ASSESSMENT OF TRACE CONTAMINANTS FROM A MODEL INDIRECT LIQUEFACTION FACILITY. VOLUME II. STREAM CHARACTERIZATION OF LURGI/FISCHER-TROPSCH COAL LIQUEFACTION

GENERAL RESEARCH CORP.
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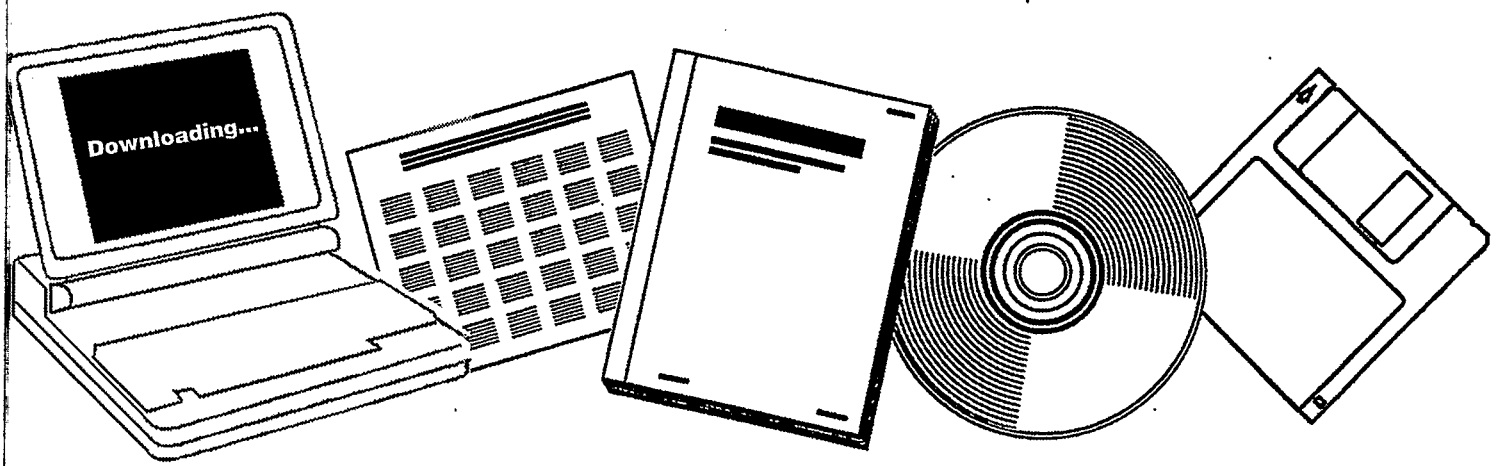

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Assessment of Trace Contaminants From a Model Indirect Liquefaction Facility

VOLUME II – STREAM CHARACTERIZATION OF LURGI/FISCHER-TROPSCH COAL LIQUEFACTION

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FOREWORD

Development and deployment of a commercial indirect liquefaction industry has been proposed as a means of reducing United States dependence on foreign sources of energy.

Deployment of a commercial industry on an environmentally acceptable basis requires identification and evaluation of potential environmental problems. This assessment is an attempt to anticipate potential environmental hazards that may be posed by commercial-scale facilities to provide an improved basis for planning and implementing environmental research.

The study comprises four major tasks: characterization of hazardous materials released from an indirect liquefaction facility; assessment of ecological hazards; assessment of public health hazards; and assessment of occupational health hazards. The report is organized in the same manner. Volume I is an overview and summary of the results; volume II presents stream characterization data; and volumes III, IV and V present assessments of ecological, public health and occupational health hazards, respectively.

This study was sponsored by the Technology Assessment Division of the Department of Energy. Organizations participating in the assessment were General Research Corporation, Oak Ridge National Laboratory, and Argonne National Laboratory.

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1 INTRODUCTION

Indirect liquefaction is a promising technology for producing synfuels. Recent studies indicate that if any portion of the national synfuels goals for 1987 and 1992 is to be met with coal liquefaction, the bulk of the production is likely to come from indirect processes. An indirect coal liquefaction industry will benefit the nation by providing a critically needed supplement to our dwindling oil and gas reserves. However, development and deployment of a commercial coal indirect liquefaciton industry is not without risks. To ensure development and deployment of indirect processes in an environmentally acceptable manner, potential hazards to the general public, occupational personnel and ecosystems must be assessed and factored into the design, siting and operation of commercial facilities. At present, the potential adverse environmental impacts of indirect liquefaction facilities are not well understood.

Especially lacking is information on the identity and quantity of trace contaminants that may be released from process and waste streams. At the present time chemical characterization data for streams from indirect liquefaction facilities are very limited. In response to these data gaps the Department of Energy (DOE) is attempting to develop preliminary estimates of the types and quantities of potential pollutants that may be released into the environment by commercial scale indirect liquefaction facilities. The purpose of these estimates is to provide a basis for estimating the types and magnitudes of potential environmental impacts of a commercial facility and a commercial industry.

The purpose of this draft report is to document the methodology, assumptions, caveats, results, and references used in developing these preliminary estimates. It is hoped that such documentation will enhance understanding of both the value and limitations of the estimates, and facilitate modification of the estimates as data become available from ongoing research.

2 METHODOLOGY

2.1 Overview

Chemical characterization data were very limited for indirect coal liquefaction; no commercial-scale facilities existed in the U.S., and data from other nations (e.g., South Africa) were generally limited and often not representative of American conditions. Because data were so limited, it was recognized that development of an information base useful for assessing environmental implications would require considerable manipulation of the data which were available. In order to minimize confusion and misinterpretation, data sources, calculations, assumptions and results were made explicit wherever possible.

Development of the data base was accomplished in several steps:

1) Choice of Indirect Liquefaction Process-

A single process was chosen to serve as the basis of the analysis to avoid the confusion which would arise from attempting to deal with several processes or a "generic" process. The Lurgi/Fischer-Tropsch process was chosen because it represented a proven, commercial technology, and more data were available for it than most other processes.

2) Development of a Conceptual Plant Configuration-

A conceptual Lurgi/Fischer-Tropsch plant, processing approximately 28,000 tons per stream day (TPSD) of low sulfur Wyoming subbituminous coal, was developed to provide the basis for estimating the types and quantities of pollutants which might be released from a commercial facility. Process operations and streams were based largely, but not exclusively, upon information in the report titled Research Guidance Studies to Assess Gasoline from Coal by Methanol-to-Gasoline and SASOL-type Fischer-Tropsch Technologies[87]. The process description and basic premises used in conceptualizing the plant are presented in Appendix A. A simplified block flow diagram, developed from the report,

is presented in Figure 1. As indicated in the diagram, the conceptual plant included environmental controls as well as process and auxiliary operations. The major process streams and environmental streams of interest in the analysis are listed in Table 1.

3) Identification of Stream Components of Interest-

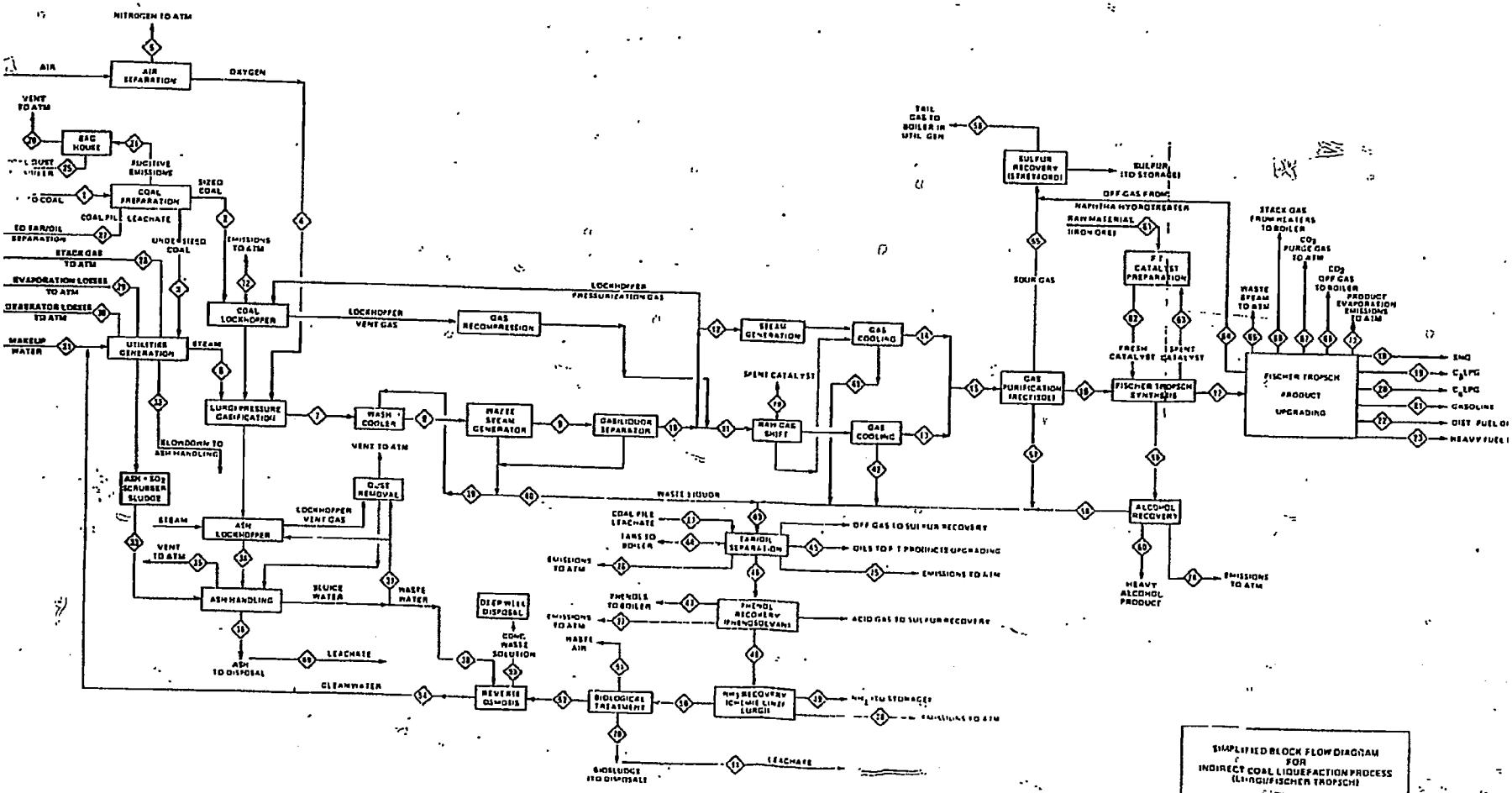
Review of the literature indicated that a variety of stream components associated with coal liquefaction would be of environmental concern. Potential stream components included in the analysis were selected by representatives of participating groups from Oak Ridge National Laboratory, Argonne National Laboratory and Battelle Pacific National Laboratory at a workshop, and are listed in Table 2. In selecting components of interest it was assumed that the plant complex would be designed to meet all existing local and federal environmental regulations, as of July 1977, for liquid and gaseous effluents. The analysis was focused largely on trace organics and trace elements.

4) Estimation of Flow Rates of Stream Components by Stream-

Flow rates of each stream component were estimated for each stream to provide initial estimates of types and quantities of compounds to be expected in each stream. Estimates of the flow rates of the major stream components were derived largely from Base Case II of the Mobil report.[87] Flow rates of the minor components (i.e., those constituting less than one percent of the stream flow rate) were estimated based on sparse information. The results are presented in Appendix B.

5) Estimation of Concentrations of Individual Trace Elements and Organic Compounds in Each Stream-

No data could be located in the literature regarding concentrations of individual trace elements and organic compounds in streams from commercial-scale Lurgi/Fischer-Tropsch plants utilizing Wyoming subbituminous coal. The types and concentrations of individual trace elements and organic compounds were estimated using data from a



SIMPLIFIED BLOCK FLOW DIAGRAM FOR INDIRECT COAL LIQUEFACTION PROCESS (LURGI/FISCHER TROPSCH)

FIGURE 1

ACKNOWLEDGMENT

The authors wish to express their appreciation to Dr. Arnold Goldberg, President, INA Loss Control Services, Inc., formerly the DOE Project Officer, and Mr. Bipin Almaula, of the U.S. Department of Energy, for their assistance and guidance throughout the project.

TABLE 1

PROCESS AND ENVIRONMENTAL STREAMS OF INTEREST*

STREAM NUMBER	STREAM NAME	SOURCE	STREAM NUMBER	STREAM NAME	SOURCE	STREAM NUMBER	STREAM NAME	SOURCE
1	Feed Coal		35	Vent Gas	Ash Handling	64	Off Gas	F-T Product Upgrading
2	Sized Coal	Coal Preparation	36	Ash/Scrubber Sludge	Ash Handling	65	Waste Stream	F-T Product Upgrading
3	Undersized Coal	Coal Preparation				66	Heater Stack Gas	F-T Product Upgrading
4	Oxygen	Air Separation	37	Sluice Water	Ash Handling	67	CO_2 Purge Gas	F-T Product Upgrading
5	Nitrogen	Air Separation	38	Waste Water	Ash Handling	68	CO_2 Off Gas	F-T Product Upgrading
6	Steam	Utilities Generation	39	Waste Liquor	Waste Steam Generator	69	Leachate from Ash	Stream 36
7	Raw Gas	Gasifier	40	Waste Liquor	Waste Steam Generator	70	Biological Sludge	Biological Treatment
8	Washed Gas	Wash Cooler						
9	Cooled Gas	Waste Steam Generator	41	Waste Liquor	Gas Cooling	71	Leachate from Biolsludge	Stream 70
10	Gas	Gas/Liquor Separator	42	Waste Liquor	Gas Cooling			
11	Gas	Gas Recompression/ Separator	43	Waste Liquor	Streams 40,41,42,57,58	72	Lockhopper vent Gas Emmissions	Coal Lockhopper
12	Gas	Gas/Liquor Seperator	44	Tars	Gas/Liquor Separation	73	Evaporative Losses	Streams 18-23
13	Cooled Shifted Gas	Gas Cooling	45	Oils	Gas/Liquor Separation			
14	Cooled Gas	Gas Cooling				74	Evaporative Losses	Stream 60
15	Combined Gas	Streams 13 &14	46	Oil/Tar Free Liquor	Gas Liquor/ Separation	75	Evaporative Losses	Stream 45
16	Purified Gas	Rectisol Unit	47	Phenols	Phenol Recovery			
17	Fischer-Tropsch Products	Fischer-Tropsch Synthesis	48	Phenol-Free Liquor	Phenol Recovery	76	Evaporative Losses	Stream 44
18	SNG	F-T Product Upgrading	49	Ammonia	Ammonia Recovery	77	Evaporative Losses	Stream 47
19	C_3LPG	F-T Product Upgrading	50	Ammonia-Free Liquor	Ammonia Recovery			
20	C_4LPG	F-T Product Upgrading				78	Evaporative Losses	Stream 49
21	Gasoline	F-T Product Upgrading	51	Waste Air	Biological Treatment			
22	Distillate Fuel Oil	F-T Product Upgrading	52	Biological Effluent	Biological Treatment	79	Spent Shift Catalyst	Raw Gas Shift
23	Heavy Fuel Oil	F-T Product Upgrading	53	Concentrated Waste	Reverse Osmosis			
24	Fugitive Emissions	Coal Preparation	54	Treated Effluent	Reverse Osmosis			
25	Coal Dust	Bag House	55	Sour Gas	Rectisol Unit			
26	Vent Gas	Bag House	56	Incineration Gas	Stretford Unit			
27	Coal Pile Leachate	Coal Preparation	57	Waste Liquor	Rectisol Unit			
28	Stack Gas	Utilities Generation	58	Waste Liquor	Alcohol Recovery			
29	Evaporative Losses	Utilities Generation	59	Aqueous Liquor	F-T Synthesis			
30	Deaerator Losses	Utilities Generation	60	Heavy Alcohol Product	Alcohol Recovery			
31	Make-up Water		61	Catalyst Raw Material				
32	Blowdown	Utilities Generation						
33	Ash & SO_2 Scrubber Sludge	Utilities Generation	62	F-T Catalyst	Catalyst Preparation			
34	Ash Slurry	Ash Lockhopper	63	Spent F-T Catalyst	F-T Synthesis			

*Stream numbers, names and sources are keyed to the flow diagram in Figure 1.

TABLE 2

STREAM COMPONENTS SELECTED FOR INCLUSION IN THE ANALYSIS

Gaseous Components

CO	C_2H_4	H_2S
CO_2	C_2H_6	COS
H_2	N_2 + Inerts	H_2O
CH_4	O_2	Others

Liquid and Solid Components

H_2O	Thiophenes	$Ni(CO)_4$
Methanol	Ammonia	Minerals
Tar	HCN	Coal
Oil	Aromatic amines	Sulfur
Naphtha	Nitrosamines	Particulates
Crude phenols	Polynuclear aromatics (PNA)	Trace elements
Mercaptans	Fatty Acids	Others

variety of sources.* Detailed descriptions of data sources and values, assumptions, and calculations are presented in Sections 2.2, 2.3, and 2.4.

6) Evaluation of Results-

Results of the effort were evaluated and compared with the results and projections from other studies to provide some insight into the reasonableness of the values.

2.2 Characterization of Liquid Streams

Review of the literature indicated that characterization data for liquid effluents for commercial-scale Lurgi/Fischer-Tropsch plants were very limited. No experimental data could be found regarding specific constituents in treated effluents from commercial-scale Lurgi/Fischer-Tropsch processing of Wyoming subbituminous coal.

Liquid streams selected for the analysis are listed in Table 3; their inter-relationships are illustrated in Figure 2.

Wash process liquor (Stream 43) was chosen as the key liquid stream of interest because it represents the largest and most highly contaminated wastewater stream in a Lurgi/Fischer-Tropsch plant.[37] It was also chosen for analysis because it is the major influent to the wastewater treatment facility in the plant; the types and quantities of constituents present in Stream 43 largely determine the types and quantities of pollutants present in the liquid and solid effluents from the wastewater treatment facility (i.e., streams 53, 54, 70 and 71).

The analysis focused on two general classes of pollutants which have been identified as primary causes of concern in liquid streams from coal conversion facilities: trace elements and organic compounds. The

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*Data from both theoretical and experimental studies were used when they were deemed appropriate and useful.

TABLE 3

LIQUID STREAMS CHARACTERIZED IN THE ANALYSIS

STREAM NUMBER	STREAM NAME
27	Coal pile leachate
31	Make-up water
38	Ash sluice water
43	Raw process water
46	Gas liquor separator effluent
48	Phenosolvan effluent
50	Ammonia stripper effluent
52	Biological treatment effluent
53	Reverse Osmosis concentrated waste solution
54	Reverse Osmosis permeate
54 & 31	Feed to cooling towers

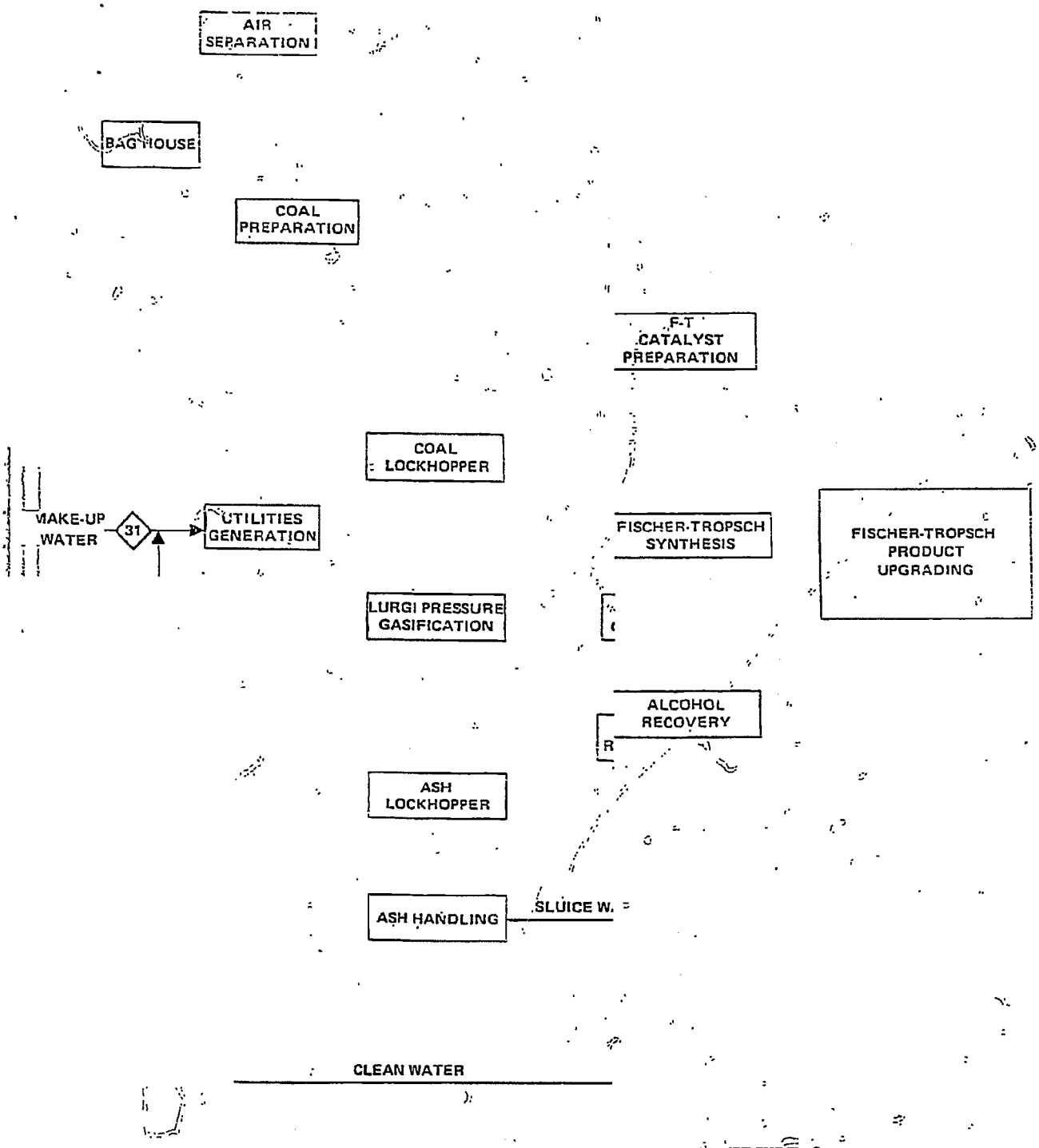

FIGURE 2

LIQUID STREAMS
FOR
OAL LIQUEFACTION PROCESS
GI-FISCHER-TROPSCH)

types and quantities of pollutants were estimated based on three sets of data. Estimates of trace elements were based largely on experimental trace element distribution coefficients developed for Lurgi at SASOL.[37] Estimates of organic compounds were based on experimental effluent data from SASOL[8] and on characterization data for coal tar produced by a bench-scale gasifier using Wyoming subbituminous coal.[19]

The types and quantities of constituents which may be present in liquid streams were estimated in 3 basic steps:

1) Identification of the types and quantities of constituents potentially present in the major raw process waste stream (Stream 43).

2) Identification or estimation of efficiency of removal of each constituent (identified in Step 1) by each wastewater treatment process specified in the flow diagram (i.e., gas/liquor separation, phenol recovery, ammonia recovery, biological treatment, and reverse osmosis).

3) Calculation of constituent concentrations in liquid effluents from the water treatment facility by sequentially applying the removal efficiencies for each constituent as the stream passed through each water treatment process. Additional pollutant loadings added to the liquid stream (via Streams 27 and 28) were estimated from literature data and incorporated into the calculations at the appropriate point.

The specific calculations, data and assumptions used in estimating the types and concentrations of trace elements and organic compounds which may be present in the liquid streams are discussed in Sections 2.2.1, 2.2.2 and 2.2.3.

2.2.1 Estimation of Trace Elements in Liquid Streams

Estimation of Trace Element Concentrations in Stream 43-

The concentrations of trace elements in Wyoming subbituminous coal on a moisture free, whole coal basis were identified in the literature. (See Table 4).

The flow rate of each trace element into the gasifier was estimated:

$$F_{TE-G} = (C_{TE})(F_{DC}) \; / \; 1{,}000{,}000$$

TABLE 4

TRACE ELEMENT CONCENTRATIONS FOR WYOMING AND ROSEBUD MONTANA SUBBITUMINOUS COALS (ppm)

Trace Elements	Wyoming Subbituminous [40]	Montana Rosebud Subbituminous [40]	Ratio of Concentrations of Trace Elements - Montana to Wyoming
Ag	.06-.43	.06	1-.14
As	.57-1.2	.08-1.2	.14-1
B	32	32	1
Ba	87	87	1
Be	.71-.8	.7-.8	.99-1
Br	-	-	-
Cd	.31-.8	.31-.8	1-1
Ce	-	-	-
Co	.55	.6-4	1.09-7.27
Cr	4.2-16	4-16	.95-1
Cs	-	-	-
Cu	8.9-10	9-10	1.01-1
F	65-67	66	.98-1.01
Ga	-	-	-
Ge	-	-	-
Hg	.11-.17	.11-.17	1-1
I	-	-	-
In	-	-	-
La	-	-	-
Li	3.6-15.0	-	-
Mo	2.2	2.2	1
Mn	2.8-3.4	2.8-3.4	1-1
Ni	1.7-14	2-14	1.18-1
P	-	-	-
Pb	.51-12	.51-12	1-1
Rb	-	-	-
Ru	-	-	-
Sb	.08-1.5	-	-
Sc	-	-	-
Se	.33	.33	1
Sn	.14	.14	1
Sr	-	-	-
Ta	-	-	-
Te	-	-	-
U	.88	.88	1
V	10-14	10-14	1
W	-	-	-
Y	-	-	-
Zn	.23-8	2-8	8.70-1
Zr	-	170	-

where-

F_{TE-G} is the flow rate of each trace element into the gasifier (in lb/hr).

C_{TE} is the concentration of each trace element in dry, whole coal (in ppm).

F_{DC} is the flow rate of dry, whole coal to the gasifier (Water-free components of Stream 2 in the flow diagram).*

The distribution of each trace element from Lurgi gasifier into ash, liquor, tar and oil streams at SASOL were identified in the literature. (See Table 5).

The distribution of trace elements in the conceptual plant was assumed to be the same as the distribution at SASOL.

The flow rate of each trace element into the gas liquor was estimated:

$$F_{TE-L} = \frac{(F_{TE-G})(D_{TE-L})}{100\%}$$

where-

F_{TE-L} is the flow rate of each trace element into the gas liquor (in lb/hr).

F_{TE-G} is the flow rate of each trace element into the gasifier (in lb/hr).

D_{TE-L} is the distribution factor of each trace element in the liquor based on SASOL data (in %) (See Table 5).

It was assumed that the total flow of each trace element into the gas liquor dissolved in the water component of the gas liquor stream, then

$$C_{TE-43} = \frac{F_{TE-L} \times 1{,}000{,}000}{F_{W-43}}$$

*Flow rates of each stream are presented in Appendix B.

TABLE 5

TRACE ELEMENT DISTRIBUTION FOR LURGI AT SASOL*,37
(Percent of Element in Coal)

Element	Ash	Liquor	Tar	Oil
Be	33.3	53.3	17.0	0.3
B	90	8.8	2.0	0.0
V	99.9	0.1	0.0	0.0
Mn	99.9	0.2	0.0	0.0
Ni	99.4	0.4	0.0	0.0
As	26.9	67.2	1.9	3.9
Cd	51.9	45.5	0.6	1.4
Sb	50.0	45.0	3.8	0.6
Ce	99.9	0.1	0.0	0.0
Hg	51.9	41.6	6.4	0.6
Pb	94.2	1.7	4.3	0.0
Br	10.0	88.9	0.1	0.0
F	56.3**	43.8**	0.0	0.0
Cl	52.6**	47.4**	0.3	0.0

*Analysis by spark source mass spectrometer (which can give a semi-quantitative analysis) for El Paso by SASOL.

**% distribution calculated on analyses as done by SASOL previously.

where-

C_{TE-43} is the concentration of each trace element in the water component of Stream 43 (in ppm).

F_{TE-L} is the flow rate of each trace element into the gas liquor (in lb/hr).

F_{W-43} is the flow rate of the water component of Stream 43, i.e., 1,993,000 lb/hr.

Estimation of Trace Element Concentrations in Stream 27-

The concentration of each trace element in coal pile leachate (Stream 27) was identified in the literature (Table 6). The literature data were assumed to be representative of Wyoming subbituminous coal.

Identification/Estimation of Efficiencies of Removal of for Each Constituent by Each Wastewater Treatment Process-

Efficiencies of removal of each constituent in the liquid streams (43 and 27) were identified or estimated from the literature for each wastewater control technology process identified in the flow diagram. Removal efficiencies assumed in the assessment are presented in Table 7.

Estimation of Trace Element Concentrations in Stream 46-

The concentration of each trace element in Stream 46 was estimated by weighting the concentrations in streams 43 and 27 by their respective flow rates, applying the efficiency of removal of each constituent by the gas liquor separator, and dividing by the flow rate of Stream 46:

$$C_{TE-46} = \frac{(C_{TE-43})(F_{W-43}) + (C_{TE-27})(F_{W-27}) \quad \frac{[100-RE_{TE-ES}]}{100}}{F_{W-46}}$$

where-

C_{TE-46} is the concentration of each trace element in the water component of Stream 46 (in ppm).

C_{TE-43} is the concentration of each trace element in the water component of Stream 43 (in ppm).

TABLE 6

LITERATURE VALUES FOR STREAM CONSTITUENTS

CONCENTRATIONS IN STREAMS / CONSTITUENTS	STREAM CONCENTRATIONS (ppm)		
	RAW GAS LIQUOR (STREAM 43)	COAL PILE LEACHATE (STREAM 27)	ASH SLUICE WATER BLOWDOWN (STREAM 38)
TRACE ELEMENTS			
Arsenic	0.55 (1)	0.01 (2)	0.02 (3)
Boron	1.9 (1)		
Beryllium	0.29 (1)	0.01 (2)	
Cadmium	0.25 (1)	0.006 (2)	0.00064 (3)
Fluorine	2.0 (1)		
Lead	0.14 (1)	0.023 (2)	0.09 (3)
Mercury	0.049 (1)	0.027 (2)	0.0003 (3)
Manganese	0.0047 (1)	110.0 (2)	0.5 (3)
Nickel	0.0036 (1)	0.32 (2)	0.35 (3)
Vanadium	0.0096 (1)		
CARBOXYLIC ACIDS			
Acetic Acid	171. (4)		
Propanoic Acid	26. (4)		
Butanoic Acid	13. (4)		
2-Methylpropionic Acid	2. (4)		
Pentanoic Acid	12. (4)		
3-Methylbutanoic Acid	1. (4)		
Hexanoic Acid	1. (4)		
BENZENE AND SUBSTITUTED BENZENES			
Biphenyl	0.7 (5)		
Ethylbenzene	15. (5)		
Indan	8.9 (5)		
Toluene	50. (5)		
1,2,4 Trimethylbenzene	6. (5)		
O-Xylene	18. (5)		
MONOHYDRIC PHENOLS			
Phenol	3100. (6)		
2-Methylphenol	340. (6)		
3-Methylphenol	420. (6)		
4-Methylphenol	300. (6)		
2,4-Xylenol	120. (6)		
3,5-Xylenol	50. (6)		
DIHYDRIC PHENOLS			
Catechol	550. (6)		
3-Methylcatechol	400. (6)		
4-Methylcatechol	385. (6)		
3,6-Dimethylcatechol	45. (6)		
Resorcinol	275. (6)		
5-Methylresorcinol	65. (6)		
4-Methylresorcinol	36. (6)		

TABLE 6 (CON'T)

CONCENTRATIONS IN STREAMS / CONSTITUENTS	STREAM CONCENTRATIONS (ppm)		
	RAW GAS LIQUOR (STREAM 43)	COAL PILE LEACHATE (STREAM 27)	ASH SLUICE WATER BLOWDOWN (STREAM 38)
POLYNUCLEAR AROMATICS			
Acenaphthylene	0.4 (5)		
Anthracene	0.1 (5)		
Benz(a) Anthracene	0.01 (5)		
Benzo(g,h,i)perylene	0.0003 (5)		
Benzo(a)pyrene	0.004 (5)		
Benzo(e)pyrene	0.004 (5)		
Chrysene	0.002 (5)		
Fluoranthene	0.2 (5)		
Fluorene	0.2 (5)		
Naphthalene	3.2 (5)		
Perylene	0.0004 (5)		
Phenanthrene	0.1 (5)		
Pyrene	0.2 (5)		
SULFUR HETEROCYCLICS			
Methylthiophene			
Thiophene			
NITROGEN HETEROCYCLICS			
Acridine	2.2 (7)		
2,4-Dimethylpyridine	1. (4)		
2,5-Dimethylpyridine	1. (4)		
2-Methylpyridine	70. (4)		
3-Methylpyridine	26. (4)		
4-Methylpyridine	6. (4)		
Pyridine	117. (4)		
Quinoline	45. (4)		
OXYGEN HETEROCYCLICS			
Benzofuran			
Dibenzofuran			
MERCAPTANS			
Methanethiol	20. (7)		
AROMATIC AMINES			
Aniline	12. (4)		

(1) Estimate based on SASOL distribution coefficients (37).
(2) Reference 18.
(3) Reference 91.
(4) Reference 8.
(5) Estimate based on RTI data (19). Limited by compound solubility.
(6) Reference 92.
(7) Estimate based on RTI data (19). Limited by compound production rate.

TABLE 7

REMOVAL EFFICIENCIES FOR LIQUID STREAM CONSTITUENTS BY CONTROL PROCESS
(Percent Removed)

COMPOUND	GAS LIQUOR SEPARATOR (RE_{X-LS})	PHENOSOLVAN (RE_{X-PH})	AMMONIA RECOVERY (RE_{X-AR})	BIOLOGICAL TREATMENT (RE_{X-BT})	REVERSE OSMOSIS (RE_{X-RO})
ALIPHATICS, ALICYCLICS AND FATTY ACIDS	0	15 (1)*	0	95 (2,3)	
Acetic Acid					51 (9)
Propanoic Acid					65 (9)
Butanoic Acid					63 (10)
2-Methylpropionic Acid					63 (10)
Pentanoic Acid					63 (10)
3-Methylbutanoic Acid					63 (10)
Hexanoic Acid					63 (10)
BENZENE AND SUBSTITUTED BENZENES		15 (1)		40-90+ (3,4,5)	63 (10)
Ethylbenzene				90 (4)	
Toluene				90 (4)	
1,2,4-Trimethylbenzene				90 (4)	
O-Xylene				90 (5)	
MONOHYDRIC PHENOLS		99.5 (1)		92-94 (6)	
Phenol				99 (7)	69 (9)
2-Methylphenol				97 (7)	74 (9)
3-Methylphenol				97 (7)	87 (9)
4-Methylphenol				97 (7)	75 (9)
2,4-Xylenol				81 (7)	90 (9)
3,5-Xylenol				37 (7)	90 (9)
DIHYDRIC PHENOLS		60 (1)		HIGH (3,7)	
Catechol				97 (7)	75 (9)
3-Methylcatechol				100 (5)	(11)
4-Methylcatechol				97 (8)	(11)
3,6-Dimethylcatechol				97 (8)	(11)
Resorcinol				98 (7)	(9)
5-Methyl Resorcinol				97 (8)	(11)
4-Methyl Resorcinol				97 (8)	(11)
TRIHYDRIC PHENOLS		60 (1)		LOW (3)	
Phloroglucinol					

*Numbers in parenthesis refer to references.

(1) Reference 78.
(2) Reference 8.
(3) Reference 15.
(4) Reference 80.
(5) Reference 102.
(6) Reference 6.
(7) Reference 93.
(8) Assumed same removal as catechol.
(9) Reference 25.
(10) Assumed value based on rejection of non-phenolic organics in reference 25.
(11) Assumed same removal as catechol and resorcinol.
(12) DOE/ECT, unpublished.
(13) Assumed same removal as nitrogen heterocyclics.
(14) Assumed values: assuming little degradation, but absorption/sedimentation removes 90% compounds (>2 rings) and 70% compounds (1,2 rings).
(15) Assumed same value as phenanthrene.
(16) Assumed same value as for pyridine.
(17) Assumed value.
(18) Reference 51.
(19) Average value, reference 34.
(20) Reference 17.
(21) Average value, reference 35.

TABLE 7 (Cont.)

COMPOUND	GAS LIQUOR SEPARATOR (RE_{X-LS})	PHENO-SOLVAN (RE_{X-PH})	AMMONIA RECOVERY (RE_{X-AR})	BIOLOGICAL TREATMENT (RE_{X-BT})	REVERSE OSMOSIS (RE_{X-RO})
POLYAROMATIC HYDROCARBONS	0	15 (1)	0	30-90+ (4,12)	99 (15)
Acenaphthylene				90 (14)	
Acridine				90 (14)	
Anthracene				90 (14)	
Benz(a)anthracene				90 (14)	
Benzo(g,h,i)perylene				90 (14)	
Benzo(a)pyrene				90 (14)	
Benzo(e)pyrene				90 (14)	
Biphenyl				70 (5)	
Chrysene				90 (14)	
Fluoranthene				90 (14)	
Fluorene				90 (14)	
Indan				70 (14)	
Indene				75 (5)	
Naphthalene				70 (14)	
Perylene				90 (14)	
Phenanthrene				90 (14)	(9)
Pyrene				90 (14)	
SULFUR HETEROCYCLICS		15 (2)			63 (10)
Methylthiophene				70 (14)	
Thiophene				70 (14)	
NITROGEN HETEROCYCLICS					74 (16)
2,4-Dimethylpyridine		99 (2)		90+ (5)	
2,5-Dimethylpyridine		99 (2)		90+ (5)	
2-Methylpyridine		99 (2)		90+ (5)	
3-Methylpyridine		99 (2)		90+ (5)	
4-Methylpyridine		99 (2)		90+ (5)	
Pyridine		99 (2)		99+ (5)	(9)
Quinoline		99 (13)		90 (13)	
OXYGEN HETEROCYCLICS					74 (13)
Benzofuran		15 (1)		90 (13)	
Dibenzofuran		15 (1)		90 (13)	
MERCAPTANS					
Methanethiol		15 (1)		90 (17)	90 (17)
AROMATIC AMINES					
Aniline		15 (1)		95 (5)	63 (10)
TRACE ELEMENTS		0		30-90 (12,18)	
Arsenic				50 (17)	89 (21)
Boron				50 (17)	90 (21)
Beryllium				50 (17)	90 (17)
Cadmium				32.5 (19)	90 (17)
Fluorine				50 (17)	93 (6)
Lead				70 (19)	60 (21)
Mercury				47.5 (19)	90 (17)
Manganese				50 (17)	100 (6)
Nickel				27.5 (19)	98 (6)
Vanadium				45 (20)	95 (21)

F_{W-43} is the flow rate of the water component of Stream 43, i.e., 1,993,000 lb/hr.

C_{TE-27} is the concentration of each trace element in the water component of Stream 27 (in ppm).

F_{W-27} is the flow rate of the water component of Stream 27, i.e., 1,030 lb/hr.

RE_{TE-LS} is the efficiency of removal of each trace element in the gas liquor separator (in %).

F_{W-46} is the flow rate of the water component of Stream 46, i.e., 1,991,000 lb/hr.

Estimation of Trace Element Concentrations in Stream 48

The concentration of each trace element in Stream 48 was estimated using the following equation:

$$C_{TE-48} = \frac{(C_{TE-46})(F_{W-46})\ \frac{[100-RE_{TE-PH}]}{100}}{F_{W-48}}$$

where-

C_{TE-48} is the concentration of each trace element in Stream 48 (in ppm).

C_{TE-46} is the concentration of each trace element in Stream 46 (in ppm).

F_{W-46} is the flow rate of the water component of Stream 46, i.e., 1,991,000 lb/hr.

RE_{TE-PH} is the efficiency of removal of each trace element by the Phenosolvan control unit (in %).

F_{W-48} is the flow rate of the water component of Stream 48, i.e., 1,990,000 lb/hr.

Estimation of Trace Element Concentrations in Stream 50

The concentration of each trace element in Stream 50 was estimated using the following equation:

$$C_{TE-50} = \frac{(C_{TE-48})(F_{W-48})\ \frac{[100-RE_{TE-AR}]}{100}}{F_{W-50}}$$

where-

C_{TE-50} is the concentration of each trace element in Stream 50, (in ppm).

C_{TE-48} is the concentration of each trace element in Stream 48, (in ppm).

F_{W-48} is the flow rate of the water component of Stream 48, i.e., 1,990,000 lb/hr.

RE_{TE-AR} is the efficiency of removal of each trace element by the Ammonia Recovery unit (in %).

F_{W-50} is the flow rate of the water component of Stream 50, i.e., 1,991,000 lb/hr.

Estimation of Trace Element Concentrations in Stream 52

The concentration of each trace element in Stream 52 was estimated using the following equation:

$$C_{TE-52} = \frac{(C_{TE-50})(F_{W-50})\ \frac{[100-RE_{TE-BT}]}{100}}{F_{W-52}}$$

where-

C_{TE-52} is the concentration of each trace element in Stream 52, (in ppm).

C_{TE-50} is the concentration of each trace element in Stream 50, (in ppm).

F_{W-50} is the flow rate of the water component of Stream 50, i.e., 1,991,000 lb/hr.

RE_{TE-BT} is the efficiency of removal of each trace element by the Biological Treatment unit, (in %).

F_{W-52} is the flow rate of the water component of Stream 52, i.e., 1,962,000 lb/hr.

Estimation of Trace Element Concentrations in Stream 38-

The concentration of each trace element in Stream 38 was assumed to be equal to the concentration of elements in column volume leachate fractions of ash from Lurgi gasification of Montana Rosebud coal.[91] The data were assumed to give a good approximation of Wyoming subbituminous coal as the concentration of almost all trace elements were essentially equal in both coals, as shown in Table 4. The concentration of each trace element in Stream 38 is presented in Table 6.

Estimation of Trace Element Concentrations in Stream 53-

The concentrations of each trace element in Stream 53 was estimated using the following equation:

$$C_{TE-53} = \frac{[(C_{TE-52})(F_{W-52}) + (C_{TE-38})(F_{W-38})]\ \frac{[RE_{TE-RO}]}{100}}{F_{W-53}}$$

where-

C_{TE-53} is the concentration of each trace element in Stream 53, (in ppm).

C_{TE-52} is the concentration of each trace element in Stream 52, (in ppm).

F_{W-52} is the flow rate of the water component of Stream 52, i.e., 1,962,000 lb/hr.

C_{TE-38} is the concentration of each trace element in Stream 38, (in ppm).

F_{W-38} is the flow rate of the water component of Stream 38, i.e., 879,000 lb/hr.

RE_{TE-RO} is the efficiency of removal of each trace element by the Reverse Osmosis unit (in %).

F_{W-53} is the flow rate of the water component of Stream 53 which is assumed to be 20% of the sum of the water components of Streams 52 and 38, i.e., 568,200 lb/hr.

Estimation of Trace Element Concentrations in Stream 54-

The concentration of each trace element in Stream 54 was estimated using the following equation:

$$C_{TE-54} = \frac{(C_{TE-52})(F_{W-52}) + (C_{TE-38})(F_{W-38})\ \frac{[100-RE_{TE-RO}]}{100}}{F_{W-54}}$$

where-

C_{TE-54} is the concentration of each trace element in Stream 54 (in ppm).

C_{TE-52} is the concentration of each trace element in Stream 52 (in ppm).

F_{W-52} is the flow rate of the water component of Stream 52, i.e., 1,962,000 lb/hr.

C_{TE-38} is the concentration of each trace element in Stream 38 (in ppm)

F_{W-38} is the flow rate of the water component of Stream 38, i.e., 879,000 lb/hr.

RE_{TE-RO} is the efficiency of removal of each trace element by the Reverse Osmosis unit (in %).

F_{W-54} is the flow rate of the water component of Stream 54, assumed to be equal to 80% of the sum of the water components of Stream 52 and 38, i.e., 2,273,000 lb/hr.

Estimation of Trace Element Concentrations in Stream 31-

The concentration of each trace element in Stream 31 (make-up water to utilities generation) was assumed to be zero.

Estimation of Trace Element Concentrations in Streams 31+54-

The concentration of each trace element in Streams 31+54 was estimated using the following equation:

$$C_{TE-(31+54)} = \frac{(C_{TE-31})(F_{W-31}) + (C_{TE-54})(F_{W-54})}{(F_{W-31}) + (F_{W-54})}$$

where-

$C_{TE-(31+54)}$	is the concentration of each trace element in Stream 31 + 54, (in ppm).
C_{TE-31}	is the concentration of each trace element in Stream 31, (in ppm).
F_{W-31}	is the flow rate of the water component of Stream 31, i.e., 1,180,000 lb/hr.
C_{TE-54}	is the concentration of each trace element in Stream 54, (in ppm).
F_{W-54}	is the flow rate of the water component of Stream 54, assumed to be equal to 80% of the sum of the water components of Streams 52 and 38, i.e., 2,273,000 lb/hr.

2.2.2 Estimation of Organic Compounds in Liquid Streams

Data on the types and concentrations of organic compounds in liquid streams were very limited. No data could be found regarding organic constituents in process waters from Lurgi/Fischer-Tropsch processing of Wyoming subbituminous coal.

In order to provide estimates of the types and concentrations of organic compounds which may be present in liquid streams from wastewater treatment units, data from two sources were used.

- A search of the literature indicated that limited data were available from the SASOL operation in South Africa and Lurgi gasifiers in Westfield, Scotland.[92] Although the coal feed type, liquid stream flow rates, and operating conditions may not be the same as those specified for the conceptual plant used in this analysis, the available data were assumed to be representative. The data are presented in Table 6.

- Ongoing studies sponsored by the Environmental Protection Agency recently have characterized the organic components of tars produced by gasification of Wyoming subbituminous coal. Although there are differences between the conceptual plant and the EPA study regarding reactor configuration and operating conditions, the EPA data were assumed to be useful in providing preliminary estimates of the types and concentrations of organic compounds which may be produced by Lurgi gasification of Wyoming subbituminous coal. Parameter values for the EPA

study, Lurgi gasifiers and the conceptual plant configuration are compared in Table 8. Data from the EPA Study which were used in estimating the types and concentrations of organic compounds in liquid streams are summarized in Table 9 (column 4).

These two sources of data were used to estimate the concentrations of organics in Stream 43. Estimates of concentrations of organics in subsequent liquid streams in the wastewater treatment units were estimated by sequentially applying removal efficiencies of control units for each organic constituent to calculate the amount of each constituent which would remain in the liquid stream, and then dividing the quanitity of constituent by the flow rate of the water component of each stream.*

Estimation of Organics Concentrations in Stream 43-

As in the case of trace elements, Stream 43 was considered to be the crucial liquid stream for the analysis; it was the largest, most highly contaminated liquid waste stream in the plant, and its composition largely determined the composition and flow rates of subsequent streams from the wastewater treatment units.

Characterization of organics in Stream 43 was accomplished using data from the SASOL and Westfield, Scotland plants [92] and gasification screening tests[19] described in the previous section. The SASOL and Westfield data, presented in Table 6, were assumed to be representative of Stream 43 and were used directly. The tar characterization data from the gasification screening tests were used in the following way to estimate quantities of organics in Stream 43.

1) It was assumed that the compounds detected in the tar produced by fixed-bed gasification of Wyoming subbituminous coal and the rates of production would be representative of Lurgi gasification of Wyoming subbituminous coal.

*The water component of each stream was used rather than the whole stream because it was assumed that the total quantity of each constituent was dissolved in the water component.

TABLE 8

COMPARISON OF PARAMETER VALUES FOR GASIFICATION REACTORS

	RTI Test #33[19]	Lurgi[19]	Conceptual Plant[87]
Air/Coal, g/g	1.5	3.0	1.2
Steam/Coal, g/g	.36	1.5	.89
Carbon Conversion, %	98.9	95	99.5
Coal Residence Time (min)	110	60	No Data
Tar Produced, g/g	.012	No Data	.019
Gas Procuded, SCF/lb	35	52	38
HHV of Raw Gas, Btu/SCF	201	195	No Data
Throughput, lb/hr/ft^2	45	248	No Data
Coal Type	Wyoming Subbit	New Mexico Subbit	Wyoming Subbit
Pressure, Psia	200	300	450
Mesh Size	8 x 16	1.75" x .08"	1/4" x 2"
Maximum Temperature ^{o}C	1040	No Data	No Data
Heatup Time to 800^{o}C, Min.	8	NA*	NA*

* NA-Not applicable

TABLE 9

ESTIMATION OF COMPOUND QUANTITIES BASED ON TAR CONSTITUENTS AND COMPOUND SOLUBILITY*

1 COMPOUND	2 Identified in Large, Tar, Oil or Liquor (T,O,L)	3 Identified in Tar from Wyoming Subbituminous Coal	4 Compound Production Rate (1) (gm/gm of Coal)	5 Compound Production (2) (lb/hr)	6 Maximum Liquor Concentration (3) (ppm)	7 Compound Solubility in Water (ppm)	8 Number of Rings in Compound	9 Assumed Percent of Saturation Level (11)	10 Assumed Concentration Due to Solubility (ppm)	11 Assumed Concentration in Stream 43
Methanethiol		✓	2.3×10^{-5}	43.7	70.6	24,000 (9)	-	-	-	30.
Ethyl Benzene	O (10)	✓	1.5×10^{-4}	285.2	134.6	152 (7)	1	10	15.	15.
Methylthiophene		✓	1.0×10^{-4}	190.1	89.7	I (5) (6)	1	10		(9.)**
Phenol	L (12)	✓	1.6×10^{-3}	3042.1	1435.7	82,000 (6)	1	10	8,200	1435.
Thiophene	O (10)	✓	3.0×10^{-5}	57.0	26.9	.1 (5) (6)	1	10		(3.)
Toluene	O (10)	✓	2.2×10^{-3}	4182.9	1974.1	500 (6)	1	10	50.	50.
1,2,4-Trimethylbenzene	O (10)	✓	-	-	-	57 (7)	1	10	5.7	6.
Xylene (O)	O (10)	✓	8.0×10^{-4}	1521.1	717.9	175 (7)	1	10	17.5	18.
Benzofuran	O (10)	✓	1.0×10^{-4}	190.1	89.7	I (5) (6)	2	10		**
Biphenyl		✓	6.3×10^{-6}	12.0	5.7	7 (4)	2	10	0.7	0.7
Indan	O (10)	✓	7.6×10^{-5}	144.5	68.1	88.9 (13)	2	10		9.0
Indene	O (10)	✓	5.5×10^{-4}	1045.7	493.5	I (5) (6)	2	10		**
Naphthalene	O (10)	✓	1.5×10^{-4}	665.5	314.1	32 (4)	2	10	3.2	3.
Quinoline		✓	5.1×10^{-5}	96.9	45.7	6,100 (4)	2	10	610.	45.
Acenaphthylene		✓	4.9×10^{-5}(8)	93.2	43.9	4 (4)	3	10	0.4	0.4
Acridine		✓	2.4×10^{-6}	4.6	2.2	vss (5) (6)	3	10	-	2.2
Anthracene		✓	8.5×10^{-5}	161.6	76.3	I (4)	3	10	0.1	0.1
Dibenzofuran	O (10)	✓	5.9×10^{-5}	112.2	52.9	I (6)	3	10	-	0.2
Fluorene		✓	5.7×10^{-5}	108.4	51.1	2 (4)	3	10	0.2	0.2
Phenanthrene		✓	4.4×10^{-5}	83.7	39.5	I (4)	3	10	0.1	0.1
Benz(a)Anthracene		✓	5.2×10^{-6}(8)	9.9	4.7	0.01 (4)	4	100	0.01	0.01
Chrysene		✓	2.0×10^{-5}	38.3	17.9	0.002 (4)	4	100	0.002	0.002
Fluoranthene		✓	1.2×10^{-5}	60.8	28.7	0.2 (4)	4	100	0.	0.
Pyrene		✓	1.5×10^{-5}	66.5	31.4	0.2 (4)	4	100	0.2	0.2
Benzo(a)Pyrene		✓	1.4×10^{-6}(8)	2.7	1.3	0.004 (4)	5	100	0.004	0.004
Benzo(e)Pyrene		✓	8.7×10^{-7}(8)	1.6	0.8	0.004 (4)	5	100	0.004	0.004
Perylene		✓	1.3×10^{-5}	24.7	11.7	0.0004(4)	5	100	0.0004	0.0004
Benzo(g,h,i)Perylene		✓	2.9×10^{-7}(8)	0.6	0.3	0.0003 (4)	6	100	0.0003	0.0003

(1) Reference 19.
(2) Total Production = (Pollutant Production Rate)(1,901,324 lb coal/hr).
(3) Maximum Concentration = (Total Production) ÷ (Flow Rate of Stream 43).
(4) Reference 9.
(5) vss = very slighly soluble; ss = slightly soluble; I = insoluble.
(6) Reference 75.
(7) Reference 4.
(8) Reference 79.
(9) Reference 113.
(10) Reference 40.
(11) Reference 45.
(12) Reference 92.
(13) Reference 2.

*Numbers in parenthesis refer to footnotes

**Estimates highly uncertain due to lack of data on compound solubility.

2) It was further assumed that the concentration of each compound in the gas liquor would be limited by either the production rate of the compound or the solubility of the compound in water.

3) The quantity of each compound produced as a function of the quantity of coal fed to the gasifier was identified in the study. The data are presented in Table 9 (column 4).

4) It was assumed that the total quantity of each organic compound in the tar dissolved in the water component of Stream 43. The resultant concentration of each organic compound in the water component of Stream 43 was calculated using the following equation:

$$C_{o-43} = \frac{(R_o)(F_{C-2})}{F_{W-43}}$$

where-

C_{o-43} is the concentration of each organic compound in the water component of Stream 43, (in ppm).

R_o is the rate of production of each organic compound per unit of coal charged to the gasifier (lb compound produced/lb of coal gasified).

F_{C-2} is the flow rate of whole coal to the gasifier, i.e., Stream 2, (1,901,324 lb/hr).

F_{W-43} is the flow rate of the water component of Stream 43, i.e., 1,993,000 lb/hr.

The results are presented in Table 9, Column 6.

5) The concentration of each compound, which would result if the limiting factor were the solubility of the compound in water, was estimated:

$$C_{o-43} = \frac{(S_{o-W})(L_{o-W})}{100\%}$$

where-

C_{o-43} is the concentration of each organic compound in Stream 43 if the solubility of the compound in water were the limiting factor (in ppm).

S_{o-W} is the solubility of the compound in water (in ppm).

L_{o-W} is the assumed level of solubility (in %) which would be attained by each compound as a function of molecular size. Based upon findings at Oak Ridge National Laboratory[45] it was assumed that for compounds with 4 or more rings L_{o-W} = 100%, and for compounds with 3 or fewer rings L_{o-W} = 10%.

The results are presented in Table 9, Column 10.

6) The concentration of each organic compound in the water component of Stream 43 was assumed to be the lesser of the two concentrations estimated in steps 4 and 5. Concentrations in Stream 43 used in the analysis are presented in Table 9, Column 11.

Estimation of Organics Concentrations in Stream 27-

Concentrations of organic compounds in Stream 27 were assumed to be zero due to lack of data on specific compounds.

Estimation of Organics Concentrations in Stream 46-

The concentration of each organic compound in the water component of stream 46 was estimated:

$$C_{o-46} = \frac{(C_{o-43})(F_{W-43}) + (C_{o-27})(F_{W-27}) \quad \frac{[100-RE_{o-LS}]}{100}}{F_{W-46}}$$

where-

C_{o-46} is the concentration of each compound in the water component of Stream 46, (in ppm).

C_{o-43} is the concentration of each compound in the water component of Stream 43, (in ppm).

F_{W-43} is the flow rate of the water component of Stream 43, i.e., 1,993,000 lb/hr.

C_{o-27} is the concentration of each organic compound in Stream 27, i.e., assumed = 0.

F_{W-27} is the flow rate of the water component of Stream 27.

RE_{o-LS} is the efficiency of removal of each compound in the tar/oil separation unit (in %).

F_{W-46} is the flow rate of the water component of Stream 46, i.e., 1,991,000 lb/hr.

Estimation of Organics Concentrations in Stream 48-

The concentration of each compound in Stream 48 was estimated using the following:

$$C_{o-48} = \frac{(C_{o-46})(F_{W-46})\ \frac{[100-RE_{o-PH}]}{100}}{F_{W-48}}$$

where-

C_{o-48} is the concentration of each compound in the water component of Stream 48 (in ppm).

C_{o-46} is the concentration of each compound in the water component of Stream 46.

F_{W-46} is the flow rate of the water component of Stream 46, i.e., 1,991,000 lb/hr.

RE_{o-PH} is the efficiency of removal of each compound in the Phenosolvan unit (in %).

F_{W-48} is the flow rate of the water component of Stream 48, i.e., 1,990,000 lb/hr.

Estimation of Organics Concentrations in Stream 50-

The concentration of each organic compound in Stream 50 was estimated using the following:

$$C_{o-50} = \frac{(C_{o-48})(F_{o-48})\ \frac{[100-RE_{o-AR}]}{100}}{F_{W-50}}$$

where-

C_{o-50} is the concentration of each compound in the water component of Stream 50 (in ppm).

C_{o-48} is the concentration of each compound in the water component of Stream 48 (ppm).

F_{W-48} is the flow rate of the water component of Stream 48, i.e., 1,990,000 lb/hr.

RE_{o-AR} is the efficiency of removal of each compound in the ammonia recovery unit (in %).

F_{W-50} is the flow rate of the water component of Stream 50, i.e., 1,991,000 lb/hr.

Estimation of Organic Consentrations in Stream 52-

The concentration of each compound in Stream 52 was estimated using the following:

$$C_{o-52} = \frac{(C_{o-50})(F_{W-50}) \quad \frac{[100-RE_{o-BT}]}{100}}{F_{W-52}}$$

where-

C_{o-52} is the concentration of each compound in the water component of Stream 52 (in ppm).

C_{o-50} is the concentration of each compound in the water component of Stream 50 (ppm).

F_{W-50} is the flow rate of the water component of Stream 50, i.e., 1,991,000 lb/hr.

RE_{o-BT} is the efficiency of removal of each compound in the Biological Treatment unit (in %).

F_{W-52} is the flow rate of the water component of Stream 52, i.e., 1,962,000 lb/hr.

Estimation of Organic Concentrations in Stream 38-

Concentrations of organic compounds in Stream 38 were assumed to be zero, due to lack of data.

Estimation of Organics Concentrations in Stream 53-

The concentration of each organic compound in Stream 53 was estimated using the following:

$$C_{o-53} = \frac{[(C_{o-52})(F_{W-52}) + (C_{o-38})(F_{W-38})] \quad \frac{[RE_{o-RO}]}{100}}{F_{W-53}}$$

where-

C_{o-53} is the concentration of each compound in the water component of Stream 53 (in ppm).

C_{o-52} is the concentration of each compound in the water component of Stream 52 (in ppm).

F_{W-52} is the flow rate of the water component of Stream 52, i.e., 1,962,000 lb/hr.

C_{o-38} is the concentration of each compound in Stream 38, assumed = 0.

F_{W-38} is the flow rate of the water component of Stream 38, i.e., 879,000 lb/hr.

RE_{o-RO} is the efficiency of removal of each compound in the Reverse Osmosis unit (in %).

F_{W-53} is the flow rate of the water component of Stream 53, assumed to be equal to 20% of the combined water flow rate of Streams 38 and 52, i.e., 568,200 lb/hr.

Estimation of Organic Concentrations in Stream 54-

Concentrations of each compound in Stream 54 were estimated using the following:

$$C_{o-54} = \frac{[(C_{o-52})(F_{W-52}) + (C_{o-38})(F_{o-38})]\ \frac{[100-RE_{o-RO}]}{100}}{F_{W-54}}$$

where-

C_{o-54} is the concentration of each compound in the water component of Stream 54 (in ppm).

C_{o-52} is the concentration of each compound in the water component of Stream 52 (in ppm).

F_{W-52} is the flow rate of the water component of Stream 52, i.e., 1,962,000 lb/hr.

C_{o-38} is the concentrations of each organic compound in Stream 38, assumed = 0.

RE_{o-RO} is the efficiency of removal of each compound in the Reverse Osmosis unit (in %).

F_{W-54} is the flow rate of the water component of Stream 54, assumed to be equal to 80% of the combined water flow rate of Stream 52 and 38, i.e., 2,273,000 lb/hr.

Estimation of Organic Concentrations in Stream 31-

Concentration of organics in treated makeup water (Stream 31) was assumed to be equal to zero.

Estimation of Organic Concentrations in Streams 31+54-

The concentration of each organic compound in Streams 31+54 was estimated using the following:

$$C_{o-(31+54)} = \frac{(C_{o-31})(F_{W-31}) + (C_{o-54})(F_{W-54})}{F_{W-31} + F_{W-54}}$$

where-

$C_{o-(31+54)}$ is the concentration of each compound in the water component of Streams (31+54).

C_{o-31} is the concentration of each compound in Stream 31, assumed = 0.

F_{W-31} is the flow rate of the water component of Stream 31, i.e., 1,179,700 lb/hr.

C_{o-54} is the concentration of each compound in the water component of Stream 54.

F_{W-54} is the flow rate of the water component of Stream 54, i.e., 2,273,000 lb/hr.

$F_{W-31}+F_{W-54}$ is the sum of the flow rate of the water component of Streams 31+54, i.e., 3,452,000 lb/hr.

2.2.3 Results

The estimated concentrations and flow rates of each stream constituent, including both trace elements and organic compounds, are presented by stream in Table 10 and 11.

TABLE 10

CONCENTRATION IN STREAM (PPM)

COMPOUNDS/ TRACE ELEMENTS	27	31	38	43	44	48	50	52	53	54	54131
Arsenic	1.0E-02	0.0	2.0E-02	5.5E-01	5.5E-01	5.5E-01	5.5E-01	2.0E-01	8.9E-01	2.0E-02	1.0E-02
Beryllium	1.0E-02	0.0	0.0	2.9E-01	2.9E-01	2.9E-01	2.9E-01	1.5E-01	4.6E-01	1.3E-02	8.5E-03
Boron	0.0	0.0	0.0	1.9E100	1.9E100	1.9E100	1.9E100	9.0E-01	3.1E100	8.5E-02	5.6E-02
Cadmium	6.0E-03	0.0	6.4E-04	2.5E-01	2.5E-01	2.5E-01	2.5E-01	1.7E-01	5.3E-01	1.5E-02	9.0E-03
Fluorine	0.0	0.0	0.0	2.0E101	2.0E101	2.0E101	2.0E101	1.0E101	3.3E101	6.2E-01	4.1E-01
Lead	2.3E-02	0.0	9.0E-02	1.4E-01	1.4E-01	1.4E-01	1.4E-01	4.3E-02	1.7E-01	2.9E-02	1.9E-02
Manganese	1.1E102	0.0	5.0E-01	4.7E-03	6.2E-02	6.2E-02	6.2E-02	3.1E-02	8.0E-01	0.0	0.0
Mercury	2.7E-02	0.0	3.0E-04	4.9E-02	4.9E-02	4.9E-02	4.9E-02	2.6E-02	8.1E-02	2.2E-03	1.5E-02
Nickel	3.2E-01	0.0	3.5E-02	3.8E-02	3.9E-02	3.9E-02	3.9E-02	2.0E-02	1.5E-01	7.6E-04	5.0E-04
Vanadium	0.0	0.0	0.0	9.6E-03	9.6E-03	9.6E-03	9.6E-03	5.4E-03	1.0E-02	2.3E-04	1.5E-04
Acetic acid	0.0	0.0	0.0	1.7E102	1.7E102	1.5E102	1.5E102	7.4E100	1.3E101	3.1E100	2.1E100
Aniline	0.0	0.0	0.0	1.2E101	1.2E101	1.2E-01	1.2E-01	6.1E-03	1.3E-02	1.9E-03	1.3E-03
Butanoic Acid	0.0	0.0	0.0	1.3E101	1.3E101	1.1E101	1.1E101	5.6E-01	1.2E100	1.0E-01	1.2E-01
Catechol	0.0	0.0	0.0	5.5E102	5.5E102	2.2E102	2.2E102	6.7E100	1.7E101	1.4E100	9.5E-01
Hexanoic Acid	0.0	0.0	0.0	1.0E100	1.0E100	8.5E-01	8.5E-01	4.3E-02	9.4E-02	1.4E-02	9.1E-03
Pentanoic Acid	0.0	0.0	0.0	1.2E101	1.2E101	1.0E101	1.0E101	5.2E-01	1.1E100	1.7E-01	1.1E-01
Phenol	0.0	0.0	0.0	3.1E103	3.1E103	1.4E101	1.4E101	1.4E-01	3.0E-01	4.2E-02	2.8E-02
Propanoic Acid	0.0	0.0	0.0	2.6E101	2.6E101	2.3E101	2.3E101	1.1E100	2.5E100	3.4E-01	2.2E-01
Pyridine	0.0	0.0	0.0	1.2E102	1.2E102	1.2E100	1.2E100	1.2E-02	3.0E-02	2.7E-03	1.0E-03
Resorcinol	0.0	0.0	0.0	2.0E102	2.0E102	1.1E102	1.1E102	2.2E100	5.0E100	4.0E-01	3.2E-01
2-Methylphenol	0.0	0.0	0.0	3.4E102	3.4E102	1.7E100	1.7E100	5.2E-02	1.3E-01	1.2E-02	7.7E-03
2-Methylpropionic Ac	0.0	0.0	0.0	2.0E100	2.0E100	1.7E100	1.7E100	8.6E-02	1.9E-01	2.0E-02	1.0E-02
2-Methylpyridine	0.0	0.0	0.0	7.0E101	7.0E101	7.0E-01	7.0E-01	7.1E-02	1.8E-01	1.6E-02	1.1E-02
2,4-Dimethylpyridine	0.0	0.0	0.0	1.0E100	1.0E100	1.0E-02	1.0E-02	1.0E-03	2.6E-03	2.3E-04	1.5E-04
2,4-Xylenol	0.0	0.0	0.0	1.2E102	1.2E102	6.0E-01	6.0E-01	1.2E-01	3.6E-01	1.0E-02	6.2E-03
2,5-Dimethylpyridine	0.0	0.0	0.0	1.0E100	1.0E100	1.0E-02	1.0E-02	1.0E-03	2.6E-03	2.3E-04	1.5E-04
3-Methylbutanoic Aci	0.0	0.0	0.0	1.0E100	1.0E100	8.5E-01	8.5E-01	4.3E-02	9.4E-02	1.4E-02	9.1E-03
3-Methylcatechol	0.0	0.0	0.0	4.0E102	4.0E102	1.6E102	1.6E102	0.0	0.0	0.0	0.0
3-Methylphenol	0.0	0.0	0.0	4.2E102	4.2E102	2.1E100	2.1E100	6.4E-02	1.9E-01	7.2E-03	4.7E-03

TABLE 10 (CONT.)

CONCENTRATION IN STREAMS (PPM)

COMPOUNDS/ TRACE ELEMENTS	27	31	38	43	44	48	50	52	53	54	54131
3-Methylpyridine	0.0	0.0	0.0	2.6E+01	2.6E+01	2.6E-01	2.6E-01	2.6E-02	6.7E-02	5.9E-03	3.9E-03
3,5-Xylenol	0.0	0.0	0.0	5.0E+01	5.0E+01	2.5E-01	2.5E-01	1.4E-01	5.0E-01	1.4E-02	9.1E-03
3,6-Dimethylcatechol	0.0	0.0	0.0	4.5E+01	4.5E+01	1.0E+01	1.0E+01	5.5E-01	1.4E+00	1.2E-01	7.0E-02
4-Methyl Resorcinol	0.0	0.0	0.0	3.6E+01	3.6E+01	1.4E+01	1.4E+01	4.4E-01	1.1E+00	9.5E-02	5.2E-02
4-Methylcatechol	0.0	0.0	0.0	3.9E+02	3.9E+02	1.5E+02	1.5E+02	4.7E+00	1.2E+01	1.0E+00	6.7E-01
4-Methylphenol	0.0	0.0	0.0	3.0E+02	3.0E+02	1.5E+00	1.5E+00	4.6E-02	1.2E-01	9.9E-03	6.5E-03
4-Methylpyridine	0.0	0.0	0.0	6.0E+00	6.0E+00	6.0E-02	6.0E-02	6.1E-03	1.6E-02	1.4E-03	9.0E-04
5-Methyl Resorcinol	0.0	0.0	0.0	6.5E+01	6.5E+01	2.6E+01	2.6E+01	7.9E-01	2.1E+00	1.7E-01	1.1E-01
Acenaphthylene	0.0	0.0	0.0	4.0E-01	4.0E-01	3.4E-01	3.4E-01	3.5E-02	1.2E-01	3.0E-04	2.0E-04
Anthracene	0.0	0.0	0.0	1.0E-01	1.0E-01	8.5E-02	8.5E-02	8.6E-03	3.0E-02	7.5E-05	4.9E-05
Benz(a)anthracene	0.0	0.0	0.0	1.0E-02	1.0E-02	8.5E-03	8.5E-03	8.6E-04	3.0E-03	7.5E-06	4.9E-06
Benzo(a)pyrene	0.0	0.0	0.0	4.0E-03	4.0E-03	3.4E-03	3.4E-03	3.5E-04	1.2E-03	3.0E-06	2.0E-06
Benzo(e)pyrene	0.0	0.0	0.0	4.0E-03	4.0E-03	3.4E-03	3.4E-03	3.5E-04	1.2E-03	3.0E-06	2.0E-06
Benzo(ghi)Perylene	0.0	0.0	0.0	3.0E-04	3.0E-04	2.6E-04	2.6E-04	2.6E-05	8.9E-05	2.2E-07	1.5E-07
Biphenyl	0.0	0.0	0.0	7.0E-01	7.0E-01	6.0E-01	6.0E-01	1.0E-01	6.2E-01	1.4E-03	1.0E-03
Chrysene	0.0	0.0	0.0	2.0E-03	2.0E-03	1.7E-03	1.7E-03	1.7E-04	5.9E-04	1.5E-06	9.8E-07
Dibenzofuran	0.0	0.0	0.0	1.0E-01	1.0E-01	8.5E-02	8.5E-02	8.6E-03	3.0E-02	1.9E-03	1.3E-03
Ethylbenzene	0.0	0.0	0.0	1.5E+01	1.5E+01	1.3E+01	1.3E+01	1.3E+00	2.9E+00	4.2E-01	2.8E-01
Fluoranthene	0.0	0.0	0.0	2.0E-01	2.0E-01	1.7E-01	1.7E-01	1.7E-02	5.9E-02	1.5E-04	9.8E-05
Fluorene	0.0	0.0	0.0	2.0E-01	2.0E-01	1.7E-01	1.7E-01	1.7E-02	5.9E-02	1.5E-04	9.8E-05
Indan	0.0	0.0	0.0	8.9E+00	8.9E+00	7.6E+00	7.6E+00	2.3E+00	7.9E+00	2.0E-02	1.3E-02
Methanethiol	0.0	0.0	0.0	2.2E+01	2.2E+01	1.9E+01	1.9E+01	1.9E+00	5.9E+00	1.4E-01	1.1E-01
Naphthalene	0.0	0.0	0.0	3.2E+00	3.2E+00	2.7E+00	2.7E+00	8.3E-01	2.8E+00	7.2E-03	4.7E-03
Perylene	0.0	0.0	0.0	4.0E-04	4.0E-04	3.4E-04	3.4E-04	3.5E-05	1.2E-04	3.0E-07	2.0E-07
Phenanthrene	0.0	0.0	0.0	1.0E-01	1.0E-01	8.5E-02	8.5E-02	8.6E-03	3.0E-02	7.5E-05	4.9E-05
Pyrene	0.0	0.0	0.0	2.0E-01	2.0E-01	1.7E-01	1.7E-01	1.7E-02	5.9E-02	1.5E-04	9.8E-05
Quinoline	0.0	0.0	0.0	9.5E+00	9.5E+00	9.5E-02	9.5E-02	9.7E-03	2.5E-02	2.2E-03	1.4E-03
Toluene	0.0	0.0	0.0	5.0E+01	5.0E+01	4.3E+01	4.3E+01	4.3E+00	9.4E+00	1.4E+00	9.1E-01
O-Xylene	0.0	0.0	0.0	1.0E+01	1.0E+01	1.5E+01	1.5E+01	1.5E+00	3.3E+00	4.0E-01	3.2E-01

TABLE 11

FLOW RATES IN STREAMS (LBS/HR)

COMPOUNDS/ TRACE ELEMENTS	27	31	38	43	46	48	50	52	53	54	54131
Arsenic	1.0E-05	0.0	1.0E-02	1.1E100	1.1E100	1.1E100	1.1E100	5.5E-01	5.1E-01	6.3E-02	6.3E-02
Beryllium	1.6E-05	0.0	0.0	5.0E-01	5.0E-01	5.0E-01	5.0E-01	2.9E-01	2.5E-01	2.9E-02	2.9E-02
Boron	0.0	0.0	0.0	3.9E100	3.9E100	3.9E100	3.9E100	1.9E100	1.7E100	1.9E-01	1.9E-01
Cadmium	6.2E-06	0.0	6.4E-04	5.0E-01	5.0E-01	5.0E-01	5.0E-01	3.4E-01	3.0E-01	3.4E-02	3.4E-02
Fluorine	0.0	0.0	0.0	4.0E101	4.0E101	4.0E101	4.0E101	2.0E101	1.9E101	1.4E100	1.4E100
Lead	2.4E-05	0.0	7.9E-02	2.0E-01	2.0E-01	2.0E-01	2.0E-01	8.4E-02	9.0E-02	6.5E-02	6.5E-02
Manganese	1.1E 01	0.0	4.4E-01	9.3E-03	1.2E-01	1.2E-01	1.2E-01	6.1E-02	5.0E-01	0.0	0.0
Mercury	2.0E-05	0.0	2.4E-04	9.7E-02	9.7E-02	9.7E-02	9.7E-02	5.1E-02	4.6E-02	5.1E-03	5.1E-03
Nickel	3.3E-04	0.0	3.1E-02	7.7E-02	7.7E-02	7.7E-02	7.7E-02	5.4E-02	0.5E-02	1.7E-03	1.7E-03
Vanadium	0.0	0.0	0.0	1.9E-02	1.9E-02	1.9E-02	1.9E-02	1.1E-02	1.0E-02	5.3E-04	5.3E-04
Acetic acid	0.0	0.0	0.0	3.4E102	3.4E102	2.9E102	2.9E102	1.4E101	7.4E100	7.1E100	7.1E100
Aniline	0.0	0.0	0.0	2.4E101	2.4E101	2.4E-01	2.4E-01	1.2E-02	7.5E-03	4.4E-03	4.4E-03
Butanoic Acid	0.0	0.0	0.0	2.6E101	2.6E101	2.2E101	2.2E101	1.1E100	6.9E-01	4.1E-01	4.1E-01
Catechol	0.0	0.0	0.0	1.1E103	1.1E103	4.4E102	4.4E102	1.3E101	9.9E100	3.3E100	3.3E100
Hexanoic Acid	0.0	0.0	0.0	2.0E100	2.0E100	1.7E100	1.7E100	8.5E-02	5.3E-02	3.1E-02	3.1E-02
Pentanoic Acid	0.0	0.0	0.0	2.4E101	2.4E101	2.0E101	2.0E101	1.0E100	6.4E-01	3.8E-01	3.8E-01
Phenol	0.0	0.0	0.0	6.2E103	6.2E103	3.1E101	3.1E101	3.1E-01	2.1E-01	9.6E-02	9.6E-02
Propanoic Acid	0.0	0.0	0.0	5.2E101	5.2E101	4.4E101	4.4E101	2.2E100	1.4E100	7.7E-01	7.7E-01
Pyridine	0.0	0.0	0.0	2.3E102	2.3E102	2.3E100	2.3E100	2.3E-02	1.7E-02	6.1E-03	6.1E-03
Resorcinol	0.0	0.0	0.0	5.5E102	5.5E102	2.2E102	2.2E102	4.4E100	3.3E100	1.1E100	1.1E100
2-Methylphenol	0.0	0.0	0.0	6.8E102	6.8E102	3.4E100	3.4E100	1.0E-01	7.5E-02	2.6E-02	2.6E-02
2-Methylpropionic Ac	0.0	0.0	0.0	4.0E100	4.0E100	3.4E100	3.4E100	1.7E-01	1.1E-01	6.3E-02	6.3E-02
2-Methylpyridine	0.0	0.0	0.0	1.4E102	1.4E102	1.4E100	1.4E100	1.4E-01	1.0E-01	3.6E-02	3.6E-02
2,4-Dimethylpyridine	0.0	0.0	0.0	2.0E100	2.0E100	2.0E-02	2.0E-02	2.0E-03	1.5E-03	5.2E-04	5.2E-04
2,4-Xylenol	0.0	0.0	0.0	2.4E102	2.4E102	1.2E100	1.2E100	2.4E-01	2.0E-01	2.3E-02	2.3E-02
2,5-Dimethylpyridine	0.0	0.0	0.0	2.0E100	2.0E100	2.0E-02	2.0E-02	2.0E-03	1.5E-03	5.2E-04	5.2E-04
3-Methylbutanoic Aci	0.0	0.0	0.0	2.0E100	2.0E100	1.7E100	1.7E100	8.5E-02	5.3E-02	3.1E-02	3.1E-02
3-Methylcatechol	0.0	0.0	0.0	8.0E102	8.0E102	3.2E102	3.2E102	0.0	0.0	0.0	0.0
3-Methylphenol	0.0	0.0	0.0	8.4E102	8.4E102	4.2E100	4.2E100	1.3E 01	1.1E-01	1.6E-02	1.6E-02

TABLE 11 (CONT.)

FLOW RATES IN STREAMS (LBS/HR)

COMPOUNDS/ TRACE ELEMENTS	27	31	38	43	46	48	50	52	53	54	54A31
3-Methylpyridine	0.0	0.0	0.0	5.2E101	5.2E101	5.2E-01	5.2E-01	5.2E-02	3.0E-02	1.3E-02	1.3E-02
3,5-Xylenol	0.0	0.0	0.0	1.0E102	1.0E102	5.0E-01	5.0E-01	3.1E-01	2.0E-01	3.1E-02	3.1E-02
3,6-Dimethylcatechol	0.0	0.0	0.0	9.0E101	9.0E101	3.6E101	3.6E101	1.1E100	8.1E-01	2.7E-01	2.7E-01
4-Methyl Resorcinol	0.0	0.0	0.0	7.2E101	7.2E101	2.9E101	2.9E101	8.6E-01	6.5E-01	2.2E-01	2.2E-01
4-Methylcatechol	0.0	0.0	0.0	7.7E102	7.7E102	3.1E102	3.1E102	9.2E100	6.9E100	2.3E100	2.3E100
4-Methylphenol	0.0	0.0	0.0	6.0E102	6.0E102	3.0E100	3.0E100	9.0E-02	6.7E-02	2.2E-02	2.2E-02
4-Methylpyridine	0.0	0.0	0.0	1.2E101	1.2E101	1.2E-01	1.2E-01	1.2E-02	8.8E-03	3.1E-03	3.1E-03
5-Methyl Resorcinol	0.0	0.0	0.0	1.3E102	1.3E102	5.2E101	5.2E101	1.6E100	1.2E100	3.9E-01	3.9E-01
Acenaphthylene	0.0	0.0	0.0	8.0E-01	8.0E-01	6.8E-01	6.8E-01	6.8E-02	6.7E-02	6.8E-04	6.8E-04
Anthracene	0.0	0.0	0.0	2.0E-01	2.0E-01	1.7E-01	1.7E-01	1.7E-02	1.7E-02	1.7E-04	1.7E-04
Benz(a)anthracene	0.0	0.0	0.0	2.0E-02	2.0E-02	1.7E-02	1.7E-02	1.7E-03	1.7E-03	1.7E-05	1.7E-05
Benzo(a)pyrene	0.0	0.0	0.0	8.0E-03	8.0E-03	6.8E-03	6.8E-03	6.8E-04	6.7E-04	6.8E-06	6.8E-06
Benzo(e)pyrene	0.0	0.0	0.0	8.0E-03	8.0E-03	6.8E-03	6.8E-03	6.8E-04	6.7E-04	6.8E-06	6.8E-06
Benzo(ghi)perylene	0.0	0.0	0.0	6.0E-04	6.0E-04	5.1E-04	5.1E-04	5.1E-05	5.0E-05	5.1E-07	5.1E-07
Biphenyl	0.0	0.0	0.0	1.4E100	1.4E100	1.2E100	1.2E100	3.6E-01	3.5E-01	3.6E-03	3.6E-03
Chrysene	0.0	0.0	0.0	4.0E-03	4.0E-03	3.4E-03	3.4E-03	3.4E-04	3.4E-04	3.4E-06	3.4E-06
Dibenzofuran	0.0	0.0	0.0	2.0E-01	2.0E-01	1.7E-01	1.7E-01	1.7E-02	1.3E-02	4.4E-03	4.4E-03
Ethylbenzene	0.0	0.0	0.0	3.0E101	3.0E101	2.6E101	2.6E101	2.6E100	1.6E100	9.5E-01	9.5E-01
Fluoranthene	0.0	0.0	0.0	4.0E-01	4.0E-01	3.4E-01	3.4E-01	3.4E-02	3.4E-02	3.4E-04	3.4E-04
Fluorene	0.0	0.0	0.0	4.0E-01	4.0E-01	3.4E-01	3.4E-01	3.4E-02	3.4E-02	3.4E-04	3.4E-04
Indan	0.0	0.0	0.0	1.0E101	1.0E101	1.5E101	1.5E101	4.5E100	4.5E100	4.5E-02	4.5E-02
Methanethiol	0.0	0.0	0.0	4.4E101	4.4E101	3.7E101	3.7E101	3.7E100	3.3E100	3.7E-01	3.7E-01
Naphthalene	0.0	0.0	0.0	6.4E100	6.4E100	5.4E100	5.4E100	1.6E100	1.6E100	1.6E-02	1.6E-02
Perylene	0.0	0.0	0.0	8.0E-04	8.0E-04	6.8E-04	6.8E-04	6.8E-05	6.7E-05	6.8E-07	6.8E-07
Phenanthrene	0.0	0.0	0.0	2.0E-01	2.0E-01	1.7E-01	1.7E-01	1.7E-02	1.7E-02	1.7E-04	1.7E-04
Pyrene	0.0	0.0	0.0	4.0E-01	4.0E-01	3.4E-01	3.4E-01	3.4E-02	3.4E-02	3.4E-04	3.4E-04
Quinoline	0.0	0.0	0.0	1.9E101	1.9E101	1.9E-01	1.9E-01	1.9E-02	1.4E-02	4.9E-03	4.9E-03
Toluene	0.0	0.0	0.0	1.0E102	1.0E102	8.5E101	8.5E101	8.5E100	5.3E100	3.1E100	3.1E100
o-Xylene	0.0	0.0	0.0	3.3E101	3.3E101	2.8E101	2.8E101	2.8E100	1.9E100	1.1E100	1.1E100

2.3 Characterization of Gaseous Streams

Characterization data in the literature were very limited. No experimental data could be found regarding specific gaseous constituents from Lurgi/Fischer-Tropsch processing of Wyoming subbituminous coal.

Gaseous streams selected for the analysis are listed in Table 12; their interrelationships are illustrated in Figure 3. These streams were selected because they may contain constituents of environmental concern and they will be released to the environment.

The analysis focused on criteria pollutants and two general classes of pollutants which have been identified as potential causes of concern in gaseous streams from coal conversion facilities: trace elements and organic compounds.

TABLE 12

GASEOUS STREAMS CHARACTERIZED FOR RISK ASSESSMENT

STREAM NUMBER*	STREAM NAME
28	Utility stack gases to atmosphere
29	Evaporative losses (incl. cooling tower drift)
72	Lockhopper vent gas emissions
73	Evaporative losses (Streams 18-23)
74	Evaporative losses (Stream 60)
75	Evaporative losses (Stream 45)
76	Evaporative losses (Stream 44)
77	Evaporative losses (Stream 47)
78	Evaporative losses (Stream 49)

*See Figure 3 on following page.

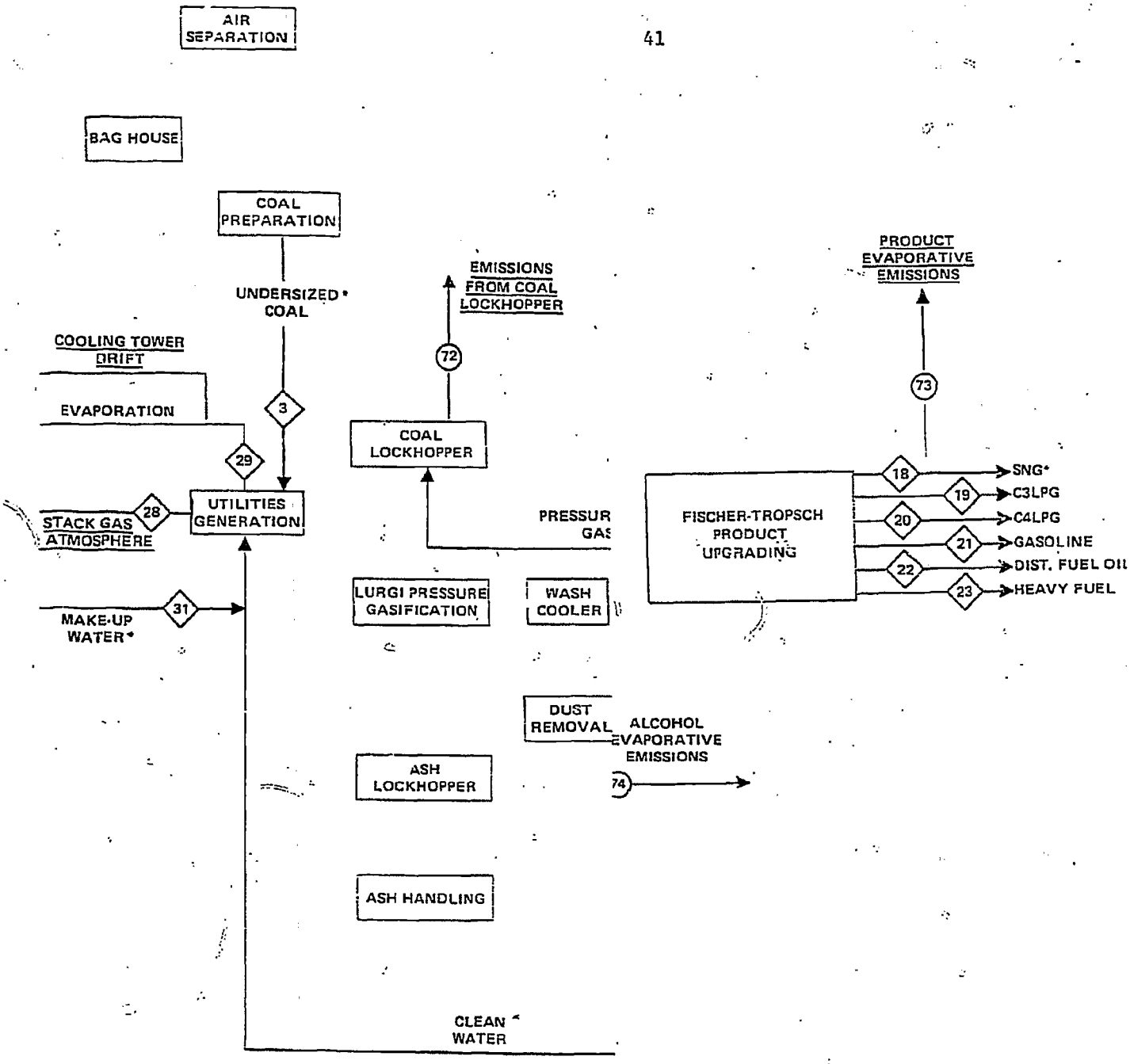

FIGURE 3

EOUS STREAMS
FOR
L LIQUEFACTION PROCESS
FISCHER-TROPSCH)

FOR CHARACTERIZING
EAMS.

In general the types and quantities of pollutants in each stream reported here have been derived from the literature and modified, as necessary, to reflect the size and feed coal of the conceptual plant used in this analysis. The types and quantities of trace elements present in the gaseous streams were estimated using the trace element characterization data for Wyoming subbituminous coal presented in Table 13. The distribution of trace elements from the gasifier was based on SASOL data[37], and is presented in Table 14. The distribution of trace elements from the utility boiler was based on data from the WESCO Coal Gasification Project[108] and is presented in Table 15.

The specific calculations, data and assumptions used in estimating the types and concentrations of trace elements and organic compounds which may be present in the gaseous streams were analyzed by stream.

Utility Stack Gases (Stream 28)

Stream Constituents:

The major and minor constituents of Stream 28 were reported by Schreiner[87], and are presented in Table 16.

Any of the trace elements found in the coal could be present in trace amounts. The flow rates of five trace elements in Stream 28 were estimated by calculating the amount of each element entering the utility boiler in the feed coal and tar from the gasifier, and then applying distribution coefficients based on the WESCO report (See Table 15).

The quantity of each trace element in the tar was estimated:

$$Q_{TE-T} = (C_{TE-DC})(F_{DC-G})(D_{TE-T})$$

where-

Q_{TE-T} is the flow rate of the trace element in the tar feed to the boiler (lb/hr).

C_{TE-DC} is the concentration of the trace element in the dry coal, ppm.

TABLE 13

TRACE ELEMENT CONCENTRATIONS FOR WYOMING AND ROSEBUD MONTANA SUBBITUMINOUS COALS (ppm)

Trace Elements	Wyoming Subbituminous [40]	Montana Rosebud Subbituminous [40]	Ratio of Concentrations of Trace Elements - Montana to Wyoming
Ag	.06-.43	.06	1-.14
As	.57-1.2	.08-1.2	.14-1
B	32	32	1
Ba	87	87	1
Be	.71-.8	.7-.8	.99-1
Br	-	-	-
Cd	.31-.8	.31-.8	1-1
Ce	-	-	-
Co	.55	.6-4	1.09-7.27
Cr	4.2-16	4-16	.95-1
Cs	-	-	-
Cu	8.9-10	9-10	1.01-1
F	65-67	66	.98-1.01
Ga	-	-	-
Ge	-	-	-
Hg	.11-.17	.11-.17	1-1
I	-	-	-
In	-	-	-
La	-	-	-
Li	3.6-15.0	-	-
Mo	2.2	2.2	1
Mn	2.8-3.4	2.8-3.4	1-1
Ni	1.7-14	2-14	1.18-1
P	-	-	-
Pb	.51-12	.51-12	1-1
Rb	-	-	-
Ru	-	-	-
Sb	.08-1.5	-	-
Sc	-	-	-
Se	.33	.33	1
Sn	.14	.14	1
Sr	-	-	-
Ta	-	-	-
Te	-	-	-
U	.88	.88	1
V	10-14	10-14	1
W	-	-	-
Y	-	-	-
Zn	.23-8	2-8	8.70-1
Zr	-	170	-

TABLE 14

TRACE ELEMENT DISTRIBUTION FOR LURGI AT SASOL*,37
(Percent of Element in Coal)

Element	Ash	Liquor	Tar	Oil
Be	33.3	53.3	17.0	0.3
B	90	8.8	2.0	0.0
V	99.9	0.1	0.0	0.0
Mn	99.9	0.2	0.0	0.0
Ni	99.4	0.4	0.0	0.0
As	26.9	67.2	1.9	3.9
Cd	51.9	45.5	0.6	1.4
Sb	50.0	45.0	3.8	0.6
Ce	99.9	0.1	0.0	0.0
Hg	51.9	41.6	6.4	0.6
Pb	94.2	1.7	4.3	0.0
Br	10.0	88.9	0.1	0.0
F	56.3**	43.8**	0.0	0.0
Cl	52.6**	47.4**	0.3	0.0

*Analysis by spark source mass spectrometer (which can give a semi-quantitative analysis) for El Paso by SASOL.

**% distribution calculated on analyses as done by SASOL previously.

TABLE 15

DISTRIBUTION OF TRACE ELEMENTS FROM UTILITY BOILER [108]

TRACE ELEMENT	DISTRIBUTION (%)			
	BOTTOM ASH	ESP FLY ASH	STACK GAS SCRUBBER	ATMOSPHERIC EMISSIONS
As	4.4	94.6	0.8	0.2
Be	16.9	82.2	0.7	0.2
Cd	16.0	82.7	1.0	0.3
F	1.2	26.8	57.6	14.4
Hg	4.4	13.0	0.1	82.5
Pb	9.7	89.3	0.8	0.2

F_{DC-G} is the flow rate of dry coal to the gasifier, i.e., 1,369,000 lb/hr.

D_{TE-T} is the fraction of the total quantity of this trace element fed to the gasifier that ends up in the tar. (Table 14).

and the total quantity of each trace element in Stream 28 due to trace element input from the feed coal and tar was estimated:

$$Q_{TE-28} = [(C_{TE-DC})(Q_{DC-B}) + (Q_{TE-T})]\ D_{TE-28}$$

where-

Q_{TE-28} is the flow rate of the trace element to the atmosphere, lb/hr

C_{TE-DC} is the concentration of the trace element in the coal feed to the boiler, ppm, dry coal basis.

Q_{DC-B} is the flow rate of dry coal to the boiler, i.e., 298,000 lb/hr.

Q_{TE-T} is the flow rate of the trace element in the tar feed to the boiler, lb/hr. (from Table 17, below)

D_{TE-28} is the fraction of the total quantity of this trace element fed to the boiler that is emitted to the atmosphere. (Table 15)

TABLE 16 - Utility Stack Gases, Stream 28

Component	lbs/hr*	Wt%
CO_2	2,739,799	39.46
N_2 + Inerts	3,632,785	52.33
O_2	71,264	1.03
H_2O	497,676	7.17
SO_x (as SO_2)	960	138 ppm
NO_x (as NO)	176	25 ppm

*Appendix B, Stream 28

The calculations are presented in Tables 17 and 18.

TABLE 17- Flow Rates of Trace Elements in the Tar

$$C_{TE-DC}^{40} \times F_{DC-G}^{87} \times D_{TE-T}^{*,37} = Q_{TE-T}$$

Trace Elements	(ppm)	(MM lb/hr)		(lb/hr)
As	.57-1.2	1.369	.019	.0148-.0312
Be	.71-.80	1.369	.17	.1652-.1862
Cd	.31-.80	1.369	.006	.0025-.0066
F	65-67	1.369	0.0	0.0
Hg	.11-.17	1.369	.064	.0096-.0149
Pb	.51-12.0	1.369	.043	.0300-.7064

TABLE 18 - Flow Rates of Trace Elements in Stream 28

$$(C_{TE-DC}^{40} \times F_{DC-B}^{87} + Q_{TE-T}^{**}) \times D_{TE-28}^{108} = Q_{TE-28}$$

Trace Elements	(ppm)	(MM lb/hr)	(lb/hr)		(lb/hr)
As	.57-1.2	.298	.0148-.0312	.002	.0004-.0008
Be	.71-.80	.298	.1652-.1862	.002	.0008-.00085
Cd	.31-.80	.298	.0025-.0066	.003	.0003-.0007
F	65-67	.298	.0000-.0000	.144	2.789-2.875
Hg	.11-.17	.298	.0096-.0149	.825	.0350-.0541
Pb	.51-12.0	.298	.0300-.7064	.002	.0004-.0086

---

* See Table 14

**From Table 17

Atmospheric Losses from Cooling Towers* (Stream 29)

Stream Constituents:

The flow rate of cooling tower atmospheric losses for the plant size studied was 2,413,000 lbs/hr. The flow rates of the constituents in the cooling tower atmospheric losses were calculated using the following equation:

$$Q_C = (C)(F_A)$$

where-

Q_C is the flow rate of the component, lbs/hr.

C is the concentration of this component in the cooling water, ppm.

F_A is the flow rate of the atmospheric losses, MM lbs/hr.

The calculations are presented in Table 19.

Feed Lockhopper Vent Gas (Stream 72)

Stream Constituents:

The following assumptions were made in calculating the composition of the feed lockhopper vent gas.

1) The feed lockhopper pressurizing gas has the same composition as the product gas stream leaving the Gas/Liquor Separator. Gas phase composition of the raw gas was assumed to be those components that remained in the product gas stream after condensation and separation of the Lurgi tar and Lurgi oil. Sound engineering practice supports this interpretation.

2) 0.1% of the total flow rate of product gas exiting the Gas/Liquor Separator was vented to the atmosphere during lockhopper depressurization.[40]

3) The list of individual organic compounds, except for the fatty acids, contained in the vent gas was derived from the literature.[19]

---

*Atmospheric losses from the cooling tower consist of two components, evaporation and drift. Make-up water to the cooling tower consists of boiler blowdown and treated gas liquor.

TABLE 19 - Atmospheric Losses from Cooling Towers, Stream 29

	C^*	x	F_A^{87}	=	Q_C
Component	(ppm)		(MM lb/hr)		(lbs/hr)
COD	501		2.413		1210
BOD	77		2.413		190
TOC**	89		2.413		220
Tars/Oils**	9		2.413		20
Other Organics**	85		2.413		210
Ammonia	508		2.413		1230
Na^{+1}	363		2.413		876
Ca^{+1}	209		2.413		504
Mg^{+2}	0		2.413		0
Alkalinity as C_aCO_3	0		2.413		0
SO_3^{-2} / SO_4^{-2}	2254		2.413		5439
Cl^-	112		2.413		270
SCN^-	1		2.413		2
TDS	3083		2.413		7439

4) It was assumed that the fatty acids present in the raw gas liquor would also be present in the product gas. The list of fatty acids contained in the gas liquor was presented in the literature.[92]

5) It was assumed that the trace elements present in the coal would also be present in the product gas. The list of trace elements contained in Wyoming subbituminous coal was derived from the literature[40] and is presented in Table 13 of this report.

The estimated composition of Stream 72 is presented in Table 20.

---

*Reference: Unpublished EPA data

**See composition of liquid stream 54 + 31 or organic compounds and trace elements possibly present in the atmospheric losses

TABLE 20-Feed Lockhopper Vent Gas, Stream 72

Component	Lbs/Hr*	Wt %**
N_2	8.4	.002
H_2O	1422	36.374
CO_2	1483	37.934
CO	602	15.399
H_2	89	2.277
CH_4	206	5.269
C_2H_4	2.5	0.064
H_2S	5.4	0.138
COS	.12	0.003
$Ni(CO)_4$	.006	1.5 ppm
Tars:	4.4	.113
Naphthalene		
Anthracene		
Phenanthrene		
Pyrene		
Cresols		
Phenol		
Xylenols		
Fluorene		
Dibenzofuran		
Chrysene		
Perylene		
Aniline		

*0.1% of Stream 10 in the flow diagram.

**Calculated using the following equation:

$$\text{wt \%} = \frac{\text{(lbs/hr of the component)}}{3909.38} \times 100$$

TABLE 20 (Cont.)

Component	Lbs/Hr	Wt%
Oils:	38.5	.985
Benzene		
Thiophene		
Toluene		
Xylenes		
Phenol		
Alkylphenols		
Naphthalene		
Indan		
Cresols		
Xylenols		
Naphtha:	15.7	.402
C_2- C_6 Aliphatics		
Benzene		
Xylene		
Ethylbenzene		
Phenols:	5.2	.133
Phenol		
Xylenols		
Cresols		
Trimethylphenol		
O-Isopropylphenol		
Mercaptans:	.02	5.1 ppm
Methanethiol		
Ethanethiol		
Thiophenes:	.016	4.1 ppm
Thiophene		
Methylthiophene		
Ammonia	8.1	.207
HCN	.008	2.0 ppm
Aromatic Amines:	.004	1.0 ppm
Aniline		
Methylaniline		
Dimethylaniline		

TABLE 20 (Concluded)

Component	Lbs/Hr	Wt %
Nitrosamines:	.002	.5 ppm
N-Nitrosamine		
PAHs	.002	.5 ppm
Chrysene		
Perylene		
Pyrene		
Fluorene		
Anthracene		
Napthalene		
Biphenyl		
Indene		
Benzofuran		
Dibenzofuran		
Fluoranthene		
Quinoline		
Acridine		
Fatty Acids:	1	.026
Acetic Acid		
Propanoic Acid		
n-Butanoic Acid		
2-Methylpropanoic Acid		
n-Pentanoic Acid		
3-Methyl Butanoic Acid		
n-Hexanoic Acid		
Trace Elements:	.002	.5 ppm
Ag		
As		
B		
Ba		
Be		
Cd		
Co		
Cr		
Cu		
F		
Hg		
Mn		
Ni		
Pb		
Se		
Sn		
U		
V		
Zn		
Total	3909.38	99.79

Evaporative Emissions (Stream 73-78)

Stream Constituents:

The contaminants believed to be found in evaporative emissions are presented in Table 21. A more detailed breakdown of gasoline in Stream 73 is presented in Table 22.

TABLE 21 - Evaporative Emissions for Product and By-Product Storage, Streams 73-78

Product/By-Product	Lbs/Hour
Diesel Oil (Stream 73)	0.513
Fuel Oil (Stream 73)*	0.014
Lurgi Oil (Stream 75)**	12.625
Lurgi Tar (Stream 76)†	6.750
Alcohol (Stream 74)††	1.500
Phenols (Stream 77)§	3.750
Ammonia (Stream 78)	No Data
C_3LPG (Stream 73)	No Data
C_4LPG (Stream 73)	No Data

*The fuel oil was reported to be all C_7 + hydrocarbons.[87]

**The folloiwng compounds were reported to be present in the Lurgi oil: benzene, thiophene, toluene, xylenes, phenol, alkyl phenols, naphthalene, cresols, benzothiophene. (EPA unpublished data.)

†The following compounds were reported to be present in the Lurgi tar: napththalene, anthracene, fluoranthene, pyrene, cresols, phenol, fluorene, dibenzofuran. (EPA unpublished data.)

††The alcohol was reported to be ethanol and C_3 + alcohols.[87]

§ The following phenolic compounds were expected to be present: phenol: catechol, resorcinol, methylcatechol, methyl resorcinol, cresols, xylenols.

TABLE 22-Evaporative Emissions of Gasoline, Stream 73

Component	lbs/Hour*
Methane	0.213
Ethylene	0.001
Propylene	0.017
Propane	0.425
Isobutane	2.071
Isobutylene	0.738
n-Butane	2.413
Cis-2-Butane	0.575
Isopentane	5.238
n-Pentane	2.450
Hexanes	0.446
Heptanes	0.188
Octanes	0.299
Total	15.055

2.4 Characterization of Solid Streams

No experimental data could be found regarding specific constituents in solid wastes from Lurgi/Fischer-Tropsch processing of Wyoming subbituminous coal.

Solid streams selected for the analysis are listed in Table 23; their interrelationships are illustrated in Figure 4. These streams were selected because they may contain constituents of environmental concern, and their disposal may result in environmental releases.

The analysis focused on two classes of pollutants which have been identified as potential causes of environmental concern in solid streams from coal conversion facilities; trace elements and organic compounds.

In general the types and quantities of pollutants in each stream either have been

- estimated from the literature and modified, as necessary, to reflect the size and feed coal of the conceptual plant used by ORNL as the basis of this analysis, or

*Unpublished EPA data

TABLE 23

SOLID STREAMS CHARACTERIZED FOR RISK ASSESSMENT

STREAM NUMBER	STREAM NAME
33	Utility ash and SO_2 scrubber sludge
34	Gasifier ash
36	Combined ash
62	Fresh Fischer-Tropsch catalyst
63	Spent Fischer-Tropsch catalyst
69*	Leachate from ash (Stream 36)
70*	Biological sludge
71*	Leachate from biosludge (Stream 70)
79	Spent shift catalyst

*Liquid stream, but emanating from a solid waste after disposal.

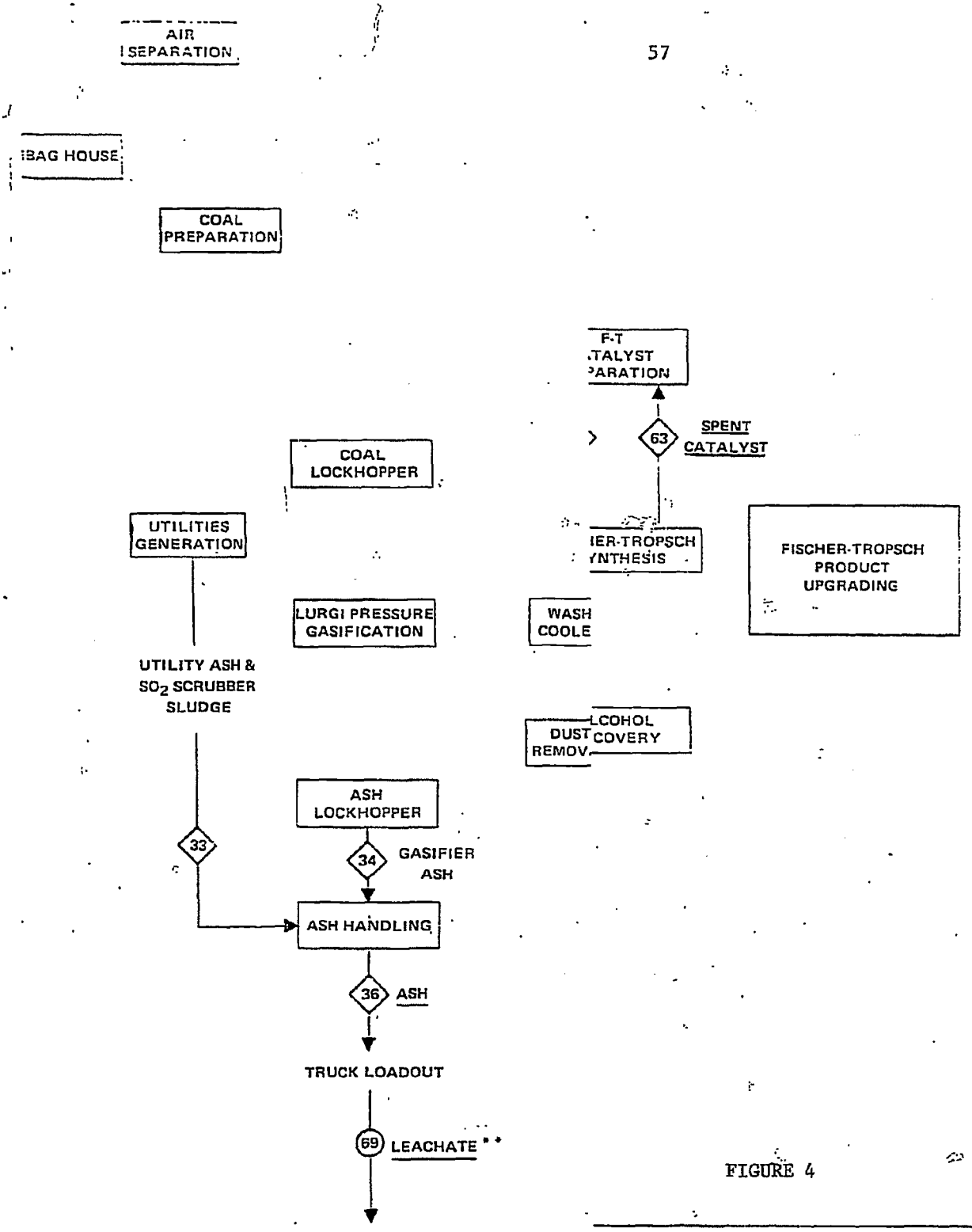

FIGURE 4

LID STREAMS
FOR
. LIQUEFACTION PROCESS
ISCHER-TROPSCH)

OR CHARACTERIZING

UMBERS WHICH ARE NOT
OW DIAGRAM.

- estimated by assuming that pollutants removed from the gaseous and liquid streams in the solid form via non-destructive mechanisms (e.g., absorption and reverse osmosis) will be present in the resultant solid wastes.

The type and quantities of trace elements present in Stream 33 (bottom ash, fly ash and scrubber sludge) were estimated using the trace element characterization data for Wyoming subbituminous coal presented in Table 24. The distribution of trace elements from the utility boiler and in the gasifier tar were calculated using distribution data from WESCO[108] and SASOL[37], respectively, presented in Tables 25 and 26.

The specific calculations, data and assumptions used in estimating the types and concentrations of trace elements and organic compounds which may be present in the solid streams are discussed in the following pages.

Boiler Bottom Ash, Fly Ash and Scrubber Sludge (Stream 33)

Stream Constituents:

The concentrations of six trace elements in Stream 33 were estimated by calculating the total input of each trace element into the utilities generation section (in coal and gasifier tar) and then applying the distribution factor for each trace element (See Table 25).

The flow rates of the trace elements in the tar feed to the boiler were first calculated using the following equation.

$$Q_{TE-T} = (C_{TE-DC})(F_{DC-G})(D_{TE-T})$$

where-

Q_{TE-T} is the flow rate of the trace element in the tar feed to the boiler, lb/hr

C_{TE-DC} is the concentration of the trace element in the dry coal, in ppm

F_{DC-G} is the flow rate of dry coal to the gasifier, MM lbs/hr

D_{TE-T} is the fraction of the total quantity of this trace element fed to the gasifier that ends up in the tar.

TABLE 24

TRACE ELEMENT CONCENTRATIONS FOR WYOMING AND ROSEBUD MONTANA SUBBITUMINOUS COALS (ppm).

Trace Elements	Wyoming Subbituminous[40]	Montana Rosebud Subbituminous[40]	Ratio of Concentrations of Trace Elements - Montana to Wyoming
Ag	.06-.43	.06	1-.14
As	.57-1.2	.08-1.2	.14-1
B	32	32	1
Ba	87	87	1
Be	.71-.8	.7-.8	.99-1
Br	-	-	-
Cd	.31-.8	.31-.8	1-1
Ce	-	-	-
Co	.55	.6-4	1.09-7.27
Cr	4.2-16	4-16	.95-1
Cs	-	-	-
Cu	8.9-10	9-10	1.01-1
F	65-67	66	.98-1.01
Ga	-	-	-
Ge	-	-	-
Hg	.11-.17	.11-.17	1-1
I	-	-	-
In	-	-	-
La	-	-	-
Li	3.6-15.0	-	-
Mo	2.2	2.2	1
Mn	2.8-3.4	2.8-3.4	1-1
Ni	1.7-14	2-14	1.18-1
P	-	-	-
Pb	.51-12	.51-12	1-1
Rb	-	-	-
Ru	-	-	-
Sb	.08-1.5	-	-
Sc	-	-	-
Se	.33	.33	1
Sn	.14	.14	1
Sr	-	-	-
Ta	-	-	-
Te	-	-	-
U	.88	.88	1
V	10-14	10-14	1
W	-	-	-
Y	-	-	-
Zn	.23-8	2-8	8.70-1
Zr	-	170	-

TABLE 25

DISTRIBUTION OF TRACE ELEMENTS FROM UTILITY BOILER[108]

TRACE ELEMENT	DISTRIBUTION (%)			
	BOTTOM ASH	ESP FLY ASH	STACK GAS SCRUBBER	ATMOSPHERIC EMISSIONS
As	4.4	94.6	0.8	0.2
Be	16.9	82.2	0.7	0.2
Cd	16.0	82.7	1.0	0.3
F	1.2	26.8	57.6	14.4
Hg	4.4	13.0	0.1	82.5
Pb	9.7	89.3	0.8	0.2

TABLE 26

TRACE ELEMENT DISTRIBUTION FOR LURGI AT SASOL*,37
(Percent of Element in Coal)

Element	Ash	Liquor	Tar	Oil
Be	33.3	53.3	17.0	0.3
B	90	8.8	2.0	0.0
V	99.9	0.1	0.0	0.0
Mn	99.9	0.2	0.0	0.0
Ni	99.4	0.4	0.0	0.0
As	26.9	67.2	1.9	3.9
Cd	51.9	45.5	0.6	1.4
Sb	50.0	45.0	3.8	0.6
Ce	99.9	0.1	0.0	0.0
Hg	51.9	41.6	6.4	0.6
Pb	94.2	1.7	4.3	0.0
Br	10.0	88.9	0.1	0.0
F	56.3**	43.8**	0.0	0.0
Cl	52.6**	47.4**	0.3	0.0

*Analysis by spark source mass spectrometer (which can give a semi-quantitative analysis) for El Paso by SASOL.

**% distribution calculated on analyses as done by SASOL previously.

The flow rates of the trace elements in the bottom ash plus fly ash stream were then calculated using the equation below.

$$Q_{TE-A} = [(C_{TE-DC})(F_{DC-B}) + (Q_{TE-T})]\ D_{TE-A}$$

where-

Q_{TE-A} is the flow rate of the trace element in the bottom ash plus fly ash, lb/hr.

C_{TE-DC} is the concentration of the trace element in the coal feed to the boiler, ppm dry coal basis.

F_{DC-B} is the flow rate of dry coal to the boiler, MM lbs/hr.

Q_{TE-T} is the flow rate of the trace element in the tar feed to the boiler, lb/hr.

D_{TE-A} is the fraction of the total quantity of this trace element fed to the boiler that is removed with the boiler bottom ash and fly ash.

The calculations are presented in Tables 27, 28, and 29.

Table 27 - Flow Rates of Trace Elements in the Tar

Trace Element	C_{TE-DC}[40] (ppm)	x	F_{DC-G}* (MM lb/hr)	x	D_{TE-T}[37]	=	Q_{TE-T} (lb/hr)
As	.57-1.2		1.369		.019		.0148-.0312
Be	.71-.80		1.369		.17		.1652-.1862
Cd	.31-.80		1.369		.006		.0025-.0066
F	65-67		1.369		0.0		0
Hg	.11-.17		1.369		.064		.0096-.0149
Pb	.51-12.0		1.369		.043		.0300-.7064

*Appendix B, Stream 2

TABLE 28 - Flow Rates of Trace Elements in the Bottom Ash and Fly Ash of Stream 33

Trace Element	$(C_{TE-DC}$ (ppm)	x F_{DC-B}* (MM lb/hr)	+ F_{TE-T}**) (lb/hr)	x D_{TE-A}	= Q_{TE-A} (lb/hr)
As	.57-1.2	.298	.0148-.0312	.99	.183-.385
Be	.71-.80	.298	.1652-.1862	.991	.373-.421
Cd	.31-.80	.298	.0025-.0066	.987	.094-.242
F	65-67	.298	0	.28	5.424-5.590
Hg	.11-.17	.298	.0096-.0149	.174	.0074-.0114
Pb	.51-12.0	.298	.0300-.7064	.99	.180-4.240

The flow rates of six trace elements in the scrubber sludge portion of Stream 33 were estimated using the following equation.

$$Q_{TE-S} = [(C_{TE-DC})(F_{DC-B}) + (F_{TE-T})]\ D_{TE-S}$$

where-

Q_{TE-S} is the flow rate of the trace element in the scrubber sludge, lb/hr.

C_{TE-DC} is the concentration of the trace element in the coal feed to the boiler, ppm, dry coal basis.

F_{DC-B} is the flow rate of dry coal to the boiler, MM lbs/hr.

F_{TE-T} is the flow rate of the trace element in the tar feed to the boiler, lb/hr.

D_{TE-S} is the fraction of the total quantity of this trace element fed to boiler that was removed with the scrubber sludge.

The calculations are presented in Table 29.

*Appendix B, Stream 3

**From Table 27

TABLE 29 - Flow Rates of Trace Elements in the Scrubber Sludge Portion of Stream 33

Trace Element	$(C_{TE-DC}$[40] (ppm)	x	F_{DC-B}* (MM lb/hr)	+	F_{TE-T}**) (lb/hr)	x	D_{TE-S}[108]	=	Q_{TE-S} (lb/hr)
As	.57-.12		.298		.0148-.0312		.008		.0015-.0031
Be	.71-80		.298		.1652-.1862		.007		.0026-.0030
Cd	.31-.80		.298		.0025-.0066		.01		.0009-.0025
F	65-67		.298		0		.576		11.157-11.500
Hg	.11-.17		.298		.0096-.0149		.001		.0000-.0001
Pb	.51-12.0		.298		.0300-.7064		.008		.0015-.0343

Gasifier Ash (Stream 34)

Stream Constituents:

Schreiner[87] reported flow rates for the materials in Stream 34, and these are presented in Table 30.

TABLE 30 - Flow Rates of Materials in Stream 34

Constituent	Flow Rate
H_2O	199,486
Minerals	96,031
Coal	7,038
Sulfur	66

The flow rates of nine trace elements in the gasifier ash were estimated using the following equation:

$$Q_{TE-34} = (C_{TE-DC})(F_{DC-G})(D_{TE-G})$$

*Appendix B, Stream 3

**From Table 27

where-

Q_{TE-34} is the flow rate of the trace element in the gasifier ash stream, lb/hr.

C_{TE-DC} is the concentration of the trace element in the coal feed to the gasifier, ppm, dry coal basis.

F_{DC-G} is the flow rate of dry coal to the gasifier, MM lbs/hr.

D_{TE-G} is the fraction of the total quantity of this trace element fed to the gasifier that was removed with the gasifier ash.

The calculations are presented in Table 31.

TABLE 31 - Flow Rates of Trace Elements in the Gasifier Ash, Stream 34

Trace Element	C_{TE-DC}[40] (ppm)	x	F_{DC-G}* (MM lb/hr)	x	D_{TE-G}[37]	=	Q_{TE-34} (lb/hr)
As	.57-1.2		1.369		.269		.2099-.4419
Be	.71-.80		1.369		.330		.3210-.3617
Cd	.31-.80		1.369		.519		.2203-.5684
F	65-67		1.369		.563		50.10-51.64
Hg	.11-.17		1.369		.519		.0782-.1208
Pb	.51-12.0		1.369		.942		.6577-15.48
B	32		1.369		.900		39.43
Ni	1.7-14.0		1.369		.994		2.313-19.05
V	10.0-14.0		1.369		.999		13.676-19.147

*Appendix B, Stream 2

Dewatered Gasifier Ash, Boiler Ash, and Scrubber Sludge to Final Disposal (Stream 36)

Stream Constituents:

Schreiner[87] reported flow rates for the materials in Stream 36, and these are presented in Table 32.

TABLE 32 - Flow Rates of Materials in Stream 36

Constituent	Flow Rate (lbs/hr)
H_2O	20,000
Minerals	116,989
Coal	7,038
Sulfur	66

The flow rates of nine trace elements in Stream 36 were estimated using the following equation.

$$Q_{TE-36} = Q_{TE-A} + Q_{TE-S} + Q_{TE-34} - (C_{TE-38})(F_{38})$$

where-

Q_{TE-36} is the flow rate of the trace element in Stream 36, lb/hr.

Q_{TE-A} is the flow rate of the trace element in the boiler bottom ash and fly ash, lb/hr.

Q_{TE-S} is the flow rate of the trace element in the scrubber sludge, lb/hr.

Q_{TE-34} is the flow rate of the trace element in the gasifier ash, Stream 34, lb/hr.

C_{TE-38} is the concentration of the trace element in the sluice water recycle, Stream 38, ppm.

F_{38} is the flow rate of Stream 38, MM lb/hr.

The calculations are presented in Table 33.

Spent F-T Catalyst (Stream 63)

Stream Constituents:

Commercial Fischer-Tropsch catalysts included cobalt (fixed-bed) and iron (fixed- and fluid-bed). Although iron was the base for both units, catalyst preparation and formulation were extremely different and very specific for each unit type.

Although spent F-T catalyst was removed periodically, not continuously, Schreiner reported the replacement rate of F-T catalyst on a continous basis to be 30 TPSD. Catalyst life was approximately 50 days.

Due to the proprietary nature of the catalyst, very limited information was available regarding chemical composition, economics of regeneration or metal recovery from spent catalysts. It appeared that the cobalt band catalyst could be economically recovered. On-site regeneration of iron band catalyst may not be practical or economical, and hence it may be either sent to metals/catalyst vendors or disposed of as a solid waste. No data was available regarding leachate characteristics.

Leachate from Solid Wastes in Stream 36 (Stream 69)

Stream Constituents:

Ash and sludge from the boiler and gasifier were slurried and pumped to the ash handling unit where the solids were dewatered. The dewatered solids, therefore, were leached before they went to final disposal. Nevertheless, the data in the following table, which represents first column volume leachate fractions of Montana Rosebud subbituminous ash, were assumed to be representative of the leachate composition from a quenched ash. Stream components are listed in Table 34. Estimation of the leachate flow rate is presented on the following two pages.

TABLE 34 - Leachate from Montana Rosebud* Ash, Stream 69

Trace Element	Concentration[91] (mg/l)
Al	.20
As	.02
Cd	.00064
Cu	.03
Fe	1.6
Hg	.0003
Mn	.50
Ni	.035
Pb	.09
Se	.06
Zn	.0029
Other Trace Elements	No data
Organics	No data

*The trace element composition of Montana Rosebud subbituminous coal was very similar to the trace element composition of Wyoming subbituminous coal as shown in Table 24.

Estimation of the Flow Rate of Leachate
From Ash and Scrubber Sludge Disposal

The flow rate of Stream 36* indicated that:

Total Dry Ash + Scrubber Sludge = 127,802 lb/hr.

With an onstream factor of 92% assumed,[87]

Days on line per year = (365 days/hr)(92%) = 336 days/year

Total dry ash and scrubber sludge:

=(127,802 lb/hr)(336 days/year)(24 hr/day) = 1,030,595,328 lb/yr

Four values were averaged for the density of dry ash/sludge[36]:

Density = [(72 + 75 + 105 + 116)lb/ft^3] ÷ 4 = 92 lb/ft^3

A density of 92 lb/ft^3 was assumed so that the total volume of waste was:

$$\text{Volume} = \frac{1{,}030{,}595{,}328 \text{ lbs/year}}{(92 \text{ lb/ft}^3)(43{,}560 \text{ ft}^2\text{/acre})} = 257 \text{ acre-feet/year}$$

This waste was assumed to be disposed of by landfill to an average thickness of 30 feet[36]. The total acreage of solid waste was:

$$\text{Acre/year} = \frac{257.2 \text{ acre-feet/year}}{30 \text{ feet}} = 8.57 \text{ acres/year}$$

Because leachate generation was directly attributable to the average net yearly precipitation/evaporation, it was best to consider rainfall levels in the U.S. as the basis for total leachate production. The range of net precipitation was from 0 to >30 inches per year. This gave a range of 0 to >815,000 gal/acre/year for leachate generation.[16]

The landfilling of ash and scrubber sludge required 8.57 acres per year, and the rate of production of leachate ranged from a low of 0 gallons per year to a high of: >6,984,550 gal/year. High leachate production = (8.57 acres)(>815,000) = >6,984,550 gal/year.

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*Appendix B, Stream 36

Biological Sludge (Stream 70)

Stream Constituents:

Flow rate of wastewater to the biotreatment unit was 1,990,190 lbs/hr.*

1,990,190 lbs/hr = 3,977 gpm

The WESCO EIS reported[108] that 6.7 TPD of dry biological solids were produced from a wastewater flow of 2,810 gpm.

6.7 TPD x 2000 lbs/ton x 1 day/24 hrs x 1 hr/60 min = 9.3 lbs/min

$$\frac{\text{9.3 lbs/min dry biological sludge}}{\text{2810 gpm wastewater}} = .0033 \text{ lbs/gal}$$

Sludge production was adjusted to flow rate from Schreiner:[87]

.0033 lbs/gal x 3977 gpm = 13 lbs/min = 780 lbs/hr. dry solids.

Vacuum filtration was assumed to produce a solid concentration of 20%:

780 ÷ 0.2 = 3,900 lbs/hr biological sludge.

Removal in the activated sludge unit was accomplished through absorption and sedimentation for the biorefractory compounds. The biorefractory compounds removed from the water were contained in the biosludge. The flow rate of biorefractory compounds removed with the biosludge was:

$$F_B = (C_{52})\ (R_{52})\ (F_{52})$$

where–

F_B is the flow rate of each biorefractory compound in the biosludge (lb/hr.)

C_{52} is the concentration of each biorefractory compound in Stream 52 (ppm_w)

R_{52} is the efficiency of removal of each compound in the biotreatment unit

F_{52} is the flow rate of Stream 52 (10^6 gal/hr.)

*Appendix B, Stream 50

Calculations are presented in Table 35.

TABLE 35 - Biological Sludge, Stream 70

Compound	C_{52} Removal (ppm)*	x R_{52} Flow Rate Efficiency**	x F_{52} Biosludge (10^6 lb/hr)	= F_B (lb/hr)
Acenaphthylene	0.3403	0.9	1.99	0.61
Anthracene	0.0851	0.9	1.99	0.15
Benz(a)anthracene	0.00851	0.9	1.99	0.015
Benzo(g,h,i)perylene	0.00026	0.9	1.99	0.00046
Benzo(a)pyrene	0.0034	0.9	1.99	0.0061
Benzo(e)pyrene	0.0034	0.9	1.99	0.0061
Chrysene	0.0017	0.9	1.99	0.003
Fluoranthene	0.1702	0.9	1.99	0.31
Fluorene	0.1702	0.9	1.99	0.31
Naphthalene	2.723	0.70	1.99	3.80
Phenanthrene	0.0851	0.90	1.99	0.15
Pyrene	0.1702	0.90	1.99	0.30
Arsenic	0.5545	0.50	1.99	0.55
Beryllium	0.2932	0.50	1.99	0.29
Cadmium	0.2503	0.325	1.99	0.16
Mercury	0.0486	0.475	1.99	0.046
Lead	0.1403	0.70	1.99	0.20

*Estimated values. See Table 10, column 8.

**See Table 7.

Leachate from Biosludge (Stream 71)

Stream Constituents:

No data available.

Spent Shift Catalyst (Stream 79)

Stream Constituents:

The average useful life of shift catalyst was 3 years.* An indirect liquefaction plant producing 45,000 BPSD fuel oil equivalent had an inventory of about 400 tons of shift catalyst.** Therefore once every 3 years 400 tons of spent shift catalyst was replaced. The spent catalyst may either be disposed of or reclaimed. Because of the high price of cobalt it is likely that spent shift catalyst will be reclaimed. The trace element content of spent shift catalyst is given in Table 36.

TABLE 36 - Spent Shift Catalyst, Stream 79

Constituent Elements	Quantity (% wt)*
Cobalt	5-15
Molybdenum	15-25
Sulfur	5-20
Carbon	5-10
Arsenic	0.7-7.0
Lead	4-10
Selenium	0.3-1
Mercury	0.2-0.8

*Unpublished EPA data

**Calculated from unpublished EPA data

3 ESTIMATION OF MAXIMUM POST-DILUTION POLLUTANT CONCENTRATIONS RESULTING FROM INDIRECT LIQUEFACTION STREAMS

3.1 Introduction

Maximum post-dilution concentrations of various pollutants resulting from discharge streams from indirect liquefaction facilities were estimated to provide a basis for subsequent analytical tasks in the risk assessment.

Due to the relatively high degree of uncertainity regarding estimated pollutant concentrations in discharge streams, and the total lack of site specific environmental information, sophisticated modeling of pollutant transport, transformation and fate was not warranted. Instead, maximum post-dilution pollutant concentrations resulting from the various facility discharges were estimated using either dilution factors based on the Source Analysis Model (SAM/I)[112] or very simple models.

Short descriptions of the assumptions and calculations used to estimate the pollutant post-dilution concentrations resulting from the release of selected facility streams are presented in Section 3.3 in addition to tables of results. A short description of the Source Analysis Model (SAM/I) is presented in Appendix C.

3.2 Caveats

These estimates of post-dilution concentrations have been prepared to provide a basis for conducting subsequent analytical tasks of the assessment of indirect liquefaction. While a considerable amount of effort has been expended in developing these estimates, users of the data are reminded and cautioned that, at best, the estimates are very rough due to a variety of problems, including but not limited to the following:

- Characterization data (qualitative and quantitative) for process and effluent streams from Lurgi/Fischer-Tropsch plants were very limited. Data used in developing these estimates came from a variety of sources and may not be representative of commercial Lurgi/Fischer-Tropsch plants.

- Dilution factors used to estimate post-dilution concentrations were not representative of any particular plant or site; they were general values derived by modeling nationwide average conditions.

- Environmental interactions and transformations were not considered in the estimates.

- Using SAM/I, dilution factors and resultant post-dilution concentrations were a function of discharge stream flow rates; discharge stream flow rates used in developing the estimates were derived from the conceptual plant flow diagram/matrix, which may or may not be truly representative of a commercial Lurgi/Fischer-Tropsch plant.

- The estimates of post-dilution concentrations presented in Tables 37 through 42 actually represent only incremental increases in pollutants due to the discharge of a single stream, i.e., the estimates did not include environmental background concentrations, nor did they include pollutant loadings from other discharge streams from the indirect liquefaction facility.

3.3 Assumptions, Calculations and Results

Estimation of Pollutant Post-Dilution Concentrations Due to Release of Stream 28 - Utility Stack Gas

Post-dilution concentrations of pollutants due to release of Stream 28 were estimated using a dilution factor from the Source Analysis Model (SAM/I). The assumptions and calculations are presented below. The results are presented in Table 37.

Assumptions:

- Ambient temperature = 25°C, pressure = 1 atm.
- Mean density of Stream 28 = Mean density of air = 1,180 gm/m^3

Calculation:

$$PC = \frac{(EC)\left(\frac{\mu g}{gm}/PPM_w\right)(\text{Density of air})}{DF}$$

where-

PC is the post-dilution concentration, in $\mu g/m^3$

EC is the emission stream concentration in PPM_w

Density of air is 1,180 gm/m^3

DF is the SAM/I dilution factor, which = 235 for a gaseous stream being discharged into the atmosphere at a flow rate of 8.75 x 10^5 gm/sec.

$$\frac{\mu g/PPM_w}{gm} = 1.0$$

TABLE 37

ESTIMATED POST-DILUTION CONCENTRATIONS DUE TO DISCHARGE OF STREAM 28-UTILITY STACK GAS

Stream Component	Emission Stream Concentration* (PPM_w)	Post-Dilution Concentration ($\mu g/m^3$)
CO_2	3.9 E+5	2.0 E+6
N_2 + Inerts	5.2 E+5	2.6 E+6
O_2	1.0 E+4	5.2 E+4
H_2O	7.2 E+4	3.6 E+5
SO_x	1.4 E+2	7.0 E+2
NO_x	2.5 E+1	1.3 E+2
Arsenic	1.2 E-4**	5.8 E-4
Beryllium	1.2 E-4**	6.1 E-4
Cadmium	1.0 E-4**	5.1 E-4
Lead	1.2 E-3**	6.0 E-3
Mercury	7.8 E-3**	3.9 E-2
Particulates	4.0 E-1	2.0 E 0

*See Section 2.3

**Based upon higher value of thee estimated range of concentration

Estimation of Pollutant Concentrations Due to Release of Stream 29 - Atmospheric Losses from Cooling Tower

The risks due to Stream 29 were analyzed differently for public health and ecosystems. Risks to public health were evaluated assuming that essentially all of the atmospheric emissions from the cooling tower were in the gaseous state. This assumption was not strictly accurate. However it appeared to be reasonable in view of the fact that drift would comprise a relatively small part (5%) of the atmospheric losses and it was assumed that the receptor population was situated close to the liquefaction facility.

The uncertainity regarding the transport and fate of drift and the partitioning of pollutants between the drift and evaporative losses appeared to be of greater importance in the ecological evaluation than in the public health evaluation. The ecological evaluation was based on pollutant emission rates rather than post-dilution concentrations.

Post-dilution Concentrations for Public Health:

Atmospheric post-dilution concentrations of pollutants due to discharge of Stream 29 were estimated using a dilution factor from the Source Analysis Model (SAM/I). Assumptions and calculations used in estimating post-dilution concentrations and emission rates are presented below. Results are presented in Table 38.

TABLE 38
ESTIMATED POST-DILUTION CONCENTRATIONS DUE TO
DISCHARGE OF STREAM 29 - ATMOSPHERIC LOSSES FROM COOLING TOWER

Stream Component	Conc. in Cooling Water (PPM_W)	Conc. in Atmospheric Emissions (PPM_W)	Public Health Post-dilution Concentration ($\mu g/m^3$)	Ecological Emmission Rate (mg/sec)
Ammonia	2.5E+1	4.9E-1	1.9E+1	4.3E+2
Arsenic	1.8E-2	3.5E-4	1.3E-2	5.5E 0
Beryllium	8.5E-3	1.7E-4	6.5E-3	2.6E 0
Boron	5.6E-2	1.1E-3	4.3E-2	1.7E+1
Cadmium	9.8E-3	1.9E-4	7.5E-3	3.0E 0
Fluorine	4.1E-1	8.0E-3	3.1E-1	1.2E+2
Lead	1.9E-2	3.7E-4	1.5E-2	5.8E 0
Mercury	1.5E-3	2.9E-5	1.1E-3	4.6E-1
Nickel	5.0E-4	9.8E-6	4.0E-4	1.5E-1
Vanadium	1.5E-4	2.9E-6	1.1E-4	4.6E-2
Acetic Acid	2.1E 0	4.1E-2	1.6E 0	6.4E+2
Aniline	1.3E-3	2.6E-5	1.0E-3	4.0E-1
Butanoic Acid	1.2E-1	2.3E-3	9.1E-2	3.6E+1
Catechol	9.5E-1	1.9E-2	7.2E-1	2.9E+2
Hexanoic Acid	9.1E-3	1.8E-4	6.9E-3	2.8E 0
Pentanoic Acid	1.1E-1	2.2E-3	8.4E-2	3.3E+1
Phenol	2.8E-2	5.5E-4	2.1E-2	8.5E 0
Propanoic Acid	2.2E-1	4.3E-3	1.7E-1	6.7E+1
Pyridine	1.8E-3	3.5E-5	1.4E-3	5.5E-1
Resorcinol	3.2E-1	6.3E-3	2.4E-1	9.7E+1
2-Methylphenol	7.7E-3	1.5E-4	5.9E-3	2.3E 0
2-Methylpropionic Acid	1.8E-2	3.5E-4	1.4E-2	5.5E 0

TABLE 38 (Continued).

Stream Component	Conc. in Cooling Water (PPM_w)	Conc. in Atmospheric Emissions (PPM_w)	Public Health Post-dilution Concentration ($\mu g/m^3$)	Ecological Emmission Rate (mg/sec)
2-Methylpyridine	1.1E-2	2.2E-4	8.4E-3	3.3E 0
2,4-Dimethylpyridine	1.5E-4	2.9E-6	1.1E-4	4.6E-2
2,4-Xylenol	6.6E-3	1.3E-4	5.0E-3	2.0E 0
2,5-Dimethylpyridine	1.5E-4	2.9E-6	1.1E-4	4.6E-2
3-Methylbutanoic Acid	9.1E-3	1.8E-4	6.9E-3	2.8E 0
3-Methylcatechol	0.0E 0	0.0E 0	0.0E 0	0.0E 0
3-Methylphenol	4.7E-3	9.2E-5	3.6E-3	1.4E 0
3-Methylpyridine	3.9E-3	7.6E-5	3.0E-3	1.2E 0
3,5-Xylenol	9.1E-3	1.8E-4	6.9E-3	2.9E+1
3,6-Dimethylcatechol	7.8E-2	1.5E-3	5.9E-2	2.4E+1
4-Methyl Resorcinol	6.2E-2	1.2E-3	4.7E-2	1.9E+1
4-Methylcatechol	6.7E-1	1.3E-2	5.1E-1	2.0E+2
4-Methylphenol	6.5E-3	1.3E-4	4.9E-3	2.0E 0
4-Methylpyridine	9.0E-4	1.8E-5	6.9E-4	2.7E-1
5-Methyl Resorcinol	1.1E-1	2.2E-3	8.4E-2	3.3E+1
Acenaphthylene	2.0E-4	3.9E-6	1.5E-4	6.1E-2
Anthracene	4.9E-5	9.6E-7	3.7E-6	1.5E-2
Benz(a)anthracene	4.9E-6	9.6E-8	3.7E-6	1.5E-3
Benzo(a)pryene	2.0E-6	3.9E-8	1.5E-6	6.1E-4

TABLE 38 (Concluded)

Stream Component	Conc. in Cooling Water (PPM_w)	Conc. in Atmospheric Emissions (PPM_w)	Public Health Post-dilution Concentration ($\mu g/m^3$)	Ecological Emmission Rate (mg/sec)
Benzo(e)pyrene	2.0E-6	3.9E-8	1.5E-6	6.1E-4
Benzo(g,h,i)perylene	1.5E-7	2.9E-9	1.4E-2	4.6E-5
Biphenyl	1.0E-3	2.0E-5	7.6E-4	3.0E-1
Chrysene	9.8E-7	1.9E-8	7.5E-7	3.0E-4
Dibenzofuran	1.3E-3	2.5E-5	1.0E-3	4.0E-1
Ethylbenzene	2.8E-1	5.5E-3	2.1E-1	8.5E+1
Fluoranthene	9.8E-5	1.9E-6	7.4E-5	3.0E-2
Fluorene	9.8E-5	1.9E-6	7.4E-5	3.0E-2
Indan	1.3E-2	2.5E-4	9.9E-3	4.0E 0
Methanethiol	1.1E-1	2.2E-3	8.4E-2	3.3E+1
Naphthalene	4.7E-3	9.2E-5	3.6E-3	1.4E 0
Perylene	2.0E-7	3.9E-9	1.5E-7	6.1E-5
Phenanthrene	4.9E-5	9.6E-7	3.7E-5	1.5E-2
Pyrene	9.8E-5	1.9E-6	7.4E-5	3.0E-2
Quinoline	1.4E-3	2.8E-5	1.1E-3	4.3E-1
Toluene	9.1E-1	1.8E-2	6.9E-1	2.8E+2
o-Xylene	3.2E-1	6.2E-3	2.4E-1	9.7E+1

Assumptions:

- Ambient temperature - 25°C, pressure - 1 atm.
- Evaporative losses accounted for essentially all of the atmospheric losses from the cooling tower.*
- Relative humidity of influent air was 0%, and of effluent air was 100%.
- Water content of air was 0.02 lb water/lb of dry air.[75]
- Density of atmospheric emission stream = density of air = 1,180 gm/m^3.

Calculation:

The total flow rate of moisture and air from the cooling tower was calculated using the following:

$$TF = WF + AF$$

where—

TF is the total flow rate of air and moisture

WF is the flow rate of moisture

AF is the flow rate of air

At 25°C and 1 ATM, the moisture content of air was 0.02 lb water/lb dry air. Therefore,

$$AF = (WF)\ (1\ lb/0.02\ lb) = 50\ WF$$

and

$$TF = WF + 50WF = 51\ WF$$

According to Schreiner, the flow rate of water out of the cooling tower was 2.413×10^6 lb/hr or 3.04×10^5 gm/sec. Therefore,

$$TF = (51)(3.04 \times 10^5\ gm/sec) = 1.55 \times 10^7\ gm/sec.$$

*According to Schreiner[87] drift accounted for 5% and evaporative losses 95%, but to simplify the estimates it was assumed that all of the atmospheric loss was evaporative in nature.

The concentration of each pollutant in the total emission stream (air + water) was calculated by the following:

$$EC = \frac{(CW)(WF)}{TF}$$

where-

EC is the pollutant concentration in the total emission stream, in PPM_w

CW is the pollutant concentration in the cooling tower feed water, in PPM_w

WF is the flow rate of the water in the atmospheric stream, 3.04×10^5 gm/sec

TF is the total flow rate of air and moisture.

But, $TF = 51 \times WF$

therefore-

$$EC = \frac{(CW)(WF)}{51\ WF} = \frac{CW}{51}$$

The post-dilution concentration of each pollutant was then calculated:

$$PC = \frac{(EC)(\frac{\mu g}{gm}/PPM_w)(\text{Density of Air})}{DF}$$

where-

PC is the pollutant post-dilution concentration, in $\mu g/m^3$

EC is the pollutant concentration in the emission stream, in PPM_w.

$\frac{\mu g}{gm}$ / PPM_w is a conversion factor, equal to 1.0

Density of air is 1,180 gm/m^3

DF is the SAM/I dilution factor, which was 30.4 for a gaseous discharge to the atmosphere at a flow rate of 1.55×10^7 gm/sec.

Emission Rates for Ecosystems:

From an ecological perspective, the partitioning of contaminants between drift and evaporation losses was important because drift tends

to settle over a more limited area, relatively close to the plant, than the evaporative losses. Thus, whatever contaminants were present in the drift would tend to become enriched on the surface of vegetation and in soils within one or two kilometers of the plant. Because data were so limited and partitioning was important, the ecological risks were evaluated on the basis of pollutant emission rates rather than post-dilution concentrations in the atmosphere. Two emission rates were calculated as follows:

$$E = (C)(F)$$

where-

E is the emission rate, in mg/sec

C is the pollutant concentration in water fed to the cooling tower, in mg/l

F is the flow rate of Stream 29, i.e., 304 l/sec.

Estimation of Pollutant Post-Dilution Concentrations Due to Disposal of Stream 53 - Reverse Osmosis Concentrated Waste Solution

Two sets of post-dilution concentrations were estimated for disposal of Stream 53. The set used to evaluate risks to public health was developed assuming that groundwater contamination would be the major concern; the set used to evaluate risks to ecosystems was developed assuming contamination of surface streams would be the primary cause of concern. The assumptions and calculations are presented below. The results are presented in Table 39.

TABLE 39

ESTIMATED POST-DILUTION CONCENTRATIONS DUE TO DISCHARGE OF STREAM 53 - REVERSE OSMOSIS WASTE SOLUTION

Stream Component	Effluent Stream Concentration (PPM_w)	Public Health Post-dilution Concentration (PPM_w)	Ecological Post-dilution Concentration (PPM_w)
Arsenic	8.9E-1	8.9E-2	2.3E-1
Beryllium	4.6E-1	4.6E-2	1.2E-1
Boron	3.1E 0	3.1E-1	7.9E-1
Cadmium	5.3E-1	5.3E-2	1.3E-1
Fluorine	3.3E+1	3.3E 0	8.3E 0
Lead	1.7E-1	1.7E-2	4.3E-2
Manganese	8.8E-1	8.8E-2	2.2E-1
Mercury	8.1E-2	8.1E-3	2.1E-2
Nickel	1.5E-1	1.5E-2	3.8E-2
Vanadium	1.8E-2	1.8E-3	4.5E-3
Acetic Acid	1.3E+1	1.3E 0	3.3E 0
Aniline	1.3E-2	1.3E-3	3.3E-3
Butanoic Acid	1.2E-0	1.2E-1	3.1E-1
Catechol	1.7E+1	1.7E 0	4.4E 0
Hexanoic Acid	9.4E-2	9.4E-3	2.4E-2
Pentanoic Acid	1.1E 0	1.1E+1	2.8E-1
Phenol	3.8E-1	3.8E-2	9.6E-2
Propanoic Acid	2.5E 0	2.5E+1	6.3E-1

TABLE 39 (Cont.)

Stream Component	Effluent Stream Concentration (PPM_w)	Public Health Post-Dilution Concentration (PPM_w)	Ecological Post-Dilution Concentration (PPM_w)
Pyridine	3.0E-2	3.0E-3	7.5E-3
Resorcinol	5.8E 0	5.8E-1	1.5E 0
2-Methylphenol	1.3E-1	1.3E-2	3.3E-2
2-Methylpropionic Acid	1.9E-1	1.9E-2	4.8E-2
2-Methylpyridine	1.8E-1	1.8E-2	4.6E-2
2,4-Dimethylpyridine	2.6E-3	2.6E-4	6.6E-4
2,4-Xylenol	3.6E-1	3.6E-2	9.1E-2
2,5-Dimethylpyridine	2.7E-3	2.6E-4	6.6E-4
3-Methylbutanoic Acid	9.4E-2	9.4E-3	2.4E-2
3-Methylcatechol	0.0E 0	0.0E 0	0.0E 0
3-Methylphenol	1.9E-1	1.9E-2	4.8E-2
3-Methylpyridine	6.7E-2	6.7E-2	1.7E-2
3,5-Xylenol	5.0E-1	5.0E-2	1.3E-1
3,6-Dimethylcatechol	1.4E 0	1.4E-1	3.6E-1
4-Methyl Resorcinol	1.1E 0	1.1E-1	2.8E-1
4-Methylcatechol	1.2E+1	1.2E 0	3.1E 0
4-Methylphenol	1.2E-1	1.2E-2	3.0E-2
4-Methylpyridine	1.6E-2	1.6E-3	4.1E-3
5-Methyl Resorcinol	2.1E 0	2.1E-1	5.3E-1
Acenaphthylene	1.2E-1	1.2E-2	3.0E-2

TABLE 39 (Concluded)

Stream Component	Effluent Stream Concentration (PPM_w)	Public Health Post-dilation Concentration (PPM_w)	Ecological Post-dilution Concentration (PPM_w)
Anthracene	3.0E-2	3.0E-3	7.6E-3
Benz(a)anthracene	3.0E-3	3.0E-3	7.6E-4
Benzo(a)pyrene	1.2E-3	1.2E-4	3.0E-4
Benzo(e)pyrene	1.2E-3	1.2E-4	3.0E-4
Benzo(g,h,i)perylene	8.9E-5	8.9E-6	2.2E-5
Biphenyl	6.2E-1	6.2E-2	1.6E-1
Chrysene	5.9E-4	5.9E-5	1.5E-4
Dibenzofuran	2.2E-2	2.2E-3	5.6E-3
Ethylbenzene	2.9E 0	2.9E-1	7.3E-1
Fluoranthene	5.9E-2	5.9E-3	1.5E-2
Fluorene	5.9E-2	5.9E-3	1.5E-2
Indan	7.9E 0	7.9E-1	2.0E 0
Methanethiol	5.9E 0	5.9E-1	1.5E 0
Naphthalene	2.8E 0	2.8E-1	7.1E-1
Perylene	1.2E-4	1.2E-5	3.0E-5
Phenanthrene	3.0E-2	3.0E-3	7.6E-3
Pyrene	5.9E-2	5.9E-3	1.5E-2
Quinoline	2.5E-2	2.5E-3	6.3E-3
Toluene	9.4E 0	9.4E-1	2.4E 0
o-Xylene	3.3E 0	3.3E-1	8.3E-1

Post-dilution Concentrations for Public Health:

The risk to public health posed by Stream 53 was assumed to originate from improper disposal of the stream and subsequent contamination of the groundwater. The dilution factor was derived from the Source Analysis Model (SAM/I). Assumptions and calculations were as follows.

Assumptions:

- Stream 53 disposed of in a sump or fill site.
- Receiving body (sump or fill site) had a base diameter $\geq$ 10m.
- SAM/I dilution factors were appropriate for estimating subsequent pollutant concentrations in groundwater.
- Local population used groundwater directly for domestic needs.
- Flow rate of Stream 53 = 569,000 lb/hr (71,700 gm/sec).

Calculations

Post-dilution concentrations of pollutants from Stream 53 for the public health analysis were calculated using the following equation:

$$PC = \frac{EC}{DF}$$

where-

PC is the post-dilution concentration in PPM_w or mg/l.

EC is the concentration in effluent Stream 53, in PPM_w.

DF is the SAM/I dilution factor, which was 10, for a liquid stream discharged into a sump or fill site with a diameter $\geq$ 10 meters.

Post-dilution Concentrations for Ecosystems:

The risk to ecosystems posed by Stream 53 was assumed to orginate from disposal of the stream and subsequent leakage of all of the stream contaminants into a small surface stream. A SAM/I dilution factor was not used.

Assumptions:

- Stream 53 was disposed of in an inadequate evaporation pond.
- All of the stream components except water were subsequently released into a small (10 cfs) surface stream through overflow or by percolation through the soil.
- Loss of stream contaminants through physical, chemical and biological processes prior to entry into the surface stream was negligible.
- Evaporation of the water components of stream 53 in the evaporation pond was significant, resulting in extreme concentration of stream contaminants prior to the entry into the surface stream.

Calculations:

Post-dilution concentrations of pollutants from Stream 53 for the ecological analysis were calculated using the following equation:

$$PC = \frac{(EC)(FR_{53})}{FR_s}$$

where-

PC is the post-dilution concentrations, in PPM_w.

EC is the constituent concentration in Stream 53, in PPM_w.

FR_{53} is the flow rate of Stream 53, 71.7 gm/sec.

FR_s is the flow rate of the surface stream, 283 l/sec.

Estimation of Pollutant Post-Dilution Concentrations Due to the Discharge of Stream 69 - Leachate from Gasifier and Utility Ash

Two sets of post-dilution concentrations were estimated for discharge of contaminants in Stream 69. The set used to evaluate risks to public health was developed assuming that groundwater contamination would be the major concern, while the set used to evaluate risks to ecosystems was developed assuming contamination of surface streams would be the primary cause for concern. The assumptions and calculations are presented below. The results are presented in Table 40.

TABLE 40

ESTIMATED POST-DILUTION CONCENTRATIONS DUE TO DISCHARGE OF STREAM 69 - ASH LEACHATE

Stream Component	Effluent Stream Concentration (PPM_w)	Public Health Post-dilution Concentration (PPM_w)	Ecological Post-dilution Concentration (PPM_w)
Aluminum	2.0E-1	2.0E-2	6.0E-4
Arsenic	2.0E-1	2.0E-3	6.0E-5
Cadmium	6.4E-4	6.4E-5	1.9E-6
Copper	3.0E-2	3.0E-3	9.0E-5
Iron	1.6E 0	1.6E-1	4.8E-3
Lead	9.0E-2	9.0E-3	2.7E-4
Manganese	5.0E-1	5.0E-2	1.5E-3
Mercury	3.0E-4	3.0E-5	9.0E-7
Nickel	3.5E-2	3.5E-3	1.1E-4
Selenium	6.0E-2	6.0E-3	1.8E-4
Zinc	2.9E-3	2.9E-4	1.8E-4

Post-dilution Concentrations for Public Health:

The risk to public health was assumed to originate from improper disposal of the stream and subsequent contamination of groundwater. The dilution factor was derived from the Source Analysis Model (SAM/I). Assumptions and calculations were as follows:

Assumptions:

- Gasfier and utility ash (Stream 36) were the source of the leachate.
- The ash was disposed of at a fill site.
- The fill site had a base diameter $\geq$ 10 meters.
- SAM/I dilution factors were appropriate for estimating subsequent pollutant concentrations in groundwater.
- The local population used the groundwater directly for domestic uses.
- Flow rate of the leachate = 7×10^6 gallons/year.*

Calculations:

Post-dilution concentrations of pollutants from Stream 69 for the public health analysis were calculated using the following equation:

$$PC = \frac{EC}{DF}$$

where-

PC is the pollutant post-dilution concentrations, in PPM_w

EC is the pollutant concentration in effluent Stream 69, in PPM_w*

DF is the SAM/I dilution factor, which was 10, for a liquid stream discharged in a fill site with a base diameter $\geq$ 10 meters.

*See Section 2.4

Post-dilution Concentrations for Ecosystems:

The risk to ecosystems posed by Stream 69 was assumed to originate from disposal of the ash and subsequent contamination of a small surface stream. A SAM/I dilution factor was not used.

Assumptions:

- Flow rate of the leachate = 7.0×10^6 gal/year* or 0.85 liters/sec.
- Pollutant concentrations in the leachate were not reduced by physical, chemical or biological processes prior to entry into a small surface stream.
- The surface stream flow rate was 10 cubic feet/sec (283 1/sec).

Calculations:

The post-dilution concentration of each pollutant due to release of Stream 69 was calculated using the following:

$$PC = \frac{(EC)(LF)}{SF} = \frac{(EC)(.85\ 1/sec)}{283\ 1/sec} = \frac{EC}{333}$$

where-

PC is the post-dilution concentrations, in PPM_w.

EC is the concentration in the effluent stream, in PPM_w.

LF is the flow rate of the leachate, equal to 0.85 1/sec.

SF is the flow rate of the small surface stream, 283 1/sec.

Estimation of Pollutant Post-Dilution Concentrations Due to Disposal of Stream 70 - Biosludge

The post-dilution concentrations of pollutants, which might result from disposal of Stream 70, biosludge, were estimated assuming that all of the trace elements and toxic organic compounds in the biosludge were made available to a small surface stream through

*See Section 2.4

leaching. Assumptions and calculations are presented below. Results are presented in Table 41.

Assumptions:

- Biosludge was disposed of in a landfill.
- All of the trace metals and toxic organics were leached out of the biosludge and enter a surface stream.
- The concentrations of leachate contaminants were not reduced by physical, chemical or biological processes prior to entry into the surface stream.
- The flow rate of the surface stream was 10 cfs.
- The water component of the leachate was negligible.

Calculations

The concentration of each pollutant in the surface stream was calculated as follows:

$$PC = \frac{(PR)(1000mg/gm)}{SF}$$

where-

PC is the post-dilution concentration, in PPM_w

PR is the production rate of the trace elements and organics in Stream 70*, in gm/sec.

SF is the flow rate of the surface stream, 283 l/sec.

*See Table 35 for pollutant production rate.

TABLE 41

ESTIMATED POST-DILUTION CONCENTRATION DUE TO DISPOSAL OF STREAM 70 - BIOSLUDGE

Stream Component	Biosludge Removal Rate (gm/sec)	Post-dilution Concentration (PPM_w)
Arsenic	6.9E-2	2.4E-1
Beryllium	3.7E-2	1.3E-1
Cadmium	2.0E-2	7.1E-2
Mercury	5.8E-3	2.0E-2
Lead	2.5E-2	8.9E-2
Acenaphthylene	7.7E-2	2.7E-1
Anthracene	1.9E-2	6.7E-2
Benz(a)anthracene	1.9E-3	6.7E-3
Benz(g,h,i)perylene	5.8E-5	2.0E-4
Benzo(a)pyrene	7.7E-4	2.7E-3
Benzo(e)pyrene	7.7E-4	2.7E-3
Chrysene	3.8E-4	1.3E-3
Fluoranthene	3.9E-2	1.4E-1
Fluorene	3.9E-2	1.4E-1
Naphthalene	4.8E-1	1.7E 0
Phenanthrene	1.9E-2	6.7E-2
Pyrene	3.8E-2	1.3E-1

Estimation of Pollutant Post-Dilution Concentrations Due to Release of Stream 72 - Lockhopper Vent Gas

The post-dilution concentrations of pollutants which may result from the discharge of Stream 72 were estimated using a dilution factor from the Source Analysis Model (SAM/I). The assumptions and calculations are presented below. The results are presented in Table 42.

Assumptions:

- Ambient temperature = 25°C, pressure = 1 atm.
- Mean density of Stream 72 = 1,180 gm/m^3 (25°, 1 atm)

Calculation:

$$PC = \frac{(EC)\left(\frac{\mu g}{gm}/PPM_w\right)(\text{Density of Air})}{DF}$$

where-

PC is the post-dilution concentration, in $\mu g/m^3$

EC is the concentration in Stream 72 in PPM_w*

$\left(\frac{\mu g}{gm}/PPM_w\right)$ is a conversion factor = 1.0

Density of air is 1,180 gm/m^3

DF is the SAM/I dilution factor, which was 24,000 for a gaseous stream being discharged into the atmosphere at a rate of 493 gm/sec.

3.4 Applications of Results

The information presented in Volume II represents estimates of maximum post-dilution concentrations for trace elements and organic compounds released by a model, commercial-scale indirect liquefaction facility. The ecological, public health and occupational health hazards posed by this model facility are based upon these estimates and are described in Volumes III, IV and V, respectively. Volume I presents a summary of Volumes II through V and overall conclusions made in the assessment.

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*See Section 2.2

TABLE 42

ESTIMATED POST-DILUTION CONCENTRATIONS DUE TO DISCHARGE OF STREAM 72 - LOCKHOPPER VENT GAS

Stream Component	Emission Stream Concentration (PPM_w)	Post-dilution Concentration ($\mu g/m^3$)
CO	1.5E+5	7.4E+3
CH_4	5.2E+4	2.5E+3
C_2H_4	6.4E+2	3.1E+1
H_2S	1.4E+3	6.6E+1
COS	3.0E+1	1.4E 0
$Ni(CO)_4$	1.5E 0	7.4E-2
Tars	1.1E+3	5.4E+1
Oils	9.9E+3	4.9E+2
Naphtha	4.0E+3	1.9E+2
Phenols	1.3E+3	6.4E+1
Mercaptans	5.1E 0	2.5E-1
Thiophenes	4.1E 0	2.0E-1
Ammonia	2.0E+3	9.8E+1
HCN	2.0E 0	9.8E-2
Aromatic amines	1.0E 0	4.9E-2
Nitrosamines	5.0E-1	2.5E-2
PAHs	5.0E-1	2.5E-2
Fatty acids	2.6E+2	1.3E+1
Trace elements	5.0E-1	2.5E-2

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APPENDIX A

LIQUEFACTION PROCESS DESCRIPTION AND BASIC PREMISES USED IN DEVELOPING THE MATERIAL BALANCE

Process Description

Sized coal (+ 1/4" to 2") was gasified in the Lurgi gasifiers at 450 psig using steam and oxygen to yield a raw synthesis gas (syngas) product. The raw syngas exitted the gasifiers at 900` F. This gas was cooled and scrubbed to remove the attendant particulates, tars, oils, phenols, and other impurities. The impurities were separated from the gas as a gas liquor in the gas/liquor separator. The partially cleaned syngas was then split into two streams; one stream was further cooled while the other stream underwent shift conversion to adjust the H_2/CO ratio in the gas such that H_2/CO ratio of the combined gas stream was in the desired range for the Fischer-Tropsch reaction. The two streams were then comingled and further purified using the Rectisol process to remove the sour gases (H_2S and CO_2) and naphtha from the syngas.

The cleaned gas from the Rectisol process was fed to the Fischer-Tropsch reactors where it was catalytically converted (over a proprietary iron catalyst) to mainly aliphatic hydrocarbon products. The raw products from the Fischer-Tropsch reactors were further processed and upgraded to yield the plant product slate consisting of SNG, C_3 and C_4 LPG, gasoline and fuel oils by using conventional petroleum refinery processes. Details of the product upgrading section have been omitted from the flowsheet because: 1) it consisted of conventional petroleum refinery-type processes, and 2) the major unknowns regarding environmental and occupational health concerns were associated with the front-end or syngas production section of the process.

The acid gases recovered in the various processing steps were taken to the sulfur recovery step where they were converted to sulfur using the Stretford process. The sulfur produced was proposed for sale as plant product. Tail gas from the Stretford process was incinerated in the plant boiler.

APPENDIX A

(cont.)

Boiler stack gas cleanup facilities for SO_2 removal were provided to reduce the SO_2 emissions to 0.2 pounds of SO_2 per million Btu of fired heat. In addition, an electrostatic precipitator was included to reduce the particulate matter to 0.1 pound per million Btu of fired heat duty.

The gas liquors recovered in the syngas cleanup steps were collected and processed further to separate the oils, dust, tars, crude phenols, and ammonia from the water. The recovered water underwent additional treatment prior to reuse in the process. Waste products recovered from the gas liquor were disposed of appropriately as indicated below.

Oils and tars were recovered from the waste water by settling and decantation. The oils were processed further in the product upgrading section to yield additional plant products; the tars were incinerated in the plant boiler. Crude phenols were recovered from the waste water by using the Phenosolvan process. The crude phenols were incinerated in the plant boiler. Anhydrous NH_3 was recovered for sale by using the Chemie-Linz/Lurgi process.

The denuded waste water from the ammonia recovery step was biologically treated to reduce its BOD and COD levels by removing the residual organics present in the water. The water was then subjected to a reverse osmosis treatment to reduce its metal salts content prior to reuse in the process. The biosludge (from the biological treatment step) was disposed of in an environmentally acceptable manner such as a landfill operation.

APPENDIX A
(cont.)

TABLE A-1- Coal analysis:

Proximate analysis, as-received basis (wt.%)

Volatile matter	33.1
Fixed carbon	33.8
Ash	5.1
Moisture	28.0
Total	100.0

Ultimate analysis, moisture and ash-free (MAF) basis (wt.%)

Carbon	74.45
Hydrogen	5.10
Oxygen	19.25
Nitrogen	0.75
Sulfur	0.45
Total	100.00

Heating value, MAF basis, Btu/lb

High heating value	12,720
Low heating value	12,236

TABLE A-2- Product slate

SNG^{86}, MMscf/sd*	173.3
C_3 LPG, BPDS**	1,1707
C_4 LPG, BPSD	146
Gasoline, BPSD	13,580
Diesel fuel, BPSD	2,307
Heavy fuel oil, BPSD	622
Mixed alcohols, BPSD	1,825
Sulfur, TPSD	61
Anhydrous, NH_3, TPSD	103
Total product, BPSD FOE†	44,950

* MMscf/sd = Million standard cubic feet per stream day

**BPSD = Barrels per stream day

†FOE = Fuel oil equivalent at 6×10^6 Btu/barrel fuel oil

APPENDIX B:

ESTIMATION OF STREAM FLOW RATES AND
CONCENTRATIONS BY INDIVIDUAL
STREAM ARE PRESENTED IN
TABLES B-1 AND B-2

TABLE B-1

Appendix B: Estimated process stream concentration for the risk assessment of Indirect (Lurgi/Fischer-Tropsch) coal liquefaction process

Component	Stream Number											
	1	2	3	4	5	6	7	8	9	10	11	12
FLOWRATE, lb mol/h												
CO 28.01							21459	21459	21459	21459	4042	17416
CO_2 44.01							33724	33724	33724	33722	6353	27370
H_2 2.02							44332	44332	44332	44332	8359	35973
CH_4 16.04							12866	12866	12866	12866	2424	10442
C_2H_4 28.05							86	86	86	86	16	69
C_2H_6 30.07							614	614	614	614	116	498
N_2 + Inerts 28.01				278	55554		310	310	310	310	59	252
O_2 32.00				14060	783							
H_2S 34.08							158	158	158	157	30	128
COS 60.07							2	2	2	2	<1	2
H_2O 18.02						94379	88481	93936				
Others												
Total gas flowrate, lb mol/h				14338	56335	94379	202032	207487	113551	113548	21400	92150
Temperature, °F	Amb.[b]	Amb.	Amb.	290	Amb.	748	900[c]	700[c]	400[c]	367	367	367
Pressure, psia	Atm.	Atm.	Atm.	480	Atm.	660	450[c]	445[c]	425[c]	414	414	414
FLOWRATE, lb/h												
H_2O	648687	532390	115917		11567				1692727	1425476	268531	1156945
Methanol												
Tar							36311	39504	39504	4438	835	3601
Oil							51911	53255	53255	38467	7246	31221
Naphtha							15675	15675	15675	2951	2951	12722
Crude phenols							15193	16189	16189	5234	986	4248
Mercaptans[d]							40	42	42	20	6	14
Thiophenes[d]							35	36	36	16	5	11
Ammonia							9812	9985	9985	8028	1522	6556
HCN[e]							8	8	8	8	2	6
Aromatic amines[g]							4	4	4	4	1	3
Nitrosamines[g]							2	2	2	2	<1	2
PNA							80	82	82	2	1	1
Fatty acids							2799	2976	2976	1029	194	835
$Ni(CO)_4$[f]							5	6	6	6	2	4
Minerals	116959	96020	20904									
Coal	1549420	1271963	277067									
Sulfur												
Particulates							4106	4516	4516			
Trace elements[g]	1158	951	201				7	8	8	2	1	1
Others												
Total liquid/solid flowrate, lb/h	2316024	1901324	414089		11567		335988	1422818	1835015	1498457	282286	1216172
TOTAL STREAM FLOWRATE, lb/h	2316024	1901324	414089	457707	1592627	1700710	4146482	4251081	4251081	3914406	737404	3177001
Radioactivity[h]	2.6	2.6					0.1	0.1	0.1	0.1	0.1	0.1

Table B-1

Appendix B (Continued)

Components	Stream Number 13	14	15	16	17	18	19	20	21	22	23	24[k]
FLOWRATE, lb mol/h												
CO 28.01	1218	17416	18634	18500	483	13						
CO_2 44.01	9177	27370	36546	2900	3102	85						
H_2 2.02	11184	35973	47156	46985	9337	719						
CH_4 16.04	2424	10442	12866	12460	14258	17055						
C_2H_4 28.05	16	69	86	21	381	188						
C_2H_6 30.07	116	498	614	277	818	445						
N_2 & Inerts 28.01	59	252	310	309	309	308						
O_2 32.00												4
H_2S 34.08	30	128	157									1
COS 60.07	<1	2	2									
H_2O 18.02												
Others				1[i]						2	1	1
Total gas flowrate, lb mol/h	24225	92150	116371	81453	28688	18813				2	1	6
Temperature, °F	86	86	86	68	100	130	100	100	100	130	130	Amb.
Pressure, psig	400	400	400	348	248	1000	350	146	142	100	100	Atm.
FLOWRATE, lb/h												
H_2O	710	2474	3184		117	36						168
Methanol				200	pp[j]							
Tar												
Oil												
Naphtha	2953	12722	15675	15675	pp							
Crude phenols					pp				16056			
Mercaptans[d]	2	4	6	<1	pp							
Thiophenes[d]	1	3	4	<1								
Ammonia	15	66	81	17								
HCN[d]	1	3	4									
Aromatic amines[d]	<1	2	3									
Nitrosamines[d]	<1	1	2									
PNA	pp	pp	pp		pp							
Fatty acids					pp					pp	pp	
$Ni(CO)_4$[f]	<1	<1	2	<1		<1						
Minerals												
Coal												25
Sulfur												310
Particulates												
Trace elements[g]	1	1	2	1	1							92
Others					185977[m]	8903[m]	8190[m]	1245[m]	124862[m]	25390[m]	7436[m]	5
Total liquid/solid flowrate, lb/h	3686	15277	18963	15696	186095	8940	8190	1245	140918	25390	7436	600
TOTAL STREAM FLOWRATE, lb/h	509687	1976108	2485795	973482	627641	315340	8190	1245	140918	25426	7454	762
Radioactivity[h]	0.1	0.1	0.1	0.05								2.6

Table B-1

Appendix B (Continued)

Component	Stream Number											
	25[k]	26[k]	27[l]	28	29	30	31	32	33	34	35	36
FLOWRATE, lb mol/h												
CO 28.01												
CO_2 44.01				62254								
H_2 2.02												
CH_4 16.04												
C_2H_4 28.05												
C_2H_6 30.07												
N_2 + Inerts 28.01		4		129696								
O_2 32.00		1		2227								
H_2S 34.08												
COS 60.07												
H_2O 18.02		1										
Others				19[m]								
Total gas flowrate, lb mol/h		6		194192								
Temperature, °F	Amb.	Amb.	60	100	Amb.	Amb.	60	70	70	180[c]	Amb.	Amb.
Pressure, psig	Atm.	Atm.	Atm.	Atm.	Atm.	Atm.	5	5	5	10[c]	Atm.	Atm.
FLOWRATE, lb/h												
H_2O	168		1030	497676	2413000	10000	1179700	878977		199486	25500	20000
Methanol												
Tar												
Oil												
Naphtha												
Crude phenols												
Mercaptans[d]												
Thiophenes[d]												
Ammonia												
HCN[n]												
Aromatic amines[o]			pp		pp							
Nitrosamines[e]			pp		pp							
PNA			pp		pp							
Fatty acids												
$Ni(CO)_4$[f]				2								
Minerals	25		2					4420	20950	96031		116989
Coal	310									7038		7038
Sulfur										66		66
Particulates	90	2		3							pp	
Trace elements[n]	4	<1	<1	2				50	200	940		1192
Others									2577[o]			2577[o]
Total liquid/solid flowrate, lb/h	597	3	1033	497683	2413000	10000	1179700	883447	23727	303561	25500	147802
TOTAL STREAM FLOWRATE, lb/h	597	165	1033	6942675	2413000	10000	1179700	883447	23727	303561	25500	147802
Radioactivity[h]	2.6			0.05					2.5	2.5		2.5

Table B-1

Appendix B (Continued)

Component		Stream Number									
		37	38	39	40	41	42	43	44	45	46
FLOWRATE, lb mol/h											
CO	28.01										
CO_2	44.01			< 1	< 1			2			2
H_2	2.02										
CH_4	16.04										
C_2H_4	28.05										
C_2H_6	30.07										
N_2 + Inerts	28.01			< 1	< 1						
O_2	32.00										
H_2S	34.08							< 1			< 1
COS	60.07										
H_2O	18.02										
Others											
Total gas flowrate, lb mol/h				2	2			3			3
Temperature, °F		70[a]	70[a]	393	393	170[a]	197[a]	160[a]	157	110	95
Pressure, psig		10[a]	10[a]	251	251	251	250	250[a]	100	80	50
FLOWRATE, lb/h											
H_2O		139579	878977	98623	982625	340413	216938	1992989	2347		1990642
Methanol				3188	31879	3603	835	36311	36311		
Tar				1344	13444	31221	7246	51911	2	51709	200
Oil				pp	pp	pp	pp	pp	pp	pp	pp
Naphtha				996	9959	4248	986	15193	pp		15191
Crude phenols				2	20	10	4	39	39	pp	pp
Mercaptans[d]				1	19	8	4	34	34	pp	pp
Thiophenes[d]				173	1734	6490	1507	9808			9808
Ammonia				pp	pp	3	1	4	pp	2	2
HCN[e]				pp	pp	1	< 1	2	pp	1	1
Aromatic amines[d]				pp	pp	1	< 1	2	pp	1	1
Nitrosamines				7	78	1	1	80	78	2	pp
PNA				177	1770	835	194	8268			8268
Fatty acids						3	1	5	1	1	
$Ni(CO)_4$											
Minerals		413	2600								
Coal											
Sulfur											
Particulates				410	4108			4108	4108		
Trace elements[g]		8	50	< 1	5			5	5		pp
Others											
Total liquid/solid flowrate, lb/h		140000	881627	104562	1045635	386837	227719	2118759	42925	51716	2024115
TOTAL STREAM FLOWRATE, lb/h		140000	881627	104634	1045707	386837	227719	2118881	42925	51716	2024237
Radioactivity[h]											

Table B-1
Appendix B (Continued)

Component	Stream Number										
	47	48	49	50	51	52	53[g]	54[g]	55	56	57
FLOWRATE, lb mol/h											
CO 28.01									134	134	
CO_2 44.01		2		2	314				33646	33646	
H_2 2.02									171	174	
CH_4 16.04										411	
C_2H_4 28.05									65	65	
C_2H_6 30.07									337	338	
N_2 + Inerts 28.01					11673				1	1	
O_2 32.00					2704				14		
H_2S 34.08		< 1		< 1	pp				157	2	
COS 60.07									2	2	
H_2O 18.02										14	
Others					2[p]						
Total gas flowrate, lb mol/h		3		3	14653				34527	34787	
Temperature, °F	266	95	95	130	Amb.	80[a]	70[a]	80[a]	95	95	58
Pressure, psig	330	157	300	50	Atm.	10[a]	100[a]	10[a]	12	6	390
FLOWRATE, lb/h											
H_2O	452	1990190	40	1990190	13981	1961947	27855	2813069	764	41992	2420
Methanol									463	463	
Tar											
Oil	200	pp		pp		pp	pp	pp			pp
Naphtha	pp	pp		pp		pp		pp			pp
Crude phenols	14606	587		587							
Mercaptans[d]	pp	pp		pp					pp		5
Thiophenes[d]	pp	pp		pp					pp		3
Ammonia		9808	8521	1287		pp					
HCN[e]	2	pp							4	4	60
Aromatic amines[d]	1	pp		pp		pp	pp	pp	pp		3
Nitrosamines[d]	1	pp		pp		pp	pp	pp	pp		2
PNA	pp	pp		pp		pp	pp	pp	pp		pp
Fatty acids		8268		pp		pp	pp	pp	pp		pp
$Ni(CO)_4$[f]									3	1	
Minerals							2100	500			
Coal											
Sulfur											
Particulates											
Trace elements[g]							45	5			
Others										61[m]	
Total liquid/solid flowrate, lb/h	15262	2008851	8561	2000292	13981	1961947	30000	2813574	1237	42523	2490
TOTAL STREAM FLOWRATE, lb/h	15262	2008975	8561	2000414	440296	1961947	30000	2813574	1507999	1546631	2494
Radioactivity[h]									0.05	0.05	

Table B-1 Appendix B (Concluded)

Component	Stream Number										
	58	59	60	61	62	63	64	65	66	67	68
FLOWRATE, lb mol/h											
CO 28.01						pp			< 1		< 1
CO_2 44.01						pp	< 1		2360	2	1635
H_2 2.02							2		30		3
CH_4 16.04							5		54		4[l]
C_2H_6 28.05							1		< 1		< 1
C_3H_8 30.07									2		1
N_2 + inerts 28.01									5235		< 1
O_2 32.00									177		
H_2S 34.08						pp	2		< 1		
COS 60.07						pp					
H_2O 18.02											
Others							1[m]	125	1351 < 1[m]	< 1	< 1[m]
Total gas flowrate, lb mol/h							12	125	9215	3	1691
Temperature, °F	130	100	100	Amb.	Amb.	Amb.	100	212	600	200	95
Pressure, psig	100	220	100	Atm.	Atm.	Atm.	12	Atm.	8	Atm.	8
FLOWRATE, lb/h											
H_2O	450593	450593		762							1810
Methanol		374									
Tar											
Oil	pp	pp									
Naphtha	pp	pp									
Crude phenols	pp	pp									
Mercaptans[d]											
Thiophenes[d]											
Ammonia	17	17									
HCN[d]											
Aromatic amines[d]	pp	pp									
Nitrosamines[d]	pp	pp									
PNA	pp	pp									
Fatty acids	pp	pp									
$Ni(CO)_4$[d]											
Minerals											
Coal											
Sulfur											
Particulates											
Trace elements											
Others	5469[m]	26703[m]	21234[m]	6854[g]	2480[g]	2480[g]					
Total liquid/solid flowrate, lb/h	456079	477687	21234	7616	2480	2482					
TOTAL STREAM FLOWRATE, lb/h	456079	477687	21234	7616	2480	2482	286	2253	281652	106	74699
Radioactivity[h]											

Table B-2

Appendix B: Detailed breakdown of liquid hydrocarbons

Component		Stream Numbers[a] 17	18	19	20	21	22	23	56	58	60	64	66	68
FLOWRATE, lb mol/h														
C_2H_6	30.07			1.06										
C_3H_6	42.08	745.30	189.49	17.71									0.50	0.50
C_3H_8	44.09	124.45	18.25	168.12										
i C_4H_8	56.10	400.30	0.24		1.55	4.68			0.18			0.18	0.07	0.05
1 C_4H_8	56.10													
i C_4H_{10}	58.12	2.60	0.06			1.32								
n C_4H_{10}	58.12	49.33	0.03		19.93	89.05			0.83			0.83		
i C_5H_{10}	70.13	231.27	0.04			7.55								
1 C_5H_{10}	70.13													
i C_5H_{12}	72.15	9.90				305.63								
n C_5H_{12}	72.15	29.71	0.01			55.53	0.02		0.07			0.07	0.14	
1 C_6H_{12}	84.16	152.51	0.01											
i C_6H_{12}	84.16					173.67								
i C_6H_{14}	86.17	11.17	0.01			30.72	0.02							
n C_6H_{14}	86.17	26.08	0.01				0.05							
C_n[b]														
C_7^+[b]		587.88	0.65				129.70	22.81						
Alkylate	102.51					332.07								
Cat. poly gasoline	118.15					350.88								
Acids	63.24									86.48				
Ethanol	46.07										254.61			
Heavy alcohols	64.69										146.92			
Total, lb mol/h		2370.45	208.80	186.89	21.48	1351.10	129.79	22.81	1.08	86.48	401.53	1.08	0.71	0.55
Total, lb/h		185977	8901	8190	1245	124862	25390	7436	61	5469	21234	61	34	23
C_7^+ mol. wt.		150.6	153.24				195.70	326.00						

[a] Stream numbers indicated correspond to stream numbers in Figure 1.

[b] See below for component molecular weight.

APPENDIX C

EPA SOURCE ANALYSIS MODEL I (SAM/I)*

The SAM/I model has been designed for intermediate screening purposes to evaluate chemical analysis data. To address these objectives, the model includes elementary treatment of pollutant dispersion or dilution to post-dilution levels, but does not incorporate post-dilution chemical reaction or transformation.

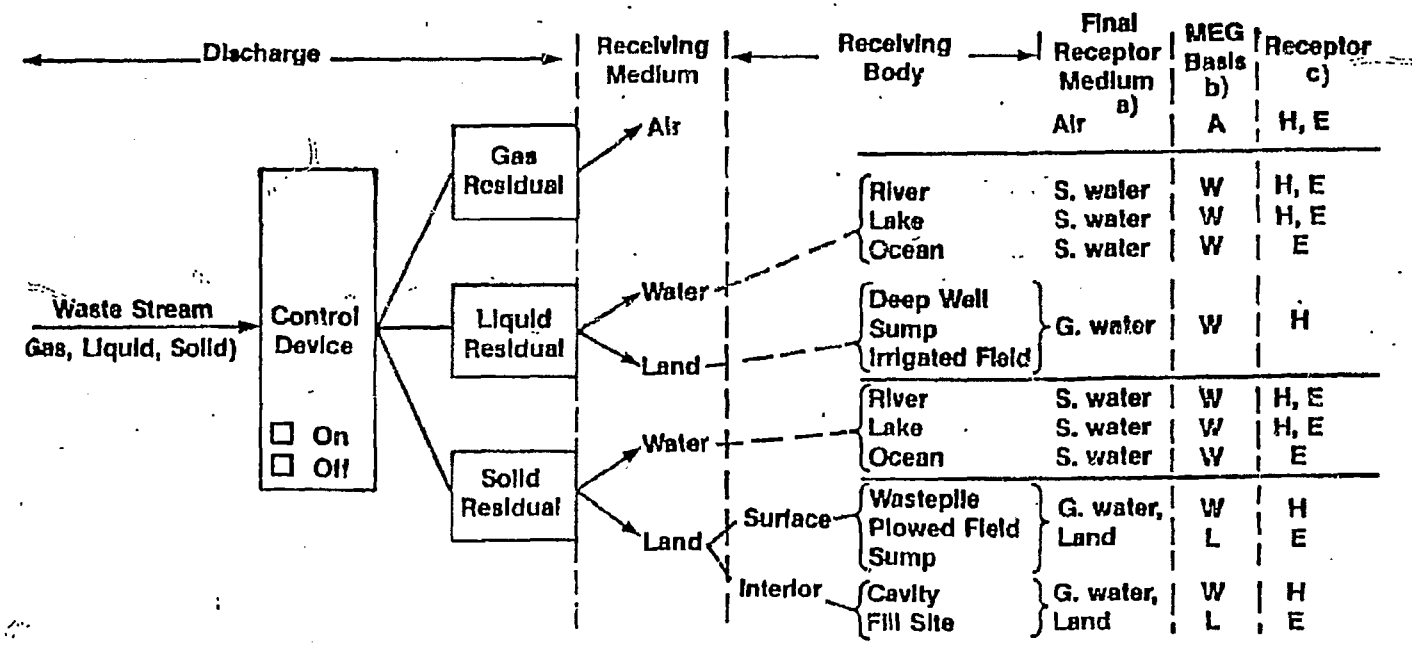
To obtain the estimated maximum post-dilution concentration of a pollutant because of the discharge stream, SAM/I employs approximate dispersion models to account for the dilution of a discharge concentration to a post-dilution concentration. Models have been developed for gaseous, liquid, and solid discharges into appropriate receiving bodies within air, water, and land media. Figure C-1 illustrates the discharge stream/receiving body combinations treated. The figure shows that any given gaseous, liquid, or solid waste stream from a source can be discharged in a number of ways to air, water, or land-receiving media.

Similarly, liquid and solid streams can be discharged to deep well, sump (or waste pond), irrigated field, wastepile, plowed field, cavity, or fill site-receiving bodies in the land medium. The underlying physical picture for all the SAM/I dispersion models is that of a discharge stream entering an entraining post-dilution flow. After mixing takes place, the pollutant stream dispersion, or dilution factor can be approximated by the ratio of the entraining stream volumetric flow rate** to the discharge stream flow rate. SAM/I defines a discharge stream dilution factor, K, in just such a manner:

$$K = \frac{\text{Entraining stream volumetric flow rate}}{\text{Discharge stream volumetric flow rate}}$$

*Information in this Appendix is excepted from reference 112.

**Entraining stream volumetric flow rate includes the discharge stream volumetric flow rate, i.e. it is the total volumetric flow rate of the two streams after they are mixed.



a) S. water: Surface water, G. water: Ground water
b) A: Air, W: Water, L: Land
c) H: Health, E: Ecological

Figure C-1 SAM/I pollutant discharge overview.

Therefore, the estimated maximum* post-dilution concentration for a pollutant species is the ratio of the discharge concentration to the dilution factor.

Dilution factors have been defined for all the receiving bodies shown in Figure C-1. In the dispersion models used to calculate these dilution factors, entraining flow characteristics and certain discharge stream characteristics have been internally parameterized based on estimates of nationwide averages of these characteristics. Thus, only discharge stream flow rate remains a model variable. Further, several model discharge stream flow rates have been defined, spanning discharge flow rate range of interest. Typical dilution factors have been assigned to each of these model streams. Therefore, the SAM/I user need only know the discharge rate of the stream under evaluation, and receiving body discharges into, to perform SAM/I calculations.

As an example, for gaseous effluent streams discharges into the atmosphere, a Gaussian plume dispersion model was used to predict maximum ground level pollutant concentrations. Here, the entraining flow is the atmosphere. The entraining flow characteristics, atmospheric stability, and wind speed are given values within the model typical of nationwide average conditions. Further, discharge stream stack height is internally parameterized by relating average stack height to average source flow rate (e.g., large utility power plants, sources with flue gas discharge rates in the Mg/s range have stack heights around 200m, whereas small commercial or industrial boilers, with flue gas flow rates in the kg/s range have about 10 m stacks). Thus, for SAM/I evaluations a user need only know discharge flow rate to be able to assign an approximate dilution factor.

The defined SAM/I dilution factors, as a function of effluent stream discharge rate, for the various effluent stream/receiving bodies is summarized in Table C-1. Details of the models used to assign these dilution factors are reported elsewhere.

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*Maximum under worst probable conditions; it does not consider extreme worst conditions.

Table 33 - Flowrates of Trace Elements in Stream 36

Trace Element	Q_{TE-A}* (lb/hr)	+ Q_{TE-S}** (lb/hr)	+ Q_{TE-34}† (lb/hr)	− [(C_{TE-38})††	(F_{38})§	] = Q_{TE-36} (lb/hr)
				(ppm)	(MM lb/hr)	
As	.183-.385	.0015-.0031	.2099-.4419	.02	.882	.377-.812
Be	.373-.421	.0026-.0030	.3210-.3617	ND	.882	<.697-.786
Cd	.094-.242	.0009-.0025	.2203-.5684	.00064	.882	.315-.812
F	5.424-5.590	11.157-11.500	50.10-51.64	ND	.882	<66.68-68.73
Hg	.0074-.0114	.0000-.0001	.0782-.1208	.0003	.882	.085-.132
Pb	.180-4.240	.0015-.0343	.6577-15.48	.09	.882	.760-19.67
B	ND§§	ND	39.43	ND	.882	>39.4
Ni	ND	ND	2.313-19.05	.035	.882	>19.02
V	ND	ND	13.676-19.147	ND	.882	>19.147

*From Table 28
**From Table 29
†From Table 31
††These data are first column volume leachate fractions of Montana Rosebud subbituminous ash from the Lurgi gasifier in Westfield, Scotland. Montana Rosebud coal has a trace element composition very similar to the trace element composition of Wyoming subbituminous. These data were published in Shriner et al., July 1979. It was assumed that the concentrations of trace elements in the sluice water would be the same as the concentrations of trace elements in the first column volume leachate.
§ Appendix B, Stream 38.
§§ No Data

TABLE C-1

SUMMARY OF MODEL STREAM DISCHARGE RATES AND DILUTION FACTORS

Discharge Stream Type	Gas		Liquid/Soluble Solid			
Receiving Body	Air		River/Lake		Ocean	
Discharge Rate Q (g/s) and Dilution Factor K	Q	K	Q	K	Q	K
	2.5×10^6 6.5×10^5 1.3×10^5 6.8×10^3 5.4×10^2	1×10^2 3×10^2 1×10^3 5×10^3 2×10^4	1×10^5 1×10^4 1×10^3 1×10^2 1×10^1	1.6×10^2 1.6×10^3 1.6×10^4 1.6×10^5 1.6×10^6	3×10^4 (Barge)	1×10^3

Discharge Stream Type	Liquid		Liquid/Soluble Solid				Leached Solid	
Receiving Body	Deep Well		Irrigated Field		Sump, Waste Pile, Plowed Field, Cavity, Fill Site		Any Land Body	
Discharge Rate Q (g/s) and Dilution Factor K	Q	K	Q	K	Q	K	Q	K
	Any	1	Any	100	Any	10^{*} 100^{**}	Any	1

* Large receiving body with base diameter d ≥ 10m.

** Large receiving body with base diameter d < 10m.