	Human	Eye and respiratory irritation and mental effects		1.9 E06		Kingsbury et al. 1979
25	(No data on respiratory toxicity.)						Kingsbury et al. 1979
26	Methyl acetate	Human	Severe toxic effects	1	1.5 E06		Kingsbury et al. 1979
	Methyl methacrylate	Rat	LC50	1	1.5 E07		Kingsbury et al. 1979
	Butyl acetate	Human	Throat irritation		9.6 E05		Kingsbury et al. 1979
		Human	Toxic effects	1	9.6 E06		Kingsbury et al. 1979
N-Amyl acetate	Human	Toxic threshold	0.5	1.0 E06		Kingsbury et al. 1979	
27	(No data on respiratory toxicity.)						Kingsbury et al. 1979

Table B-3. (continued)

RAC	Representative chemical	Test organism ^a	Response ^b	Exposure		Notes	Reference
				Duration (h)	Concentration ($\mu\text{g}/\text{m}^3$)		
28	Acetonitrile	Rat	Lethal threshold	4	1.3 E07		Kingsbury et al. 1979
		Human	Bronchial effects		2.7 E05		Kingsbury et al. 1979
	Acrylonitrile	Rat	Lethal threshold	4	1.1 E06		Kingsbury et al. 1979
29	(No data on respiratory toxicity)						Kingsbury et al. 1979
30	Fly ash	Monkey	Slight lung fibrosis	13,390	4.6 E+02		National Research Council 1979c
31	Arsenic trioxide	Rat	Weight lag and physiological effects	24	2.5 E+01		National Research Council 1977c
32	Mercury (metal)	Human	Toxic threshold		1.0 E+03	40-year exposure	Cassidy and Furr 1978
		Rabbit	Toxic threshold		2.9 E+04		Cassidy and Furr 1978
		Human	Central nervous system effects		1.7 E+02		Kingsbury et al. 1979
33	Nickel carbonyl	Rat	LC ₅₀	0.5	2.4 E+05		National Research Council 1975
34	Cadmium oxide fumes	Human	Lethality	8	5.0 E+03	20-year exposure Occupational exposure	Hammons et al. 1978
	Cadmium oxide dust	Human	Impaired lung function		3.15 E+03		Hammons et al. 1978
	Cadmium	Human	Pulmonary and renal effects		1.0-27 E+01		Kingsbury et al. 1979
35	Lead	Human	Threshold of overt poisoning		5.0 E+02	Occupational exposure	National Research Council 1972

^aLatin binomials are listed in Appendix C.

^bLC₅₀/LC₁₀₀ = concentration required to kill 50%/100% of test organisms.
 LT₅₀ = time to lethality for 50% of organisms tested.

APPENDIX C

Common and Scientific Names of Animals and Plants

Common and Scientific Names of Animals and Plants
Animals

<u>Common name</u>	<u>Scientific name</u>
Bigmouth buffalo	<u>Ictiobus cyprinellus</u>
Black crappie	<u>Pomoxis nigromaculatus</u>
Bluegill	<u>Lepomis macrochirus</u>
Brook trout	<u>Salvelinus fontinalis</u>
Brown trout	<u>Salmo trutta</u>
Canary	<u>Serinus canarius</u>
Carp	<u>Cyprinus carpio</u>
Channel catfish	<u>Ictalurus punctatus</u>
Chicken	<u>Gallus gallus</u>
Chinook salmon	<u>Oncorhynchus tshawytscha</u>
Coho salmon	<u>Oncorhynchus kisutch</u>
Dog	<u>Canis familiaris</u>
Fathead minnow	<u>Pimephales promelas</u>
Goldfish	<u>Carassius auratus</u>
Green sunfish	<u>Lepomis cyanellus</u>
Guinea pig	<u>Cavia cobaya</u>
Human	<u>Homo sapiens</u>
Largemouth bass	<u>Micropterus salmoides</u>
Monkey	<u>Macaca sp.</u>
Mosquitofish	<u>Gambusia affinis</u>
Mouse	<u>Mus musculus</u>
Northern pike	<u>Esox lucius</u>
Pig	<u>Sus scrofa</u>
Pink salmon	<u>Oncorhynchus gorbuscha</u>
Pumpkinseed	<u>Lepomis gibbosus</u>
Rabbit	<u>Oryctolagus cuniculus</u>
Rainbow trout	<u>Salmo gairdneri</u>
Rat	<u>Rattus rattus</u>
Smallmouth buffalo	<u>Ictiobus bulbalus</u>
White bass	<u>Morone chrysops</u>

Plants

<u>Common name</u>	<u>Scientific name</u>
African marigold	<u>Tagetes sp.</u>
Alfalfa	<u>Medicago sativa</u>
Apple	<u>Malus sylvestris</u>
Barley	<u>Hordeum vulgare</u>
Bean	<u>Phaseolus vulgaris</u>
Broadbean	<u>Vicia faba</u>
Bush bean	<u>Phaseolus vulgaris</u>
Cabbage	<u>Brassica oleracea</u>
Carnation	<u>Dianthus caryophyllus</u>
Carrot	<u>Daucus carota</u>
Chickweed, common	<u>Stellaria media</u>
Cocksfoot	<u>Dactylis glomerata</u>

Appendix C (continued)
Plants

<u>Common name</u>	<u>Scientific name</u>
Coleus	<u>Coleus blumei</u>
Corn	<u>Zea mays</u>
Cotton	<u>Gossypium hirsutum</u>
Cowpea	<u>Vigna sinensis</u>
Cress	<u>Lepidium sativum</u>
Cucumber	<u>Cucumis sativus</u>
Durum wheat	<u>Triticum durum</u>
Endive	<u>Cicorium endivia</u>
English ivy	<u>Hedera helix</u>
Gram	<u>Cicer arietinum</u>
Grapefruit	<u>Citrus paradisi</u>
Green bean	<u>Phaseolus vulgaris</u>
Lettuce	<u>Lactuca sativa</u>
Loblolly pine	<u>Pinus taeda</u>
Lucerne	<u>Medicago sativa</u>
Meadowgrass	<u>Poa pratensis</u>
Mustard	<u>Brassica alba</u>
Norway spruce	<u>Picea abies</u>
Oat	<u>Avena sativa</u>
Oat, wild	<u>Avena fatua</u>
Pea	<u>Psoralea corylifolia</u>
Pepper	<u>Capsicum frutescens</u>
Petunia	<u>Petunia sp.</u>
Pinto bean	<u>Phaseolus vulgaris</u>
Popinac	<u>Acacia farnesiana</u>
Poppy	<u>Papaver sp.</u>
Radish	<u>Raphanus sativus</u>
Red clover	<u>Trifolium pratense</u>
Rice	<u>Oryza sativa</u>
Ricinus	<u>Ricinus communis</u>
Rose	<u>Rosa sp.</u>
Runner bean	<u>Phaseolus vulgaris</u>
Ryegrass, Italina	<u>Lolium multiflorum</u>
Soybean	<u>Glycine max</u>
Spruce	<u>Picea abies</u>
Squash	<u>Cucurbita sp.</u>
Sugar beet	<u>Beta vulgaris</u>
Sunflower	<u>Helianthus annuus</u>
Sycamore	<u>Platanus occidentalis</u>
Thevetia	<u>Thevetia neriifolca</u>
Tobacco	<u>Nicotiana tabacum</u>
Tomato	<u>Lycopersicon esculentum</u>
Turnip	<u>Brassica napus</u>
Wheat	<u>Triticum durum</u>
White pine	<u>Pinus strobus</u>

APPENDIX D

Species-Specific Results of the Analysis of Extrapolation Error

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

RAC	PGMATC ^a (mg/L)									
	Carp	Buffalo	Channel catfish	White bass	Green sunfish	Bluegill sunfish	Largemouth bass	Black crappie	Rainbow trout	Brook trout
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 Nonheterocyclic 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

^aPGMATCs were not calculated for RACs 1-3.

^bNo data.

Table D-2. Probabilities of chronic toxic effects on fish populations due to RAC 4 at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0345	0.0649	Class
Bigmouth buffalo	0.0345	0.0649	Class
Smallmouth buffalo	0.0345	0.0649	Class
Channel catfish	0.0261	0.0597	Class
White bass	0.0915	0.1068	a
Green sunfish	0.0451	0.0468	Genus
Bluegill sunfish	0.0980	0.0927	Species
Largemouth bass	0.1186	0.1336	Family
Black crappie	0.1940	0.2261	Family
Western site:			
Rainbow trout	0.0839	0.1117	Class
Brook trout	0.0839	0.1117	Class

^aBluegill - Perciformes

Table D-3. Probabilities of chronic toxic effects on fish populations due to RAC 5 at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0069	0.0097	Class
Bigmouth buffalo	0.0069	0.0097	Class
Smallmouth buffalo	0.0069	0.0097	Class
Channel catfish	0.0092	0.0196	Class
White bass	0.0168	0.0185	Class
Green sunfish	0.0168	0.0185	Class
Bluegill sunfish	0.0168	0.0185	Class
Largemouth bass	0.0168	0.0185	Class
Black crappie	0.0168	0.0185	Class
Western site:			
Rainbow trout	0.0144	0.0090	Species
Brook trout	0.0149	0.0149	Family

Table D-4. Probabilities of chronic toxic effects on fish populations due to RAC 15 at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0016	0.0019	Class
Bigmouth buffalo	0.0016	0.0019	Class
Smallmouth buffalo	0.0016	0.0019	Class
Channel catfish	0.0022	0.0047	Class
White bass	0.0038	0.0018	a
Green sunfish	0.0025	0.0006	Genus
Bluegill sunfish	0.0030	0.0004	Species
Largemouth bass	0.0035	0.0015	Family
Black crappie	0.0136	0.0262	Family
Western site:			
Rainbow trout	0.0030	0.0021	Class
Brook trout	0.0030	0.0021	Class

^aBluegill - Perciformes

Table D-5. Probabilities of chronic toxic effects on fish populations due to RAC 22 at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0238	0.0392	Class
Bigmouth buffalo	0.0238	0.0392	Class
Smallmouth buffalo	0.0238	0.0392	Class
Channel catfish	0.0258	0.0540	Class
White bass	0.0617	0.0783	Class
Green sunfish	0.0282	0.0266	Genus
Bluegill sunfish	0.0559	0.0494	Species
Largemouth bass	0.0372	0.0296	Species
Black crappie	0.1263	0.1711	Family
Western site:			
Rainbow trout	0.0550	0.0538	Species
Brook trout	0.0507	0.0628	Family

Table D-6. Probabilities of chronic toxic effects on fish populations due to RAC 26 at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0092	0.0062	Family
Bigmouth buffalo	0.0011	0.0007	Class
Smallmouth buffalo	0.0011	0.0007	Class
Channel catfish	0.0019	0.0031	Class
White bass	0.0023	0.0010	Class
Green sunfish	0.0075	0.0040	Genus
Bluegill sunfish	0.0114	0.0051	Species
Largemouth bass	0.0132	0.0117	Family
Black crappie	0.0374	0.0667	Family
Western site:			
Rainbow trout	0.0015	0.0002	Species
Brook trout	0.0023	0.0009	Family

Table D-7. Probabilities of chronic toxic effects on fish populations due to RAC 32 at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0088	0.0130	Class
Bigmouth buffalo	0.0088	0.0130	Class
Smallmouth buffalo	0.0088	0.0130	Class
Channel catfish	0.0112	0.0242	Class
White bass	0.0216	0.0252	Class
Green sunfish	0.0216	0.0252	Class
Bluegill sunfish	0.0216	0.0252	Class
Largemouth bass	0.0216	0.0252	Class
Black crappie	0.0216	0.0252	Class
Western site:			
Rainbow trout	0.0186	0.0132	Species
Brook trout	0.0184	0.0197	Family

Table D-8. Probabilities of chronic toxic effects on fish populations due to RAC 32A at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0259	0.0428	Class
Bigmouth buffalo	0.0259	0.0428	Class
Smallmouth buffalo	0.0259	0.0428	Class
Channel catfish	0.0277	0.0575	Class
White bass	0.0675	0.0853	Class
Green sunfish	0.0675	0.0853	Class
Bluegill sunfish	0.0675	0.0853	Class
Largemouth bass	0.0675	0.0853	Class
Black crappie	0.0675	0.0853	Class
Western site:			
Rainbow trout	0.0948	0.0964	Species
Brook trout	0.0498	0.0478	Species

Table D-9. Probabilities of chronic toxic effects on fish populations due to RAC 33 at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0032	0.0012	Family
Bigmouth buffalo	0.0003	0.0001	Class
Smallmouth buffalo	0.0003	0.0001	Class
Channel catfish	0.0007	0.0009	Class
White bass	0.0007	0.0001	Class
Green sunfish	0.0021	0.0005	Genus
Bluegill sunfish	0.0024	0.0003	Species
Largemouth bass	0.0027	0.0011	Family
Black crappie	0.0115	0.0225	Family
Western site:			
Rainbow trout	0.0004	0.0000	Species
Brook trout	0.0008	0.0001	Family

Table D-10. Probabilities of chronic toxic effects on fish populations due to RAC 34 at annual median ambient concentrations for unit release

Species	Ratio of ambient concentration to PGMATC	Probability of exceeding the PGMATC	Level of extrapolation
Eastern site:			
Carp	0.0271	0.0192	Species
Bigmouth buffalo	0.1957	0.2235	Class
Smallmouth buffalo	0.1957	0.2235	Class
Channel catfish	0.1516	0.2052	Class
White bass	0.5739	0.3908	Class
Green sunfish	0.0039	0.0008	Species
Bluegill sunfish	0.0053	0.0014	Species
Largemouth bass	0.0059	0.0036	Family
Black crappie	0.0204	0.0388	Family
Western site:			
Rainbow trout	1.1682	0.5332	Species
Brook trout	0.7237	0.4308	Species

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 the selection of appropriate toxicity data and association of the data with components of the Standard Water Column Model (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 ten algal populations if no other information is available. If data are available on diatoms and blue-green algae, a further division is possible, based on physiological parameters in the model and past experience with SWACOM. Like diatoms, species 1 to 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 are 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 increase in blue-green algae growth is one of our endpoints, we assign the greatest sensitivity to the consumer (i.e., 15) that is most abundant during the summer of the simulated year.

LC₅₀ 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, an 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 Categories (RACs), 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 involves 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 the response of organisms 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 GSS. However, some organics might have a "narcotic," effect which would be opposite to the reaction assumed here.

The GSS 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 the 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 (microcosm simulation). 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 we alter the parameters simultaneously in the direction indicated by the GSS until we duplicate the original experiment. Thus, for an LC_{50} (96 h), we find the percentage change that halves the population in 4 d.

At the conclusion of the Microcosm simulations, we have the percentage change in the parameters that 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 that is one-fifth 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 $\pm 100\%$. 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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