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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 analyzes the risks associated with two indirect coal liquefaction technologies: Lurgi gasification with Fischer-Tropsch synthesis and Koppers-Totzek gasification with Fischer-Tropsch synthesis. The plant configurations evaluated were adapted from design information provided by the developers of the technologies. Both configurations reflect a feed coal capacity of  $2.72 \times 10^7$  kg (30,000 tons) per day. Source terms for atmospheric and aqueous waste streams were based 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.

A reference environment resembling eastern Kentucky or West Virginia was employed in the risk analyses. Estimates of concentrations of released contaminants in the air, soil, 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.

Risk to the five ecological endpoints were estimated using one or more of three techniques: the quotient method, analysis of extrapolation error, and ecosystem uncertainty analysis. In the quotient method, estimated environmental concentrations were simply compared to toxicological benchmarks such as  $LC_{50}$ '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 all RACs in terms of a common unit, the 96-h  $LC_{50}$  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 two 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, which can magnify or offset the direct effects of contaminants of organisms.

With respect to fish, nine RACs were determined to be significant for one or both technologies. RAC 5 (ammonia) and RAC 34 (cadmium) were the only RACs found to be significant for both technologies and all risk analysis methods. RAC 4 (acid gases) was significant for both technologies, according to the quotient method and analysis of extrapolation error; however, this RAC could not be addressed using ecosystem uncertainty analysis. The whole effluent from the

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\* $LC_{50}$  = lethal dose to 50% of population exposed.

Lurgi-based technology appeared to be somewhat more acutely toxic than the corresponding effluent from the Koppers-Totzek technology. For both technologies, conventional pollutants such as ammonia, cadmium, and hydrogen sulfide appear to be substantially more hazardous to fish than the complex organic contaminants usually associated with synfuels.

Algal toxicity data were available for only ten RACs. Because of the diversity of experimental designs and test endpoints used in algal bioassays, it was not possible to rank the RAC using the quotient method. However, most of the toxicity quotients calculated for algae were lower than the corresponding quotients for fish. Only RACs 33 (nickel) and 34 (cadmium) would be judged significant for any technology using the quotient method. Ecosystem uncertainty analysis suggested greater risks of effects on algae than did the quotient method, primarily because of reductions in grazing intensity related to the effects of contaminants on zooplankton and fish.

Conventional pollutants, especially  $\text{SO}_2$  and  $\text{NO}_2$ , were found to have the greatest potential effects on terrestrial biota. Ground-level  $\text{SO}_2$  concentrations for both 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) appear of greatest concern for phytotoxicity. However, observable effects are unlikely unless these trace elements are deposited on soils having preexisting high concentrations of these elements and chemical properties favoring the solution phase.

## ABSTRACT

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This report presents an analysis of the risks to fish, water quality (due to noxious algal blooms), crops, forests, and wildlife of two technologies for the indirect liquefaction of coal: Lurgi and Koppers-Totzek gasification of coal for Fischer-Tropsch synthesis. A variety of analytical techniques were used to make maximum use of the available data to consider effects of effluents on different levels of ecological organization. The most significant toxicants to fish were found to be ammonia, cadmium, and acid gases. An analysis of whole-effluent toxicity indicated that the Lurgi effluent is more acutely toxic than the Koppers-Totzek effluent. Six effluent components appear to pose a potential threat of blue-green algal blooms, primarily because of their effects on higher trophic levels. The most important atmospheric emissions with respect to crops, forests, and wildlife were found to be the conventional combustion products  $\text{SO}_2$  and  $\text{NO}_2$ . Of the materials deposited on the soil, arsenic, cadmium, and nickel appear of greatest concern for phytotoxicity.



## 1. INTRODUCTION

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

For purposes of risk analysis, the thousands of potentially significant contaminants 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 populations that detract from water use, (3) reductions in timber yield or undesirable changes in forest composition, (4) reductions in agricultural production, and (5) reductions in wildlife populations. Rather than descriptions of specific sites, the risk analyses employ generalized reference environments, with characteristics representative of regions in which synfuels plants may be sited. Two reference environments are being used in the research for USEPA: an eastern environment resembling

Table 1-1. Risk Analysis Categories (RACs)

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

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

This report analyzes risks associated with two indirect coal liquefaction technologies: Lurgi gasification with Fischer-Tropsch synthesis and Koppers-Totzek gasification with Fischer-Tropsch synthesis. The analyses assumed commercial-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 risk associated with different technologies; (3) to compare the risks of the indirect 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 (1) estimates of aqueous and atmospheric source terms for four commercial-scale indirect coal liquefaction plants, and (2) estimates of exposure concentrations for aquatic and terrestrial biota near 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 Energy Technology Division (TRW 1983) described commercial-scale plant configurations for two indirect coal liquefaction processes: Lurgi gasification with Fischer-Tropsch synthesis and Koppers-Totzek gasification with Fischer-Tropsch synthesis. The plant configurations evaluated by TRW were adapted from design information provided by the developers of the two 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.

Both plant configurations reflect a feed coal capacity of  $2.72 \times 10^7$  kg (30,000 tons) per day. TRW estimated quantities and compositions of all uncontrolled and controlled waste streams, expressed in Risk Analysis Categories (RACs), (Sect. 1). For aqueous waste streams, two alternative control options were considered:

1. Phenol extraction, ammonia recovery, biological oxidation, chemical precipitation, and carbon adsorption.
2. Option 1, followed by forced evaporation and surface impoundment. This implies zero discharge to surface water.

Because of the large number of atmospheric effluent sources associated with each technology, the atmospheric source terms are not presented in this report. They are given in Tables 2-8 and 3-8 of the report by TRW (1983). The aqueous source terms for option 1 are summarized in Table 2.1-1. They include process-generated wastewaters, coal pile runoff, and cooling tower blowdown. Control option 2 is a zero-discharge control strategy; consequently, no source terms are presented.

## 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 was 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 the 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 ( $\text{m}^3/\text{s}$ ), stream width (m), reach length (m), sediment load (mg/L), sediment density ( $\text{g}/\text{m}^3$ ), the depth of the biologically active sediment (cm), the fraction of organic carbon in the sediment (unitless), stream temperature (K), current velocity (m/s), wind velocity (m/s), and the radius of sediment particles (cm). Estimates of stream flow, temperature, and suspended solids for the

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

RAC	Lurgi/Fischer-Tropsch	Koppers-Totzek/Fischer-Tropsch
4	4.3	1.8-3.8
5	59	18
6	0	0
7	0	0
8	0	0
9	35	320
10	4.4 E-05	0
11	0	0
12	4.2 E-03	1.7 E-04
13	2.8 E-04	5.9 E-03
14	2.3 E-02	3.4 E-04
15	3.4 E-02	1.4 E-04
16	0	0
17	0	0
18	0	0
19	8.9 E-03	0
20	3.5	0
21	0.19	6.9 E-04
22	6.7 E-05	6.3 E-04
23	0	0
24	1.7 E-02	0.23
25	0	0
26	7.6 E-06	7.0 E-05
27	0	0
28	0	0
31	3.8	1.2-1.3
32	4.0 E-02	3.6 E-03
33	0.40-0.46	0.08-0.22
34	4.2 E-02	2.4 E-02
35	0.48	0.10-0.11
36	8.4	200

eastern site were set within ranges observed by the U.S. Geological Survey (USGS) for the Big Sandy River at Louisa, Kentucky, and the Monongahela River at Braddock, Pennsylvania (USGS 1977, 1979). Values for the other stream parameters were taken from Southworth (1979). Irradiance values [ $\text{photons}/(\text{cm}^2 \cdot \text{s})$ ] for estimating photolysis rates were obtained from Zepp and Cline (1977).

Probability distributions for flow, temperature, and suspended solids were generated, based on the means, minima, and maxima of these parameters observed at the USGS stations. Normal distributions for particle radius, organic carbon fraction, current velocity, and wind velocity were derived from ranges used by Southworth (1979). Because current velocity and sediment load are influenced by stream flow, a correlation coefficient of 0.7 was specified between flow and velocity and between flow and suspended solids. All environmental parameters used in the exposure analysis are presented in Table 2.2-1.

#### 2.2.2 Contaminant Characteristics

For determining the characteristics of organic contaminants (Table 2.2-2), the chemical properties used were molecular weight ( $\text{g/mol}$ ), aqueous solubility ( $\text{g/L}$ ), octanol-water partition coefficient (unitless), quantum yield of direct photolysis (unitless), molar extinction coefficient [ $(\text{cm} \cdot \text{L})/\text{mol}$ ], and vapor pressure ( $\text{mmHg}$ ). 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); 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).

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 <sup>3</sup> /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 <sup>3</sup>	1.02	0	1.02	1.02
Fraction of 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 <sup>a</sup> (g/mol)	Aqueous solubility <sup>b</sup> (g/L)	Octanol-water partition coefficient (log P)	Quantum yield of photolysis (unitless)
4	Hydrogen sulfide	34.06			
5	Ammonia	17.03			
6	Butane	58.12	6.1 E-02		
7	Formaldehyde	30.03			
8	Methylene chloride	84.93	1.67 E+01		
9	Acetic acid	60.05	3.80 E-02	-0.17 <sup>c</sup>	
10	Thiophene	84.14	4.43 E-01	1.81 <sup>c</sup>	
11	Pyridine	79.10	3.00 E-02	0.650 <sup>c</sup>	
12	Benzene	78.12	1.78 E+00	2.13 <sup>c</sup>	
13	Cyclohexane	84.16	5.5 E-02	4.0 <sup>c</sup>	
14	Toluene	92.15	5.15 E-01	2.69 <sup>c</sup>	
15	Anthracene	178.24	7.50 E-05	4.45 <sup>c</sup>	0.003 <sup>d</sup>
17	Aniline	93.13	3.40 E+01	0.90 <sup>c</sup>	
19	Dibenzofuran	168.21	3.00 E-03	4.12 <sup>c</sup>	
20	Butanoic acid	88.1	5.62 E+01	0.79 <sup>c</sup>	
21	Phenol	94.11	8.20 E+01	1.46 <sup>c</sup>	
22	Acrolein	56.07	9.74 E-01	0.90 <sup>e</sup>	
23	Methanethiol	48.11	4.00 E-05	-0.660 <sup>c</sup>	
24	Methanol	32.04	2.7 E-01	-0.74 <sup>c</sup>	
25	Nitrobenzene	123.11	1.9 E+00	2.31 <sup>e</sup>	
26	Methyl phthalate	194.19	5.0 E+00		
28	Acrylonitrile	53.06	3.83 E-01	-0.92 <sup>c</sup>	
31	Arsenic	74.92			
32	Mercury	200.59			
33	Nickel	58.71			
34	Cadmium	112.40			
35	Lead	207.19			
36	Fluorine	19.00			

<sup>a</sup>Weast (1980).<sup>b</sup>Verschuieren (1977).<sup>c</sup>Leo et al. (1971).<sup>d</sup>Zepp and Schlotzhauer (1979).<sup>e</sup>Briggs (1981).

Mass transfer rates and dissolved fractions were calculated using the method of Southworth (1979). Particulate-settling velocities were calculated from Stoke's Law (Weast 1980). Direct photolysis rate constants for anthracene were calculated using the method of Zepp and Cline (1977). Adsorption and desorption coefficients were approximated using the method of Karickhoff et al. (1979).

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

### 2.2.3 Results

Model runs were conducted for the reference stream, using the source terms presented in Table 2.1-1. 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 and 2.2-4. For all practical purposes, the concentrations computed using contaminant-specific removal rates are identical to concentrations computed from dilution alone. Thus, at least in the immediate vicinity of contaminant sources located on rivers such as the eastern reference stream, 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 was summarized by Travis et al. (1983), who also described the method for

Table 2.2-3. Estimated ambient contaminant concentrations, eastern reference stream, Lurgi/Fischer-Tropsch process

RAC	Reference compound	Mean (g/L)	Median (g/L)	Upper 95% <sup>a</sup> (g/L)
4	Hydrogen sulfide	9.99 E-06	8.77 E-06	1.97 E-05
5	Ammonia	1.36 E-04	1.20 E-04	2.69 E-04
6	Butane	0	0	0
7	Formaldehyde	0	0	0
8	Methylene chloride	0	0	0
9	Acetic acid	8.10 E-05	7.11 E-05	1.59 E-04
10	Thiophene	1.02 E-10	8.94 E-11	2.00 E-10
11	Pyridine	0	0	0
12	Benzene	9.72 E-09	8.54 E-09	1.91 E-08
13	Cyclohexane	6.47 E-10	5.68 E-10	1.27 E-09
14	Toluene	5.32 E-08	4.67 E-08	1.05 E-07
15	Anthracene	6.94 E-08	6.45 E-08	1.19 E-07
16	Methylamine	0	0	0
17	Aniline	0	0	0
18	Quinoline	0	0	0
19	Dibenzofuran	2.06 E-08	1.81 E-08	4.05 E-08
20	Butanoic acid	8.10 E-06	7.11 E-06	1.59 E-05
21	Phenol	4.40 E-07	3.86 E-07	8.65 E-07
22	Acrolein	1.55 E-10	1.36 E-10	3.13 E-10
23	Methanethiol	0	0	0
24	Methanol	3.93 E-08	3.45 E-08	7.73 E-08
25	Nitrobenzene	0	0	0
26	Methyl phthalate	1.76 E-11	1.54 E-11	3.46 E-11
27	Acetamide	0	0	0
28	Acrylonitrile	1.2 E-05	1.1 E-05	2.5 E-05
31	Arsenic	8.85 E-06	7.78 E-06	1.74 E-05
32	Mercury	9.52 E-08	8.36 E-08	1.88 E-07
33	Nickel	1.06 E-06	9.31 E-07	2.09 E-06
34	Cadmium	9.69 E-08	8.51 E-08	1.91 E-07
35	Lead	1.12 E-06	9.83 E-07	2.20 E-06
36	Fluorine	1.96 E-05	1.72 E-05	3.85 E-05

<sup>a</sup>Concentration expected to be equaled or exceeded on 5% of days.

Table 2.2-4. Estimated ambient contaminant concentrations, eastern reference stream, Koppers-Totzek/Fischer-Tropsch process

RAC	Reference compound	Mean (g/L)	Median (g/L)	Upper 95% <sup>a</sup> (g/L)
4	Hydrogen sulfide	8.9 E-06	7.8 E-06	1.8 E-05
5	Ammonia	4.2 E-05	3.7 E-05	8.3 E-05
6	Butane	0	0	0
7	Formaldehyde	0	0	0
8	Methylene chloride	0	0	0
9	Acetic acid	7.4 E-04	6.5 E-04	1.5 E-03
10	Thiophene	0	0	0
11	Pyridine	0	0	0
12	Benzene	3.9 E-100	3.5 E-10	7.7 E-10
13	Cyclohexane	1.4 E-08	1.2 E-08	2.7 E-08
14	Toluene	7.9 E-10	6.9 E-10	1.5 E-09
15	Anthracene	2.9 E-10	2.7 E-10	4.9 E-10
16	Methylamine	0	0	0
17	Aniline	0	0	0
18	Quinoline	0	0	0
19	Dibenzofuran	0	0	0
20	Butanoic acid	0	0	0
21	Phenol	1.6 E-09	1.4 E-09	3.1 E-09
22	Acrolein	1.5 E-09	1.3 E-09	2.9 E-09
23	Methanethiol	0	0	0
24	Methanol	5.3 E-07	4.7 E-07	1.0 E-07
25	Nitrobenzene	0	0	0
26	Methyl phthalate	1.6 E-10	1.4 E-10	3.2 E-10
27	Acetamide	0	0	0
28	Acrylonitrile	0	0	0
31	Arsenic	3.1 E-06	2.7 E-06	6.1 E-06
32	Mercury	9.1 E-09	8.0 E-09	1.8 E-08
33	Nickel	5.2 E-07	4.5 E-07	1.0 E-06
34	Cadmium	6.0 E-08	5.2 E-08	1.2 E-07
35	Lead	2.4 E-07	2.2 E-07	4.8 E-07
36	Fluorine	4.7 E-04	4.1 E-04	9.2 E-04

<sup>a</sup>Concentration expected to be equaled or exceeded on 5% of days.

calculating accumulation in soil. Soil concentrations were 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. This calculation is performed using the food chain model TERREX.

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

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

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

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

$K_d$  = the distribution coefficient ( $\text{L/kg}$ ).

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

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

where

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

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

$\rho$  = soil bulk density ( $\text{g}/\text{cm}^3$ ),

$\theta$  = volumetric water content ( $\text{cm}^3/\text{cm}^3$ ),

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

$r$  = soil volumetric water content ( $\text{mL}/\text{cm}^3$ ).

If  $C_{iss}$  calculated via Eq. (1) exceeds  $C^{\text{max}}$  calculated via Eq. (2), then  $C_{iss}$  is set equal to  $C^{\text{max}}$ . The value of  $\theta$  used in Eq. (2) is very important in providing a reasonable estimate of  $C^{\text{max}}$ . Since measured values of  $K_d$  are usually under saturated conditions,  $\theta$  in Eq. (2) represents total soil porosity.

These calculations generate sector-average ground-level concentrations in air, soil, and soil solution in 16 directions at 500 m intervals from 1,500 to 50,000 m from the source. The highest annual average concentrations in air and the highest soil and soil solution concentrations after 35 years of deposition are presented in Tables 2.3-1 and 2.3-2.

Table 2.3-1. Maximum ambient atmospheric and soil concentrations of RACs for the Lurgi/Fischer-Tropsch process

RAC	Name	Annual average concentration in air ( $\mu\text{g}/\text{m}^3$ )	Concentration in soil ( $\mu\text{g}/\text{kg}$ )	Concentration in soil solution ( $\mu\text{g}/\text{L}$ )
1	Carbon monoxide	4.63 E-01	a	a
2	Sulfur oxides	8.5 E-01	a	a
3	Nitrogen oxides	3.69	a	a
4	Acid gases	8.41 E-03	a	a
5	Alkaline gases	3.65 E-03	a	a
6	Hydrocarbon gases	39.1	15.7	16.3
7	Formaldehyde	b	b	b
8	Volatile organochlorines	b	b	b
9	Volatile carboxylic acids	b	b	b
10	Volatile O & S heterocyclics	7.86 E-04	3.22 E-05	2.69 E-05
11	Volatile Nheterocyclics	b	b	b
12	Benzene	1.18 E-02	4.90 E-03	3.77 E-03
13	Aliphatic/alicyclic hydrocarbons	5.34	1.38	9.86
14	Mono- or diaromatic hydrocarbons	5.29	3.07	6.14 E-01
15	Polycyclic aromatic hydrocarbons	1.14 E-02	1.02	1.58 E-02
16	Aliphatic amines	b	b	b
17	Aromatic amines	b	b	b
18	Alkaline N heterocyclics	b	b	b
19	Neutral N, O, S heterocyclics	4.73 E-04	1.79 E-05	4.72 E-06
20	Carboxylic acids	b	b	b
21	Phenols	4.74 E-03	1.21	1.79
22	Aldehydes and ketones	0.910	1.51	3.11
23	Nonheterocyclic organosulfur	8.18 E-04	9.79 E-04	4.45 E-04
24	Alcohols	3.95	43.7	90.1
25	Nitroaromatics	b	b	b
26	Esters	b	b	b
27	Amides	b	b	b
28	Nitriles	b	b	b
29	Tars	b	b	b
30	Respirable particles	28.9	a	a
31	Arsenic	7.66 E-04	3700	18.5
32	Mercury	1.91 E-05	3.04 E-03	3.04 E-04
33	Nickel	1.06 E-03	4920	32.8
34	Cadmium	1.39 E-05	9.90	1.52
35	Lead	1.28 E-02	1.29 E-04	14.3
36	Other trace elements	7.25 E-03	a	a
37	Radioactive materials	6.33 E-04	a	a

<sup>a</sup>No accumulation in soil.

<sup>b</sup>No emissions.

Table 2.3-2. Maximum ambient atmospheric and soil concentrations of RAUs for the Koppers-Totzek/Fischer-Tropsch process

RAC	Name	Annual average concentration in air ( $\mu\text{g}/\text{m}^3$ )	Concentration in soil ( $\mu\text{g}/\text{kg}$ )	Concentration in soil solution ( $\mu\text{g}/\text{L}$ )
1	Carbon monoxide	22.4	a	a
2	Sulfur oxides	6.87	a	a
3	Nitrogen oxides	5.92	a	a
4	Acid gases	0.135	a	a
5	Alkaline gases	3.70 E-05	a	a
6	Hydrocarbon gases	50.0	20.1	20.8
7	Formaldehyde	b	b	b
8	Volatile organochlorines	b	b	b
9	Volatile carboxylic acids	b	b	b
10	Volatile O & S heterocyclics	b	b	b
11	Volatile N heterocyclics	b	b	b
12	Benzene	5.71 E-05	2.38 E-05	1.83 E-05
13	Aliphatic/alicyclic hydrocarbons	6.55	169	12.1
14	Mono- or diaromatic hydrocarbons	6.52	3.78	0.757
15	Polycyclic aromatic hydrocarbons	0.0173	1.55	0.0239
16	Aliphatic amines	b	b	b
17	Aromatic amines	b	b	b
18	Alkaline N heterocyclics	b	b	b
19	Neutral N, O, S heterocyclics	b	b	b
20	Carboxylic acids	b	b	b
21	Phenols	b	b	b
22	Aldehydes and ketones	0.986	2.13	4.39
23	Nonheterocyclic organosulfur	0.397	0.475	0.216
24	Alcohols	10.3	1680	3450
25	Nitroaromatics	b	b	b
26	Esters	b	b	b
27	Amides	b	b	b
28	Nitriles	b	b	b
29	Tars	b	b	b
30	Respirable particles	127	a	a
31	Arsenic	1.52 E-04	360	1.80
32	Mercury	4.28 E-03	6.83 E-01	6.83 E-02
33	Nickel	1.90 E-03	3000	20
34	Cadmium	5.68 E-05	17.6	2.71
35	Lead	1.83 E-03	976	1.08
36	Other trace elements	4.39 E-02	a	a
37	Radioactive materials	1.18 E-03	a	a

aNo accumulation in soil.

bNo emissions.