

OAK RIDGE NATIONAL LABORATORY

MARTIN MARIETTA

Environmental Risk Analysis for Direct Coal Liquefaction

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ENVIRONMENTAL SCIENCES DIVISION

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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 Categories (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 risk analysis of four direct coal liquefaction technologies: Exxon Donor Solvent (EDS), Solvent Refined Coal-I (SRC-I), Solvent Refined Coal-II (SRC-II), and H-Coal. All four technologies had equal capacites (2.72 x 10⁴ Mg coal/d) and the same waste treatments. All were located in a reference environment resembling eastern Kentucky. Estimates of concentrations of released contaminants in the air, and surface water of the reference environment were obtained, using a simple Gaussian-plume atmospheric dispersion and deposition model and a steady-state surface water fate model. Concentrations in soil and soil solution were obtained from a terrestrial food chain model.

Risk to the five ecological end points were estimated using one or more of three methods: 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 LC_{50} '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 reference environment. Taxonomic extrapolations were used to express the acute effects of RACs in terms of a common unit, the 96-h ${\rm LC}_{50}$ for largemouth bass. The extrapolated LC_{50} 's and the source-term estimates were then combined and used to assess the acute toxicities of the whole effluents from the four technologies. 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 respect to fish, nine RACs were determined to be significant for one or more technologies. RAC 5 (ammonia) was the only RAC found to be significant for all technologies, waste water treatment options and analysis methods. RAC 34 (cadmium) was significant for all technologies and water treatment options according to the quotient method and by all three methods for EDS and H-Coal. The whole effluent from the H-Coal technology with conventional water treatment appeared to be the most acutely toxic. For all technologies, conventional pollutants appear to be more hazardous to fish than the complex organic contaminents usually associated with synfuels.

Algal toxicity data were available for only 10 RACs. Because of the diversity of experimental designs and test end points used in algal bioassays, it was not possible to rank the RACs using the quotient method. However, most of the toxicity quotients calculated for algae were lower than the corresponding quotients for fish. Ecosystem uncertainty analysis suggested greater risks of effects on algae than

did the quotient method, primarily because reductions in grazing intensity related to effects of contaminants of zooplankton and fish. Both methods indicate that RAC 21 (phenols) and RAC 34 (cadmium) posed a significant risk to algal communities.

Conventional pollutants, especialy SO_2 and NO_2 , were found to have the greatest potential effects on terrestrial biota. Ground-level SO_2 concentrations for all technologies were within 1 to 2 orders of magnitude of phytotoxic levels, even excluding background concentrations. Gaseous pollutant levels were well below toxic concentrations for terrestrial mammals; however, it was not possible to assess risks to nonmammalian wildlife (e.g., birds). Of the materials deposited on soil, RACs 31 (arsenic), 33 (nickel), and 34 (cadmium) pose the greatest threat of toxicity. However, observable effects are unlikely unless these trace elements are deposited on soils with high background concentrations and chemical properties favoring the solution phase.

ABSTRACT

SUTER, G. W. II, L. W. BARNTHOUSE, C. F. BAES III,
S. M. BARTELL, M. G. CANVENDISH, R. H. GARDNER,
R. V. O'NEILL, and A. E. ROSEN. 1984. Environmental
risk analysis for direct coal liquefaction. ORNL/TM-9074.
Oak Ridge National Laboratory, Oak Ridge, Tennessee.
166 pp.

This document presents an analysis of the risks to fish, water quality (due to noxious algal blooms), crops, forests, and wildlife of four technologies for the direct liquefaction of coal: Exxon Donor Solvent (EDS), Solvent Refined Coal-I (SRC-I), Solvent Refined Coal-II (SRC-II), and H-Coal. A variety of risk analysis techniques were used to make maximum use of the available data while considering effects of effluents on different levels of ecological organization. The primary objective of the analysis was to identify potentially significant effluent components. Ammonia, cadmium, and phenols were identified as presenting the highest risk to fish. An analysis of whole-effluent toxicity indicates that the H-Coal effluent poses the highest risk of the aqueous effluents examined. Six effluent components appear to pose risks of algal blooms, primarily because of their effects on higher trophic levels. The most important atmospheric emissions for crops, forests, and wildlife appear to be the conventional combustion products SO_2 , NO_{x} , and respirable particles. the materials deposited on the soil, arsenic, cadmium, and nickel appear to be of greatest concern for phytotoxicity.

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. The methods employed in this project were described by Barnthouse et al. (1982a). 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 quide 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 in waste streams and products of synthetic liquid fuels technologies have been grouped into the 38 categories, termed Risk Analysis Categories (RACs) listed in Table 1-1. Five ecological endpoints are used: (1) reductions in fish populations, (2) development of algal communities that detract from water use, (3) reductions in timber yield due to reduced growth or changes in forest composition, (4) reductions in agricultural production, and (5) reductions in wildlife populations. Rather than descriptions of specific sites, we use reference environments, with characteristics representative of regions in which synfuels plants may be sited. Two reference environments are being used in the research for EPA: an eastern environment resembling eastern Kentucky or West Virginia, and a

Table 1-1. Risk Analysis Categories (RACs)

2 Su 3 Ni 4 Ac 5 Al 6 Hy 7 Fo 8 Vo 9 Vo 10 Vo 11 Vo 12 Be 13 Al 14 Mo 15 Po 16 Al 17 Ar 18 Al 19 Ne 20 Ca 21 Ph 22 Al 25 Ni 26 Es 27 Am 28 Ni 19 Ni 10	arbon monoxide alfur oxides atrogen oxides aid gases kaline gases armaldehyde alatile organochlorines alatile carboxylic acids alatile O & S heterocyclics alatile N heterocyclics and a server eliphatic/alicyclic hydrocarbons	CO SO _X NO _X H ₂ S, HCN NH ₃ C ₁ -C ₄ alkanes, alkynes, and cyclocompounds; bp < \20°C HCHO To bp \120°C; CH ₂ Cl ₂ , CHCl ₃ , CCl ₄ To bp \120°C; formic and acetic acids only To bp \120°C; furan, THF, thiophene To bp \120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines Benzene C ₅ (bp \40°C) and greater; paraffins,
2 Su 3 Ni 4 Ac 5 Al 6 Hy 7 Fo 8 Vo 9 Vo 10 Vo 11 Vo 12 Be 13 Al 14 Mo 15 Po 16 Al 17 Ar 18 Al 19 Ne 20 Ca 21 Ph 22 Al 25 Ni 26 Es 27 Am 28 Ni 19 Ni 10	trogen oxides id gases kaline gases drocarbon gases branddehyde blatile organochlorines blatile carboxylic acids blatile O & S heterocyclics blatile N heterocyclics enzene liphatic/alicyclic hydrocarbons	SO _X NO _X H ₂ S, HCN NH ₃ C ₁ -C ₄ alkanes, alkynes, and cyclocompounds; bp < \sim 20°C HCHO To bp \sim 120°C; CH ₂ Cl ₂ , CHCl ₃ , CCl ₄ To bp \sim 120°C; formic and acetic acids only To bp \sim 120°C; furan, THF, thiophene To bp \sim 120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines Benzene
4 Ac 5 A1 6 Hy 7 Fo 8 Vo 9 Vo 10 Vo 11 Vo 12 Be 13 A1 14 Mo 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni 19 Ni	id gases kaline gases drocarbon gases rmaldehyde platile organochlorines platile carboxylic acids platile O & S heterocyclics platile N heterocyclics enzene liphatic/alicyclic hydrocarbons	NO _x H ₂ S, HCN NH ₃ C ₁ -C ₄ alkanes, alkynes, and cyclocompounds; bp < \20°C HCHO To bp \120°C; CH ₂ Cl ₂ , CHCl ₃ , CCl ₄ To bp \120°C; formic and acetic acids only To bp \120°C; furan, THF, thiophene To bp \120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines Benzene
5 A1 6 Hy 7 Fo 8 Vo 9 Vo 10 Vo 11 Vo 12 Be 13 A1 14 Mo 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	kaline gases drocarbon gases rmaldehyde platile organochlorines platile carboxylic acids platile 0 & S heterocyclics platile N heterocyclics enzene liphatic/alicyclic hydrocarbons	H ₂ S, HCN NH ₃ C ₁ -C ₄ alkanes, alkynes, and cyclocompounds; bp < \20°C HCHO To bp \120°C; CH ₂ Cl ₂ , CHCl ₃ , CCl ₄ To bp \120°C; formic and acetic acids only To bp \120°C; furan, THF, thiophene To bp \120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines Benzene
6 Hy 7 Fo 8 Vo 9 Vo 10 Vo 11 Vo 12 Be 13 A1 14 Mo 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	drocarbon gases ormaldehyde platile organochlorines platile carboxylic acids platile 0 & S heterocyclics platile N heterocyclics enzene iphatic/alicyclic hydrocarbons	C1-C4 alkanes, alkynes, and cyclocompounds; bp < √20°C HCHO To bp √120°C; CH ₂ Cl ₂ , CHCl ₃ , CCl ₄ To bp √120°C; formic and acetic acids only To bp √120°C; furan, THF, thiophene To bp √120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines Benzene
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8	platile organochlorines platile carboxylic acids platile 0 & S heterocyclics platile N heterocyclics enzene liphatic/alicyclic hydrocarbons	HCHO To bp ∿120°C; CH ₂ Cl ₂ , CHCl ₃ , CCl ₄ To bp ∿120°C; formic and acetic acids only To bp ∿120°C; furan, THF, thiophene To bp ∿120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines Benzene
9 Vo 10 Vo 11 Vo 11 Vo 12 Be 13 A1 14 Mo 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	platile carboxylic acids platile 0 & S heterocyclics platile N heterocyclics enzene iphatic/alicyclic hydrocarbons	To bp ∿120°C; formic and acetic acids only To bp ∿120°C; furan, THF, thiophene To bp ∿120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines Benzene
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11 Vo 12 Be 13 A1 14 Mo 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	elatile N heterocyclics enzene liphatic/alicyclic hydrocarbons	To bp ∿120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines Benzene
12 Be 13 A1 14 Mo 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	enzene liphatic/alicyclic hydrocarbons	pyrrolidine, alkyl pyridines Benzene
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14 Mo 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	hydrocarbons	C ₅ (bp √40°C) and greater; paraffins.
15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Pr 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	ono- or diaromatic hydro-	olefins, cyclocompounds, terpenoids, waxes
15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	carbons (excluding	hydroaromatics Toluene, xylenes, naphthalenes, biphenyls, alkyl derivatives
16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	benzene) Dlycyclic aromatic hydrocarbons	Three rings and greater; anthracene, BaA, BaP, alkyl derivatives
17 Ar 18 A1 19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	liphatic amines (excluding N heterocyclics)	Primary, secondary, and tertiary nonhetero- cyclic nitrogen, MeNH ₂ , diMeNH, triMeN
19 Ne 20 Ca 21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	romatic amines (excluding N heterocyclics)	Anilines, napthylamines, amino pyrenes; nonheterocyclic nitrogen
20 Ca 21 Pr 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	kaline N heterocyclics ("azaarenes")	Quinolines, acridines, benzacridines (excluding pyridines)
21 Ph 22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	(excluding "volatiles") eutral N, O, S hetero- cyclics (excluding "volatiles")	Indoles, carbazoles, benzofurans, dibenzo- thiophenes
22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	arboxylic acids (excluding "volatiles")	Butyric, benzoic, phthalic, stearic
22 A1 23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	ienols	Phenol, cresols, catechol, resorcinol
23 No 24 A1 25 Ni 26 Es 27 Am 28 Ni	dehydes and ketones ("carbonyls") (excluding- formaldehyde)	Acetaldehyde, acrolein, acetone, benzaldehyd
25 Ni 26 Es 27 An 28 Ni	onheterocyclic organo- sulfur	Mercaptans, sulfides, disulfides, thiophenols, CS ₂
25 Ni 26 Es 27 An 28 Ni	Icohols	Methanol, ethanol
26 Es 27 Am 28 Ni	itroaromatics	Nitrobenzenes, nitropyrenes
27 Am 28 Ni	sters	Acetates, phthalates, formates
28 Ni	nides	Acetamide, formamide, benzamides
	itriles	Acrylonitrile, acetonitrile
29 Ta	ars	
	espirable particles	•
	rsenic	As, all forms
	ercury	Hg, all forms
	ickel	Ni, all forms
	admium	Cd, all forms
	ead	Pb, all forms
	ther trace elements	. Eg a.i i oimo
		226 _{Ra}
38 Ot	adioactive materials	11 99

western environment resembling the western slope of the Rocky Mountains in north-western Colorado. Descriptions of the meteorology, hydrology, demography, land-use patterns, and biota of these two reference environments have been developed by Travis et al. (1983). The direct coal liquefaction plants are assumed to be located in the east.

This report analyzes risks associated with four direct coal liquefaction technologies: Exxon Donor Solvent, Solvent Refined Coal-I, Solvent Refined Coal-II, and H-Coal. We assumed commerical-scale facilities, with identical feed coal capacities and similar environmental control technologies, sited in the eastern reference environment. The objectives of the risk analyses were:

- 1. to identify the RACs of greatest concern for each technology,
- 2. to compare, as far as possible, the risks associated with different technologies.
- to compare the risks of the direct coal liquefaction technology to the five ecological endpoints described above, and
- 4. to compare the magnitudes of uncertainty concerning risks of different RACs and different components of risk for each RAC.

2. SOURCE TERMS AND EXPOSURE

This section presents (a) estimates of aqueous and atmospheric source terms for four commercial-scale direct coal liquefaction plants, and (b) estimates of exposure concentrations for aquatic and terrestrial biota in the vicinity of a hypothetical plant site with environmental characteristics that roughly correspond to those of proposed sites for coal liquefaction facilities in eastern Kentucky and West Virginia.

2.1 SOURCE TERMS

Under a subcontract with Oak Ridge National Laboratory, TRW Inc. (TRW) described commerical-scale plant configurations for four direct coal liquefaction processes: Exxon Donor Solvent (EDS). Solvent Refined Coal-II (SRC-II), and H-Coal (TRW 1983). The plant configurations evaluated by TRW were adapted from design information provided by the developers of the four technologies. The source term estimates developed by TRW were based largely on published process conceptual designs and test data obtained from bench-scale, pilot, or demonstration units. Control technology efficiencies were extrapolated from similar applications in other industries.

All four plant configurations reflect a feed coal capacity of 2.72×10^4 Mg (30,000 tons) per day. TRW estimated quantities and compositions of all uncontrolled and controlled waste streams, expressed in terms of Risk Analysis Units (RACs, Sect. 1). For aqueous waste streams, two alternative control options were considered:

- Steam stripping/ammonia recovery, followed by phenol extraction and biological oxidation, and
- 2. Option 1, followed by carbon adsorption.

Because of the large number of atmospheric effluent sources associated with each technology, the atmopheric source terms are not presented in this report. They are in Tables 2-8, 3-8, 4-8, and 5-8 of TRW (1983).

The aqueous source terms are summarized in Tables 2.1-1 and 2.1-2. They include process-generated wastewaters, coal pile runoff, and cooling tower blowdown.

2.2 AQUATIC EXPOSURE ASSESSMENT

Estimates of contaminant concentrations in the surface waters of the eastern reference environment were computed based on the source terms described in the preceding section. The model used for this purpose is described by Travis et al. (1983). The model used for the synfuels risk analyses is similar in concept to the EXAMS model (Baughman and Lassiter 1978), but is simpler in process chemistry and environmental detail. A river is represented as a series of completely mixed reaches. Within each reach, steady-state contaminant concentrations are computed, based on dilution and on physical/chemical removal of contaminants from the water column. Ranges and variances can be placed on all of the environmental and chemical parameters in the model to compute frequency distribution of environmental concentrations. For this analysis, frequency distributions were computed for all RACs, based on observed variability in environmental parameters affecting contaminant transport and transformation.

2.2.1 Stream Characteristics

The environmental parameters used in the surface water exposure analysis were: stream flow (m^3/s) , stream width (m), reach length (m), sediment load (mg/L), sediment density (g/m^3) , depth of the biologically active sediment (cm), fraction of organic carbon in the sediment (unitless), stream temperature (K), current velocity (m/s), wind velocity (m/s), and 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 for the Big Sandy River at Louisa, Kentucky, and the Monongahela River at Braddock, Pennsylvania (USGS 1977, 1979). Values for the other stream parameters were taken from Southworth (1979). Irradiance values $(photons\ cm^2\ s^{-1})$ for estimating photolysis rates were obtained from Zepp and Cline (1977).

Table 2.1-1. Aqueous source terms (kg/h) for four direct coal liquefaction technologies, control option 1

Exxon Donor RAC Solvent		Solvent Refined Coal-I	Solvent Refined Coal-II	H-Coal		
4	0	0	0	0		
5	5.5	9	5	5		
6	0	0	0.002-0.017	0		
7	0	0	0.79-1.8	4.8		
8	0	0	0.017-0.96	0		
9	0	0	0.15	0		
10	0.41	0	0.0097	0.05		
11	0.066	0	0.0047	0.0083		
12	0.26	0	0.0016-0.8	0.033		
13	35	35	0.0063-0.12	45		
14	2.6	1.2	2.2-7.2	3.2		
15	0.011	0.11	0.093-0.26	0.014		
16	0	0	0	0		
17	0.23	0	0.023	0.25		
18	Q	0	0	0		
19	5.7	0.11	9.5-14	7.2		
20	81	0	0	100		
21	9	43	7.7-16	46		
22	1.3	0	0	1.6		
23	0.32	4.1	0.0077-0.09	0.4		
24	0	0	0.011	0		
25	0	0	0.12	0		
26	0	0	0.08-0.72	0		
27	0	0	0	0		
28	5.4	0	0	0		
31	0.0033-0.0042	0.0065	0.0045-0.0071	0.0083		
32	0.00202	0.0115	0.000518-0.008018	0.0005		
33	0.0308-0.035	0.0363	0.0076-0.0086	0.0132-0.0572		
34	0.038	0.0033	0.0025-0.003	0.01062-0.01962		
35	0.0382-0.0402	0.5607	0.0029-0.0039	0.01762-0.08762		
36	3.52	1.226	0.46-7.79	0.353		

Table 2.1-2. Aqueous source terms (kg/h) for four direct coal liquefaction technologies, control option 2 $\,$

RAC	Exxon Donor Solvent	Solvent Refined Coal-I	Solvent Refined Coal-II	H-Coal
4	0	0	0	0
5	5.5	9	5	5
6	0	0	0.0002-0.0017	0
7	0	0	0.079-0.18	0.48
8	0	0	0.0017-0.096	0
9	0	0	0.015	0
10	0.041	0	0.00097	0.005
11	0.0066	0	0.00047	0.00083
12	0.026	0	0.00016-0.08	0.0033
13	3.5	3.5	0.00063-0.012	4.5
14	0.26	0.12	0.22-0.72	0.32
15	0.0011	0.011	0.0093-0.0256	0.0014
16	0	0	0	0
17	0.023	0	0.0023	0.028
18	0	0	0	10
19	0.57	0.011	0.95-1.4	0.72
20	8.1	0	0	10
21	0.9	4.3	0.77-1.6	4.6
22	0.13	0	0	0.16
23	0.032	0.41	0.00077-0.009	0.04
24	0	0	0.0011	0
25	0	0	0.012	0
26	0	0	0.008-0.072	0
27	0	0	0	0
28	0.54	0	0	0.68
31	0.0033-0.0042	0.0065	0.0045-0.0071	0.0083
32	0.00202	0.0115	0.000518-0.008018	3 0.0005
33	0.0308-0.035	0.0363	0.0076-0.0086	0.0132-0.0572
34	0.038	0.0033	0.0025-0.003	0.01062-0.01962
35	0.0382-0.0402	0.5607	0.0029-0.0039	0.01762-0.08762
36	3.52	1.226	0.46-7.79	0.353

Probability distributions for flow, temperature, and suspended solids were determined from 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 analysis are presented in Table 2.2-1.

2.2.2 Contaminant Characteristics

For organic contaminants, the chemical properties (Table 2.2-2) 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 were used for this assessment.

Molecular weights of organic compounds were obtained from Weast (1980); aqueous solubility data were obtained from Verschueren (1977); and 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 (280-310 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), while particulate settling velocities were calculated from Stoke's Law (Weast 1980). Direct photolysis rate constants for anthracene were calculated using the method of Zepp and Cline (1977), and adsorption/desorption coefficients were approximated using the method of Karickhoff et al. (1979).

Table 2.2-1. 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 2.2-2. 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 chlori	de 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	Pheno1	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).

^bVerschueren (1977).

^CLeo et al. (1971).

dZepp and Schlotzhauer (1979).

^eBriggs (1981).

Because of their complex environmental chemistry, removal processes for trace elements were not directly modeled. Rates of removal by sedimentation were estimated, using an adsorption/desorption coefficient of 200. Schell and Sibley's (1982) study of K_d 's for radionuclides suggests that this is probably a conservative estimate for most trace elments under most environmental conditions.

2.2.3 Results

Model runs were performed for the reference stream using the source rates presented in Tables 2.1-1 and 2.1-2. 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 Tables 2.2-3 through 2.2-6. For all practical purposes, the concentrations computed using contaminant-specific removal rates are identical to concentrations computed from pure dilution rates. 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.

2.3 ATMOSPHERIC DISPERSION AND DEPOSITION

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 by 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 values for soil bulk density, precipitation, evapotranspiration, and irrigation and taking into account removal by leaching, biological degradation, and chemical degradation.

Table 2.2-3. Estimated ambient contaminant concentrations, eastern reference stream, Exxon Donor Solvent process

RAC	Reference compound	Treatment option	Mean (g/L)	Median (g/L)	95% (g/L)
4	Hydrogen sulfide	1 2	0 0	0	0 0
5	Ammonia	l 2	1.3 E-05 1.3 E-05	1.1 E-05 1.1 E-05	2.5 E-05 2.5 E-05
6	Butane	1 2	0 0	0 0	0 0
7	Formaldehyde	1 2	0 0	0 0	0
8	Methylene chloride	1 2	0 0	0 0	0 0
9	Acetic acid	1 2	0 0	0 0	0
10	Thiophene	. 1 2	9.5 E-07 9.5 E-08	8.3 E-07 8.3 E-08	1.9 E-06 1.9 E-07
11	Pyridine	1 2	1.5 E-07 1.5 E-08	1.3 E-07 1.3 E-08	3.0 E-07 3.0 E-08
12	Benzene	1 2	6.0 E-07 6.0 E-08	5.3 E-07 5.3 E-08	1.2 E-06 1.2 E-07
13	Cyclohexane	1	8.1 E-05 8.1 E-06	7.1 E-05 7.1 E-06	1.6 E-04 1.6 E-05
14	Toluene	1 2	6.0 E-06 6.0 E-07	5.3 E-06 5.3 E-07	1.2 E-05 1.2 E-06
15	Anthracene	1 2	2.2 E-08 2.2 E-09	2.1 E-08 2.1 E-09	3.8 E-08 3.8 E-09
16	Methylamine	1 2	0 0	0 0	0 0
17	Aniline	1 2	5.3 E-07 5.3 E-08	4.7 E-07 4.7 E-08	1.0 E-06 1.0 E-07
18	Quinoline	1 2	0	0	0 0

Table 2.2-3. (continued)

RAC	Reference compound	Treatment option	Mean (g/L)	Median (g/L)	95% (g/L)
19	Dibenzofuran	1 2	1.3 E-05 1.3 E-06	1.2 E-05 1.2 E-06	2.6 E-05 2.6 E-06
20	Butanoic acid	1 2	1.9 E-04 1.9 E-05	1.6 E-04 1.6 E-05	3.7 E-04 3.7 E-05
21	Phenol	1 2	2.1 E-05 2.1 E-06	1.8 E-05 1.8 E-06	4.1 E-05 4.1 E-06
22	Acrolein	1 2	3.0 E-06 3.0 E-07	2.6 E-06 2.6 E-07	5.9 E-06 5.9 E-07
23	Methanethiol	1 2	7.4 E-07 7.4 E-08	6.5 E-07 6.5 E-08	1.5 E-06 1.5 E-07
24	Methanol	1 2	0 0	0 0	0 0
25	Nitrobenzene	1 2	0 0	0 0	0 0
26	Methyl pntnalate	1 2	0 0	0 0	0 0
27	Acetamide	. 1	0 U	0 0	0 0
28	Acrylonitrile	1 2	1.2 E-05 1.2 E-06	1.1 E-05 1.1 E-06	2.5 E-05 2.5 E-06
31	Arsenic	1 2	9.7 E-09 9.7 E-09	8.5 E-09 8.5 E-09	1.9 E-08 1.9 E-08
32	Mercury	1 2	4.7 E-09 4.7 E-09	4.1 E-09 4.1 E-09	9.2 E-09 9.2 E-09
33	Nickel	1 2	8.1 E-08 8.1 E-08	7.1 E-08 7.1 E-08	1.6 E-07 1.6 E-07
34	Cadmium	1 2	8.8 E-08 8.8 E-08	7.7 E-08 7.7 E-08	1.7 E-07 1.7 E-07
35	Lead	1 2	9.3 E-08 9.3 E-08		1.8 E-07 1.8 E-07
36	Fluorine	1 2	8.1 E-06 8.1 E-06		1.6 E-05 1.6 E-05

Table 2.2-4. Estimated ambient contaminant concentrations, eastern reference stream, SRC-I process

RAC	Reference compound	Treatment option	Mean (g/L)	Median (g/L)	95% (g/L)
4	Hydrogen sulfide	1 2	0	0	0
5	Ammonia	1 2	2.1 E-05 2.1 E-05	1.8 E-05 1.8 E-05	4.1 E-05 4.1 E-05
6	Butane	1 2	0	0 0	0 0
7	Formaldenyde	1 2	0 0	0 0	0 0
8	Metnylene chloride	1 2	0 0	0 0	0 0
9	Acetic acid	1 2	0 0	0 0	0 0
10	Thiophene	1 2	0	0 0	0 0
11	Pyridine	1 2	0 0	0 0	0 0
12	Benzene	1 2	0 0	0	0 0
13	Cyclonexane	1-	8.1 E-05 8.1 E-06	7.1 E-05 7.1 E-06	1.6 E-04 1.6 E-05
14	Toluene	1 2	2.8 E-06 2.8 E-07	2.4 E-06 2.4 E-07	5.5 E-06 5.5 E-07
15	Anthracene	1 2	2.2 E-07 2.2 E-08	2.1 E-07 2.1 E-08	3.8 E-07 3.8 E-08
16	Methylamine	1 2	0 0	0 0	0 0
17	Aniline	1 2	0 0	0 0	0 0
18	Quinoline	1 2	0 0	0 0	0

Table 2.2-4. (continued)

R AC	Reference compound	Treatment option	Mean (g/L)	Median (g/L)	95% (g/L)
19	Dibenzofuran	1 2	2.5 E-07 2.5 E-08		5.0 E-07 5.0 E-08
20	Butanoic acid	1 2	0 0	0 0	0 0
21	Pheno l	1 2	9.9 E-05 9.9 E-06	8.7 E-05 8.7 E-06	2.0 E-04 2.0 E-05
22	Acrolein	1 2	0 0	0 0	0 0
23	Methanethiol	1 2	9.5 E-06 9.5 E-07	8.3 E-06 8.3 E-07	1.9 E-05 1.9 E-06
24	Methanol	1 2	0 0	0 0	0
25	Nitrobenzene	1 2	0 0	0 0	0 0
26	Metnyl phthalate	1 2	0 0	0 0	0 0
27	Acetamide	1 2	0 0	0 0	0 0
28	Acrylonitrile	1 2	0 0	0 0	0 0
31	Arsenic	1 2	1.5 E-08 1.5 E-08	1.3 E-08 1.3 E-08	3.0 E-08 3.0 E-08
32	Mercury	1 2	2.7 E-08 2.7 E-08	2.3 E-08 2.3 E-08	5.2 E-08 5.2 E-08
33	Nickel	1 2	8.4 E-08 8.4 E-08		1.7 E-07 1.7 E-07
34	Cadmium	1 2	7.6 E-09 7.6 E-09		1.5 E-08 1.5 E-08
35	Lead	1 2	1.3 E-06 1.3 E-06		2.6 E-06 2.6 E-06
36	Fluorine	1 2	2.8 E-06 2.8 E-06		5.6 E-06 5.6 E-06

Table 2.2-5. Estimated ambient contaminant concentrations, eastern reference stream, SRC-II process

RAC	Reference compound	Treatment option	Mean (g/L)	Median (g/L)	95% (g/L)
4	Hydrogen sulfide	1 2	0	0	0
5	Ammonia	1 2	1.2 E-05 1.2 E-05	1.0 E-05 1.0 E-05	2.3 E-05 2.3 E-05
б	Butane	1 2	3.9 E-08 3.9 E-09	3.5 E-08 3.5 E-09	7.8 E-08 7.8 E-09
7	Formaldehyde	1 2	4.2 E-06 4.2 E-07	3.7 E-06 3.7 E-07	8.2 E-06 8.2 E-07
8	Metnylene chloride	1 2	2.2 E-06 2.2 E-07	2.0 E-06 2.0 E-07	4.4 E-06 4.4 E-07
9	Acetic acid	1 2	3.5 E-07 3.5 E-08	3.1 E-07 3.1 E-08	6.8 E-07 6.8 E-08
10	Tniophene	1 2	2.2 E-08 2.2 E-09	2.0 E-08 2.0 E-09	4.4 E-08 4.4 E-09
11	Pyridine	1 2	1.1 E-08 1.1 E-09	9.6 E-09 9.6 E-10	2.1 E-08 2.1 E-09
12	Benzene	1 2	1.9 E-06 1.9 E-07	1.6 E-06 1.6 E-07	3.6 E-06 3.6 E-07
13	Cyclohexane	1.	2.8 E-07 2.8 E-08	2.4 E-07 2.4 E-08	5.5 E-07 5.5 E-08
14	Toluene	1 2	1.7 E-05 1.7 E-06	1.5 E-05 1.5 E-06	3.3 E-05 3.3 E-06
15	Anthracene	1 2	5.3 E-07 5.3 E-08	4.9 E-07 4.9 E-08	9.1 E-07 9.1 E-08
16	Metnylamine	1 2	0 0	0 0	0 0
17	Aniline	1 2	5.3 E-08 5.3 E-09	4.7 E-08 4.7 E-09	1.1 E-07 1.1 E-08
18	Quinoline	1 2	0 0	0 0	0 0

Table 2.2-5. (continued)

RAC	Reference compound	Treatment option	Mean (g/L)	Median (g/L)	95% (g/L)
19	Dibenzofuran	1 2	3.2 E-05 3.2 E-06	2.8 E-05 2.8 E-06	6.4 E-05 6.4 E-06
20	Butanoic acid	1 2	0 0	0 0	0 0
21	Phenol	1 2	3.7 E-05 3.7 E-06	3.3 E-05 3.3 E-06	7.3 E-05 7.3 E-06
22	Acrolein	1 2	0 0	0 0	0 0
23	Metnanethiol	1 2	2.1 E-07 2.1 E-08	1.8 E-07 1.8 E-08	4.1 E-07 4.1 E-08
24	Methanol	1 2	2.5 E-08 2.5 E-09	2.2 E-08 2.2 E-09	5.0 E-08 5.0 E-09
25	Nitrobenzene	1 2	2.8 E-07 2.8 E-08	2.4 E-07 2.4 E-08	5.5 E-07 5.5 E-08
26	Methyl phthalate	1 2	1.7 E-06 1.7 E-07	1.5 E-06 1.5 E-07	3.3 E-06 3.3 E-07
27	Acetamide	1 2	0 0	0	0 0
28	Acrylonitrile	1 2	0 0	0 0	0 0
31	Arsenic	1 2	1.6 E-08 1.6 E-08	1.4 E-08 1.4 E-08	3.2 E-08 3.2 E-08
32	Mercury	1 2	1.9 E-08 1.9 E-08	1.6 E-08 1.6 E-08	3.7 E-08 3.7 E-08
33	Nickel	1 2	2.0 E-08 2.0 E-08		3.9 E-08 3.9 E-08
34	Cadmium	1 2	6.9 E-09 6.9 E-09	6.1 E-09 6.1 E-09	1.4 E-08 1.4 E-08
35	Lead	1 2	9.0 E-09 9.0 E-09		1.8 E-08 1.8 E-08
36	Fluorine	1 2	1.8 E-05 1.8 E-05	1.6 E-05 1.6 E-05	3.6 E-05 3.6 E-05

Table 2.2-6. Estimated ambient contaminant concentrations, eastern reference stream, H-Coal process.

RAC	Reference compound	Treatment option	Mean (g/L)	Median (g/L)	95% (g/L)
4	Hydrogen sulfide	1 2	0	0	0
5	Ammonia	1 2	1.2 E-05 1.2 E-05	1.0 E-05 1.0 E-05	2.3 E-05 2.3 E-05
6	Butane	1 2	0 0	0	0
7	Formaldehyde	1 2	1.1 E-05 1.1 E-06	9.8 E-06 9.8 E-07	2.2 E-05 2.2 E-06
8	Methylene chloride	1 2	0 0	0 0	0 0
9	Acetic acid	1 2	0 0	0 0	0 0
10	Thiophene	1 2	1.2 E-07 1.2 E-08	1.0 E-07 1.0 E-08	2.3 E-07 2.3 E-08
11	Pyridine	1 2	1.9 E-08 1.9 E-09	1.7 E-08 1.7 E-09	3.8 E-08 3.8 E-09
12	Benzene	1 2	7.6 E-08 7.6 E-09	6.7 E-08 6.7 E-09	1.5 E-07 1.5 E-08
13	Cyclonexane	1	1.0 E-04 1.0 E-05	9.1 E-05 9.1 E-06	2.0 E-04 2.0 E-05
14	Toluene	1 2	7.4 E-06 7.4 E-07	6.5 E-06 6.5 E-07	1.5 E-05 1.5 E-06
15	Anthracene	1 2	2.9 E-08 2.9 E-09	2.7 E-08 2.7 E-09	4.9 E-08 4.9 E-09
16	Methylamine	1 2	0 0	0 0	0 0
17	Aniline	1 2	6.5 E-07 6.5 E-08	5.7 E-07 5.7 E-08	1.3 E-06 1.3 E-07
18	Quinoline	1 2	0 0	0 0	0

Table 2.2-6. (continued)

R AC	Reference compound	Treatment option	Mean (g/L)	Median (g/L)	95% (g/L)
19	Dipenzofuran	1 2	1.7 E-05 1.7 E-06	1.5 E-05 1.5 E-06	3.3 E-05 3.3 E-06
20	Butanoic acid	1 2	2.3 E-04 2.3 E-05	2.0 E-04 2.0 E-05	4.6 E-04 4.6 E-05
21	Phenol	1 2	1.1 E-04 1.1 E-05	9.3 E-05 9.3 E-06	2.1 E-04 2.1 E-05
22	Acrolein	1 2	3.7 E-06 3.7 E-07	3.3 E-06 3.3 E-07	7.3 E-06 7.3 E-07
23	Methanethiol	1 2	9.3 E-07 9.3 E-08	8.1 E-07 8.1 E-08	1.8 E-06 1.8 E-07
24	Methanol	1 2	0 0	0 0	0 0
25	Nitrobenzene	1 2	0 0	0 0	0 0
26	Metnyl phthalate	1 2	0 0	0 0	0 0
27	Acetamide	1 2	0 0	0 0	0 0
28	Acrylonitrile	1 2	1.6 E-05 1.6 E-06	1.4 E-05 1.4 E-06	3.1 E-05 3.1 E-06
31	Arsenic	1 2	1.9 E-08 1.9 E-08	1.7 E-08 1.7 E-08	3.8 E-08 3.8 E-08
32	Mercury	1 2	1.2 E-09 1.2 E-09	1.0 E-09 1.0 E-09	2.3 E-09 2.3 E-09
33	Nickel	1 2	1.3 E-07 1.3 E-07	1.2 E-07 1.2 E-07	2.6 E-07 2.6 E-07
34	Cadmium	1 2	4.5 E-08 4.5 E-08		8.9 E-08 8.9 E-08
35	Lead	1 2	2.0 E-07 2.0 E-07		
36	Fluorine	1 2	8.2 E-07 8.2 E-07		1.6 E-00 1.6 E-00

Because most phytotoxicity studies are done in solution culture, we 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:

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

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

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

 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 . 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

$$C_{iss}^{max} = \frac{D_{i}[1 - exp(-\lambda_{si} t_{b})]}{10 \rho \theta d \lambda_{si}} , \qquad (2)$$

where

 D_i = the ground-level deposition rate of compound i ($\mu g m^{-2} s^{-1}$),

 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 $cm^2/1$ m^2) (1 kg/1000 g)],

```
\rho = soil bulk density (g/cm<sup>3</sup>),

\theta = volumetric water content (cm<sup>3</sup>/cm<sup>3</sup>),

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

r = soil volumetric water content (mL/cm<sup>3</sup>).
```

If C_{iss} calculated using Eq. (1) exceeds C^{max} calculated using 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 measured values of K_d are usually determined 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 m to 50,000 m from the source. The highest annual average concentrations in air and the highest soil and soil solution concentrations after 35 years of deposition are presented in Tables 2.3-1 through 2.3-4.

Table 2.3-1. Maximum ambient atmospheric and soil concentrations for Exxon Donor Solvent process.

KAC	RAC name	Annual average concentration in air $(\mu g/m^3)$	Concentration soil (µg/kg		oncentration in solution (µg/L)
1	Carbon monoxide	17.4	No	accumulation in	soil
2	Sulfur oxides	6.61	No	accumulation in	soil
3	Nitrogen oxides	7.57	No	accumulation in	soil
	Acid gases			No emissions	
	Alkaline gases			No emissions	
	Hydrocarbon gases	5.92	2.38		2.47
	Formaldehyde			No emissions	
8 9	Volatile organochlorines			No emissions No emissions	
_	Volatile carboxylic acids Volatile 0 & S heterocyclics	4.43 E-02	1.82 E-03	NO CHIISSIONS	1.51 E-03
11	Volatile N heterocyclics	4.43 E-02	1.02 E-U3	No emissions	1.51 L-03
12	Benzene	2.47 E-02	1.03 E-02	NO CM13310113	7.91 E-03
	Aliphatic/alicyclic hydrocarbons	1.37	35.4		2.53
	Mono- or diaromatic hydrocarbons	3.19	1.85		0.37
	Polycyclic aromatic hydrocarbons	0.415	37.3		0.573
	Aliphatic amines			No emissions	
	Aromatic amines	7.14 E-03	3.79 E-02		7.81 E-02
	Alkaline N heterocyclics	0.261	2.39		0.919
	Neutral N, O, S heterocyclics	1.09	4.14 E-02		1.09 E-02
20 21	Carboxylic acids	0.52	133	No emissions	196
	Phenols Aldehydes and ketones	9.96 E-03	1.65 E-02		3.4 E-02
	Nonheterocyclic organosulfur	9.38 E-06	1.12 E-05		5.1 E-06
-	Alcohols	3.30 E-00	1112 6-03	No emissions	3.1 2 00
	Nitroaromatics			No emissions	
26	Esters			No emissions	
27	Amides			No emissions	
	Nitriles			No emissions	
	Tars			No emissions	
	Respirable particles	45.4			
	Arsenic	1.85 E-04	330		1.65
	Mercury	1.54 E-05	2.46 E-03	•	2.46 E-04
	Nickel	8.57 E-04	2460		16.4 7.56
	Cadmium Lead	1.32 E-04 1.32 E-03	49.1 981		7.50 1.09
	Other trace elements	0.0287	301		1.03
	Radioactive materials	0.0287			

Table 2.3-2. Maximum ambient atmospheric and soil concentrations for SRC-I

2 Su 3 Ni 4 Ac 5 Al 6 Hy 7 Fc 8 Vo 10 Vo 11 Vo 12 Be 13 Al 14 Mc 15 Pc 16 Al 17 Ar 18 No 20 Ca 22 Al 22 Al 22 No 22 No 2	rbon monoxide lfur oxides trogen oxides id gases kaline gases	2.61 5.40 7.86		Но асси	
3 Ni 4 Acc 5 Al 6 Hy 7 Fc 8 Vo 9 Vo 11 Vo 12 Be 13 Al 14 Mc 15 Pc 16 Al 17 Ar 18 Al 19 Ne 22 Pr 22 Al 22 No 24 Al	trogen oxides id gases kaline gases				mulation in soil
4 Acc 5 Al 6 Hy 7 Fc 8 Vo 9 Vc 10 Vc 112 Be 13 Al 14 Mc 15 Pc 16 Al 17 Ar 18 Al 19 Ne 20 Ca 21 Pr 22 Al 22 Al 22 Ni 25 Ni 12 N	id gases kaline gases	7.86		No accui	mulation in soil
5 Al 6 Hy 7 Fc 8 Vo 9 Vc 10 Vc 11 Vc 11 An 12 Be 113 Al 14 Mo 15 Pc 16 Al 17 Ar 18 Al 19 Ne 20 Ca 21 Pr 22 Al 22 Al 22 Ni	kaline gases				mulation in soil
6 Hy 7 FC 8 VO 9 VC 10 VC 11 VC 11 VC 11 AN 114 MC 15 PC 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Pr 22 A1 23 Nc 24 A1 25 Nc		1.79 E-02			emissions
7 FC 8 VO 9 VC 10 VC 11 VC 112 Be 113 A1 114 MC 115 PC 16 A1 117 Ar 118 A1 119 Ne 20 Ca 21 Pr 223 Nc 24 A1 25 Ni		3.11 E-01		No	emissions
8 Vo 9 Vo 10 Vo 11 Vo 12 Be 13 A1 14 Mo 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Pr 22 A1 22 A1 22 Ni	drocarbon gases	4.77	1.92		1.99
9 Voll 10 Voll 11 Voll 12 Be 13 Al 14 Mod 15 Po 16 Al 17 Ar 18 Al 19 Ne 20 Ca 21 Pr 22 Al 22 Al 22 Al 25 Ni	rmaldehyde				emissions
10 Vol 11 Vol 12 Be 13 A1 14 Mol 15 Po 16 A1 17 Ar 18 A1 19 Ne 20 Ca 22 A1 23 No 24 A1 25 Ni 12 Vol 12 No 25 Ni 12	latile organochlorines				emissions
11 Vc 12 Be 13 A1 14 Mc 15 Pc 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Pr 22 A1 22 A1 23 No 24 A1 25 No	latile carboxylic acids				emissions
12 Bee 13 A1	latile 0 & S heterocyclics				emissions
13 A1 14 Mo 15 Pc 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Pr 22 A1 23 Nc 24 A1 25 Ni	olatile N heterocyclics				emissions
14 Mo 15 Pc 16 Al 17 Ar 18 Al 19 Ne 20 Ca 21 Pr 22 Al 23 No 24 Al 25 Ni	nzene			No	emissions
15 Pc 16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Pr 22 A1 23 No 24 A1 25 Ni	iphatic/alicyclic hydrocarbons	1.29	33.4		2.38
16 A1 17 Ar 18 A1 19 Ne 20 Ca 21 Pr 22 A1 23 No 24 A1 25 Ni	no- or diaromatic hydrocarbons	2.96	1.72		3.44 E-
17 Ar 18 A1 19 Ne 20 Ca 21 Pr 22 A1 23 No 24 A1 25 Ni	lycyclic aromatic hydrocarbons	1.48	133		2.05
18 A1 19 Ne 20 Ca 21 Pr 22 A1 23 No 24 A1 25 Ni	iphatic amines			No	emissions
19 Ne 20 Ca 21 Pr 22 A1 23 No 24 A1 25 Ni	omatic amines	8.71 E-01	4.62		9.53
20 Ca 21 Pr 22 A1 23 No 24 A1 25 No	kaline N heterocyclics			No	emissions
21 Pr 22 A1 23 No 24 A1 25 Ni	eutral N, O, S heterocyclics	8.32 E-01	3.16 E-02		8.31 E-
22 A1 23 No 24 A1 25 No	rboxylic acids		• • • •	No	emissions
23 No 24 Al 25 Ni	enols	1.82	466		686
24 A1 25 Ni	dehydes and ketones				emissions
25 Ni	onheterocyclic organosulfur				emissions
	cohols				emissions
ひん ト c	troaromatics				emissions
	ters				emissions
	ides				emissions
	triles				emissions emissions
	ars	96.7			nulation in soil
	spirable particles senic	96.7 1.23 E-03	2200	no accur	nutation in Soil
•					
	ercury ickel	1.44 E-05 1.01	2.30 E-03 32000		2.30 E-0 213
		1.99 E-05	4.74		7.29 E-0
-	admium ead	1.01 E-03	766		7.29 E-1 8.51 E-1
•	her trace elements	0.0287		No accim	mulation in soil
	ner trace elements adioactive materials	0.0287			mulation in soil

Table 2.3-3. Maximum ambient atmospheric and soil concentrations for SRC-II Process.

RAC	RAC name	Annual average concentration in air (µg/m ³)	Concentration in soil (µg/kg)	Concentration i soil solution (µg	
1	Carbon monoxide	1.67	No ac	cumulation in soil	
2	Sulfur oxides	1.53		cumulation in soil	
3	Nitrogen oxides	8.30		cumulation in soil	
4	Acid gases			No emissions	
5	Alkaline gases			No emissions	
6	Hydrocarbon gases	3 . 72	1.50	1.55	
7	Formaldehyde			No emissions	
8	Volatile organochlorines			No emissions	
9	Volatile carboxylic acids			No emissions	
10	Volatile 0 & S heterocyclics	0.0622	2.55 E-03	2.13 E-	-03
11	Volatile N heterocyclics	0.234	1.18	2.43	
12	Benzene	0.12	0.0498	0.0383	
	Aliphatic/alicyclic hydrocarbons	2.10	54.3	3.88	
	Mono- or diaromatic hydrocarbons	2.07	1.20	0.241	
	Polycyclic aromatic hydrocarbons	0.463	41.6	0.640	
16	Aliphatic amines	0.00006	0.0005	No emissions 0.0422	
17	Aromatic amines	0.00386	0.0205	0.0422	
18 19	Alkaline N heterocyclics	0.0564 0.235	0.516 0.00892	0.198	5
	Neutral N, O, S neterocyclics	0.235	0.00692	No emissions	J
20 21	Carboxylic acids Phenols	0.784	201	295	
22	Aldenydes and ketones	0.704	201	No emissions	
23	Nonheterocyclic organosulfur			No emissions	
24	Alcohols			No emissions	
	Nitroaromatics			No emissions	
	Esters			No emissions	
27	Amides			No emissions	
28	Nitriles			No emissions	
29	Tars			No emissions	
30	Respirable particles	63.3	No a	ccumulation in soil	
31	Arsenic	4.84 E-04	14.5	7.24 E	
	Mercury	1.35 E-05	2.16 E-03	2.16 E	
33	Nickel	3.57 E-04	10.4	6.93 E	
34	Cadmium	1.68 E-05	8.41 E-02	1.29 E	
35	Lead	2.27 E-04	1.92	2.13 E	03
	Other trace elements	2.40 E-02	No a	ccumulation in soil	
37	Radioactive materials			No emissions	

Table 2.3-4. Maximum ambient atmospheric and soil concentrations for H-Coal Process

RAC	RAC name	Annual average concentration in air $(\mu g/m^3)$	Concentrati soil (μg,			.,	ration in tion (μg/L)
1	Carbon monoxide	0.679		No	accumulation in	soil	
2	Sulfur oxides	2.50		No	accumulation in	soi1	
3	Nitrogen oxides	3.18		No	accumulation in	soil	
4	Acid gases	7.65 E-03		No	accumulation in	soil	
5	Alkaline gases				No emissions		
	Hydrocarbon gases	5.74	2.31				2.39
7	Formaldehyde				No emissions		
8	Volatile organochlorines				No emissions		
9	Volatile carboxylic acids				No emissions		
10	Volatile 0 & S heterocyclics				No emissions		
11	Volatile N heterocyclics	0.103	0.516				1.06
12	Benzene				No emissions		
13	Aliphatic/alicyclic hydrocarbons	0.946	24.4				1.75
	Mono- or diaromatic hydrocarbons	4.63	2.69				0.537
15	Polycyclic aromatic hydrocarbons	0.0658	5.91				0.0909
	Alipnatic amines				No emissions		
	Aromatic amines	0.0285	0.152				0.313
	Alkaline N heterocyclics	0.0960	0.877				0.337
19	Neutral N, O, S heterocyclics	0.175	0.00664				0.00175
20	Carboxylic acids	0.556	8.86				7.38
21	Phenols	0.959	245			3	61
	Aldehydes and ketones				No emissions		
23	Nonheterocyclic organosulfur	0.0485	0.0581				0.0264
	Alcohols				No emissions		
25	Nitroaromatics				No emissions		
26	Esters				No emissions		
27	Amides				No emissions		
	Nitriles				No emissions		
29	Tars	50.4			No emissions		
	Respirable particles	58.4 3.10 E-04	307	NO	accumulation in	501 l	1 60
31	Arsenic						1.53
32 33	Mercury	1.77 E-05 1.12 E-03	2.83 E-03 1130				2.83 E-04
33 34	Nickel	1.12 E-03 1.84 E-04	23.2				7.51 3.57
34 35	Cadmium Lead	1.89 E-03	23 . 2 776				0.863
აი 36	Other trace elements	4.73 E-02		No	accumulation in	coil	0.003
30 37	Radioactive materials	1.20 E-02			accumulation in		

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 EPA water quality criteria (USEPA 1980a-p), EC_{20} (the effective concentration causing a designated effect on 20% of the test organisms), LOTC (lowest observed toxic concentration), TL_{m} (median tolerance limit), and LC_{50} (the concentration required to kill 50% of the test organisms).

Because this report compares potential toxic differences amoung groups of chemicals (RACs), benchmarks common to as many of the RACs as possible were preferred. The LC_{50} and TL_{m} (which are equivalent), were selected to represent acute toxicity (Table A-1). Chronic effects are presented as GMATCs (geometric mean maximum allowable toxicant concentrations, 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, a variety of 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, with the 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 (<u>Daphnia</u> species), with insect data presented when available. The fish species selected

are those usually used in toxicity testing, namely, fathead minnows (<u>Pimephales promelas</u>), bluegills (<u>Lepomis macrochirus</u>), and rainbow trout (<u>Salmo gairdneri</u>). Data for algal assays are sparse, so all species appearing in the literature, to our knowledge, were included in Table A-3.

Tables 3.1-1 to 3.1-4 present the highest quotients for each RAC and category of effect for the four direct liquefaction technologies. The acute toxicity quotients were calculated using the upper 95th percentile concentration (an estimate of the worst acute exposure, assuming stable plant operation). The chronic quotients were calculated using the annual median concentration, and the algal quotients were calculated for both concentrations because 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 in the reference stream.

Quotients are interpreted according to the best judgment of the analyst (Barnthouse et al. 1982a). A value of 0.01 (1.0 E-02) or less indicates little apparent environmental significance; 0.01 to 10 (1.0 E+01) suggests possible or potential adverse effects; and greater than 10 describes a chemical of probable environmental concern. The utility of these screening criteria must be confirmed by further experience in risk analysis and by field studies.

Ammonia (alkaline gases-RAC 5) appears to be the most serious ichthyotoxin in the effluents of all four technologies, with quotients for fish acute toxicity of 0.23 to 0.60 for both effluent treatments. Cadmium (RAC 34) also appears to be a general problem with fish quotients greater than 0.01 for acute toxicity in all technologies. Quotients greater than 0.01 for acute or chronic toxicity appeared in three technologies for aliphatic/alicyclic hydrocarbons (RAC 13) and phenols (RAC 21); in two technologies for mono- or diaromatic hydrocarbons (RAC 14), aldehydes and ketones (RAC 22), and mercury (RAC 32); and in one technology for polycyclic aromatic hydrocarbons (RAC 15) and esters (RAC 26). SRC-II has the most RACs (8) that appear problematical for effects on fish.

Table 3.1-1. Toxicity quotients for toxicity to fish and algae (ambient contaminant concentration/toxic benchmark concentration) for the Exxon Donor Solvent process

				lighest quotient ^a		
RAC No.	RAC name	Treatmentb	Fish acute 95%	Fish chronic Median	Median Al	gae 95%
1	Carbon monoxide		No effluent			
2	Sulfur oxides		No effluent			
3	Nitrogen oxides		No effluent			
4	Acid gases		No effluent			
5	Alkaline gases	1	3.69 E-01	No toxicity data	No toxicity	data
	•	2	3.69 E-01			
6	Hydrocarbon gases		No effluent			
7	Formaldehyde		No effluent			
8	Volatile organochlorines		No effluent			
9	Volatile carboxylic acids		No effluent			
10 11	Volatile 0 & S heterocyclics		No toxicity data			
12	Volatile N-heterocyclics	,	No toxicity data	No. 402024 do40	1 01 5 06	2.25 E-06
12	Benzene	1 2	2.23 E-04 2.23 E-05	No toxicity data	1.01 E-06 1.01 E-07	2.25 E-07
13	Aliphatic/alicyclic	ĺ	1.14 E-02	No toxicity data	No toxicity	
13	hydrocarbons	2	1.14 E-02	No coxicity data	NO LUXICILY	data
14	Mono- or diaromatic	ĺ	5.15 E-03	8.52 E-03	1.60 E-04	3.59 E-04
1.7	hydrocarbons	2	5.15 E-04	8.52 E-04	1.60 E-05	3.59 E-05
15	Polycyclic aromatic	ì	9.60 E-04	No toxicity data	3.84 E-07	7.06 E-07
	hydrocarbons	ż	9.60 E-05	no contenty data	3.84 E-08	7.05 E-08
16	Aliphatic amines	~	No effuent		0.0 00	7.00 - 00
17	Aromatic amines	1 2	No toxicity data	No toxicity dat.	4.67 E-02 4.67 E-03	1.05 E-01 1.05 E-02
18	Alkaline N heterocyclics		No effluent			
19	Neutral N, O, S heterocyclics		No toxicity data			
20	Carpoxylic acids	1	2.05 E-03	No toxicity data	No toxicity	data
		2	2.05 E-04		•	
21	Pheno1s	1	5.29 E-03	8.35 E-03	9.15 E-04	2.05 E-03
		2	5.29 E-04	8.35 E-04	9.15 E-05	2.05 E-04
22	Aldehydes and ketones	j	1.29 E-01	1.26 E-01	No toxicity	data
0.3	Newboden 15	2	1.20 E-02	1.25 E-02		
23 2 4	Nonheterocyclic organosulfur Alcohols		No toxicity data			
25	Nitroaromatics		No effluent No effluent			
26	Esters		No effluent			
27	Amides		No effluent			
28	Nitriles	1	2.43 E-03	4.22 E-03	No toxicity	data
		2	2.43 E-04	4.22 E-04	NO COXICICY	uata
29	Tars	-	No effluent	1122 2 04		
30	Respirable particles		No effluent			
31	Arsenic	1	1.43 E-06	1.71 E-06	3.68 E-06	8.25 E-06
		2	1.43 E-06	1.71 E-06	3.68 E-06	8.25 E-06
32	Mercury	1	3.84 E-04	1.79 E-02	5.13 E-05	1.15 E-04
		2	3.84 E-04	1.79 E-02	5.13 E-02	1.15 E-04
33	Nickel	1	3.47 E-05	6.53 E-04	7.12 E-04	1.60 E-03
2.4	Cadadaa	2	3.47 E-05	6.53 E-04	7.12 E-04	1.60 E-03
34	Cadmium	1	1.73 E-01	4.55 E-02	1.55 E-02	3.46 E-02
25	Load	2	1.73 E-01	4.55 E-02	1.55 E-02	3.46 E-02
35	Lead	1	3.05 E-04	4.30 E-03	1.63 E-04	3.66 E-04
36	Other trace elements	2	3.05 E-04	4.30 E-03	1.63 E-04	3.66 E-04
JU	Other trace elements (fluorine)	1 2	6.97 E-03 6.97 E-03	6.33 E-05 6.33 E-05	No toxicity	data

althe quotients are calculated using the lowest acute LC_{50} 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 (Tables 2.2-3 through 6).

 $^{^{\}mathrm{D}}$ The alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Table 3.1-2. Toxicity quotients for toxicity to fish and algae (ambient contaminant concentration/toxic benchmark concentration) for the SRC-I process

			F	lighest quotient ^a		
RAC No.	RAC Name T	reatmentb	Fish acute 95%	Fish chronic Median	Alg Median	95%
1	Carbon monoxide		No offloor		···	
2	Sulfur oxides		No effluent No effluent			
3	Nitrogen oxides		No effluent			
4	Acid gases		No effluent			
5	Alkaline gases	1	6.03 E-01	No toxicity data	No toxicity	data
•		2	6.03 E-01	no soxyovey ages	(nutrient)	
5	Hydrocarbon gases	-	No effluent		(1,221,121,17)	
7	Formaldehyde		No effluent			
8	Volatile organochlorines		No effluent			
9	Volatile carboxylic acids		No effluent			
10	Volatile 0 & S heterocyclics		No effluent			
11	Volatile N heterocyclics		No effluent			
12 13	Benzene	1	No effluent	No. Acres de Santa de Arre	No. 4-14-44.	
13	Alipnatic/alicyclic	1	1.14 E-02	No toxicity data	No toxicity	data
14	hydrocarbons Mono- or diaromatic	2 1	1.14 E-03 2.38 E-03	3.93 E-03	7.39 E-05	1.66 E-04
14	hydrocarbons	2	2.38 E-04	3.93 E-03	7.39 E-05 7.39 E-06	1.66 E-05
15	Polycyclic aromatic hydrocarbor		9.60 E-03	No toxicity data	3.84 E-06	7.06 E-06
13	Totycyclic alomacic hydrocarbon	2	9.60 E-04	no toxicity data	3.84 E-07	7.06 E-07
16	Aliphatic amines	_	No effluent		0.01 = 01	
17	Aromatic amines		No effluent			
18	Alkaline nitrogen heterocyclics	5	No effluent			
19	Neutral N, O, S heterocyclics		No toxicity data			
20	Carboxylic acids		No effluent			
21	Phenols]	2.53 E-02	3.99 E-02	4.37 E-03	9.79 E-03
	43 to to do a contra de cons	2	2.53 E-03	3.99 E-03	4.37 E-04	9.79 E-04
22 23	Aldehydes and ketones		No effluent No toxicity data			
24	Nonheterocyclic organosulfur Alcohols		No effluent			
25	Nitroaromatics		No effluent			
26	Esters		No effluent			
27	Amides		No effluent			
28	Nitriles		No effluent			
29	Tars		No effluent			
30	Respirable particles		No effluent			
31	Arsenic	1	2.22 E-06	2.64 E-06	5.70 E-06	1.28 E-05
		2	2.22 E-06	2.64 E-06	5.70 E-06	1.28 E-05
32	Mercury	1	2.18 E-03	1.02 E-01	2.92 E-04	6.55 E-04
		2	2.18 E-03	1.02 E-01	2.92 E-04	6.55 E-04
33	Nickel	1	3.60 E-05	6.77 E-04	7.38 E-04	1.65 E-03
		2	3.60 E-05	6.77 E-04	7.38 E-04 1.34 E-03	1.65 E-03 3.01 E-03
34	Cadmium	1	1.50 E-02	3.95 E-03 3.95 E-03	1.34 E-03	3.01 E-03
25	Land	2 1	1.50 E-02 4.26 E-03	6.00 E-02	2.28 E-03	5.11 E-03
35	Lead	2	4.26 E-03	6.00 E-02	2.28 E-03	5.11 E-03
26	Other trace elements	ì	2.43 E-03	2.21 E-05	No toxicity	
36	(fluorine)	2	2.43 E-03	2.21 E-05		·

 $^{^{}m a}$ The quotients are calculated using the lowest acute LC $_{
m 50}$ or TL $_{
m m}$ 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 (Table 2.2-4).

 $^{^{\}text{D}}$ The alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

 $\label{thm:concentration} \begin{tabular}{ll} Table 3.1-3. & Toxicity quotients for toxicity to fish and algae (ambient contaminant concentration/toxic benchmark concentration) for the SRC-II process \\ \end{tabular}$

				lighest quotient ^a		
RAC No.	RAC name	Treatment ^b	Fish acute 95%	Fish chronic Median	Median	95%
 1	Carbon monoxide		No effluent			
2	Sulfur oxides		No effluent			
3	Nitrogen oxides		No effluent			
4	Acid gases		No effluent			
5	Alkaline gases	1	3.35 E-01	No toxicity data	No toxicity	data
	•	2	3.35 E-01	_		
5	Hydrocarbon gases	1	1.57 E-08	No toxicity data	No toxicity	data
	3	2	1.57 E-09			
7	Formaldehyde	1	1.64 E-04	No toxicity data	No toxicity	data
	•	2	1.64 E-05			
8	Volatile organochlorines	1	1.60 E-04	1.63 E-03		
		2	1.60 E-05	1.63 E-04		
9	Volatile carboxylic acids	1	7.76 E-06	No toxicity data	No toxicity	data
	·	2	7.76 E-07			
10	Volatile O & S heterocyclics		No toxicity data			
11	Volatile N heterocyclics		No toxicity data			
12	Benzene	1	6.87 E-04	No toxicity data	3.10 E-06	6.93 E-06
		2	6.87 E-05		3.10 E-07	6.93 E-07
13	Aliphatic/alicyclic	1	3.90 E-05	No toxicity data	No toxicity	data
		2	3.90 E-06			
14	Mono- or diaromatic hydrocarbo	ns 1	1.43 E-02	2.36 E-02	4.43 E-04	9.94 E-04
		2	1.43 E-03	2.36 E-03	4.43 E-05	9.94 E-05
15	Polycyclic aromatic hydrocarbo		2.27 E-02	No toxicity data	9.07 E-06	1.67 E-05
		2	2.27 E-03		9.07 E-07	1.67 E-06
16	Aliphatic amines		No toxicity data			
17	Aromatic amines		No toxicity data			
18	Alkaline N heterocyclics		No effluent			
19	Neutral N, O, S heterocyclics		No toxicity data			
20	Carboxylic acids		No effluent			
21	Phenols	1	9.40 E-03	1.48 E-02	1.63 E-03	3.64 E-03
00		2	9.40 E-04	1.48 E-03	1.63 E-04	3.64 E-04
22 23	Aldehydes and ketones		No effluent			
24	Nonheterocyclic organosulfur		No toxicity data			
24 25	Alconols Nitroaromatics		No toxicity data			
26	Esters	,	No toxicity data	3 02 5 03	1 00 E 00	0 00 5 00
20	Esters	1 2	4.49 E-03	1.83 E-01	1.33 E-02	2.98 E-02
27	Amides	2	4.49 E-04	1.83 E-02	1.33 E-03	2.98 E-03
28	Nitriles		No effluent No effluent			
29	Tars		No effluent			
30	Respirable particles		No effluent			
31	Arsenic	1		3 00 5 06	C 00 C 06	1 20 5 05
31	Arsenic	2	2.43 E-06 2.43 E-06	2.89 E-06	6.22 E-06	1.39 E-05
32	Mercury	1		2.89 E-06	6.22 E-06	1.39 E-05
JŁ	riei cui y	2	1.58 E-03 1.58 E-03	7.09 E-02	2.04 E-04	4.57 E-04
33	Nickel	ĺ		7.00 E-02	2.04 E-04	4.57 E-04
33	HICKET	2	8.52 E-06 8.52 E-06	1.60 E-04	1.75 E-04	3.92 E-04 3.92 E-04
34	Cadmium	1		1.60 E-04	1.75 E-04	
JŦ	Caum Fulli	2	1.37 E-02	3.59 E-03	1.22 E-03	2.73 E-03
35	Lead	1	1.37 E-02	3.59 E-03	1.22 E-03	2.73 E-03
33	Lead	2	2.96 E-05 2.96 E-05	4.17 E-04	1.59 E-05	3.55 E-05 3.55 E-05
36	Other trace elements	1	1.54 E-02	4.17 E-04	1.59 E-05	
50	(fluorine)	2	1.54 E-02	1.40 E-04 1.40 E-04	No toxicity	uava

 $^{^{}a}$ The quotients are calculated using the lowest acute LC $_{50}$ 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 (Table 2.2-5).

 $^{^{\}text{D}}$ The alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Table 3.1-4. Toxicity quotients for toxicity to fish and algae (ambient contaminant concentration/toxic benchmark concentration) for the H-Coal process

	_	Highest quotient ^a					
RAC No.	RAC name	[reatmentb	Fish_acute 95%	Fish chronic Median	Algae Median 95%		
1	Carbon monoxide		No effluent				
ż	Sulfur oxides		No effluent				
3	Nitrogen oxides		No effluent				
4	Acid gases		No effluent				
5	Alkaline gases	1	3.35 E-01	No toxicity data	No toxicity data		
		2	3.35 E-01	-	_		
5	Hydrocarbon gases	_	No effluent				
7	Formaldehyde	1	4.37 E-04	No toxicity data	No toxicity data		
	V-1-423	2	4.37 E-05				
8	Volatile organochlorines		No effluent				
10	Volatile carboxylic acids		No effluent				
11	Volatile 0 & S heterocyclics		No toxicity data				
12	Volatile N heterocyclics Benzene	1	No toxicity data	No toudoitu data	1.28 E-07 2.86 E-07		
12	benzene	1 2	2.83 E-05 2.83 E-06	No toxicity data	1.28 E-07 2.86 E-03 1.28 E-08 2.86 E-08		
13	Aliphatic/alicyclic hydrocarbo		1.46 E-02	No tovicity data	No toxicity data		
13	Airpriatic/aircyclic nyurocarbo	2	1.46 E-02	No toxicity data	NO COXICILY data		
14	Mono-or diaromatic hydrocarbon		6.33 E-03	1.05 E-02	1.97 E-04 4.42 E-04		
14	mono-or diaromatic hydrocaroon	2	6.33 E-04	1.05 E-03	1.97 E-05 4.42 E-05		
15	Polycyclic aromatic hydrocarbo	-	1.22 E-03	No toxicity data	4.88 E-07 8.99 E-07		
13	rolycyclic aromatic nydlocarbo	2	1.22 E-04	No toxicity data	4.88 E-08 8.99 E-08		
16	Aliphatic amines	2	No effluent		4.00 1-00 0.99 1-00		
17	Aromatic amines	1		No toxicity data	5.69 E-02 1.28 E-0		
1.7	Al oliacic allities	2	no toxicity data	no toxicity data	5.69 E-03 1.28 E-02		
18	Alkaline N heterocyclics	L	No effluent		3.03 2-00 1.20 2 0.		
19	Neutral N. O. S heterocyclics		No toxicity data				
20	Carboxylic acids	7	2.53 E-03	No toxicity data	No toxicity data		
20	darboxy ric deras	ż	2.53 E-04	no commency comm	,,,,,,		
21	Phenols	ī	2.70 E-02	4.27 E-02	4.67 E-03 1.05 E-03		
21	Thenot 3	ż	2.70 E-03	4.27 E-03	4.67 E-04 1.05 E-0		
22	Aldehydes and ketones	ī	1.58 E-01	1.55 E-01	No toxicity data		
	madified and negoties	ż	1.58 E-02	1.55 E-02	,		
23	Nonheterocyclic organosulfur		No toxicity data				
24	Alcohols		No effluent				
25	Nitroaromatics		No effluent				
26	Esters		No effluent				
27	Amides		No effluent				
28	Nitriles	1	3.05 E-03	5.31 E-03	No toxicity data		
		2	3.05 E-04	5.31 E-04			
29	Tars		No effluent				
30	Respirable particles		No effluent				
31	Arsenic	l l	2.84 E-06	3.38 E-06	7.28 E-06 1.63 E-0		
31	711 30.110	2	2.84 E-06	3.38 E-06	7.28 E-06 1.63 E-0		
32	Mercury	ī	9.49 E-05	4.42 E-03	1.27 E-05 2.85 E-0		
02		2	9.49 E-05	4.42 E-03	1.27 E-05 2.85 E-0		
33	Nickel	ī	5.67 E-05	1.07 E-03	1.16 E-03 2.61 E-0		
33		ż	5.67 E-05	1.07 E-03	1.16 E-03 2.61 E-0		
34	Cadmium	ī	8.94 E-02	2.35 E-02	7.98 E-03 1.79 E-0		
J7	owani will	ż	8.94 E-02	2.35 E-02	7.98 E-03 2.79 E-0		
35	Lead	ī	6.66 E-04	9.38 E-03	3.56 E-04 7.99 E-0		
55		2	6.66 E-04	9.38 E-03	3.56 E-04 7.99 E-0		
36	Other trace elements	ī	7.00 E-04	6.35 E-06	No toxicity data		
50	(fluorine)	ż	7.00 E-04	6.35 E-06			

^aThe quotients are calculated using the lowest acute LC_{50} 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 (Table 2.2-6).

 $^{^{\}mathrm{D}}$ The alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Fewer RACs appear to be important for algal toxicity due to both the shortage of algal toxicity data and the relative insensitivity of algae to several tested RACs. Aromatic amines (RAC 17) may be toxic in EDS and H-Coal effluents, with quotients greater than 0.1 for acute exposures and 0.01 for chronic exposures. Cadmium may also be toxic in EDS and H-Coal effluents, and phenols (RAC 21) and esters (RAC 26) may be toxic in effluents from H-Coal and SRC-II, respectively.

Barnthouse et al. (1982a) 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 (RACs 33, 34, and 35), water hardness is important in determining the concentrations of these metals required to elicit a toxic response (Table 3.1-1), a fact reflected in the EPA 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 field exposures requires a series of extrapolations, each of which is made with some error (Barnthouse et al. 1982a; Suter et al. 1983). 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 et al. (1983). Acute toxicity data from the Columbia National Fisheries Research Laboratory (Johnson and Finley 1980) are used for the extrapolation between species. Life-cycle toxicity data (Suter et al., 1983) were used to develop a regression relationship between acute and chronic toxicity data. Variances associated with extrapolating acute toxicity between taxa and acute to chronic toxicity are accumulated to provide an estimate of the variability associated with the estimate of chronic toxicity and used in obtaining estimates of risk, given estimates of the distribution of the ambient contaminant concentrations.

All of the emitted RACs for which $96-h\ LC_{50}$'s could be found (Table A-1) have been analyzed by the extrapolation error method. The quotient of the ratio of the ambient concentration of an RAC to its predicted GMATC (PGMATC) is presented as an estimate of the hazard of 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 (Tables 2.2-3 through 6).

In general, the extrapolation between species was done 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 datum available for hydrogen sulfide (RAC 4) and for fluoranthene (RAC 15) was for bluegill sunfish (Lepomis macrochirus); and the only acute toxicity datum available for indan (RAC 13) and for quinoline (RAC 18) was for fathead minnow (Pimephales promelas). Difficulties also arose with RAC 15 for estimating the acute toxicity of white bass (Morone chrysops) and with RAC 13 for estimating the acute toxicity of bigmouth and smallmouth buffalo (Ictiobus cyprinellus and I. bubalus). The problem arose because no fish in the family Percichthyidaea or in the genus Ictiobus were tested at the Columbia National Fisheries Research Laboratory. The genus Ictiobus is in the family Catostomidae, members of which were 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 with all Perciformes other than bluegills ($R^2 = 0.91$) and fathead minnow with all Cypriniformes other than fathead minnow ($R^2 = 0.92$).

3.2.2 Results

The species-specific values of the predicted GMATCs, quotients, and the risks of exceeding the GMATC for the annual median ambient contaminant concentrations are presented in Appendix D. These species-specific values are only presented for those RACs with a hazard greater than or equal to 0.01. They are summarized in Tables 3.2-1 through 3.2-4 for the four technologies. Ammonia (RAC 5) appears to present the most consistent threat of chronic toxicity to fish, with quotients and risks greater than 0.1 for all species, technologies, and water treatments. For SRC-I, the predicted GMATC for ammonia slightly exceeds the ambient median concentration for five out of nine fish

Table 3.2-1. Ranges of ratios of ambient concentrations to PGMATCs and probabilities of exceeding the PGMATC for Exxon Donor Solvent $^{\mathtt{a}}$

	Ambient concentrat	ion/PGMATC	Probability of ex	ceeding the PGMATC
RAC	treatment1 ^b	treatment2	treatmentl	treatment2
1	No effluent			
2	No effluent			
3 4	No effluent No effluent			
5	0.2572-0.6205	0.2572-0.6205	0.2616-0.4039	0.2616-0.4039
6	No effluent	0.23/2-0.0203	0.2010-0.4039	0.2010-0.4039
6 7 8	No effluent			
8	No effluent			
9	No effluent			
10	No fish toxicity data			
11	No fish toxicity data			
12	0.0013-0.0046	0.0001-0.0005	0.0003-0.0072	0.0000-0.0003
13	0.2786-1.0832	0.0279-0.1083	0.2530-0.5145	0.0312-0.1557
14	0.0362-0.0813	0.0036-0.0081	0.0497-0.1063	0.0021-0.0121
15 16	0.0001-0.0010 No effluent	0.0000-0.0001	0.0000-0.0008	0.0000-0.0000
17	No fish toxicity data			
18	No effluent			
19	No fish toxicity data			
20	0.0034-0.1147	0.0003-0.0115	0.0047-0.3107	0.0001-0.1540
21	0.0396-0.3539	0.0040-0.0354	0.0478-0.3230	0.0020-0.0698
22	0.2082-1.1049	0.0208-0.1105	0.2241-0.5182	0.0225-0.1561
23	No fish toxicity data			
24	No effluent			
25	No effluent			
26	No effluent			
27	No effluent		2 2442 2 2225	0.0010.0.0540
28	0.0282-0.2706	0.0028-0.0271	0.0449-0.2805	0.0013-0.0542
29	No effluent			
30	No effluent	0.0000 0.0001	0.0000-0.0000	0.0000-0.0000
31	0 0000-0.0001	0.0000-0.0001 0.0001-0.0003	0.0000-0.0001	0.0000-0.0001
32 32A	0.0001-0.0003 0.0004-0.0009	0.0004-0.0009	0.0001-0.0003	0.0001-0.0003
32A 33	0.0004-0.0009	0.0001-0.0027	0.0001-0.0003	0.0000-0.0040
33 34	0.0010-0.1468	0.0010-0.1468	0.0000-0.1692	0.0000-0.1692
35	0.0002-0.0015	0.0002-0.0015	0.0000-0.0017	0.0000-0.0017
55	0,000 0101.0			

aSpecies-specific values are provided in Appendix D.
bThe alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Table 3.2-2. Ranges of ratios of ambient concentrations to PGMATCs and probabilities of exceeding the PGMATC for SRC-I $^{\rm a}$

	Ambient concentrat	TOTT/ PGMATC	Probability of exceeding the PGMA			
R AC	treatmentl ^b	treatment2	treatment1	treatment2		
1	No effluent					
2 3 4 5 6	No effluent					
3	No effluent					
4	No effluent	0 420 3 02	0 242 0 5021	0.342-0.5031		
5	0.420-1.02	0.420-1.02	0.342-0.5031	0.342-0.5031		
6	No effluent					
7	No effluent					
8	No effluent					
9	No effluent					
10	No effluent					
11 12	No effluent No effluent					
13	0.2786-1.0832	0.0279-0.1083	0.2530-0.5145	0.0312-0.1557		
		0.0279-0.1083	0.0199-0.0565	0.0005-0.0048		
14 15	0.0167-0.0375 0.0011-0.0095	0.0001-0.0010	0.0199-0.0363	0.0000-0.0008		
16	No effluent	0.0001-0.0010	0.0002-0.0171	0.0000-0.0000		
17	No effluent					
18	No effluent					
19	No fish toxicity data					
20	No effluent					
21	0.1890-1.6908	0.0189-0.1691	0.1951-0.5918	0.0203-0.2150		
22	No effluent					
23	No fish toxicity data					
24	No effluent					
25	No effluent					
26	No effluent					
27	No effluent					
28	No effluent					
29	No effluent					
30	No effluent	0 0000 0 0000				
31	0.0000-0.0002	0.0000-0.0002	0.0000-0.0001	0.0000-0.0001		
32 32A	0.0007-0.0017 0.0020-0.0052	0.0007-0.0017	0.0003-0.0010	0.0003-0.0010		
32A 33	0.0001-0.0028	0.0020-0.0052	0.0017-0.0038	0.0017-0.0038		
33 34	0.0001-0.0028	0.0001-0.0028 0.0001-0.0128	0.0000-0.0042	0.0000-0.0042		
35	0.0001-0.0128	0.0001-0.0128	0.0000-0.0147	0.0000-0.0147		
J	0.0020-0.0212	0.0028-0.0212	0.0005-0.0380	0.0005-0.0380		

^aSpecies-specific values are provided in Appendix D.

^bThe alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Table 3.2-3. Ranges of ratios of ambient concentrations to PGMATCs and probabilities of exceeding the PGMATC for SRC-IIa

	Ambient concentrat	ion/PGMATC	Probability of exceeding the PGM		
RAC	treatment1 ^b	treatment2	treatmentl	treatment2	
1	No effluent				
2	No effluent				
3	No effluent				
4	No effluent				
5 6	0.2334-0.5639	0.2334-0.5639	0.2472-0.3851	0.2472-0.3851	
6	0.0000-0.0000	0.0000-0.0000	0.0000-0.0073	0.0000-0.0020	
7	No fish toxicity data	0.0000 0.0010	0 0004 0 0400	0 0000 0 0000	
8 9	0.0016-0.0177 0.0000-0.0003	0.0002-0.0018 0.0000-0.00000	0.0004-0.0402 0.0000-0.0000	0.0000-0.0030 0.0000-0.0000	
10	No fish toxicity data	0.0000-0.00000	0.0000-0.0000	0.0000-0.0000	
ii	No fish toxicity data				
12	0.0039-0.0140	0.0004-0.0014	0.003-0.0251	0.0000-0.0015	
13	0.0010-0.0037	0.0001-0.0004	0.0001-0.0054	0.0000-0.0002	
14	0.1002-0.2251	0.0100-0.0225	0.1335-0.2242	0.0100-0.0353	
15	0.0026-0.0225	0.0003-0.0022	0.0011-0.0421	0.0000-0.0028	
16	No effluent				
17	No fish toxicity data				
18	No effluent				
19	No fish toxicity data				
20	No effluent		0.0055.0.4300	0 0050 0 1107	
21	0.0704-0.6293	0.0070-0.0629	0.0856-0.4189	0.0053-0.1107	
22	No effluent				
23	No fish toxicity data				
24	No fish toxicity data				
25 26	No fish toxicity data 0.0051-0.1813	0.0005-0.0181	0.0070-0.2178	0.0002-0.0336	
27	No effluent	0.0003-0.0181	0.00/0-0.21/0	0.0002-0.0330	
28	No effluent				
29	No effluent				
30	No effluent				
31	0.0000-0.0002	0.0000-0.0002	0.0000-0.0001	0.0000-0.0001	
32	0.0005-0.0012	0.0005-0.0012	0.0002-0.0006	0.0002-0.0006	
32A	0.0014-0.0036	0.0014-0.0036	0.0010-0.0022	0.0010-0.0022	
33	0.0000-0.0007	0.0000-0.0007	0.0000-0.0005	0.0000-0.0005	
34	0.0001-0.0116	0.0001-0.0116	0.0000-0.0131	0.0000-0.0131	
35	0.0000-0.0001	0.0000-0.0001	0.0000-0.0000	0.0000-0.0000	

aSpecies-specific values are provided in Appendix D. bThe alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Table 3.2-4. Ranges of ratios of ambient concentrations to PGMATCs and probabilities of exceeding the PGMATC for H-Coal^a

	Ambient concentrat	ion/PGMATC	Probability of ex	ceeding the PGMATC
RAC	treatment1 ^b	treatment2	treatmentl	treatment2
1	No effluent			
2 3 4	No effluent			
<u>ح</u>	No effluent			
4 5	No effluent 0.2338-0.05639	0.2338-0.5639	0.2472-0.3851	0.2472-0.3851
5	No effluent	0.2330-0.3039	0.24/2-0.3031	0.2472-0.3031
6 7	No fish toxicity data			
8	No effluent			
9	No effluent			
10	No fish toxicity data			
ii	No fish toxicity data			
12	0.0002-0.0006	0.0000-0.0001	0.0000-0.0004	0.0000-0.0000
13	0.3582-1.3927	0.0358-0.1393	0.2966-0.5599	0.0416-0.1847
14	0.0445-0.1001	0.0045-0.0100	0.0620-0.1239	0.0030-0.0152
15	0.0001-0.0012	0.0000-0.0001	0.0000-0.0011	0.0000-0.0000
16	No effluent			
17	No fish toxicity data			
18	No effluent			
19	No fish toxicity data	0.0004.0.0140		
20	0.0042-0.1416	0.0004-0.0142	0.0063-0.3278	0.0002-0.1657
21 22	0.2022-1.8089 0.2563-1.3601	0.0202-0.1809 0.0256-0.1360	0.2048-0.6034 0.2592-0.5561	0.0221-0.2248 0.0292-0.1800
23	No fish toxicity data	0.0230-0.1300	0.2392-0.3301	0.0292-0.1800
24	No effluent			
25	No effluent			
26	No effluent			
27	No effluent			
28	0.0355-0.3407	0.0036-0.0341	0.0586-0.3160	0.0021-0.0664
29	No effluent			
30	No effluent			
31	0.0000-0.0003	0.0000-0.0003	0.0000-0.0001	0.0000-0.0001
32	0.0000-0.0001	0.0000-0.0001	0.0000-0.0000	0.0000-0.0000
32A	0.0001-0.0002	0.0001-0.0002	0.0000-0.0000	0.0000-0.0000
33 34	0.0001-0.0044	0.0001-0.0044	0.0000-0.0075	0.0000-0.0075
3 4 35	0.0005-0.0758 0.0004-0.0033	0.0005-0.0758	0.0000-0.0990	0.0000-0.0990
33	0.0004-0.0033	0.0004-0.0033	0.0000-0.0048	0.0000-0.0048

^aSpecies-specific values are provided in Appendix D.

^bThe alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

species so the risk is greater than 0.5. Four organic RACs, aliphatic/alicyclic hydrocarbons (RAC 13), mono- or diaromatic hydrocarbons (RAC 14). phenols (RAC 21), and aldehydes and ketones (RAC 22), have high quotients and risks for treatment 1 for at least 2 of the technologies. However, use of treatment 2 reduces the concentration of all of these RACs by an order of magnitude so that only RACs 13, 21, and 22 have hazards exceeding 0.1 and none exceed 1. The only other RAC with hazard or risk values exceeding 0.1 for both treatments is cadmium (RAC 34) for EDS. The only other RACs with hazard or risk values greater than 0.1 for any combination of species, technology, and treatment are carboxylic acids (RAC 20) for EDS and H-Coal, esters (RAC 26) for SRC-II, and nitriles (RAC 28) for EDS and H-Coal.

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 tested for a particular chemical, (2) differences in sensitivity of the site species expressed as biases in the extrapolation between the test species and site species, and (3) the variance associated with the extrapolation.

3.2.3 Toxicity of the Whole Effluent

Tables 3.2-5 to 3.2-8 present a consideration of the acute toxicity of the whole effluent. Only acute toxicity is considered because there is no accepted theory for modeling addition of effects expressed as toxic thresholds such as GMATCs. The acute effects are expressed in a common unit, the 96-h LC_{50} to largemouth bass, which is generated by taxonomic extrapolation from LC_{50} data for a variety of species (Appendix A) using the method of Suter et al. (1983).

The possible modes of joint action of chemicals are synergism, concentration addition, independent action (response addition), and antagonism (Muska and Weber 1977). Concentration addition is generally accepted to be the best general model for combined effects of mixed chemicals on fish (Alabaster and Lloyd 1982; EIFAC 1980; SGOMSEC, in press). In a recent review, Lloyd (in press) stated "There is no evidence for synergism (i.e., more-than-additive action) between the

Table 3.2-5. Estimated acute LC $_{50}$ for largemouth bass and ratio of upper 95th percentile of the ambient concentration to the LC $_{50}$ for Exxon Donor Solvent

RAC		Concentration/LC ₅₀				
	LC ₅₀ (μg/L)	Treatment la	Treatment 2			
]	No toxicity data					
2 3 4 5 6 7	No toxicity data					
3 1	No toxicity data 36.3	No effluent				
5	444	5.64 E-02	5.64 E-02			
6	5,716,048	No effluent				
7	No toxicity data					
8	52,048	No effluent				
9	10,511	No effluent				
10	No toxicity data					
11	No toxicity data	0.45 5.04	2 46 5 05			
12	4,815	2.46 E-04	2.46 E-05			
13	2,324	6.85 E-02 5.16 E-03	6.85 E-03 5.16 E-04			
14 15	2,296 3,310	1.16 E-05	1.16 E-06			
16	No toxicity data	1.10 L=03	1.10 L=00			
17	No toxicity data					
18	6,171	No effluent				
19	No toxicity data					
20	184,876	1.99 E-03	1.99 E-04			
21	14,282	2.87 E-03	2.87 E-04			
22	160	3.70 E-02	3.70 E-03			
23	No toxicity data					
2 4 25	No toxicity data					
25 26	No toxicity data 601	No effluent				
27	No toxicity data	no errident				
28	9,437	2.60 E-03	2.60 E-04			
29	No toxicity data	2000 2 00	2,000 2 0.			
30	No toxicity data					
31	22,236	8.61 E-07	8.61 E-07			
32	321	2.87 E-05	2.87 E-05			
32A	74.6	1.23 E-04	1.23 E-04			
33	4,496	3.55 E-05	3.55 E-05			
34 ∙35	1,696 20,865	1.02 E-04	1.02 E-04			
J J	20,003	8.78 E-06	8.78 E-06			
Total		1.75 E-01	6.85 E-02			

^aThe alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Table 3.2-6. Estimated acute LC $_{50}$ for largemouth bass and ratio of upper 95th percentile of the ambient concentration to the LC $_{50}$ for SRC-I

RAC		Concentration/LC ₅₀				
	LC ₅₀ (μg/L)	Treatment 1a	Treatment 2			
1	No toxicity data					
2 3 4 5 6 7	No toxicity data					
3	No toxicity data					
4	36.3	No effluent	0.00 = 00			
5	444	9.23 E-02	9.23 E-02			
6	5,716,048	No effluent				
	No toxicity data	N = - CC1				
8	52,048	No effluent				
9	10,511	No effluent				
10 11	No toxicity data					
12	No toxicity data 4,815	No effluent				
13	2,324	6.85 E-02	6.85 E-03			
14	2,296	2.38 E-03	2.38 E-04			
15	3,310	1.16 E-04	1.16 E-05			
16	No toxicity data	1010 2 01	2 00			
17	No toxicity data					
18	6,171	No effluent				
19	No toxicity data					
20	184,876	No effluent				
21	14,282	1.37 E-02	1.37 E-03			
22	160	No effluent				
23	No toxicity data					
24	No toxicity data					
25	No toxicity data	No offloort				
26	601	No effluent				
27	No toxicity data	No effluent				
28	9,437 No toxicity data	NO ETT TUETO				
29	No toxicity data					
30 31	22,236	1.33 E-06	1.33 E-06			
32	321	1.63 E-04	1.63 E-04			
32A	74.6	7.02 E-04	7.02 E-04			
33	4,496	3.68 E-05	3.68 E-05			
34	1,696	8.87 E-06	8.87 E-06			
35	20,865	1.22 E-04	1.22 E-04			
Total		1.78 E-01	1.02 E-01			

aThe alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Table 3.2-7. Estimated acute LC50 for largemouth bass and ratio of upper 95th percentile of the ambient concentration to the LC50 for SRC-II

RAC		Concentration/LC ₅₀				
	LC ₅₀ (µg/ L)	Treatment 1ª	Treatment 2			
1	No toxicity data					
2 3 4 5 6 7 8	No toxicity data No toxicity data					
4	36.3	No effluent				
5	444	5.13 E-02	5.13 E-02			
6	5,716,048	1.36 E-08	1.36 E-09			
7	No toxicity data	0 40 7 05	0 40 5 00			
8	52,048	8.40 E-05	8.40 E-06 6.50 E-06			
9 10	10,511 No toxicity data	6.50 E-05	0.30 E-00			
10	No toxicity data					
12	4,815	7.56 E-04	7.56 E-05			
13	2,324	2.35 E-04	2.35 E-05			
14	2,296	1.43 E-02	1.43 E-03			
15	3,310	2.74 E-04	2.74 E-05			
16	No toxicity data					
17 18	No toxicity data	No effluent				
19	6,171 No toxicity data	No errident				
20	184,876	No effluent				
21	14,282	5.10 E-03	5.10 E-04			
22	160	No effluent				
23	No toxicity data					
24	No toxicity data					
25 26	No toxicity data 601	5.45 E-03	E 4E F 04			
27	No toxicity data	5.45 E-US	5.45 E-04			
28	9,437	No effluent				
29	No toxicity data					
30	No toxicity data					
31	22,236	1.45 E-06	1.45 E-06			
32	321	1.14 E-04	1.14 E-04			
32A 33	74.6	4.90 E-04	4.90 E-04			
34	4,496 1,696	8.72 E-06 8.06 E-06	8.72 E-06 8.06 E-06			
35	20,865	8.52 E-07	8.52 E-07			
Total		7.82 E-02	5.45 E-02			

^aThe alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

Table 3.2-8. Estimated acute LC_{50} for largemouth bass and ratio of upper 95th percentile of the ambient concentration to the LC_{50} for H-Coal

RAC		Concentration/LC ₅₀			
	LC ₅₀ (µg/L)	Treatment la	Treatment 2		
1	No toxicity data				
2 3 4 5 6 7 8 9	No toxicity data				
3	No toxicity data	N= -661			
4	36.3	No effluent	E 12 E 02		
5	444	5.13 E-02	5.13 E-02		
0 7	5,716,048	No effluent			
0	No toxicity data 52,048	No effluent			
Q Q	10,511	No effluent			
10	No toxicity data	No critacit			
11	No toxicity data				
12	4,815	3.12 E-05	3.12 E-06		
13	2,324	8.81 E-02	8.81 E-03		
14	2,296	6.35 E-03	6.35 E-04		
15	3,310	1.48 E-05	1.48 E - 06		
16	No toxicity data				
17	No toxicity data				
18	6,171	No effluent			
19	No toxicity data	2 46 5 02	2 46 5 04		
20	184,876	2.46 E-03 1.47 E-02	2.46 E-04 1.47 E-03		
21 22	14 , 282 160	4.55 E-02	4.55 E-03		
23	No toxicity data	4.55 L-02	4.55 £ 65		
24	No toxicity data				
25	No toxicity data				
26	601	No effluent			
27	No toxicity data				
28	9,437	3.28 E-03	3.28 E-04		
29	No toxicity data				
30	No toxicity data		05		
31	22,236	1.70 E-06	1.70 E-06		
32	321	7.10 E-06	7.10 E-06		
32A	74.6	3.05 E-05	3.05 E-05 5.80 E-05		
33	4,496	5.80 E-05	5.27 E-05		
34	1,696	5.27 E-05 1.91 E-05	1.91 E-05		
35	20,865	1.91 L=05	1.51 6-05		
Total		2.12 E-01	6.75 E-02		

aThe alternate effluent treatments are: (1) steam stripping/ammonia recovery, phenol extraction, and biological oxidation; and (2) treatment 1 plus carbon adsorption.

common pollutants; at toxic concentrations the joint action is additive and at concentrations below those considered 'safe' there is circumstantial evidence for less-than-additive joint action." Furthermore, Parkhurst et al. (1981) found that when ammonia speciation was accounted for, the toxicity of the major components of synfuels effluents was concentration additive. Therefore, we use the concentration addition model to examine the potential toxicity of the combined RACs.

The analysis was performed by calculating the total toxic units (ΣTU) of the effluent, where a toxic unit is the concentration of a toxiciant divided by the threshold LC_{50} (Sprague and Ramsey 1965). We used the upper 95th percentile of the predicted ambient concentration since the concern in this case is with acute lethality, and we use the 96-h LC_{50} as a reasonable approximation of the threshold LC_{50} (Ruesink and Smith 1975). The ΣTU values for the eight combinations of liquefaction technologies and effluent treatment ranged from 0.0545 to 0.212. The highest value is for treatment 1 of H-Coal effluent and is primarily due to the summation of RACs 5, 13, and 22 (alkaline gases, aliphatic/alicyclic hydrocarbons, phenols, and aldehydes and ketones). While these values do not suggest that acute lethality of post-larval fish would be caused by these effluents, they indicate that the toxicity of the total effluent could be considerably higher than that of any one RAC and suggest that sublethal effects or mortality of sensitive life stages due to direct liquefaction effluents may be a problem.

These results can be compared with results of tests for <u>Daphnia</u> acute lethality in diluted SRC and H-Coal effluent treated in bench-scale facilities (Bostick et al. 1982). The <u>Daphnia magna</u> 48-h LC_{50} for steam-stripped and bio-oxidized SRC effluent (equivalent to treatment 1 but without phenol extraction) was 2.4% effluent and for effluent additionally ozonated and carbon filtered (treatment 2 only adds carbon filtration) was 4.7% effluent. The <u>D. magna</u> LC_{50} for steam-stripped and solvent-extracted H-Coal effluent (only roughly equivalent to treatment 1) was 4.4% effluent and with additional ozonation and carbon filtration was 3.2% effluent (ozonation increased

the toxicity). For comparison, our model generates an exposure in the first river reach equivalent to 0.4% effluent. Thus our predicted exposure is approximately an order of magnitude lower than the acute toxic concentration to <u>Daphnia</u> of bench-treated effluent. This result is consistent with the ΣTU values shown in Tables 3.2-5 to 3.2-8 which are approximately one-tenth of those for a largemouth bass LC_{50} .

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 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 10 phytoplankton, 5 zooplankton, 3 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 are primarily in the form of mortalities. Therefore, assumptions about the mode of action of the toxicant are required to determine appropriate changes in model parameters. We assumed that organisms respond to all chemicals according to a general stress syndrome (GSS). That is, they increase respiration rates, decrease photosynthetic and grazing rates, become more susceptible to predation, etc. This assumption permits us to define percent changes in model parameters that cause the same mortality as that 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 for the EUA are shown in Table 3.3-1. Estimates of risk can be made for nine RAC. These RACs were the only chemical groups for which adequate data exist.

3.3.2 Results of Ecosystem Uncertainty Analysis

Results of the risk analysis for the direct liquefaction technologies are shown in Fig. 3.3-1 to 3.3-4 and deterministic results are shown in Table 3.3-2. None of the technologies produces measureable amounts of quinoline (RAC 18), and this risk assessment unit will not be considered in the analysis. Environmental concentrations of benzene (RAC 12), arsenic (RAC 31), and nickel (RAC 33) were very low and did not result in significant risks. Therefore, results for these three chemicals are not shown on the graphs.

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 chosen as indicative of minimal effects that could be noticed in the field. Risk values were calculated for these endpoints across a range of environmental concentrations that encompass the 5th to 95th percentile exposures. The range of exposures for each technology is shown at the bottom of the figures.

The lines on the graph do not pass through the origin because there is a risk of an increase in algae (0.086) or a decrease in fish biomass (0.038), even as the environmental concentrations of the toxicants approach zero. This reflects residual uncertainty in simulating ecosystem effects. For example, there is always some probability of a small decrease in fish biomass due to natural variability.

Results for naphthalene, phenol, mercury, and lead show a similar pattern. In all of these cases, there is an upturn in the risk curves,

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

Trophic Level	Model species	Ammonia	Benzene	Naphthalene	Quinoline	Phenol	Arsenic	Nickel	Cadmium	Lead	Mercury
Algae	1-3	420.0	525.0	33.0	25.0	258.0	2.32	0.50	0.16	0.50	0.01
	4-7	420.0	525.0	33.0	25.0	20.0	2.32	0.50	0.06	0.50	0.01
	8-10	420.0	525.0	33.0	117.0	95.0	2.32	0.50	0.06	0.50	0.01
Zooplankton	11	8.0	450.0	8.6	57.2	300.0	4.47	9.67	0.5	40.8	0.78
	12	8.0	380.0	8.6	28.5	36.4	5.28	0.85	0.0099	0.45	0.005
	13	8.0	300.0	6.5	48.2	58.1	1.35	1.93	0.14	27.4	0.53
	14	8.0	233.8	4.5	39.3	157.0	2.49	4.91	0.25	14.0	0.27
	15	8.0	17.6	2.5	30.3	14.0	0.51	0.15	0.0035	0.67	0.01
Forage fish	16	1.1	33.0	6.6	1.5	36.0	15.6	4.87	0.63	4.61	0.15
	17	8.2	22.0	78.3	1.5	16.4	41.8	5.27	1.94	23.8	0.24
	18	23.7	34.0	150.0	1.5	34.9	26.0	4.45	1.63	31.5	0.50
Game fish	19	0.41	5.3	2.3	11.0	9.0	13.3	0.05	0.002	1.17	0.25

aValues taken from following documents: ammonia - Hohreiter (1980); benzene - USEPA (1980c); naphthalene - USEPA (1980e); quinoline - O'Neill et al. (1982); phenol - USEPA (1980g); arsenic - USEPA (19801); nickel - USEPA (1980n); cadmium - USEPA (1980o); lead - USEPA (1980p); and mercury - USEPA (1980m).

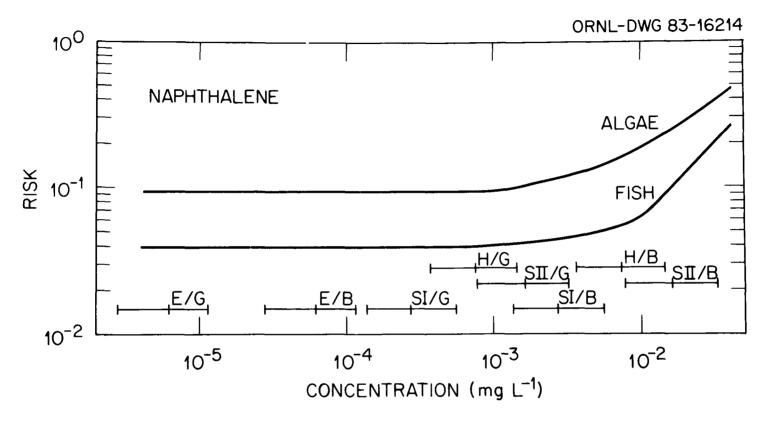


Fig. 3.3-1. Risk estimates for naphthalene (RAC 14) over a range of environmental concentrations. The 5th percentile, mean, and 95th percentile concentrations associated with the Exxon (E), H-Coal (H), SRC-I (SI), and SRC-II (SII) technologies are shown at the bottom of the graph. The notation /B and /G refer to the biologic and GAC methods (treatment options 1 and 2) for each technology. The plotted values are the probability of a quadrupling of the blue-green algal bloom and a 25% reduction in game fish biomass.

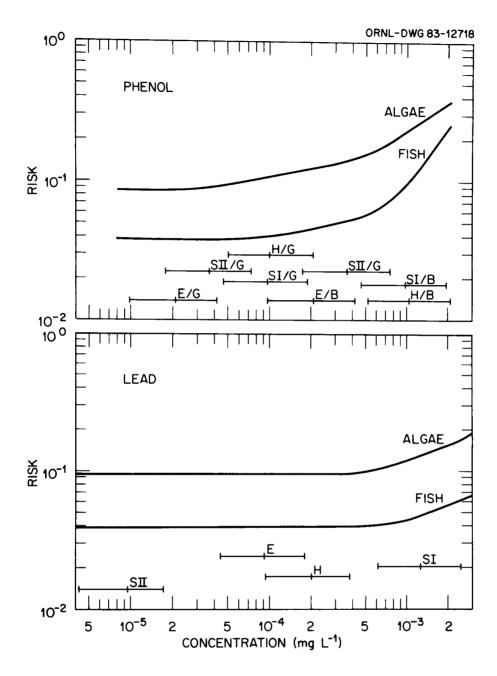


Fig. 3.3-2. Risk estimates for phenol (RAC 21) and lead (RAC 35) over a range of environmental concentrations. The 5th percentile, mean, and 95th percentile concentrations associated with the Exxon (E), H-Coal (H), SRC-I (SI), and SRC-II (SII) technologies are shown at the bottom of the graph. The notation /B and /G refer to the biologic and GAC methods (treatment options 1 and 2) for each technology. The plotted values are the probability of a quadrupling of the blue-green algal bloom and a 25% reduction in game fish biomass.

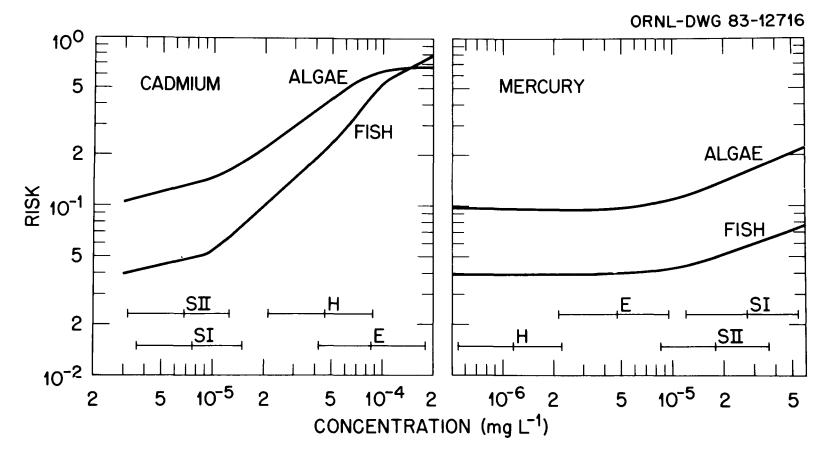


Fig. 3.3-3. Risk estimates for cadmium (RAC 34) and mercury (RAC 32) over a range of environmental concentrations. The 5th percentile, mean, and 95th percentile concentrations associated with the Exxon (E), H-Coal (H), SRC-I (SI), and SRC-II (SII) technologies are shown at the bottom of the graph. The plotted values are the probability of a quadrupling of the blue-green algal bloom and a 25% reduction in game fish biomass.

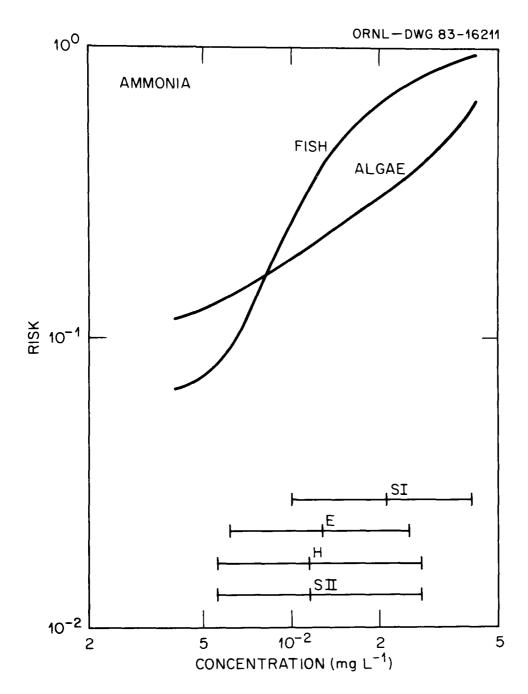


Fig. 3.3-4. Risk estimates for ammonia (RAC 5) over a range of environmental concentrations. The 5th percentile, mean, and 95th percentile concentrations associated with the Exxon (E), H-Coal (H), SRC-I (SI), and SRC-II (SII) technologies are shown at the bottom of the graph. The plotted values are the probability of a quadrupling of the blue-green algal bloom and a 25% reduction in game fish biomass.

Table 3.3-2. Deterministic results of ecosystem uncertainty analyses. Values are percent increases in maximum algal bloom and percent decrease in game fish biomass at the mean environmental concentration for each of the direct liquefaction technologies. When two values are given, the first is for treatment 1 and the second value (in parentheses) is treatment 2.

	Algae	EXXON	H-Coal	SRC-I	SRC-II
Ammonia	Algae	80	66	176	66
	Fish	17	14	32	14
Benzene	Algae	a (a)	a (a)	b] (a)
	Fish	a (a)	a (a)	b	a (a)
Naphthalene	Algae	42 (2)	53 (3)	17 (a)	124 (9)
	Fish	2 (^a)	3 (^a)	1 (a)	6 (^a)
Pheno l	Algae	14 (a)	87 (6)	77 (6)	25 (2)
	Fish	2 (a)	8 (^a)	8 (^a)	3 (^a)
Arsenic	Algae	a	a	a	a
	Fish	a	a	a	a
Mercury	Algae	4	a	26	17
	Fish	a	a	2	1
Nickel	Algae	4	5	4	l
	Fish	a	a	a	a
Cadmium	Algae	351	250	22	20
	Fish	20	13	3	2
Lead	Algae	l	3	18	a
	Fish	a	a	2	a

apercent change is less than 1.

bSRC-I has no effluent for this chemical.

showing significant risks at the higher concentrations reached by at least one of the technologies. The increased risk of an effect to game fish populations seems intuitively reasonable. However, the increasing risk of a blue-green algal bloom with increasing concentration is counterintuitive. This is an example of the indirect effects which EUA is capable of showing. Even though each of the chemicals is toxic to the algae, the reduction in sensitive grazing organisms more than compensates for the direct effect on phytoplankton.

Results for ammonia and cadmium show both higher risk values and more complex response curves. Because of the wide range of environmental concentrations, cadmium tends to be more important for some technologies than for others. Environmental concentrations for ammonia overlap broadly so that this chemical takes on major importance for all of the technologies. The results indicate that these two risk assessment units should be of primary concern in evaluating the environmental hazards of direct coal liquefaction.

All of the graphs illustrate the complexity of the ecosystem responses simulated by EUA. The relationship between concentration of toxicant and risk is not simply linear or exponential. The complexity of these responses results from the nonlinear interactions considered in the analysis.

3.3.3 Comparison of Risks across RACs

The importance of cadmium and ammonia is further emphasized in Figure 3.3-5. The graph shows the maximum risk associated with each of the nine RACs. The maximum risk is defined as the risk associated (1) with the upper 95th percentile concentration for whichever technology showed the highest concentrations and (2) with either algal blooms or a reduction in game fish biomass, whichever showed the higher risk. Thus, the maximum risk attempts to separate RACs that never show a significant risk from those that are significant in at least one of the relevant calculations.

The figure shows that there is a very reasonable probability that cadmium and ammonia could cause significant effects in the aquatic ecosystem. In addition, the graph indicates that mercury (RAC 32)

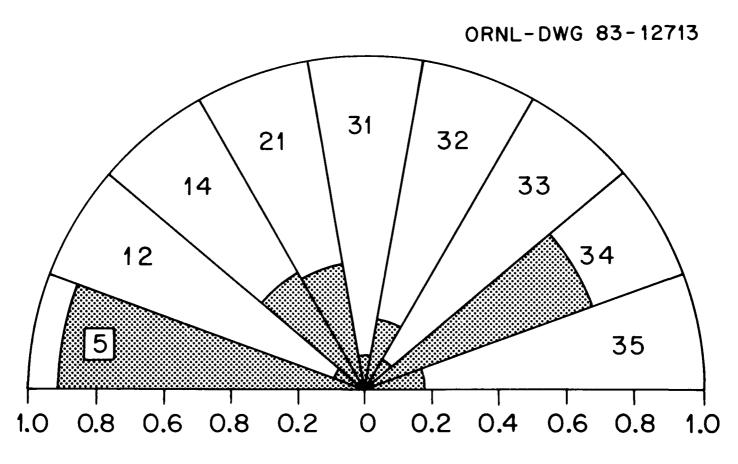


Fig. 3.3-5. Maximum risk estimates. The numbers represent each of the nine RACs. The risk values are associated with either algal blooms or reductions in fish biomass, whichever is larger, at the 95th percentile concentration of the technology with the highest concentration.

could also cause problems, though only in the SRC processes.

Naphthalene (RAC 14) and phenol (RAC 21) show significant maximum risks, but this appears only in treatment option 1.

3.3.4 Comparison of Risks between Technologies

Figure 3.3-6 compares risks across the nine RACs for the four technologies. The risk values are those associated with the upper 95th percentile concentrations. For each RAC, moving in a clockwise direction, results are given first for the risk of algal blooms and then for the risk of a reduction in game fish.

Application of treatment option 2 would largely eliminate the risks associated with naphthalene (RAC 14) and phenol (RAC 21). This would seem to be particularly important for H-Coal and SRC processes.

The Exxon and H-Coal methods show high risks for emissions of cadmium (RAC 34). The SRC processes show much lower risks associated with cadmium, with smaller significant risks for the other heavy metals (RACs 31-35). However, all four technologies have high risks for ammonia (RAC 5). The risk of reduction in game fish populations is particularly high.

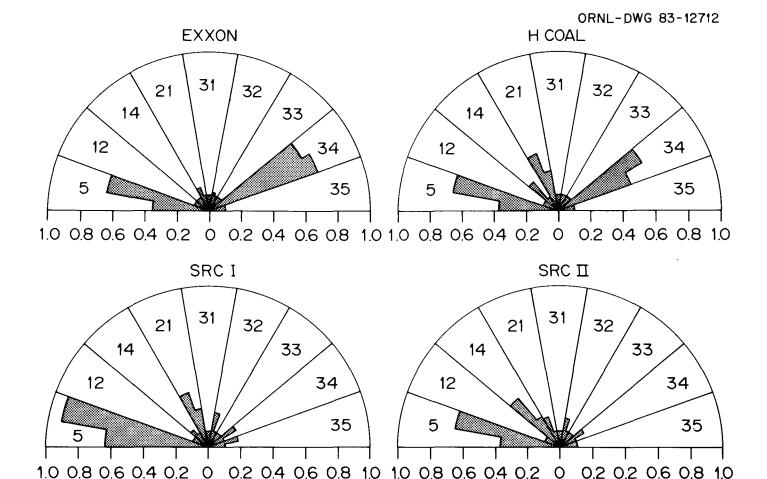


Fig. 3.3-6. Comparison of risks among technologies. Risks at the 95th percentile concentration are shown first for the algae and then for game fish, for each of the nine RACs (indicated by numbers).

4. TERRESTRIAL ENDPOINTS

The quotient method, as discussed in Sect. 3.1, consists of dividing the ambient concentrations of toxicants by the concentration at which some toxic effect is induced. It is used in this section to provide an indication of the likelihood of effects due to emissions of the individual RACs. The other risk analysis methods are not readily applicable to terrestrial organisms because of the limited data for most terrestrial taxa, the lack of standard tests and toxicological benchmarks in the data base, and the lack of agreed-upon standard responses for terrestrial biota.

4.1 VEGETATION

The phototoxicity data for the gaseous and volatile RACs are presented in Table B-1, the concentrations in ambient ground-level air are in Tables 2.3-1 through 4, and the quotients of the ratios of these values are in Table 4.1-1 through 4.1-3. The ambient concentrations are the increment of the entire RAC to the background concentration at the point of maximum ground-level concentration (Sect. 2.3). 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 yield.

The worst atmospheric toxicant in the emissions of all technologies is hydrocarbon gases (RAC 6). This rank is misleading because the worst-case representative chemical (ethylene) is a plant hormone whereas most members of this RAC are essentially inert (NRC 1976). However, because atmospheric ethylene has caused significant damage to crops near urban areas and in the vicinity of petrochemical plants (NRC 1976), the emission rate of this gas should be specifically considered in the future. The most serious phytotoxicants in air

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

RAC	RAC name	Air concentration/ lowest toxic concentration	Range of air concentration/ growth effects concentration	Soil concentration/ lowest toxic concentration	Range of soil concentration/ growth effects concentration
	Carbon monoxide Sulfur oxides	9.67 E-03 1.02 E-01	1.58 E-06 1.69 E-02 - 5.08 E-02		ation in soil ation in soil
	Nitrogen oxides	3.60 E-02	1.89 E-03 - 3.60 E-02		ation in soil
	Acid gases		emissions		
	Alkaline gases		emissions		
	Hydrocarbon gases Formaldehyde	5.15	2.48 E-03 - 8.64 E-03		
	Volatile organochlorines		emissions emissions		
9	Volatile carboxylic acids		emissions		
	Volatile O&S neterocyclics		toxicity data		
	Volatile N-heterocyclics		emissions		
	Benzene	8.23 E-07			
	Aliphatic/alicyclic hydrocarbons	1.22 E-12		1.00 E-04	
	Mono- or diaromatic hydrocarbons	1.70 E-05		3.7 E-06	3.7 E-06 [
	Polycyclic aromatic hydrocarbons			3.73	1.15-3.73 ^b
	Aliphatic amines Aromatic amines	2.64 E-05	emissions		
	Alkaline nitrogen heterocyclics		toxicity data		
	Neutral N. O. S heterocyclics	No phyto	coxicity data	1.09 E-06	1.09 E-07 - 1.09 E-06
	Carboxylic acids	No.	emissions	1.03 1.00	1.03 2-07 - 1.03 2-00
	Phenols		CIII (3 3 1 0 1 3	9.8 E-05	
	Aldehydes and ketones	3.98 E-05		3.4·E-07	3.4 E-07
	Nonheterocyclic organosulfur	3.47 E-09	1.91 E-08	2.67 E-11b	
	Alcohols		emissions		
	Nitroaromatics		emissions		
	Esters		emissions		
	Amides		emissions		
	Nitriles Fars		emissions		
	ders Respirable particles		emissions		
	respirable particles Arsenic	No phyto	toxicity data	1.1 E-01 ^b	5.16 E-03 ^b - 1.1 E-01 ^b
	Mercury	1.54 E-06		2.46 E-07	2.26 E-09 - 2.46 E-07
	vickel	113. 2-00		4.92 E-02b	5.34 E-05 - 4.92 E-02b
	Cadmium			3.78 E-02	8.4 E-04 - 3.78 E-02
35 L	_ead			1.96 E-03 ^b	1.76 E-05 - 1.96 E-03 ^b

^aAmbient air concentrations and soil and soil solution concentrations are presented in Table 2.3-1. Toxic concentrations are presented in Appendix B. ^bQuotients calculated from concentrations in soil and results of tests performed in soil. Quotients without superscript were calculated from concentrations in soil solution and results of tests performed in nutrient solution.

Table 4.1-2. Toxicity quotients for terrestrial plants for SRC-I Process. Ambient concentrations in air (annual, median, ground-level) and soil (soil solution or whole dry soil basis) are divided by concentrations causing reductions in growth, yield, or other toxic responses^a

			xicity in air		city in air
RAC	RAC Name	Air concentration/ lowest toxic concentration	Range of air concentration/ growth effects concentration	Soil concentration/ lowest toxic concentration	Range of soil concentration, growth effects concentration
1	Carbon monoxide	1.45 E-03	2.37 E-07	No accumula	ation in soil
2	Sulfur oxides	8.31 E-02	1.38 E-02 - 4.15 E-02		ation in soil
3	Nitrogen oxides	3.74 E-02	1.97 E-03 - 3.74 E-02	No accumula	ation in soil
4	Acid gases	6.39 E-05	6.39 E-05		ation in soil
5	Alkaline gases	1.48 E-04		No accumula	ation in soil
6	Hydrocarbon gases	4.15	2.0 E-03 - 6.96 E-03		
	Formaldehyde		emissions		
	Volatile organochlorines		emissions		
	Volatile carboxylic acids		emissions		
	Volatile 0 & S heterocyclics		emissions		
	Volatile N heterocyclics		emissions		
	Benzene		emissions		
	Aliphatic/alicyclic hydrocarbons	1.15 E-12		9.44 E-05	0.44.5.05
	Mono- or diaromatic hydrocarbons	1.57 E-05		3.44 E-06	3.44 E-06
15 16	Polycyclic aromatic hydrocarbons			13.3 ^b	4.1-13.3 ^b
	Aliphatic amines		emissions		
	Aromatic amines Alkaline N heterocyclics	3.23 E-03			
19		NC	emissions	8.31 E-07	8.31 E-08 - 8.31 E-07
	Neutral N, O, S heterocyclics	No	emissions	8.31 E-0/	8.31 E-08 - 8.31 E-07
21	Carboxylic acids Phenols	NO	enits tons	3.43 E-04	
	Aldehydes and ketones	No	emissions	3.43 L-04	
23	Nonheterocyclic organosulfur		emissions		
	Alcohols		emissions		
25	Nitroaromatics		emissions		
	Esters		emissions		
27	Amides	No	emissions		
28	Nitriles	No	emissions		
29	Tars	No	emissions		
30	Respirable particles			No accumula	ition in soil
31	Arsenic			7.33 E-01 ^D	3.44 E-02 ^b - 7.33 E-01 ^b
32	Mercury	2.3 E-05		2.3 E-07	2.11 E-09 - 2.3 E-07
33	Nickel			6.4 E-01 ^b	7.58 E-04 - 6.4 E-01 ^b
34	Cadmium			3.65 E-03	8.1 E-05 - 3.65 E-03
35	Lead			1.53 E-03 ^b	1.37 E-05 - 1.53 E-03 ^b

^aAir, soil and soil solution concentrations are presented in Table 2.3-2. Toxic concentrations are presented in Appendix B.

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

Table 4.1-3. Toxicity quotients for terrestrial plants for SRC-II Process. Ambient concentrations in air (annual, median, ground-level) and soil (soil solution or whole dry soil basis) are divided by concentrations causing reductions in growth, yield, or other toxic responses^a

RAC	RAC Name	Air concentration/ lowest toxic concentration	Range of air concentration/ growth effects concentration	Soil concentration/ lowest toxic concentration	Range of soil concentration/ growth effects concentration
1 2 3 4	Carbon monoxide Sulfur oxides Nitrogen oxides Acid qases	9.28 E-04 2.35 E-02 3.95 E-02	1.52 E-07 3.92 E-03 - 1.18 E-02 2.08 E-03 - 3.95 E-02 emissions	No accumul	ation in soil ation in soil ation in soil
5 6 7	Alkaline gases Hydrocarbon gases Formaldehyde	3.23 E+00 No	emissions 1.56 E-03 - 5.43 E-03 emissions		
8 9 10 11	Volatile organochlorines Volatile carboxylic acids Volatile O & S heterocyclics Volatile N heterocyclics	No	emissions emissions vtoxicity data	2.61 E-05	2.61 E-05
12 13 14 15	Benzene Aliphatic/alicyclic hydrocarbons Mono- or diaromatic hydrocarbons Polycyclic aromatic hydrocarbons	4.0 E-06 1.88 E-12 1.10 E-05		1.54 E-04 2.41 E-06 4.16 ^b	2.41 E-06 1.28-4.16 ^b
16 17 18	Aliphatic amines Aromatic amines Alkaline N heterocyclics Neutral N, O, S heterocyclics	1.43 E-05	emissions ctoxicity data	2.35 E-07	2.35 E-08 - 2.35 E-07
20 21	Carboxylic acids Phenols Aldehydes and ketones		emissions emissions	1.48 E-04	2.35 E-06 - 2.35 E-07
24 25	Nonheterocyclic organosulfur Alcohols Nitroaromatics Esters	No No	emissions emissions emissions emissions		
28	Amides Nitriles Tars Kespirable particles	No	emissions emissions emissions	No accumul	ation in soil
31 32 33 34	Arsenic Mercury Nickel Cadmium	1.35 E-06		4.83 E-03 ^b 2.16 E-07 2.08 E-04 ^b 6.45 E-05	2.27 E-04 ^b - 4.83 E-03 ^b 1.98 E-09 - 2.16 E-07 2.47 E-07 - 2.08 E-04 ^b 1.43 E-06 - 6.45 E-05
35 36 37	Lead Other trace elements Radioactive materials	No	emissions	3.84 E-06 ^b	3.44 E-08 - 3.84 E-06 ^b lation in soil

^aAir, soil and soil solution concentrations are presented in Table 2.3-3. Toxic concentrations are presented in Appendix B.

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

(ignoring ethylene) are ${\rm SO}_{\rm X}$ and ${\rm NO}_{\rm X}$. The maximum annual average concentrations predicted for ${\rm SO}_2$ (RAC 2) from EDS emissions are within a tenth of those that cause visible injury to needles of sensitive white pines, and, for both ${\rm SO}_2$ and ${\rm NO}_{\rm X}$ (RAC 3) emissions from all technologies, those concentrations are greater than a hundredth of those that reduce growth or yield of several plant species.

Because of its ubiquity and importance as a phytotoxicant, sulfur dioxide (RAC 2) has been relatively well studied for its effects on crop yield and can be analyzed in greater detail than other RACs. McLaughlin and Taylor (in press) have put forward the following dose-response relationship for yield reduction of beans as a function of SO_2 exposure:

% yield reduction = -17.4 + 29.2 (log dose-ppmh).

This empirical relationship is based on a regression of 20 points from five field experiments on soybeans and snap beans. Eighty percent of the variation in yield reduction was associated with variation in dosage, and the equation was significant at $\alpha = 0.0001$.

Because SO_2 appears to be the most serious phytotoxic air pollutant, we used this relationship to examine the potential effects of full growing-season exposure to SO_2 on crop yield. If we assume a 200-d growing season for soybeans on the eastern site and a 12 h exposure day, the SO_2 dose from EDS at 6.61 $\mu g/m^3$ SO_2 is 5.95 ppmh. Sulfur dioxide concentrations from EDS are 1.2 times those from SRC-I, 2.6 times those from H-Coal, and 4.3 times those from SRC-II. That dose results in a 5.6% reduction in yield using McLaughlin and Taylor's formula.

This predicted effect is remarkable in that it results from an SO_2 concentration that is more than 10 times lower than the lowest concentration reported to affect yield. This anomaly is due to the great length of a growing season relative to the length of experiments. The longest fumigation available to McLaughlin and Taylor was 337 h. Thus, use of their formula for a full growing season requires an extrapolation of almost a factor of 10 in the duration

component of the dose. Because the experimental field fumigations are typically carried out in the most sensitive stage (assumed to be the pod-fill in the case of beans), use of the formula for the full growing season probably overestimates effects.

We might place a lower bound on the level of effect by assuming that effects only occur during pod-fill. If that stage is assumed to last 30 d, the dose is 0.89 ppmh. This is less than a quarter of the threshold dose for effects on yield (3.92 ppmh).

For a real synfuels plant, this SO_2 emission would be added to a background SO_2 concentration that may reach 80 $\mu\mathrm{g/m}^3$ under the current annual average ambient air quality standard. The SO_2 would also interact with ozone, which reaches phytotoxic levels in many areas of the United States. This analytical exercise emphasizes the need for the full season field experiments on effects of SO_2 and SO_2 + O_3 originally planned for the EPA's National Crop Loss Assessment Network.

The phytotoxicity of materials deposited on the landscape is a more complex phenomenon than that of gases and vapors. Because the atmospheric transport model AIRDOS-EPA has a deposition velocity of zero for inorganic gases and does not model the formation of aerosols, RACs 1 through 5 are assumed to not accumulate in the soil. assumption is likely to be acceptable except in the case of ${\rm SO}_4$ deposition in forests with acid soils. The effects of ${\rm SO}_{\Lambda}$ deposition in forests result from regional-scale emissions and atmospheric processes, and therefore are well beyond the scope of this report. Deposited nongaseous RACs were assumed to accumulate in the soil over the 35-year life of the liquefaction plant. Losses due to decomposition and leaching from the root zone were calculated by the terrestrial food chain model (Sect. 2.3). 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. Whereas the results of tests conducted in soil can be directly compared with concentrations in the whole soil, results of tests conducted in solution must be compared with 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, solution concentrations are less reliable. In addition, as with the gases and vapors, the toxicity data concern 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.

For all four technologies, the most phytotoxic RAC deposited in soil was polycyclic aromatic hydrocarbons (RAC 15). The high rank of RAC 15 is suspect because benzo(a)pyrene and some other PAHs appear to act as plant hormones and can stimulate growth at very low concentrations. While PAHs can modify plant growth at concentrations as low as 0.5 ng/g soil and alteration of growth patterns can affect survival, there is no evidence that they reduce plant growth or cause injury, even at relativity high experimental concentrations (Edwards, 1983). Phytotoxic concentrations are more than 10 times those in soil or soil solution for all other RACs from all technologies, except arsenic (31) and nickel (33) for SRC-I. They are within a factor of 100 for arsenic (31), nickel (33), and cadmium (34) from EDS; phenols (21) from SRC II; and phenols, arsenic, and cadmium from H-Coal. The results for phenols are highly uncertain since only one test result has been found, inhibition of wheat seed germination. More data on the phytotoxicity of nonhalogenated phenols would be desirable. While the trace elements arsenic, nickel, and cadmium do not appear to be serious problems on the basis of this simple analysis, their concentrations are high enough to warrant greater attention in future research and risk analysis methods development.

4.2 WILDLIFE

Table 4.2-1 through 4 present the lowest quotients for the two technologies for toxicity to terrestrial animals. The quotients are 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 average ground-level concentration in

Table 4.2-1. Toxicity quotients for terrestrial animals for Exxon Donor Solvent. Concentrations in air (annual, median, ground-level) are divided by lethal concentrations and the lowest toxic concentrations^a

RAC	RAC name	Lowest lethal concentration	
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 25 26 26 27 27 27 27 27 27 27 27 27 27 27 27 27	Carbon monoxide Sulfur oxides Nitrogen oxides Acid gases Alkaline gases Hydrocarbon gases Formaldehyde Volatile organochlorines Volatile carboxylic acids Volatile 0 & S heterocyclics Volatile N heterocyclics Benzene Aliphatic/alicyclic hydrocarbons Mono- or diaromatic hydrocarbons Polycyclic aromatic hydrocarbons Aliphatic amines Aromatic amines Alkaline N heterocyclics Neutral N, O, S heterocyclics Carboxylic acids Phenols Aldehydes and ketones Nonheterocyclic organosulfur Alcohols Nitroaromatics	1.89 E-08 3.67 E-04 3.29 E-04 No 6	concentration 4.05 E-04 6.61 E-02 8.05 E-03 emissions emissions emissions emissions 1.6 E-08 emissions emissions 1.48 E-09 emissions 1.3 E-07 9.79 E-07 4.04 E-05 respiratory toxicity emissions 9.65 E-09 respiratory toxicity
25 26 27 28	Alcohols	No e No e No e No e	emissions
	· ····	No e No e	emissions
33 34 35	Nickel Cadmium Lead	3.57 E-09 2.64 E-08	3.57 E-09 1.32 E-05 2.64 E-06

 $^{^{}m a}$ Ambient air concentrations are presented in Table 2.3-1. Toxic concentrations are presented in Appendix B.

Table 4.2-2. Toxicity quotients for terrestrial animals for SRC-I Process. Concentrations in air (annual, median, ground-level) are divided by lethal concentrations and the lowest toxic concentrations^a

RAC	RAC name	Lowest lethal concentration	Lowest toxic concentration
1	Carbon monoxide	2.84 E-09	6.07 E-05
2	Sulfur oxides	3.0 E-04	5.4 E-02
3	Nitrogen oxides	3.42 E-04	8.36 E-03
4	Acid gases	8.52 E-08	2.56 E-07
5 6	Alkaline gases	4.44 E-07	2.39 E-05
6	Hydrocarbon gases		1.29 E-08
7	Formaldehyde	No e	emissions
8	Volatile organochlorines	No e	emissions
9	Volatile carboxylic acids	No (emissions
10	Volatile 0 & S heterocyclics	No e	emissions
11	Volatile N heterocyclics	No (emissions
12	Benzene	No e	emissions
13	Aliphatic/alicyclic hydrocarbons	1.40 E-08	9.21 E-07
14	Mono- or diaromatic hydrocarbons	1.97 E-06	3.75 E-05
15	Polycyclic aromatic hydrocarbons		
16	Aliphatic amines		emissions
17	Aromatic amines	1.18 E-06	1.18 E-06
18	Alkaline N heterocyclics	No (emissions
19	Neutral N, O, S heterocyclics		_
20	Carboxylic acids	No (emissions
21	Phenols		
22	Aldehydes and ketones		emissions
23	Nonheterocyclic organosulfur		emissions
24	Alcohols		emissions
25	Nitroaromatics		emissions
26	Esters		emissions
27	Amides		emissions
28	Nitriles		emissions
29	Tars	No	emissions
30	Respirable particles		2.10 E-01
31	Arsenic		4.92 E-05
32	Mercury	4 03 5 06	8.47 E-08
33	Nickel	4.21 E-06	4.21 E-06
34	Cadmium	3.98 E-09	1.99 E-06 2.02 E-06
35	Lead		2.U2 E-U0

^aAmbient air concentrations are presented in Table 2.3-2. Toxic concentrations are presented in Appendix B.

Table 4.2-3. Toxicity quotients for terrestrial animals for SRC-II Process. Concentrations in air (annual, median, ground-level) are divided by lethal concentrations and the lowest toxic concentrations^a

RAC	RAC name	Lowest lethal concentration	Lowest toxic concentration
1	Carbon monoxide	1.82 E-09	3.88 E-05
2	Sulfur oxides	8.5 E-05	1.53 E-02
3	Nitrogen oxides	3.61 E-04	8.83 E-03
4	Acid gases	No emis	
5	Alkaline gases	No emi	
6	Hydrocarbon gases	No emi	1.01 E-08
7 8	Formaldehyde	No emi:	
9	Volatile organochlorines Volatile carboxylic acids	No emi:	
10	Volatile 0 & S heterocyclics	2.07 E-09	2.07 E-09
11	Volatile N heterocyclics	1.8 E-08	1.8 E-08
12	Benzene	6.32 E-07	6.32 E-07
13	Aliphatic/alicyclic hydrocarbons	2.28 E-08	1.5 E-06
14	Mono- or diaromatic hydrocarbons	1.38 E-06	2.62 E-05
15	Polycyclic aromatic hydrocarbons		
16	Aliphatic amines	No emi	
17	Aromatic amines	5.22 E-09	5.22 E-09
18	Alkaline N heterocyclics		
19 20	Neutral N, O, S heterocyclics	8)	
21	Carboxylic acids Phenols	No emis	SSIONS
	Aldehydes and ketones	No emi	ecione
23	Nonheterocyclic organosulfur	No emi	
24	Alcohols	No emi:	
25	Nitroaromatics	No emi	
	Esters	No emi	
	Amides	No emis	ssions
	Nitriles	No emi:	
29	Tars	No emis	
30	Respirable particles		1.38 E-01
31 32	Arsenic		1.94 E-05
	Mercury Nickel	1 40 5 00	7.94 E-08
	Cadmium	1.49 E-09	1.49 E-09
35	Lead	3.36 E-09	1.68 E-06 4.54 E-07
			4.34 C=U/

 $^{^{\}mathrm{a}}$ Ambient air concentrations are presented in Table 2.3-3. Toxic concentrations are presented in Appendix B.

air. Data from all species are lumped because there were not enough data on the nonmammalian taxa for separate treatment. Carcinogenesis and other genotoxic effects were not included.

Lethality is considered because it is a consistent and frequently determined response that has clear population implications, but all predicted concentrations were well below lethal levels. 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 that are as low as one ten-thousandth of lethal concentrations. These responses range from increased airway resistance in one-hour exposures of guinea pigs to impaired lung and liver function in human occupational exposures. The most toxic RACs for all technologies by this sublethal criterion are the conventional combustion products: sulfur oxides (2) and respirable particulates (30). Whereas these concentrations may constitute a locally significant increment to the background concentration of these major pollutants, the significance of ambient air pollution to wildlife is largely unknown. While the predicted sulfur oxide and respirable particle concentrations are below the annual primary ambient air quality standards for SO₂ $(1.5-6.6 \, \mu g/m^3 \, vs \, 80 \, \mu g/m^3)$ and total particulates (45.4-63.3) $\mu q/m^3$ vs 75 $\mu q/m^3$), there is little scientific basis for the assumption that protection of human health will automatically protect wildlife.

5. EVALUATION OF RISKS

5.1 EVALUATION OF RISKS TO FISH

Table 5.1-1 lists, for each technology and wastewater treatment option, the RACs determined to be potentially ecologically significant by one or more of the three methods employed in this report. The significance criterion for the quotient method is an acute effects quotient greater than 0.01 (i.e., a lowest observed LC_{50} or TLM_{96} less than a hundred times the estimated environmental concentration). For analysis of extrapolation error, RACs are considered to be significant if the risk that the environmental concentration may exceed the PGMATC of one or more of the reference fish species is greater than 0.1. For ecosystem uncertainty analysis, RACs are considered to be significant if the risk of a 25% reduction in game fish biomass is greater than 0.1.

A total of nine RACs were determined to be significant for one or more technologies. RAC 5 (ammonia) was the only RAC found to be significant for all technologies, all treatment options, and all risk analysis methods. RAC 34 (cadmium) was significant for all technologies and treatment options according to the quotient method; RAC 21 (phenols) was significant for all technologies according to analysis of extrapolation error (AEE). AEE ranked five RACs as significant for at least one combination of technology and waste treatment that was not picked by the other two methods, and AEE found cadmium (RAC 34) to be significant less often than the other methods. These differences can be largely accounted for by the fact that while the other methods use the responses of the species that are tested, AEE predicts the responses of a specific fish fauna. Several members of this fauna are significantly more sensitive to most chemicals than are the species used to test those five RACs. However, in the case of cadmium, data are available for the other methods on rainbow trout, which is more sensitive to this metal than are the warm-water species used in AEE. Thus, differences in sensitivity among fish taxa appear to account for most of the variation between methods in the lists of significant RACs.

Table 5.1-1. RACs determined to pose potentially significant risks to fish populations by one or more of three risk analysis methods

Exxon Donor Solvent		SRC-I		SRC	-II	H-Coal		
ηa	5p	1	2	1	2	1	2	
5 (QM, AEE, EUA) ^C	5 (QM, AEE, EUA)	5 (QM, AEE, EUA)	5 (QM, AEE, EUA)	5 (QM, AEE, EUA)	5 (QM, AEE, EUA)	5 (QM, AEE, EUA)	5 (QM, AEE, EUA)	
13 (QM, AEE)	13 (AEE)	13 (QM, AEE)	13 (AEE)	14 (QM, AEE, EUA)	21 (AEE)	13 (QM, AEE)	13 (QM, AEE)	
14 (AEE)	20 (AEE)	21 (QM, AEE, EUA)	21 (AEE)	21 (AEE)	34 (QM)	14 (QM, AEE)	20 (AEE)	
20 (AEE)	22 (QM, AEE)	34 (QM)	34 (QM)	26 (AEE)		20 (AEE)	21 (AEE)	
21 (AEE)	34 (QM, AEE, EUA)			34 (QM)		21 (QM, AEE, EUA)	22 (QM, AEE)	
22 (QM, AEE)						22 (QM, AEE)	34 (QM, EUA)	
28 (AEE)						28 (AEE)		
34 (QM, AEE, EUA)						34 (QM, EUA)		

aWastewater treatment option 1.

bWastewater treatment option 2.

CQM = quotient method; AEE = analysis of extrapolation error, EUA = ecosystem uncertainty analysis.

The exposure analyses, the significance criteria, and the methods themselves are conservative, and therefore it would be premature to conclude that adverse consequences would result from the contaminant releases assessed in this report. These nine RACs should, however, be foci for future refinements of the risk analyses and for future toxicological and ecological research. In addition to the RACs listed in Table 5.1-1, there are eight RACs for which no applicable toxicity data were available. These are RACs 10 (volatile 0 & S heterocyclics), 11 (volatile N heterocyclics), 16 (aliphatic amines), 17 (aromatic amines), 23 (nonheterocyclic organosulfur compounds), 24 (alcohols), 25 (nitroaromatics), and 27 (amides).

There are two ways to compare the four technologies for ecological risk. It was shown using the toxic units approach (Sect. 3.2-3) that, for treatment option 1, the H-Coal effluent has the greatest potential for acute toxicity to fish; for option 2, the Exxon Donor Solvent effluent appears to be the most acutely toxic. SRC-I's total toxicity is almost entirely due to ammonia while H-Coal also has large emissions of organics and cadmium. By the other criterion, number of potentialy significant RACs in the effluent (Table 5.1-1), H-Coal and EDS appear to pose the greatest risk to fish.

5.2 EVALUATION OF RISKS OF ALGAL BLOOMS

Algal toxicity data were available for only 10 RACs. Moreover, because of the diversity of experimental designs and test endpoints used in algal bioassays, it is not meaningful to rank the RACs using the quotient method. Finally, as noted in Sect. 3.1, there is no clear distinction between acute effects and chronic effects in algal bioassays.

It does appear, however, that most of the quotients that can be calculated are lower for algae than for fish; only RACs 17, 21, 26, and 34 would be judged significant for any technology using the quotient method. For treatment option 2, only RAC 34 is significant.

Ecosystem uncertainty analysis suggests greater risks of effects on algae than does the quotient method. Risks of 10% or more of a fourfold increase in algal biomass, for one or more technologies and

for treatment options, were estimated for six of the nine RACs examined: 5, 14, 21, 32, 34, and 35. It is important to note that the effects pathway postulated in ecosystem uncertainty analysis is indirect rather than direct. All of the RACs are toxic to algae. The increases in algal biomass are caused by reductions in grazing intensity resulting from effects of contaminants on zooplankton and fish.

5.3 EVALUATION OF RISKS TO VEGETATION AND WILDLIFE

Gases and vapors emitted by direct coal liquefaction processes appear to pose a minor threat to terrestrial plants and animals. The most serious problems appear to arise from conventional products of combustion: sulfur oxides, nitrogen oxides, and respirable particles that may already be present in high concentrations at synfuels plant sites. Of the materials deposited on the soil, the trace elements arsenic, cadmium, and nickel cause the greatest concern. However, they are unlikely to be a problem except when deposited on acid soils with preexisting high concentrations of heavy metals.

5.4 VALIDATION NEEDS

There are no uniquely correct methods of quantifying ecological risks. There are several plausible ways to combine uncertainties concerning differential sensitivities of fish taxa and acute-chronic relationships. Similarly, there are 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 by examining 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, 1984), 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

R AC	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</u> pseudolimnaeus)	LC ₅₀	96	0.022		Oseid and Smith 1974
		Bluegill (adults) (juveniles) (fry, 35-d-old) (eggs)	TL _m TL _m TL _m TL _m	96 96 96 72	0.0448 0.0478 0.0131 0.0190	Flow-through test Flow-through test Flow-through test Flow-through test	Smith et al. 1976 Smith et al. 1976 Smith et al. 1976 Smith et al. 1976
		Northern pike (eggs) (fry)	TL _m TL _m	96 96	0.034-0.037 0.009-0.026	DO = 2-6 ppm DO = 2-6 ppm	Adelman and Smith 1970 Adelman and Smith 1970
5	Ammonia	Rainbow trout (fry, 85-d-old) (adults) Rainbow trout Rainbow trout Rainbow trout (fry) (fingerlings)	TL _m TL _m LC ₅₀ LC ₅₀ LC ₅₀ LC ₅₀	24 24 24 24 24 24	0.068 0.097 0.50 0.47 0.2		Rice and Stokes 1975 Rice and Stokes 1975 Herbert and Shurben 1963 Lloyd and Orr 1969 EIFAC 1970 EIFAC 1970
б	Heptane	Mosquitofish	TLm	96	4924		Wallen et al. 1957
7	Formaldehyde	Several fish species	LC ₅₀	24	50-120		National Research Council 1981

Table A-1. (continued)

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

Table A-1. (continued)

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

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>T</u> . <u>pyriforma</u>)	LC ₅₀	72	125.7	50% growth	Schultz et al. 1980
		D. magna Fathead minnow Fathead minnow	LC ₅₀ LC ₅₀ LC ₅₀	48 48 96	30.28 1.50 46.0		Millemann et al. 1984 Millemann et al. 1984 Mattson et al. 1976
	2-Methylquinoline	Ciliate (<u>T. pyriforma</u>)	EC ₅₀	72	48.7	50% growth inhibition	Schultz et al. 1980
	2,6-Dimethylquinoline	Ciliate (<u>T</u> . <u>pyriforma</u>)	EC ₅₀	72	33.0	50% growth inhibition	Schultz et al. 1980
19	Neutral N-,0-,S- neterocyclics					No toxicity data	
20	Benzoic acid	Mosquitofish	TL _m	96	180		Wallam et al. 1957
21	Phenol	D. magna D. magna D. magna (Young) Copepod (Mesocyclops leukarti)	LC ₅₀ LC ₅₀ TL _m LC ₅₀	48 50	19.79 9.6 7.0 108.0		Millemann et al. 1984 US EPA 1980g Dowden and Bennett 1965 US EPA 1980g
		Fathead minnow Fathead minnow	LC ₅₀ LC ₅₀	48 96	25.6 24.0-67.5	4 tests	Millemann et al. 1984 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-Methyphenol	D. magna D. magna Fathead minnow	LC ₅₀ LC ₅₀ TL _m	48 48 96	9.2 23.5 12.55	Soft water	US EPA 1980g US EPA 1980g Pickering and
		Fathead minnow	TL _m	96	13.42	Hard water	Henderson 1966a Pickering and
		Bluegill	TL _m	96	20.78	Soft water	Henderson 1966a Pickering and
	4-Methylphenol	Fathead minnow	TL _m	96	19.0		Henderson 1966a Mattson et al. 1976

Table A-1. (continued)

R AC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^C	Reference
	Mixed cresol isomers	Aquatic life	TLm	96	1.0-10.0		Kingsbury et al. 1979
	2,4-Dimethylphenol	D. magna	LC ₅₀	48	2.12		US EPA 1980h
		Fathead minnow (juvenile) Bluegill	LC ₅₀ LC ₅₀	96 96	16.75 7.75	Flow-through test	US EPA 1980h US EPA 1980h
	3,4-Dimethylphenol	Fathead minnow	LC ₅₀	96	14.0		Mattson et al. 1976
	2,5-Dimethylphenol	D. magna	LC ₅₀	48	0.96		Millemann et al. 1984
22	Acrolein	D. magna D. magna Mosquitofish Bluegill	LC ₅₀ LC ₅₀ LC ₅₀	48 48 48	0.057 0.080 0.061		US EPA 19801 US EPA 19801 National Research Council 1981 US EPA 19801
		Bluegill Brown trout	LC ₅₀ LC ₅₀	96 24	0.090 0.046		US EPA 1980i National Research Council 1981
		Rainbow trout	LC ₅₀	24	0.065		National Research Council 1981
	Acetaldehyde	Largemouth bass Bluegill	LC50 LC50	96 96	0.160 53.0		US EPA 1980i National Research Council 1981
	Acetone	D. magna	LC ₅₀	48	12,600		Canton and Adema 1978
23	Nonheterocylic 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)

AC	Representative chemical(s)	Test organism ^a	Test type ^b	Duration (h)	Concentration (mg/L)	Notes ^C	Reference
	Diethyl phthalate	D. magna Bluegill	LC ₅₀ LC ₅₀		52.1 98.2	_	US EPA 1980j US EPA 1980j
	Butylbenzl phthalate	D. magna	LC ₅₀		92.3		US EPA 1980j
		D. magna	LCEO	48	3.7		Gledhill et al. 1980
		Fathead minnow Fathead minnow	LC ₅₀ LC ₅₀	96 96	5.3 2.1	Hardness: 160 Hardness: 40	Gledhill et al. 1980 Gledhill et al. 1980
		Bluegill	LC50	90	43.3	naruness. 40	US EPA 1980j
		Bluegill	LUSA	96	1.7		Gledhill et al. 1980
		Rainbow trout	LC ₅₀	96	3.3		Gledhill et al. 1980
	Di-n-butyl phthalate	Scud (G. <u>pseudo-</u> limnaeus)	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
	Amides					No toxicity data	
	Acrylonitrile	D. magna	LC ₅₀		7.55		US EPA 1980k
		Fathead minnow	LC50	96 96	14.3 18.1		US EPA 1980k US EPA 1980k
		Fathead minnow Fathead minnow	LC ₅₀ LC ₅₀	96 96	10.1	Flow-through test	US EPA 1980k
		Bluegill	LC50	96	11.8	r row-carough test	US EPA 1980k
		Bluegill	LC ₅₀	30	10.1		US EPA 1980k
	Tars					No aquatic emission	ıs
	Respirable particles					No aquatic emission	S
	Arsenic	D. magna	TL _m	48	7.4		Hohreiter 1980
		D. <u>magna</u>	EC ₅₀	48	5.28	Immobilization	Anderson 1946
		Daphnia pulex	EC50	48	1.04	Immobilization	Sanders and Cope 1966
		Stonefly (Pteronarcys californica)	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) Bluegill	LC ₅₀	96	41.76 15.37	Flow-through test	Cardwell et al. 1976
		Rainbow trout	LC ₅₀ LC ₅₀		13.34		US EPA 19801 US EPA 19801
		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	Duration (h)	Concentration (mg/L)	Notes	Reference
32	Mercury (inorganic)	D. magna	LC ₅₀	48	0.005		Biesinger and Christensen 1972
		Stonefly (<u>Acroneuria</u> lycorius)	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	LCSO		0.24		US EPA 1980m
		Rainbow trout (juvenile)	LC ₅₀ LC ₅₀		0.155-0.4	4 tests	US EPA 1980m
	Methylmercury	Rainbow trout Rainbow trout	LC ₅₀		0.03		Hohreiter 1980
		(sac fry)	LC ₅₀	96	0.024		Hohreiter 1980
		(fingerling)	LC50	96	0.042		Hohreiter 1980
		(Juvenile) Brook trout	LC50		0.025		US EPA 1980m
		(juvenile)	LC ₅₀	96	0.084	Flow-through test	McKim et al. 1976
		(yearling)	LC50	96	0.065	Flow-through test	McKim et al. 1976
3	Nickel	D. <u>magna</u> D. magna	LC ₅₀		1.81	Hardness: 51	US EPA 1980n
		D. magna	LC ₅₀		2.34	Hardness: 100	US EPA 1980n
		Mayfly (Ephemerella subvaria)	TLm	96	4.0	Hardness: 42	Warnick and Bell 1969
		Stonefly (A. lycorius)	TL_m	96	33.5	Hardness: 40	Warnick and Bell 1969
		Damselfly (unidentified)	TLm	96	21.2	Hardness: 50	Rehwoldt et al. 1973
		Midge (Chironomus sp.)	TL _m	96	8.6	Hardness: 50	Rehwoldt et al. 1973
		Caddisfly (unidentified)	TL _m	96	30.2	Hardness: 50	Rehwoldt et al. 1973
		Fàthead minnow	LC ₅₀		4.58-5.18	Hardness: 20 2 flow-through tests	US EPA 1980n
		Fathead minnow	TLm	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	TLm	96	39.6	Hardness: 360	Pickering and

Table A-1. (continued)

RAC	Representative chemical(s)	Test organism ^a	Test type	Duration (h)	Concentration (mg/L)	Notes	Reference
							Henderson 1966b
		Rainbow trout	LC ₅₀	96	35.5	Flow-through test	Hale 1977
		Fish sp., general	LC ₅₀	96	4.6-9.8	Soft water	Hohreiter 1980
		Fish sp., general	LC50	96	39.2-42.4	Hard water	Hohreiter 1980
34	Cadmium	<u>D. magna</u>	LC ₅₀		0.0099	Hardness: 51	US EPA 1980o
		D. magna	LC ₅₀		0.033	Hardness: 104	US EPA 1980o
		D. magna	LC ₅₀		0.049	Hardness: 209	US EPA 1980o
		Mayfly (Ephemerella grandis grandis)	TLm	96	28.0		Clubb et al. 1975
		Mayfly (E. subvaria)	TL _m	96	2.0	Hardness: 54	Warnick and Bell 1969
		Stonefly (<u>Pteronarcella</u> badia)	TL'''	96	18.0		Clubb et al. 1975
		Dadia) Damselfly (unidentified)	TL _m	96	8.1	Hardness: 50	Rehwoldt et al. 1973
		Midge	TL_{m}	96	1.2	Hardness: 50	Rehwoldt et al. 1973
		(Chironomus) Caddisfly (unidentified)	TL _m	96	3.4	Hardness: 50	Rehwoldt 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	LC50	96	0.001-	Hardness: 23	US EPA 1980o
		(swim-up and parr)			0.00175	2 flow-through tests	
		Rainbow trout	LC ₅₀	96	0.00175	Hardness: 31; flow-through test	US EPA 1980o
		Carp	LC ₅₀		0.24	Hardness: 55	US EPA 1980o
		Chinook salmon (Parr)	LC50		0.0035	Hardness: 23	US EPA 1980o
		Brook trout	LC ₅₀		0.0024	Hardness: 44 (sodium sulfate)	US EPA 1980o
		Green sunfish	LC50		2.84	Hardness: 20	US EPA 1980o
		Pumpkinseed	LC ₅₀		1.5	Hardness: 55	US EPA 1980o

Table A-1. (continued)

AC	Representative chemical(s)	Test organism ^a	Test type	Duration (h)	Concentration (mg/L)	Notes	Reference
5	Lead	D. magna	LCso		0.612	Hardness: 54	US EPA 1980p
		D. magna	LC ₅₀ LC ₅₀ LC ₅₀		0.952	Hardness: 110	US EPA 1980p
		Fathead minnow	LC50	96	2.4	Hardness: 20	US EPA 1980p
		Fathead minnow	TLm	96	482.0	Hardness: 360	Pickering and Henderson 1966b
		Bluegill	TL _m	96	23.8	Hardness: 20	Pickering and Henderson 1966b
		Bluegill	TLm	96	442.0	Hardness: 360	Pickering and Henderson 1966b
		Rainbow trout (fry)	LC ₅₀	96	0.6		Hohreiter 1980
		Rainbow trout	LC50	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
86	Fluorine	D. magna		48	270.0	"Toxic threshold"	Hohreiter 1980
		Goldfish		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	TLm	240	2.3-7.5	TL _m varies with temperature	Angelovic et al. 1961

aLatin binomials are listed in Appendix C.

 $^{^{}b}LC_{50}$ = concentration required to kill 50% of test organisms. TL_{m} = median tolerance limit. EC_{20} = effective concentraton causing a designated effect on 20% of test organismsn.

^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	uration (d)	Concentration (mg/L)	Notes	Reference
8	Carbon tetrachloride Chloroform	Fathead minnow Rainbow trout	Embryo-larval Embryo-larval	27	>3.4	200 mg/L water	U.S. EPA, 1980a U.S. EPA, 1980b
		Rainbow trout	Embryo-larval	27	2.0	50 mg/L water hardness	U.S. EPA, 1980b
		Rainbow trout	Embryo	23	10.6	40% teratogenesis	U.S. EPA, 1980b
12	Benzene	<u>Daphnia</u> magna	Life cycle		>98.0		U.S. EPA, 1980c
14	Naphtnalene	Fathead minnow	Embryo-larval		0.62		U.S. EPA, 1980e
21	Phenol 2,4-Dimethylphenol	Fathead minnow Fathead minnow Fathead minnow	Embryo-larval Embryo-larval Embryo-larval		2.56 2.191 2.475		U.S. EPA, 1980g U.S. EPA, 1980h U.S. EPA, 1980h
22	Acrolein	D. magna D. magna	Life cycle Life cycle		0.024 0.034	Survival reduced after 64 days	U.S. EPA, 1980i National Research Council, 1981
		Fathead minnow	Life cycle		0.021	arcer of days	U.S. EPA, 1980i
	Di-2-ethylhexyl phthalate	<u>D. magna</u> Rainbow trout	Life cycle Embryo-larval		<0.003 0.008		U.S. EPA, 1980j U.S. EPA, 1980j
	Butylbenzyl phthalate	<u>D. magna</u> Fathead minnow	Life cycle Embryo-larval		0.44 0.22		U.S. EPA, 1980j U.S. EPA, 1980j
28	Acrylonitrile	<u>D. magna</u> Fathead minnow	Life cycle LC ₅₀	30	>3.6 2.6		U.S. EPA, 1980k U.S. EPA, 1980k
31	Arsenic	D. magna D. magna Bass sp., general Pink salmon	Life cycle TLm	21 10 10	0.912 2.85 7.60 5.00	Toxic Lethal	U.S. EPA, 19801 Hohreiter, 1980 Hohreiter, 1980 Hohreiter, 1980
	Mercuric chloride	D. magna	Life cycle		0.001 - 0.0025	4 tests	U.S. EPA, 1980m
	Methylmercuric chloride	D. magna Fathead minnow Brook trout	Life cycle Life cycle		0.001 0.00023 0.00052	92% dead, 3 months	U.S. EPA, 1980m Hohreiter, 1980 U.S. EPA, 1980m

Table A-2. (continued).

RAC	Representative chemical(s)	Test organism ^a	Test type	Duration (d)	Concentration (mg/L)	Notes	Reference
33	Nickel	D. magna	Life cycle		0.015	Hardness: 51 (mg/L as CaCO ₃)	U.S. EPA, 1980n
		D. magna Caddisfly	Life cycle		0.123	Hardness: 105	U.S. EPA, 1980n
		(<u>Clistoronia</u> magnifica)	Life cycle		0.465	Hardness: 50	U.S. EPA, 1980m
		Fathead minnow	Embryo-larva	1	0.109	Hardness: 44	U.S. EPA, 1980n
		Fathead minnow	Life cycle	•	0.527	Hardness: 210	U.S. EPA, 1980n
		Rainbow trout	Embryo-larva	ì	0.350	Hardness: 50	U.S. EPA, 1980n
34	Cadmium	<u>D</u> . magna	Life cycle		0.00015	Hardness: 53	U.S. EPA, 1980o
		D. magna	Life cycle		0.00021	Hardness: 103	U.S. EPA, 1980o
		<u>D. magna</u> Midge (Tanytarsus	Life cycle		0.00044	Hardness: 209	U.S. EPA, 1980o
		dissimilis)			0.0031		U.S. EPA, 1980d
		Fathead minnow	Life cycle		0.046	Hardness: 201	U.S. EPA, 1980c
		Bluegill	Life cycle		0.050	Hardness: 207	U.S. EPA, 1980c
		Brook trout	Embryo-larva	1	0.0017	Hardness: 36	U.S. EPA, 1980o
		Brook trout	Embryo-larva	1	0.0092	Hardness: 187	U.S. EPA, 1980o
35	Lead	D. magna	Life cycle		0.012	Hardness: 52	U.S. EPA, 1980p
		D. magna Stonefly (Acroneuria	Life cycle		0.128	Hardness: 151	U.S. EPA, 1980p
		lycorias) Mayfly (Ephemerella	LC ₅₀	14	64.0		Hohreiter, 1980
		subvaria) Caddisfly (Hydropsyche	LC ₅₀	7	16.0		Hohreiter, 1980
		betteri)	LC ₅₀	7	32.0		Hohreiter, 1980
		Bluegill Bluegill	Embryo-larva		0.092	Hardness: 41	U.S. EPA, 1980p
		Rainbow trout	Embryo-larva		0.019	Hardness: 28	U.S. EPA, 1980p
		Rainbow trout	Embryo-larva		0.102	Hardness: 35	U.S. EPA, 1980p
36	Fluorine	Rainbow trout		21	113.0	100% kill, 45 mg/L CaCO ₃	Hohreiter, 1980
		Rainbow trout		21	250.0	100% kill, 320 mg/L CaCO ₃ , yearling trout	Hohreiter, 1980

aLatin binomials are listed in Appendix C.

Table A-3. Toxicity of synfuels chemicals to algae.

RAC	Representative chemical(s)	Test organism	Test type	Duration (h)	Concentration (mg/L)	Notes	Reference
12	Benzene	Chlorella vulgaris	EC ₅₀	48	525.0	Reduction in cell numbers	U.S. EPA, 1980c
14	Toluene	C. vulgaris	EC ₅₀	24	245.0	Reduction in cell numbers	U.S. EPA, 1980d
		Selenastrum <u>capricornu</u> tum	EC ₅₀	96	433.0	Reduction in cell numbers and chlorophyll <u>a</u>	U.S. EPA, 1980d
	Naphthalene	C. vulgaris	EC ₅₀	48	33.0	production Reduction in extrapolated cell numbers	U.S. EPA, 1980e
		<u>Chalamydomonas</u> <u>angulosa</u>	EC ₆₁	24	34.4	61% mortality of cells	U.S. EPA, 1980e
15	Fluoranthene	S. capricornutum	EC ₅₀	96	54.4	Reduction in cell	U.S. EPA, 1980f
		S. capricornutum	EC ₅₀	96	54.6	Reduction in chlorophyll <u>a</u> production	U.S. EPA, 1980f
17	Aniline	Agmenellum quadrupTicatum			0.010	Diffusion from disk onto algal lawn inhibited growth for 3-7 days	Batterton et al., 1978
	p-Toluidene	A. quadruplicatum			0.010	Same as above for all 4 species	Batterton et al.,
		Coccochloris elabens Eucapsis sp. Oscillatoria williamsii			0.010 0.010 0.010	Tot all 4 species	1370
1	Pheno l	S. capricornutum			20.0	Growth inhibition of 12-66% depending on time (2-3 d) and temperature (20, 24, 28°C)	U.S. EPA, 1980g
		S. capricornutum	EC ₅₀	24	40.0	Reduction in cell	U.S. EPA, 1980g
		Nitzschia <u>linearis</u>	EC ₅₀	120	258.0	Reduction in cell numbers	U.S. EPA, 1980g
		Chlorella pyrenoidosa	EC ₁₀₀	48	1500.0	Complete destruction of chlorophyll	U.S. EPA, 1980g
	2,4-Dimethylphenol	C. vulgaris C. pyrenoidosa	EC ₂₀ EC ₁₀₀	80 48	470.0 500.0	Growth inhibition Complete destruction of chlorophyll	U.S. EPA, 1980g U.S. EPA, 1980g

Table A-3. (continued).

RAC	Representative chemical(s)	Test organism	Test type	Duration (h)	Concentration (mg/L)	Notes	Reference
26	Butylbenzyl phthalate	S. capricornutum	EC ₅₀	96	0.11	Reduction in chlorophyll a	U.S. EPA, 1980j
		S. capricornutum	EC ₅₀	96	0.13	Reduction in cell numbers	U.S. EPA, 1980j
		Microcystis aeruginosa	EC ₅₀	96	1000.0	Reduction in cell	U.S. EPA, 1980j
		Navicula pelliculosa	EC50	96	0.60	Reduction in cell	U.S. EPA, 1980j
	Dimethyl phthalate	S. capricornutum	EC ₅₀	96	42.7	Reduction in chlorophyll a	U.S. EPA, 1980j
		S. capricornutum	EC ₅₀	96	39.8	Reduction in cell	U.S. EPA, 1980j
	Diethyl phthalate	S. capricornutum	EC50	96	90.3	Reduction in chlorophyll a	U.S. EPA, 1980j
		S. capricornutum	EC ₅₀	96	85.6	Reduction in cell numbers	U.S. EPA, 1980j
31	Arsenic	Cladophora, Spirogyra, Zygnema sp. Scenedesmus sp.	EC ₁₀₀	336 96	2.32 20.0	l00% kill Threshold effects	U.S. EPA, 19801 Cushman et al., 1977
32	Mercuric chloride	C. vulgaris	EC50	768	1.03	Cell division inhibition	U.S. EPA, 1980m
		Spring diatom assemblages	EC ₅₀	2	0.08	Reduction in photo- synthetic activity	U.S. EPA, 1980m
	Methylmercuric chloride	Coelastrum microporum	EC ₅₀		2.4-4.8	Growth inhibition	U.S. EPA, 1980m
33	Nickel	Chlamydomonas, Chlorella, Haematococcus, Scenedesmus sp.			0.1-0.7	Growth reduced in all cultures in water with 50 mg/L	U.S. EPA, 1980n
		Phormidium ambiguum Scenedesmus	EC16	336	0.5-10.0 1.5	CaCO ₃ Growth inhibition Threshold effects	Cushman et al., 1977 Cushman et al., 1977
34	Cadmium	Scenedesmus sp.			0.0061	Reduction in cell	U.S. EPA, 1980o
		Scenedesmus sp. C. pyrenoidosa C. vulgaris S. capricornutum Mixed species	EC ₅₀		0.05-0.5 0.25 0.06 0.05 0.005	Growth inhibition Growth inhibition Growth reduction Growth reduction Population reduction	Cushman et al., 1977 U.S. EPA, 1980o U.S. EPA, 1980o U.S. EPA, 1980o U.S. EPA, 1980o

Table A-3. (continued).

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

APPENDIX B Terrestrial Toxicity Data

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

					kposure		
RAC	Representative chemical	Test organism ^a	Response	Duration (hours)	Concentration (µg/m³)	Notes ^b	Reference
1	Carbon monoxide	Grapefruit	-CO ₂ uptake		1.8 E03	Detached leaves	National Research
		Red clover	-20% N fixation		1.1 E05		Council, 1977a National Research
		Several species	-Growth	552	1.1 E07		Council, 1977a National Research
		Popinac	Defoliation	24	2.3 E07		Council, 1977a National Research Council, 1977a
2	Sulfur dioxide ^C	Barley	-44% yield	72/wk	3.9 E02	Field, growing season	U.S. EPA, 1982
		Durum wheat Alfalfa	-42% yield -26% foliage	72/wk	3.9 E02	Field, growing season	U.S. EPA, 1982
				100	1.3 E02	5 hr/d, 5 d/wk, 4 wk	U.S. EPA, 1982
		Tobacco, Bel W3 Cocksfoot	-22% foliage -40% total wt.	100 2070	1.3 E02	5 hr/d, 5 d/wk, 4 wk	U.S. EPA, 1982
		Broadbean	Reduced net	2070 8	1.78 E02 9.2 E01	103.5 hr/wk, 20 wk	U.S. EPA, 1982
			photosynthesis				U.S. EPA, 1982
		White pine	Needle damage threshold	6	6.5 E01	sensitive clone	U.S. EPA, 1982
		Norway spruce	-25% volume growt	h 1680	1.3 E02		U.S. EPA, 1982
3	Nitrogen dioxide	Wheat	-12% straw yield	334	2 E03		Zahn, 1975
		Bush bean	-27% yield	639	2 E03		Zahn, 1975
		Spruce	-7% linear growth	1900	2-3 E03	-17% linear growth in following year	Zahn, 1975
		Endive	-37% yield	620	2 E03		Zahn, 1975
		Carrot	-30% yield	357	4 E03		Zahn, 1975
		Tobacco, bean, tomato, radish, oat, soybean	Visible foliar injury	4	3.8 E03		Heck and Tingey, 1979
		Cocksfoot and meadow grass	-Yield	2070	2.1 E02	103.5 h/wk, 20 wk	Ashenden and Mansfield, 1978
4	Hydrogen sulfide	Green bean	-20% photosynthes	is 3	7.0 E02		Taylor, in press
		Green bean	-25% whole plant vield	64	2.8 E02	4 h/d, 4 d/wk for 4 wk	Taylor, in press
		Alfalfa		672-840	4.2 E02	continuous fumigation	Thompson and Kats, 1978
		Lettuce	-66% yield	2112	4.2 E02	continuous fumigation	Thompson and Kats, 1978
		Douglas-fir	-weight and linear growth	5904	4.2 E02	continuous fumigation	Thompson and Kats, 1978
		Sugar beets	-38% sugar	3216	4.2 E02	continuous fumigation	Thompson and Kats, 1978
		addi pecas	+43% sugar	3216	4.2 E01	continuous fumigation	Thompson and Kats, 1978
5	Ammonía	Mustard	Injury	4	2.1 E03		National Research Council, 1979b

Table B-1. (continued).

RAC	Representative chemical	Test organism ^a	_	uration ours)	xposure Concentration (μg/m ³)	Notes ^b	Reference
6	Ethylene	African marigold	Epinasty	20	1.15 E00		National Air Pollution Control
		Carnation	Flowers do not open	72	1.15 E02		Administration, 1970 National Air Pollution Control
		Cotton	Growth inhibition	720	6.85 E02		Administration, 1970 National Air Pollution Control Administration, 1970
		Lily family	Growth inhibition	168	8.60 E02		National Air Pollution Control
		Various plants	Growth inhibition	240	2.39 E03		Administration, 1970 National Air Pollution Control Administration, 1970
7	Formaldehyde	Alfalfa	Injury	5	4.9 E02		National Research
		Petunia	Necrosis and leaf symptoms	48	2.47 E02		Council, 1981 Kingsbury et al., 1979
8	Vinyl chloride	Cowpea, cotton, squash	Injury	168	2.6 E05		Heck and Pires, 1962
12	Benzene	Pinto bean	Red-bordered spots	0.6	3.0 E04		Kingsbury et al., 1979
13	Cyclohexene	Runner bean	LD ₅₀ , toxicity to leaves	1	1.12 E12		Ivens, 1952
14	Toluene	Pinto bean	Bronze color	0.6	1.88 E05		Kingsbury et al., 1979
17	Aniline	Loblolly pine	Damage	3	2.7 E02		Cheeseman and Perry, 1977
22	Acrolein	Alfalfa	Oxident-type damage	9	2.5 E02		Kingsbury et al., 1979
23	Carbonyl sulfide	Runner bean	LD ₅₀ , toxicity to leaves	1	2.7 E03		Ivens, 1952
		Green bean	-13% growth	64	4.9 E02	4 h/d, 4 d/w for 4 wk	Taylor, in press

Table 8-1. (continued).

	Representative	Test		Duration E	xposure Concentration		
RAC	chemical	organism ^a	Response	(hours)	(µg/m ³)	Notes ^b	Reference
32	Mercury (metalic)	Rose	Severe damage		1.0 E01		Stahl, 1969
		Sugar beet English ivy	Damage Damage	5 12	2.8 E02 1.5 E04		Waldron and Terry, 1975 Waldron and Terry, 1975
		Coleus, Thevetia and Ricinus	Abscision	168	1.0 E01		Siegel and Siegel, 1979
	Mercuric chloride	Thevetia and Ricinus	Necrosis	168	1.0 E01		Siegel and Siegel, 1979
	Dimethylmercury	Coleus, Thevetia and Ricinus	Abscision	36	1.0 E01		Siegel and Siegel, 1979

^aLatin binomials are listed in Appendix C.

 $^{^{\}mathrm{b}}$ Unless "field" is noted, results are for laboratory studies.

^CSee also Table 4.

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

RAC	Representative chemical	Test organism* and life stage	Test medium	Response	Duration	Concentration (µg/g)	Reference
9	Acetic acid	Barley (seedling)	Solution in sand	Root growth inhibition	5d	600	Lynch, 1977
11	Metnyl pyridine	Alfalfa (sprout)	Solution	Koot growth inhibition	4d	93.1	Naik et al.,1972
13	Hexene	Oat (seedling)	Solution	Mortality		25.2	Chen and Elofson, 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	6h	0.0005	Deubert et al., 1979
	3,4-benzopyrene	Tobacco (seedling)	Soil	78% growth stimulation	60d	0.01	Graf and Nowak, 1966
	1,2-benzanthracene	Topacco (seedling)	Soil	80% growth stimulation	60d	0.02	Graf and Nowak, 1966
	1,2,5-b-di- benzanthrancene	Tobacco (seedling)	Soil	130% growth stimulation	60d	0.02	Graf and Nowak, 1966
16	Dimethylalkylamine	Gram, rice	Solution	Mortality		7.0	Dutta et al., 1972
19	Benzothiopnene	Cucumber (sprout)	Solution	9% root growth inhibition	4d	10	Schlesinger and Mowry, 1951
	Indole, 3-ethyl-lH	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	11d	35	Hilton and Nomura, 1964
		Pea (sprout)	Solution	Germination reduced by >50%	8h	10	Shukla, 1972
20	Benzoic acid	Lettuce (seedling)	Solution on filter paper	23% growth inhibition		25	Chou and Patrick, 1976
	2-nydroxy -benzoic acid	Rice (seedling)	Soil	Seedling growth inhibition	5d	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	4d	2000	Badilescu et al., 1967
22	4-hydroxy -benzaldehyde	Lettuce (seedling)	Solution on filter paper	26% growth inhibition		100	Chou and Patrick, 1976

Table B-2. (continued).

RAC	Representative cnemical	Test organism* and life stage	Test medium	Response	Duration	Concentration (µg/g)	n Reference
22	Acrolein	Alfalfa		Oxidant-type damage	9h	0.1	Kingsbury et al., 1979
23	Carbon disulfide	Apple	Soil	Root injury		420	Underhill and Cox, 1940
24	Etnanol	Lettuce (seed)	Solution	Germination inhibition	44h	1,000,000	Meyer and Mayer, 1971
27	N,N-dimethyl- formamide	Lettuce (seed)	Solution	Nearly total suppression of germination	24h	1,000,000	Meyer and Mayer, 1971
	2-methyl -benzamide	Poppy, chickweed, carrot, ryegrass corn, lucerne (mature)	Soil	13-87% reduction in yield	3-5w	220,000	Pizey and Wain, 1959
31	Arsenica	Corn (seedling)	Soil	10% growth reduction (wet tissue weight)	4w	64	Woolson, et al., 1971
		Cotton (mature)	Soil (fine sandy loam)	Approx. 55% reduction in yield	6w	8 b	Deuel and Swoboda, 1972
		Cotton (mature)	Soil (clay)	Approx. 40% reduction in yield	6w	28 ^b	Deuel and Swoboda, 1972
		Soybean (mature)	Soil (fine sandy loam)	Approx. 45% reduction in yield	6w	3 b	Deuel and Swoboda, 1972
		Soybean (mature)	Soil (clay)	Approx. 40% reduction in yield	6 w	12 ^b	Deuel and Swoboda, 1972
		Cowpea	-	Retarded growth	-	16	Albert and Arndt, 1932
32	Mercury	Barley (seed-sprout)	Solution	12% growth reduction (fresh weight)	7d post germination	5 (as Hg ⁺⁺)	Mukniya et al., 1983
		Barley (seed-sprout)	Solution	12% growth reduction (fresh weight)	7d post germination		Mukhiya et al., 1983
		Lettuce (seed-sprout)	Solution	68% reduction in elongation of lettuce hypocotyl	5d 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	7d	0.8	Carlson et al., 1975

Table B-2. (continued).

RAC	Representative chemical	Test organism* and life stage	Test medium	Response	Duration	Concentration (µg/g)	Reference
33		Oats (seeds-seedlings)	Solution in coarse sand	Stunted growth	Up to 22d 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	3w	281 (NiSO ₄ •7H ₂ O)	Agarwala et al., 1977
34	Cadmium	Corn (mature)	Solution	10% decrease in net photosynthesis	7 d	0.9	Carlson et al., 1975
		Sunflower (mature)	Solution	10% decrease in net photosynthesis	7d	0.45	Carlson et al., 1975
		Soybeans (mature)	Solution in sand and vermiculite	35% decrease in fresh weight of pods	90d	2	Huang et al., 1974
		Bean (5 weeks old)	Solution	50% growth reduction	3 w	0.2	Page et al., 1972
		Beet (5 weeks old)	Solution	50% growth reduction	3w	0.2	Page et al., 1972
		Turnip (5 weeks old)	Solution	50% growth reduction	3w	0.2	Page et al., 1972
		Corn (5 weeks old)	Solution	50% growth reduction	3w	1.2	Page et al., 1972
		Lettuce (5 weeks old)	Solution	50% growth reduction	3w	0.9	Page et al., 1972
		Tomato (5 weeks old)	Solution	50% growth reduction	3w	4.8	Page et al., 1972
		Barley (5 weeks old)	Solution	50% growth reduction	3w	5.6	Page et al., 1972
		Pepper (5 weeks old)	Solution	50% growth reduction	3w	2.0	Page et al., 1972
		Cabbage (5 weeks old)	Solution	50% growth reduction	3w	9.0	Page et al., 1972
		Soybean (seedling)	Soil (silty clay loam)	15% reduction in yield (dry weight)	5w	2.5	Haghiri, 1973
		Wheat (seedling)	Soil (silty clay loam)	20% reduction in yield (dry weight)	5₩	2.5	Haghiri, 1973
		Lettuce (mature)	Soil (silty clay loam)	40% reduction in yield (fresh weight)	Whole life	2.5	Hagniri, 1973

Table B-2. (continued).

RAC	Representative chemical	Test organism* and life stage	Test medium	Response	Duration	Concentration (µg/g)	Reference
34		Sycamore (sapling)	Soil (6:1 silty clay loam & perlite)	25% reduction in new stem growth	90d	39	Carlson and Bazzaz, 1977
35	Lead	Soybeans (mature)	Solution in sand and vermiculite	35% decrease in fresh weight of pods	90d	62	Huange et al., 1974
		Lettuce (44d old)	Soil (silty clay loam)	25% reduction in yield	30d	1000 (Pb(NO ₃) ₂	John and VanLaerhoven 1972
		Corn (25d seedling)	Vermiculite and solution	20% decrease in photosynthesis	11-21d	1000	Bazzaz et al., 1974
		Soybean (25d seedling)	Vermiculite and solution	20% decrease in photosynthesis	11-21d	2000	Bazzaz et al., 1974
		Sycamore (sapling)	Soil (6:1 silty clay loam & perlite)	25% reduction in new stem growth	90d	500	Carlson and Bazzaz, 1977

^{*}Latin binomials are listed in Appendix C.

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

 $^{^{\}rm b}$ Concentration of contaminant available in solution.

C(PMA-Phenyl mercuric acetate).

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

RAC	Representative chemical	Test organism ^a	Response	Duration (hours)	concentration (µg/m ³)	Notes	Reference
1	Carbon monoxide	Rabbit	Aortic lesions	4	1.51 E05		National Research Council, 1977a
		νog	Heart damage	1008	4.3 E04		National Research Council, 1977a
		Chicken	75% egg hatch	432	4.9 E05	egg exposed	National Research Council, 1977a
		Rabbit	90% neonate survival	720	1.0 E05	mother exposed	National Řesearch Council, 1977a
		Human	Lethality		9.2 E08		Cleland and Kingsbury, 1977
2	Sulfur dioxide	Guinea pig	Increased airway resistance	1	4.2 E02		U.S. EPA, 1982
		Guinea pig Dog	LT ₅₀ Increased airway resistance	1.1 5,400	5.8 E06 1.3 E04		U.S. EPA, 1982 U.S. EPA, 1982
		Chicken .	Modified nasal clearance		3.7 E03	Intermittent exposure, 7 d	Wakabayashi et al., 1977
	Sulfuric acid	Guinea pig	Respiratory function	1	1.0 E02		Wakabayashi et al., 1977
		Guinea pig	Lethality	8	1.8 E04		Wakabayashi et al., 1977
		Dog	Respiratory function	4,725	8.9 E02		Wakabayashi et al., 1977
3	Nitrogen dioxide	Guinea pig	LC ₅₀	1	1.5 E05		National Research Council, 1977b
		Rat	11% lethality	5,120	2.3 E04		National Research Council, 1977b
		Rat	Bronchial damage	24	2.8 E04		National Research Council, 1977b
		Mouse	Defects in pulmonary microbial defense	24	3.8 E03		National Ŕesearch Council, 1977b
		Rat and mouse	Pulmonary pathologies	Chronic	9.4 E02	Also decreased resistance to infection	National Research Council, 1977b
4	Hydrogen sulfide	Canaries, rats and dogs	Pulmonary irritation	Subacute	7.0 E04	No established chronic effects	National Research Council, 1979a

Table 8-3. (continued).

				Ex	posure				
RAC	Representative chemical	Test organism ^a	Response	Duration (hours)	Concentration (µg/m ³)	Notes	Reference		
5	Аплопіа	Chicken	Increased disease susceptibility	72	1.3 E04	Newcastle virus	National Research Council, 1979b		
		Pig	Respiratory irritation	840	4.3 E04		National Research Council, 1979b		
		Rabbit	LT ₅₀	33	7.0 E06		National Research Council, 1979b		
		Mouse	Lethal threshold	16	7.0 E05		National Research Council, 1979b		
		Human	Throat irritation	Immediate	2.8 E05		National Research Council, 1979b		
6	Acetylene	Human	Unconsciousness	0.08	3.7 E08		National Research Council, 1976		
7	Formaldenyde	Rat	LC ₅₀	4	5.7 E05		National Research Council, 1981		
		Guinea pigs	Increased airway resistance	1	3.6 E02		National Research Council, 1981		
		Rat	Respiratory and eye irritation and liver weight loss	1400	1.0 E03		National Research Council, 1981		
8	Chloroform	Mouse Human	LC50 Enlarged liver	Chronic	1.4 E05 4.9 E04	In workplace air	Kîngsbury et al., 1979 Kingsbury et al., 1979		
9	Acetic acid	Mouse Human Human	LC50 Irritation Respiratory, stomach and skin irritation	l 0.05 Chronic	1.4 E07 2.0 E06 1.5 E05	7-12 years, workplace exposure	Kingsbury et al., 1979 Kingsbury et al., 1979 National Research Council, 1976		
10	Furan Thiophene	Rat Mouse	Lethal threshold Lethal threshold	8~48 8~48	2.4 E08 3.0 E07		Kingsbury et al., 1979 Kingsbury et al., 1979		
11	Pyridine 2-Ethylpyridine	Rat Rat	LC ₅₀ LC ₁₀₀	4 3	1.3 E07 2.4 E07		Kingsbury et al., 1979 Kingsbury et al., 1979		
12	Benzene	Human	Lethal threshold	Chronic	1.9 E05	Workplace exposure	National Research Council, 1976		

Table B-3. (continued).

RAC	Representative chemical	Test organism ^a	Response	Duration (hours)	Concentration (µg/m ³)	Notes	Reference
13	Pentane	Mouse	Lethality		3.8 E08		Kingsbury et al., 1979
	Cyclopentane	Mouse	Lethality		1.1 E08		Kingsbury et al., 1979
	Hexane	Mouse	Lethality		1.2 E08		Kingsbury et al., 1979
		Human	Dizziness	0.17	1.8 E07		Kingsbury et al., 1979
	Cyclohexane	Rabbit	Lethality	1	9.2 E07		Kingsbury et al., 1979
		Rabbit	Narcosis and convulsi		4.5 E07		Kingsbury et al., 1979
	Heptane	Human	Dizziness	0.10	4.1 E06		Kingsbury et al., 1979
	Butadiene	Human	Respirtory and eye irritation	8	1.8 E07		Kingsbury et al., 1979
	Cyclopentadine	Rat	Liver and kidney damage	245	1.4 E06	expsoure = 7 hr/day for 35 days	Kingsbury et al., 1979
14	Toluene	Rat	Lethal threshold	4	1.5 E07		Kingsbury et al., 1979
		Human	Psychological effects		3.8 E05		Kingsbury et al., 1979
	Ethyl benzene	Rat	Lethal threshold	4	1.7 E07		Kingsbury et al., 1979
		Human	Eve irritation	<0.08	8.8 E05		Kingsbury et al., 1979
	p-Xylene	Mouse	Lethal threshold	4	1.5 E07		Kingsbury et al., 1979
	Tetrahydro-			•	110 207		Kingsbary co arr, 1979
	naphthalene	Guinea pig	Lethal threshold	136	1.5 E06	8 hours for 17 days	Kingsbury et al., 1979
	Naphthalene	Human	Eye irritation and damage		7.9 E04		Kingsbury et al., 1979
15	(No data on respira	tory toxicity but	several members of this	RAC are card	inogens)		Kingsbury et al., 1979
16	Ethylamine	Rat	Lethal threshold	4	5.5 E06		Kingsbury et al., 1979
		"Animals"	Lung, liver and	1008	1.8 E05		Kingsbury et al., 1979
			kidney damage		110 200		Kingsbury et ur., 1919
	l-Aminopropane	Rat	LC ₅₀	4	5.6 E06		Kingsbury et al., 1979
17	Aniline	Rat	LC ₅₀	4	9.5 E05		Kingsbury et al., 1979
	Dimethylanaline	Mouse	LC ₅₀ LC ₅₀	7	7.4 E05	Mixed isomers	Kingsbury et al., 1979
18	(No data on respirat	tory toxicity)					
19	(No data on respirat	tory toxicity)					
20	(No data on respirat	cory toxicity)					
21	(No data on respirat	tory toxicity)					

Table B-3. (continued).

RAC	Representative chemical	Test organism ^ā	Response	Duration (hours)	xposure Concentration (μg/m ³)	Notes	Reference
22	Acrolein	Rat	LC ₅₀	4	1.8 E04		National Research
		Monkey	Respiratory system	2,160	5.1 E02		Council, 1981 National Research
	Acetaldehyde	Mice, rabbits and	damage LC ₅₀	4	2.0 E06		Council, 1981 National Research
	Proprionaldehyde	guinea pigs Rat	LC ₅₀	0.5	6.2 E07		Council, 1981 National Research
		Rat	Reduced weight gain	36	3.1 E06	6 h/d x 6 d	Council, 1981 National Research Council, 1981
	Butyraldehyde	Rat	LC ₅₀	0.5	1.7 E08		National Research Council, 1981
	Butanone	Mouse	LC ₅₀	0.75	6.1 E08		National Research Council, 1981
23	Methyl mercaptan Ethyl mercaptan	Rat Rat Human	Lethal threshold LC ₅₀ Central nervous system effects	 	2.0 E07 1.1 E07 1.0 E04		Kingsbury et al., 1979 Kingsbury et al., 1979 Kingsbury et al., 1979
	n-Butyl mercaptan	Rat Human	LC ₅₀ "Toxic effect"	4 3	1.5 E07 1.0 E04		Kingsbury et al., 1979 Kingsbury et al., 1979
	Thiophenol Carbon disulfide	Rat Human	LC ₅₀ Central nervous system effects	4	1.5 E05 5.0 E04	7 years exposure	Kingsbury et al., 1979 Cleland and Kingsbury, 1977
24	Methanol	Monkey Human	LC ₅₀ Central nervous system effects		1.3 E06 7.5 E04		Kingsbury et al., 1979 Kingsbury et al., 1979
	Ethanol	Human	Eye and respiratory irritation and mental effects		1.9 E06		Kingsbury et al., 1979
25	(No data on respirat	ory toxicity)					Kingsbury et al., 1979
26	Methyl acetate Methyl methacrylate Butyl acetate	Human Rat Human Human	Severe toxic effects LC ₅₀ Throat irritation Toxic effects	1 1	1.5 E06 1.5 E07 9.6 E05 9.6 E06		Kingsbury et al., 1979 Kingsbury et al., 1979 Kingsbury et al., 1979 Kingsbury et al., 1979
	n-Amyl acetate	Human	Toxic threshold	0.5	1.0 E06		Kingsbury et al., 1979
27	(No data on respirat	ory toxicity)					Kingsbury et al., 1979
28	Acetonitrile	Rat Human	Lethal threshold Bronchial effects	4	1.3 E07 2.7 E05		Kingsbury et al., 1979 Kingsbury et al., 1979
	Acrylonitrile	Rat	Lethal threshold	4	1.1 E06		Kingsbury et al., 1979

Table B-3. (continued).

				F	xposure		
RAC	Representative chemical	Test organism ^a	Response	Duration (hours)	Concentration (µg/m ³)	Notes	Reference
29	(No data on respira	tory toxicity)					Kingsbury et al., 1979
30	Fly ash	Monkey	Slight lung fibrosis	13,390	4.6 E02		National Research Council, 1979c
31	Arsenic trioxide	Rat	Weight lag and physiological effec	2 4 :ts	2.5 EOl		National Research Council, 1977c
32	Mercury (metal)	Human Rabbit Human	Toxic threshold Toxic threshold Central nervous system effects		1.0 E03 2.9 E04 1.7 E02	40 yr. exposure	Cassidy and Furr, 1978 Cassidy and Furr, 1978 Kingsbury et al., 1979
33	Nickel carbonyl	Rat	LC ₅₀	0.5	2.4 E05		National Research Council, 1975
34	Cadmium oxide fumes Cadmium oxide dust Cadmium	Human Human Human	Lethality Impaired lung functic Pulmonary and renal effects	8 on	5.0 E03 3.15 E03 1.0-27 E01	20 yr. exposure Occupational exposure	Hammons et al., 1978 Hammons et al., 1978 Kingsbury et al., 1979
35	Lead	Human	Threshold of overt poisoning		5.0 E02	Occupational exposure	National Research Council, 1972

^aLatin binomials are lised in Appendix C.

APPENDIX C

Common and Scientific Names of Animals and Plants

Animals

Common name

Bigmouth buffalo Black crappie Bluegill Brook trout Brown trout Canary Carp Channel catfish Chicken

Chinook salmon Coho salmon

Dog

Fathead minnow

Goldfish Green sunfish Guinea pig Human

Largemouth bass

Monkey

Mosquitofish

Mouse

Northern pike

Pig

Pink salmon **Pumpkinseed**

Rabbit

Rainbow trout

Rat

Smallmouth buffalo

White bass

Scienfitic name

Ictiobus cyprinellus Pomoxis nigromaculatus Lepomis macrochirus Salvelinus fontinalis

Salmo trutta Serinus canarius Cyprinus carpio Ictalurus punctatus Gallus gallus

Oncorhynchus tshawytacha Oncorhynchus kisutch

Canis familiaris Pimephales promelas Carassius auratus Lepomis cyanellus

Cavia cobaya Homo sapiens

Micropterus salmoides

Macaca sp.

Gambusia affinis Mus musculus Esox lucius Sus scrofa

Oncorhynchus gorbuscha

Lepomis gibbosus

Orvetolagus cuniculus

Salmo gairdneri Rattus rattus Ictiobus bulbalus Morone chrysops

Plants

Common name

African marigold Alfalfa Apple Barlev Bean Broadbean Bush bean

Carrot Chickweed, common

Cabbage

Carnation

Cocksfoot Coleus Corn Cotton Cowpea Cress Cucumber Durum wheat Endive English ivy Gram

Grapefruit Green bean Lettuce

Loblolly pine Lucerne Meadowgrass

Mustard Norway spruce

0at Oat, wild Pea Pepper Petunia Pinto bean

Popinac Poppy Radish Red clover Rice

Ricinus Rose

Squash

Runner bean

Ryegrass, Italina Sovbean Spruce

Scientific name

Tagetes sp. Medicago sativa Malus sylvestris Hordeum vulgare Phaseolus vulgaris

Vicia faba

Phaseolus vulgaris Brassica oleracea Dianthus caryophyllos

Daucus carota Stellaria media Dactylis glomerata Coleus blumei

Zea mays

Gossypium hirsutum Vigna sinensis Lepidium sativum Cucumis sativus Triticum durum Cicorium endivia Hedera helix Cicer arietinum Citrus paradisi Phaseolus vulgaris Lactuca sativa Pinus taeda

Medicago sativa Poa pratensis Brassica alba Picea abies Avena sativa Avena fatua

Psoralea corylifolia Capsicum frutescens Petunia sp.

Phaseolus vulgaris Acacia farnesiana

Papaver sp. Raphanus sativus Trifolium pratense Oryza sativa

Ricinus communis Rosa sp.

Phaseolus vulgaris Lolium multiflorum

Glycine max Picea abies Cucurbita sp.

Plants (continued)

Common name Scientific name

Sugar beet Beta vulgaris Helianthus annuus Platanus occidentalis Sunflower Sycamore Thevetia Thevetia neriifolca Nicotiana tabacum Lycopersicon esculentum Tobacco Tomato Brassica napus Triticum durum Turnip

Wheat Pinus strobus White pine

APPENDIX D

Species-specific Results of the Analysis of Extrapolation Error

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

							PGMATC	(µg/1)				
	RAC	Carp	В	uffalo	Channel Catfish	White Bass	Green Sunfish	Bluegill Sunfish	Largemouth Bass	Black Crappie	Rainbow Trout	Brook Trout
1	Carbon monoxide											
2	Sulfur oxides											
3	Nitrogen oxides	0.0		0.0	11.6	2 2						
4	Acid gases	8.8		8.8	11.6	3.3	6.7	3.1	2.5	1.6	2.6	2.6
5 6	Alkaline gases	43.5	1.565	43.5	32.9	18.0	18.0	18.0	18.0	18.0	15.3	14.9
9	Hydrocarbon gases 1, Formaldehyde	565,162	1,565	, 102	11,313	29,185	29,185	29,185	29,185	29,185	19,705	19,705
8	Volatile organochlorines	533	No data	1245	600	135	705	814	744	110	566	566
9	Volatile organochiorines Volatile carboxylic acids	941		933	518	213	705 213	814 213	744 213	213	252	252
10	Volatile O&S heterocyclics		No data	933	316	213	213	213	213	213	232	232
11	Volatile N heterocyclics		No data									
iż	Benzene	421	10 3464	252	144	116	116	116	116	116	125	86
13	Aliphatic/alicyclic hydrocarbon			255	166	66	66	66	66	66	68	68
14	Mono/diaromatic hydrocarbons	120		146	91	65	65	65	65	65	65	50
15	Polycyclic aromatic nydrocarbon	s 190		190	134	79	121	98	86	22	74	74
16	Aliphatic amines		No data									
17	Aromatic amines	ı	No data									
81	Alkaline N neterocyclics	562		590	590	347	141	141	141	141	159	159
19	Neutral N. O&S heterocyclics	i	No data									
20	Carboxylic acids	48,548	48	,548	1435	2001	2001	2001	2001	2001	1317	1317
21	Phenois	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	Nonneterocylic organosulfur		No data									
24	Alcohols		No data									
25	Nitroaromatics		No data									
26	Esters	33.0		287.4	160.9	133.0	40.5	26.6	22.8	8.1	145.9	97.6
27	Amides		No data									3.60
28	Nitriles	215		389	237	65	236	220	196	41	160	160
29	Tars		No data									
30	Respirable particles		No data	470	047	229	409	424	383	67	257	281
31	Arsenic	238		479 34.2	247 26.9	14.0	409 14.0	14.0	383 14.0	14.0	257 11.9	12.0
32	Mercury (inorganic)	34.2		34.2	26.9 10.9	4.5	4.5	4.5	4.5	4.5	2.3	4.4
32A	Mercury (methyl)	11.7 94		876	410	433	147	124	110	26	552	296
33	Nickel	94 11.1		1.5	2.0	433 0.5	76.7	57.0	51.3	14.8	0.2	0.3
34	Cadmium	54		171	104	77	393	404	364	65	61	102
35	Lead	24		171	107	, ,	3,3	707	331			

Table D-2. Probabilities of chronic toxic effects on fish populations due to RAC 5 at annual median ambient concentrations for EDS.

		ient PGMATC	Probabi exceeding	Level of	
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.2572 0.2572 0.2572 0.3397 0.6205 0.6205 0.6205 0.6205	0.2572 0.2572 0.2572 0.3397 0.6205 0.6205 0.6205 0.6205	0.2616 0.2616 0.2616 0.3177 0.4039 0.4039 0.4039 0.4039 0.4039	0.2616 0.2616 0.2616 0.3177 0.4039 0.4039 0.4039 0.4039	Class

Table D-3. Probabilities of chronic toxic effects on fish populations due to RAC 13 at annual median ambient concentrations for EDS.

	Ambient conc/PGMATC		Probability of exceeding the PGMATC		Level of
Species	TMT 1	TMT2	TMTl	TMT2	extrapolation
Carp	0.3257	0.0326	0.2786	0.0366	Family
Bigmouth buffalo	0.2786	0.0279	0.2530	0.0312	*
Smallmouth buffalo	0.2786	0.0279	0.2530	0.0312	*
Channel catfish	0.4281	0.0428	0.3419	0.0652	Class
White bass	1.0832	0.1083	0.5145	0.1557	Class
Green sunfish	1.0832	0.1083	0.5145	0.1557	Class
Bluegill sunfish	1.0832	0.1083	0.5145	0.1557	Class
Largemouth bass	1.0832	0.1083	0.5145	0.1557	Class
Black crappie	1.0832	0.1083	0.5145	0.1557	Class

^{*}Fathead minnow - Cypriniformes.

Table D-4. Probabilities of chronic toxic effects on fish populations due to RAC 14 at annual median ambient concentrations for EDS.

Species	Ambient conc/PGMATC		Probabi exceeding		Level of
	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0440 0.0362 0.0362 0.0580 0.0813 0.0813 0.0813 0.0813	0.0044 0.0036 0.0036 0.0058 0.0081 0.0081 0.0081 0.0081	0.0497 0.0603 0.0603 0.1063 0.1010 0.1010 0.1010 0.1010	0.0021 0.0043 0.0043 0.0121 0.0072 0.0072 0.0072 0.0072	Family Class Class Class Class Class Class Class

Table D-5. Probabilities of chronic toxic effects on fish populations due to RAC 20 at annual median ambient concentrations for EDS.

	Ambient conc/PGMATC		Probabi exceeding		Level of
Species	ТМТ	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0034 0.0034 0.0034 0.1147 0.0823 0.0823 0.0823 0.0823 0.0823	0.0003 0.0003 0.0003 0.0115 0.0082 0.0082 0.0082 0.0082	0.0047 0.0047 0.0047 0.3107 0.1229 0.1229 0.1229 0.1229 0.1229	0.0001 0.0001 0.0001 0.1540 0.0129 0.0129 0.0129 0.0129 0.0129	Class

Table D-6. Probabilities of chronic toxic effects on fish populations due to RAC 21 at annual median ambient concentrations for EDS.

	Ambient conc/PGMATC			lity of the PGMATC	Level of
Species	TMT1	TMT2	TMTl	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0396 0.0473 0.0473 0.0885 0.1003 0.0594 0.0606 0.0675 0.3539	0.0040 0.0047 0.0047 0.0089 0.0100 0.0059 0.0061 0.0068 0.0354	0.0478 0.0783 0.0783 0.1455 0.1226 0.0669 0.0568 0.0824 0.3230	0.0022 0.0065 0.0065 0.0198 0.0100 0.0032 0.0020 0.0050 0.0698	Family Class Class Class Class Genus Species Family Family

Table D-7. Probabilities of chronic toxic effects on fish populations due to RAC 22 at annual median ambient concentrations for EDS.

Consina	Ambient conc/PGMATC		Probability of exceeding the PGMATC		Level of
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.2082 0.2082 0.2082 0.2258 0.5397 0.2466 0.4890 0.3255 1.1049	0.0208 0.0208 0.0208 0.0226 0.0540 0.0247 0.0489 0.0325 0.1105	0.2301 0.2301 0.2301 0.2566 0.3769 0.2241 0.3412 0.2601 0.5182	0.0342 0.0342 0.0342 0.0479 0.0689 0.0225 0.0422 0.0249 0.1561	Class Class Class Class Class Genus Species Species Family
					, amily

Table D-8. Probabilities of chronic toxic effects on fish populations due to RAC 28 at annual median ambient concentrations for EDS.

Species	Ambient conc/PGMATC		Probabi exceeding		Level of
	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0509 0.0282 0.0282 0.0462 0.1690 0.0464 0.0500 0.0560 0.2706	0.0051 0.0028 0.0028 0.0046 0.0169 0.0046 0.0050 0.0056 0.0271	0.0596 0.0566 0.0566 0.0968 0.2090 0.0509 0.0449 0.0680 0.2805	0.0029 0.0046 0.0046 0.0115 0.0316 0.0021 0.0013 0.0037 0.0542	Family Class Class Class Class Genus Species Family Family

Table D-9. Probabilities of chronic toxic effects on fish populations due to RAC 34 at annual median ambient concentrations for EDS.

Species	Ambient conc/PGMATC		Probabi exceeding	Level of	
	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0069 0.0501 0.0501 0.0388 0.1468 0.0010 0.0014 0.0015 0.0052	0.0069 0.0501 0.0501 0.0388 0.1468 0.0010 0.0014 0.0015 0.0052	0.0022 0.0814 0.0814 0.0782 0.1692 0.0000 0.0001 0.0003 0.0086	0.0022 0.0814 0.0814 0.0782 0.1692 0.0000 0.0001 0.0003 0.0086	Species Class Class Class Class Genus Species Family Family

Table D-10. Probabilities of chronic toxic effects on fish populations due to RAC 5 at annual median ambient concentrations for SRC-I.

	Ambient conc/PGMATC		Probabi exceeding		Level of
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.4208 0.4208 0.4208 0.5558 1.0152 1.0152 1.0152 1.0152	0.4208 0.4208 0.4208 0.5558 1.0152 1.0152 1.0152 1.0152	0.3420 0.3420 0.3420 0.3982 0.5031 0.5031 0.5031 0.5031	0.3420 0.3420 0.3420 0.3982 0.5031 0.5031 0.5031 0.5031	Class

Table D-11. Probabilities of chronic toxic effects on fish populations due to RAC 13 at annual median ambient concentrations for SRC-I.

	Ambient conc/PGMATC		Probabi exceeding		Level of
Species	TMT1	TMT2	TMT 1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.3257 0.2786 0.2786 0.4281 1.0832 1.0832 1.0832 1.0832	0.0326 0.0279 0.0279 0.0428 0.1083 0.1083 0.1083 0.1083	0.2786 0.2530 0.2530 0.3419 0.5145 0.5145 0.5145 0.5145	0.0366 0.0312 0.0312 0.0652 0.1557 0.1557 0.1557 0.1557	Family * Class Class Class Class Class Class

^{*}Fathead minnow-Cypriniformes.

Table D-12. Probabilities of chronic toxic effects on fish populations due to RAC 14 at annual median ambient concentrations for SRC-I.

Species	Ambient conc/PGMATC		Probabi exceeding	Level of	
	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0203 0.0167 0.0167 0.0268 0.0375 0.0375 0.0375 0.0375	0.0020 0.0017 0.0017 0.0027 0.0038 0.0038 0.0038 0.0038	0.0199 0.0278 0.0278 0.0565 0.0475 0.0475 0.0475 0.0475	0.0005 0.0014 0.0014 0.0048 0.0023 0.0023 0.0023 0.0023	Family Class Class Class Class Class Class Class

^{*}Fathead minnow-Cypriniformes.

Table D-13. Probabilities of chronic toxic effects on fish populations due to RAC 21 at annual median ambient concentrations for SRC-I.

Species	Ambient conc/PGMATC		Probabi exceeding	Level of	
	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp	0.1890	0.0189	0.1951	0.0203	Family
Bigmouth buffalo	0.2257	0.0226	0.2449	0.0393	Class
Smallmouth buffalo	0.2257	0.0226	0.2449	0.0393	Class
Channel catfish	0.4229	0.0423	0.3539	0.0841	Class
White bass	0.4792	0.0479	0.3550	0.0624	Class
Green sunfish	0.2836	0.0284	0.2517	0.0293	Genus
Bluegill sunfish	0.2896	0.0290	0.2422	0.0228	Species
Largemouth bass	0.3226	0.0323	0.2799	0.0383	Family
Black crappie	1.6908	0.1691	0.5918	0.2159	Family

Table D-14. Probabilities of chronic toxic effects on fish populations due to RAC 35 at annual median ambient concentrations for SRC-I.

	Ambient conc/PGMATC		Probabi exceeding		Level of
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0212 0.0067 0.0067 0.0109 0.0148 0.0029 0.0028 0.0031 0.0177	0.0212 0.0067 0.0067 0.0109 0.0148 0.0029 0.0028 0.0031 0.0177	0.0203 0.0096 0.0096 0.0241 0.0162 0.0010 0.0005 0.0015	0.0203 0.0096 0.0096 0.0241 0.0162 0.0010 0.0005 0.0015 0.0380	Family Class Class Class Class Genus Species Family

Table D-15. Probabilities of chronic toxic effects on fish populations due to RAC 5 at annual median ambient concentrations for SRC-II.

Species	Ambient conc/PGMATC		Probability of exceeding the PGMATC		Level of
	TMTl	TMT2	TMT 1	TMT2	extrapolation
Carp	0.2334	0.2334	0.2472	0.2472	Class
Bigmouth buffalo	0.2334	0.2334	0.2472	0.2472	Class
Smallmouth buffalo	0.2334	0.2334	0.2472	0.2472	Class
Channel catfish	0.3087	0.3087	0.3028	0.3028	Class
White bass	0.5639	0.5639	0.3851	0.3851	Class
Green sunfish	0.5639	0.5639	0.3851	0.3851	Class
Bluegill sunfish	0.5639	0.5639	0.3851	0.3851	Class
Largemouth bass	0.5639	0.5639	0.3851	0.3851	Class
Black crappie	0.5639	0.5639	0.3851	0.3851	Class

Table D-16. Probabilities of chronic toxic effects on fish populations due to RAC 8 at annual median ambient concentrations for SRC-II.

Species	Ambient conc/PGMATC		Probabi exceeding		Level of
	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass	0.0037 0.0016 0.0016 0.0033 0.0145 0.0028 0.0024 0.0026	0.0004 0.0002 0.0002 0.0003 0.0014 0.0003 0.0002 0.0003	0.0020 0.0023 0.0023 0.0066 0.0273 0.0010 0.0004 0.0012	0.0000 0.0001 0.0001 0.0003 0.0015 0.0000 0.0000	Family Class Class Class Class Genus Species Family
Black crappie	0.0177	0.0018	0.0402	0.0030	Family

Table D-17. Probabilities of chronic toxic effects on fish populations due to RAC 12 at annual median ambient concentrations for SRC-II.

	Ambient conc/PGMATC		Probabi exceeding	Level of	
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp	0.0039	0.0004	0.0020	0.0000	Family
Bigmouth buffalo	0.0064	0.0006	0.0094	0.0003	Class
Smallmouth buffalo	0.0064	0.0006	0.0094	0.0003	Class
Channel catfish	0.0113	0.0011	0.0251	0.0015	Class
White bass	0.0140	0.0014	0.0153	0.0004	Class
Green sunfish	0.0140	0.0014	0.0153	0.0004	Class
Bluegill sunfish	0.0140	0.0014	0.0153	0.0004	Class
Largemouth bass	0.0140	0.0014	0.0153	0.0004	Class
Black crappie	0.0140	0.0014	0.0153	0.0004	Class

Table D-18. Probabilities of chronic toxic effects on fish populations due to RAC 14 at annual median ambient concentrations for SRC-II.

	Ambient conc/PGMATC		Probabi exceeding	lity of the PGMATC	Level of
Species	TMT1	TMT2	TMT 1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.1219 0.1002 0.1002 0.1606 0.2251 0.2251 0.2251 0.2251	0.0122 0.0100 0.0100 0.0161 0.0225 0.0225 0.0225 0.0225	0.1335 0.1410 0.1410 0.2117 0.2242 0.2242 0.2242 0.2242 0.2242	0.0100 0.0157 0.0157 0.0353 0.0269 0.0269 0.0269 0.0269	Family Class Class Class Class Class Class Class

Table D-19. Probabilities of chronic toxic effects on fish populations due to RAC 15 at annual median ambient concentrations for SRC-II.

Constant	Ambient conc/PGMATC		Probabi exceeding	lity of the PGMATC	Level of
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0026 0.0026 0.0026 0.0037 0.0062 0.0041 0.0050 0.0057	0.0003 0.0003 0.0003 0.0004 0.0006 0.0004 0.0005 0.0006	0.0036 0.0036 0.0036 0.0081 0.0037 0.0014 0.0011 0.0032 0.0421	0.0001 0.0001 0.0001 0.0004 0.0000 0.0000 0.0000 0.0000	Class Class Class Class * Genus Species Family Family

^{*}Bluegill-Perciformes.

Table D-20. Probabilities of chronic toxic effects on fish populations due to RAC 21 at annual median ambient concentrations for SRC-II.

Consider	Ambient conc/PGMATC			ility of the PGMATC	Level of
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0704 0.0840 0.0840 0.1574 0.1783 0.1055 0.1078 0.1201 0.6293	0.0070 0.0084 0.0084 0.0157 0.0178 0.0106 0.0108 0.0120 0.0629	0.0856 0.1252 0.1252 0.2103 0.1918 0.1162 0.1044 0.1373 0.4189	0.0053 0.0133 0.0133 0.0353 0.0209 0.0078 0.0053 0.0113 0.1107	Family Class Class Class Class Genus Species Family Family

Table D-21. Probabilities of chronic toxic effects on fish populations due to RAC 26 at annual median ambient concentrations for SRC-II.

	Ambient conc/PGMATC		Probabi exceeding	Level of	
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0444 0.0051 0.0051 0.0091 0.0110 0.0361 0.0551 0.0641 0.1813	0.0044 0.0005 0.0005 0.0009 0.0011 0.0036 0.0055 0.0064	0.0486 0.0070 0.0070 0.0201 0.0112 0.0362 0.0482 0.0751 0.2178	0.0020 0.0002 0.0002 0.0011 0.0003 0.0012 0.0014 0.0041 0.0336	Family Class Class Class Class Genus Species Family Family

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

	Ambient conc/PGMATC		Probability of exceeding the PGMATC		Level of
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp	0.2338	0.2338	0.2472	0.2472	Class
Bigmouth buffalo	0.2338	0.2338	0.2472	0.2472	Class
Smallmouth buffalo	0.2338	0.2338	0.2472	0.2472	Class
Channel catfish	0.3087	0.3087	0.3028	0.3028	Class
White bass	0.5639	0.5639	0.3851	0.3851	Class
Green sunfish	0.5639	0.5639	0.3851	0.3851	Class
Bluegill sunfish	0.5639	0.5639	0.3851	0.3851	Class
Largemouth bass	0.5639	0.5639	0.3851	0.3851	Class
Black crappie	0.5639	0.5639	0.3851	0.3851	Class

Table D-23. Probabilities of chronic toxic effects on fish populations due to RAC 13 at annual median ambient concentrations for H-Coal.

	Ambient conc/PGMATC		Probability of exceeding the PGMATC		Level of
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp	0.4187	0.0419	0.3244	0.0485	Family
Bigmouth buffalo Smallmouth buffalo	0.3582 0.3582	0.0358 0.0358	0.2966 0.2966	0.0416 0.0416	* *
Channel catfish	0.5504	0.0550	0.3872	0.0820	Class
White bass Green sunfish	1.3927 1.3927	0.1393 0.1393	0.5599 0.5599	0.1847 0.1847	Class Class
Bluegill sunfish Largemouth bass	1.3927 1.3927	0.1393	0.5599	0.1847	Class
Black crappie	1.3927	0.1393 0.1393	0.5599 0.5599	0.1847 0.1847	Class Class

^{*}Fathead minnow-Cypriniformes.

Table D-24. Probabilities of chronic toxic effects on fish populations due to RAC 14 at annual median ambient concentrations for H-Coal.

Species	Ambient conc/PGMATC		Probabi exceeding	lity of the PGMATC	Level of
Speciles	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp	0.0542	0.0054	0.0620	0.0030	Family
Bigmouth buffalo	0.0445	0.0045	0.0728	0.0057	Class
Smallmouth buffalo	0.0445	0.0045	0.0728	0.0057	Class
Channel catfish	0.0714	0.0071	0.1239	0.0152	Class
White bass	0.1001	0.0100	0.1209	0.0096	Class
Green sunfish	0.1001	0.0100	0.1209	0.0096	Class
Bluegill sunfish	0.1001	0.0100	0.1209	0.0096	Class
Largemouth bass	0.1001	0.0100	0.1209	0.0096	Class
Black crappie	0.1001	0.0100	0.1209	0.0096	Class

Table D-25. Probabilities of chronic toxic effects on fish populations due to RAC 20 at annual median ambient concentrations for H-Coal.

	Ambient conc/PGMATC		Probabi exceeding		Level of
Species	TMT 1	TMT2	TMT1	TMT2	extrapolation
Carp	0.0042	0.0004	0.0063	0.0002	Class
Bigmouth buffalo	0.0042	0.0004	0.0063	0.0002	Class
Smallmouth buffalo	0.0042	0.0004	0.0063	0.0002	Class
Channel catfish	0.1416	0.0142	0.3278	0.1657	Class
White bass	0.1015	0.0102	0.1439	0.0165	Class
Green sunfish	0.1015	0.0102	0.1439	0.0165	Class
Bluegill sunfish	0.1015	0.0102	0.1439	0.0165	Class
Largemouth bass	0.1015	0.0102	0.1439	0.0165	Class
Black crappie	0.1015	0.0102	0.1439	0.0165	Class

Table D-26. Probabilities of chronic toxic effects on fish populations due to RAC 21 at annual median ambient concentrations for H-Coal.

	Ambient conc/PGMATC		Probabi exceeding	Level of	
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.2022 0.2415 0.2415 0.4524 0.5126 0.3034 0.3098 0.3451 1.8089	0.0202 0.0242 0.0242 0.0452 0.0513 0.0303 0.0310 0.0345 0.1809	0.2048 0.2548 0.2548 0.3649 0.3678 0.2633 0.2542 0.2917 0.6034	0.0221 0.0420 0.0420 0.0888 0.0667 0.0317 0.0250 0.0413 0.2248	Family Class Class Class Class Genus Species Family

Table D-27. Probabilities of chronic toxic effects on fish populations due to RAC 22 at annual median ambient concentrations for H-Coal.

Curatas	Ambient conc/PGMATC		Probabi exceeding	lity of the PGMATC	Level of
Species	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.2563 0.2563 0.2563 0.2780 0.6644 0.3035 0.6019 0.4006 1.3601	0.0256 0.0256 0.0256 0.0278 0.0664 0.0304 0.0602 0.0401 0.1360	0.2608 0.2608 0.2608 0.2869 0.4177 0.2592 0.3858 0.3001 0.5561	0.0423 0.0423 0.0423 0.0577 0.0840 0.0292 0.0540 0.0327 0.1800	Class Class Class Class Genus Species Species Family

Table D-28. Probabilities of chronic toxic effects on fish populations due to RAC 28 at annual median ambient concentrations for H-Coal.

Species	Ambient conc/PGMATC		Probability of exceeding the PGMATC		Level of
	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp Bigmouth buffalo Smallmouth buffalo Channel catfish White bass Green sunfish Bluegill sunfish Largemouth bass Black crappie	0.0641 0.0355 0.0355 0.0582 0.2127 0.0584 0.0629 0.0705 0.3407	0.0064 0.0036 0.0036 0.0058 0.0213 0.0058 0.0063 0.0070 0.0341	0.0753 0.0692 0.0692 0.1145 0.2404 0.0651 0.0586 0.0850 0.3160	0.0041 0.0061 0.0061 0.0148 0.0398 0.0031 0.0021 0.0052 0.0664	Family Class Class Class Class Genus Species Family

Table D-29. Probabilities of chronic toxic effects on fish populations due to RAC 34 at annual median ambient concentrations for H-Coal.

Species	Ambient conc/PGMATC		Probability of exceeding the PGMATC		Level of
	TMT1	TMT2	TMT1	TMT2	extrapolation
Carp	0.0036	0.0036	0.0006	0.0006	Species
Bigmouth buffalo	0.0259	0.0259	0.0442	0.0442	Class
Smallmouth buffalo	0.0259	0.0259	0.0442	0.0442	Class
Channel catfish	0.0200	0.0200	0.0440	0.0440	Class
White bass	0.0758	0.0758	0.0990	0.0990	Class
Green sunfish	0.0005	0.0005	0.0000	0.0000	Genus
Bluegill sunfish	0.0007	0.0007	0.0000	0.0000	Species
Largemouth bass	0.0008	0.0008	0.0001	0.0001	Family
Black crappie	0.0027	0.0027	0.0037	0.0037	Family

APPENDIX E

Detailed Methods and Assumptions for Ecosystem Uncertainty Analysis

APPENDIX E

DETAILED METHODS AND ASSUMPTIONS FOR ECOSYSTEM UNCERTAINTY ANALYSIS

E.1 ORGANIZING TOXICITY DATA

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

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

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

LC₅₀ data for fathead minnow (<u>Pimephales</u> sp.), bluegill (<u>Lepomis macrochirus</u>), and guppy (<u>Poecilia reticulata</u>) are assigned to forage fish (species 16, 17 and 18). When data on these species are not available, others are substituted, such as goldfish or mosquitofish. The game fish (species 19) was identified as rainbow trout.

E.2 TRANSFORMING TOXICITY DATA

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

E.2.1 The General Stress Syndrome (GSS)

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

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

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

E.2.2 The MICROCOSM Simulations

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

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

E.2.3 Choosing Uncertainties

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

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- 108. Library, Food and Agriculture, Organization of the United Nations, Fishery Resources and Environment Division, via delle Termi di Caracalla 001000, Rome, Italy
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