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SAMPLING AND ANALYTICAL STRATEGIES FOR COMPOUNDS IN PETROLEUM REFINERY STREAMS

Volume II



**Industrial Environmental Research Laboratory
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Research Triangle Park, North Carolina 27711**

**SAMPLING AND ANALYTICAL STRATEGIES
FOR COMPOUNDS IN
PETROLEUM REFINERY STREAMS**

Volume II. Process Analysis of Petroleum Refinery Streams

by

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APPENDIX B
PROCESS ANALYSIS OF PETROLEUM
REFINERY STREAMS

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1.0 INTRODUCTION

The objective of this analysis is to determine from available literature and through engineering analysis the potentially hazardous components in five selected effluents from a typical refinery. These stream characterizations are then to be used in developing a comprehensive sampling and analytical strategy for specific hazardous components in these streams.

The streams were selected as typical major contributors to the total refinery emissions. They are representative of the different types of refinery effluents that might be encountered. The following are the five streams studied:

- fugitive atmospheric emissions from atmospheric crude distillation,
- aqueous condensate from the atmospheric crude still,
- effluent water from the API separator,
- tail gas from the sulfur recovery unit, and
- atmospheric emissions from the fluid catalytic cracking regenerator.

Methodology

As a starting point, a literature survey is made to determine as completely as possible: (1) all known components in the selected refinery streams and (2) available toxicity data

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for the components. The result of this work is given in Table A and B of this appendix. The toxicity data given in Table A is by no means an exhaustive collection of available toxicity data, nor for data on mutagenicity, teragenicity, and tumorigenicity. Section 5.3 lists additional references which can be used to develop a much more complete base for describing the biological effects of the various refinery effluent stream components. The information given in Table A, however, is believed to be adequate for the scope of this report as a starting point in describing the toxicity of the components.

Next, each of the selected refinery streams are examined for processing characteristics which can be used later to determine the fate of components in the effluent streams. These characteristics include operating conditions, type of equipment used, and identification of the feed stream sources.

With the data given in Table B and from the processing characteristics, the compositions of the selected refinery streams are estimated. Where specific information concerning the fate of certain components is not available, engineering judgement is applied. In all cases, both stream compositions and process conditions are considered before making final estimates of effluent compositions. The complete list of components is compared to the compounds given in Table A to determine which are potentially hazardous. The result of the comparison is a final list of potentially hazardous pollutants within each stream. In addition to the list, the process conditions at each point of sampling are specified as an aid for planning the sampling procedures.

The lists of hazardous components derived from the process analysis are used in several ways. First, they are used in the development of the sampling and analytical strategy.

This strategy includes specification of sampling techniques, sample preservation methods, sample preparation and separation methods, analytical equipment, laboratory test procedures, and data interpretation. Costs for the sampling and analytical program are estimated to determine whether it is a cost effective approach.

Another important use of the data from the process analysis will be in preparation for the actual field tests. The lists of hazardous pollutants will be used as guidelines for determining the components for which analyses will be required and the number of individual tests required. This information will lead to a more accurate estimate of the total cost of the field tests.

Fugitive Emission Analysis

The approach suggested in this report for describing the fugitive emissions from the atmospheric still is unique. The method assumes fugitive losses from the distillation unit can be simulated by analyzing product streams from the column and by defining emission rates at points where emission losses occur. Ambient temperature at the emission location and the vapor pressures of the components at ambient conditions are also factors considered in characterizing fugitive emissions. The result is a simulated source emission of fugitive losses.

This method is presented as an alternative to various atmospheric monitoring methods. It provides a means of identifying potentially hazardous emissions at their sources, where sampling and analysis are simpler. It is also less costly than are the direct fugitive emission sampling methods. Details of this development are given in Section 3.0.

Crude Oil Analysis

Complete and well-documented stream analyses for crude oil are available from the literature. This information, used in conjunction with engineering assessment and process examination, is useful in predicting the components in the many refinery streams. A discussion of crude oil composition is presented in Section 4.0 and also in Table B.

2.0 CHARACTERIZATION OF SELECTED REFINERY STREAMS

This section begins by describing the process analysis used in defining a typical complete refinery. The process flows were all based on average flows in domestic refineries. Following the definition of the entire refinery, characterizations of the five refinery streams selected for this study are given. These characterizations include descriptions of the processes from which the selected effluent streams are derived and identification of hazardous components which are known to be present or suspected of being present in the effluent streams. The compounds which have been identified as potentially hazardous are given in Section 5.0 of this appendix.

The process descriptions consist of a listing of operating conditions, a process flow scheme, a listing of sampling conditions and stream compositions. Descriptions of the methods used to ascertain the presence of hazardous materials in each of the five effluent streams are also presented. The concentrations and toxicity data of the hazardous components in the selected streams are given wherever possible.

2.1 Refinery Flow Sheet

The first step in the process analysis is to define a representative refinery from which refinery stream samples might be obtained for analysis. A flow sheet based on this refinery serves as a reference in identifying hazardous components in individual refinery streams. Process units and capacities in such a refinery are similar to those found in medium to large size refineries in the United States today. Therefore, a sample team could expect to enter most domestic refineries and obtain samples similar to those described in this report. The following basic assumptions were used in developing the refinery flow sheet:

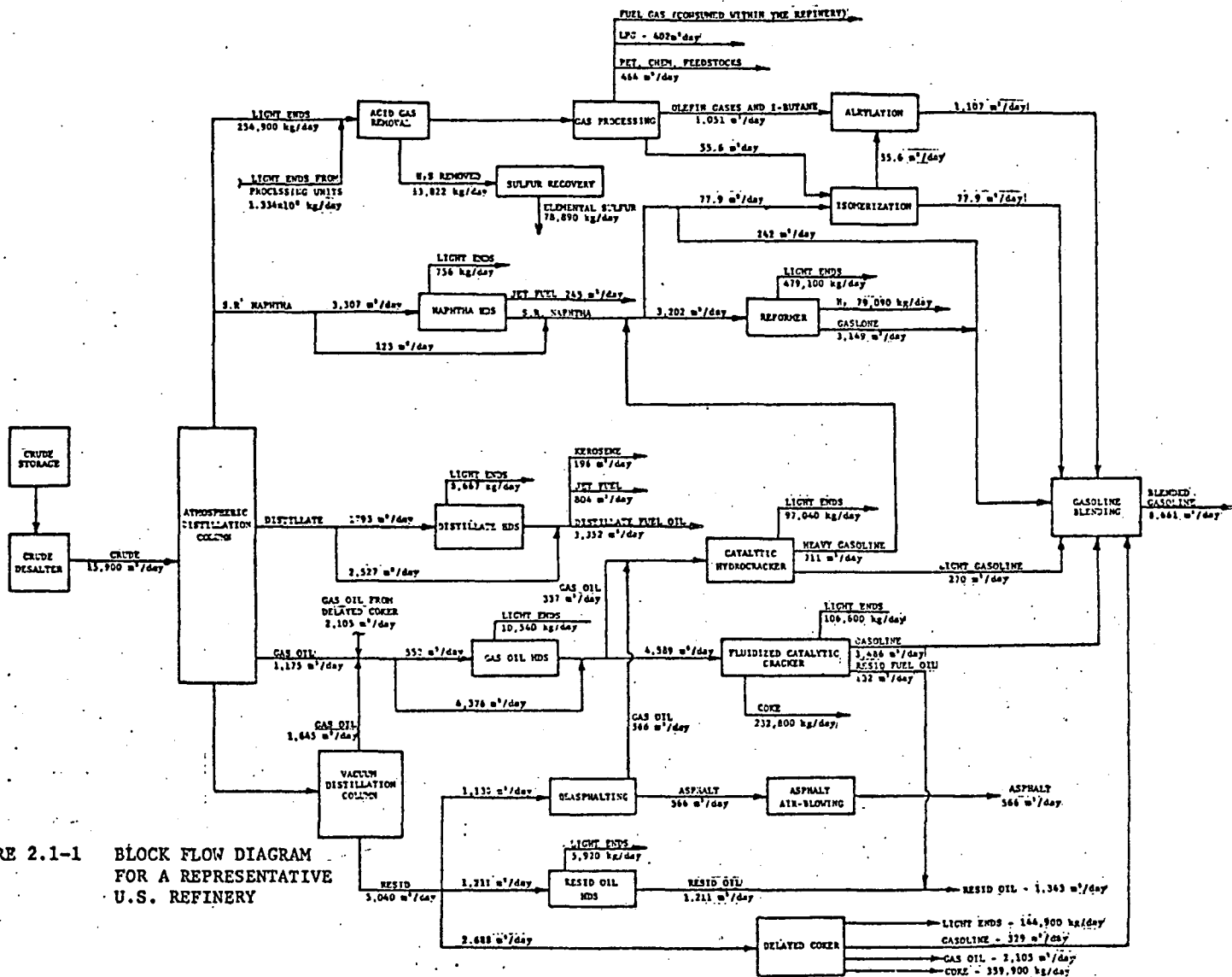
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- the refinery is located in the continental United States,
- the refinery processes 15,900 m³/day (100,000 bbl/day) of crude (this is a convenient rate for scaling process flows and capacities to actual refineries which might be selected for sampling),
- the process unit capacities are consistent with actual capacities in the United States in 1974,
- the process units selected are those in most common use in the industry today, and
- the refinery product slate represents the national average product slate for the refining industry in 1974.

To satisfy the above assumptions, the amount of crude processed during 1974 (US-209), the refinery product yields during 1974 (US-209), and the capacities of major processing units for 1974 (CA-236) are used to describe the representative refinery. Using this information, a refinery flow sheet has been prepared showing the major process equipment, major refinery stream flow rates, and the refinery products all as functions of current information about U.S. refinery operations. A block flow diagram for the representative refinery is presented in Figure 2.1-1.

The representative refinery includes the following major processing operations: crude and vacuum distillation; crude desalting; wastewater treatment (API separator); sour water

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stripping; acid gas removal; sulfur recovery; hydrodesulfurization units for naphtha, distillate, gas oil and residual oils. Other facilities included are gas processing; isomerization; alkylation; reforming; hydrocracking; fluid catalytic cracking; deasphalting; asphalt blowing; delayed coking; and associated storage and blending operations.

The representative refinery product slate is compared with the U.S. total refinery product slate with each product as a volume percent of the total refinery products in Table 2.1-1. In Table 2.1-2, the representative refinery process unit capacities are also compared with average process unit capacities in U.S. refineries.

The trend in modern refineries is toward increased hydrodesulfurization because of: (1) environmental protection laws limiting the sulfur levels in fuels; (2) reduction in the availability of low sulfur crudes; and (3) the undesirable properties of sulfur compounds including corrosiveness, odor, instability, and catalyst poisoning tendencies. This flow scheme, however, uses hydrodesulfurization only to the extent it is currently practiced in domestic refineries, which is somewhat less than might be expected in future operations. From information on performance of process units, the sulfur removal efficiencies in various HDS and cracking operations were estimated.

The fate of hazardous materials contributing to the five selected process streams can be determined using the representative process flow scheme. Using the estimated compositions and the specified flow rates, the relative environmental impacts of the five selected effluents can be approximated. In Section 2.2, each of the five streams is examined in this manner.

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TABLE 2.1-1
COMPARISON OF "REPRESENTATIVE" REFINERY PRODUCT
SLATE WITH TOTAL ACTUAL U.S. PRODUCTION

Product	Volume Percent of Total Refinery Products	
	Representative Refinery Production	*Total U.S. Production
Gasoline	50.3	49.0
Kerosine	1.2	1.2
Jet Fuel,		
Naphtha type	1.5	1.5
Kerosine type	5.0	4.9
Distillate Fuel Oil	20.4	20.4
Asphalt	3.4	3.4
Residual Fuel Oil	8.2	8.2
Marketable Coke	1.4	1.3
LPG	2.4	2.4
Petrochemical Feedstocks	2.8	2.8
Other (Fuels, misc.)	<u>3.4</u>	<u>4.9</u>
	100.0	100.0

*Source: (US-209)

TABLE 2.1-2
REFINERY PROCESS UNIT CAPACITIES
"REPRESENTATIVE" COMPARED TO AVERAGE OF U.S. REFINERIES

<u>Unit</u>	<u>Volume Percent of Crude Feedstock</u>	
	<u>Representative Refinery</u>	<u>*Average of U.S. Refineries</u>
Reformer	24.6	27.3
Fluid Cat Cracker	28.9	33.9
Hydrocracker	5.6	6.9
Coking	1.4	1.7
Asphalt	3.6	5.4
Isomerization	0.8	1.0
Alkylation	5.6	6.8
Naphtha HDS	20.8	25.2
Distillate HDS	11.3	13.7
Gas Oil HDS	3.5	4.2
Resid. Oil HDS	0.04	.05

*Source: (CA-236)

2.2 Selected Refinery Streams

This section contains descriptions of the processes from which the five selected effluent streams are derived. The manner in which materials are separated, transformed, heated, combusted, and otherwise treated in each process is discussed. The ultimate effects of these treatments with regard to the fate of potentially hazardous effluents are considered. Finally, a characterization of the selected refinery effluent streams is made with respect to hazardous compounds which are known or suspected to be present.

2.2.1 Fugitive Atmospheric Emissions From Atmospheric Crude Distillation

Process Analysis

Atmospheric crude distillation is the initial major processing step in refinery operations. The process involves the separation of hydrocarbon components of the crude petroleum into fractions of specified boiling point ranges. The type of separation made is largely governed by the crude petroleum characteristics and the products required (VA-064).

The representative refinery product slate was discussed in Section 2.1. The crude oil used in the representative refinery is a composite of crudes from the major oil fields currently supplying crudes to domestic refineries. The explanation of how the crude oil characteristics were chosen is given in Section 4.0.

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Based on the desired product slate and the representative crude processed, the fractions produced in the atmospheric crude distillation unit were determined. These fractions and their boiling ranges are presented in Table 2.2-1.

TABLE 2.2-1
TYPICAL ATMOSPHERIC CRUDE TOWER FRACTIONS
AND BOILING RANGES

<u>Fraction</u>	<u>Boiling Range</u>
Light Ends	<40°C
Naphtha	40°C - 177°C
Distillate	177°C - 304°C
Gas Oil	304°C - 402°C
Topped Crude	>402°C

Atmospheric crude distillation is usually accomplished in one fractionation stage. The raw crude is desalted and then heated in a direct-fired furnace to approximately 340°- 370°C before being fed to the fractionation unit (WA-074).

The fugitive atmospheric emissions from the atmospheric crude distillation unit are of interest since all of the hazardous components in crude petroleum are potential atmospheric emissions at the crude tower. Also, since the general housekeeping at these units is not always good, the quantity of the fugitive emissions from this source can be significant.

The potential fugitive emissions at the atmospheric distillation unit exist at many points in the unit. The major sources of fugitive emissions are expected to include leaks from the following types of equipment:

- valve stems (i.e., control valves, block valves, and other valves in the unit),
- pump seals,
- drain vent and sample valves,
- relief valves and blowdown systems,
- gas compressor seals, and
- flanges and fittings.

The location of these fugitive emissions sources and suggested sampling points are illustrated in Figure 2.2-1 for a typical atmospheric crude still.

Definition of Fugitive Emissions Basis

Potentially hazardous components in fugitive emissions from the atmospheric distillation unit are characterized by the components originally present in the crude oil feedstock. Therefore, an essential input for definition of such emissions from the atmospheric still, and from other downstream process units as well, involves inspection of the crude oil. The crude oil composition is defined in Section 4.0 and in Table B of this appendix. The determination of the hazardous components is discussed in Section 5.0.

Fugitive emissions are defined in this study as a composite of all fugitive emission sources at the crude tower. It was assumed that these emissions could be simulated by compositing selected process streams in and around the tower. The process streams examined are: light ends, naphtha, distillate, gas oil, and topped crude.

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The major sources of fugitive emissions, such as valves, pump seals, and compressor seals are indicated on this flow sheet.

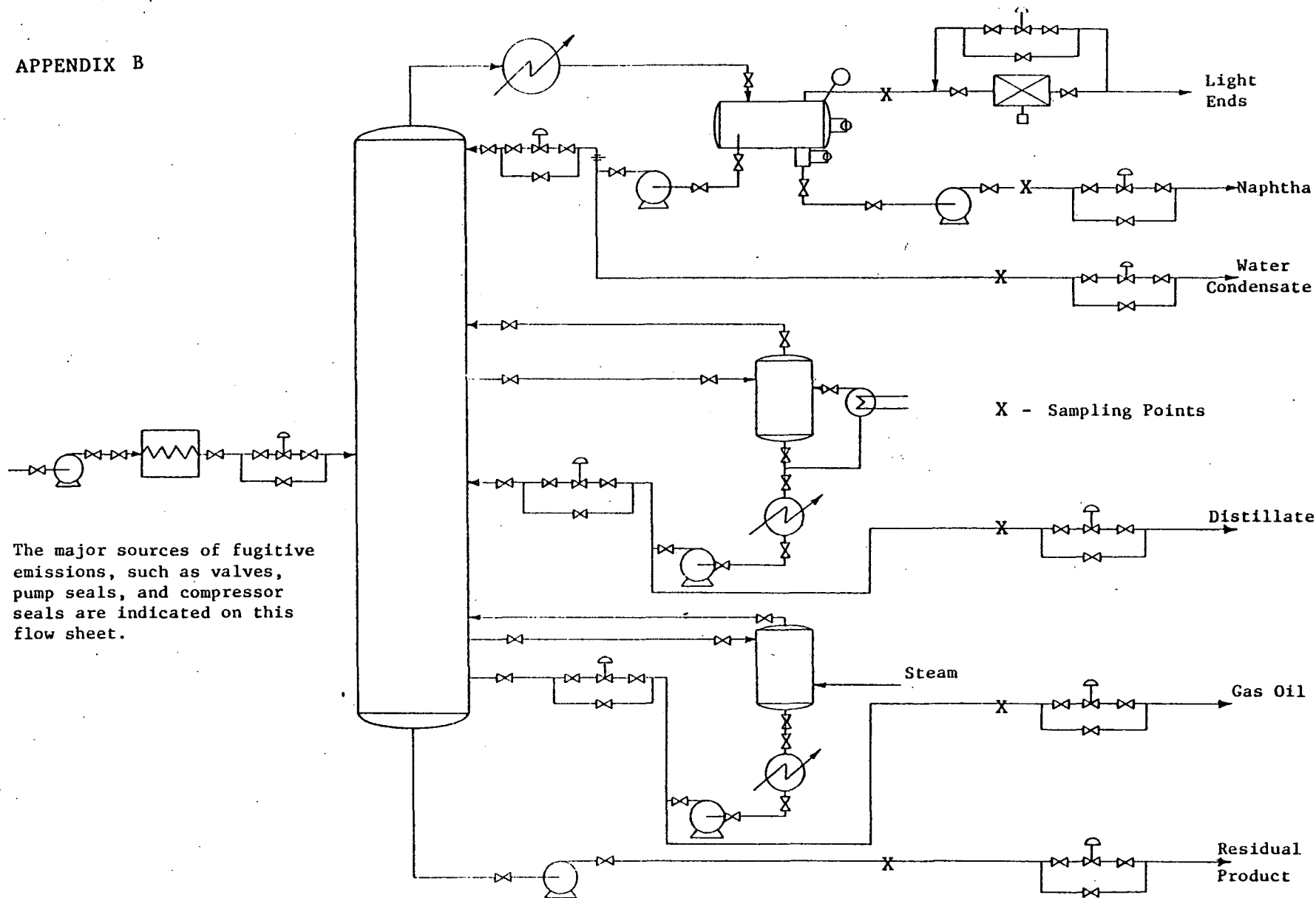


FIGURE 2.2-1 ATMOSPHERIC CRUDE TOWER FUGITIVE EMISSION SOURCES

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There are many factors affecting the amount of emissions from the crude unit that actually become fugitive emissions. Some of these factors are:

- the ambient temperature at the location of the emission,
- the utilization of an adequate organic recovery system for leaks, and
- the vapor pressure effects of hazardous components at ambient conditions.

Crude oil components with boiling points greater than 260°C were not considered to be among the fugitive emissions. Inspection of the component list indicates that the higher boiling hazardous materials will not be present in fugitive emissions above their TLV concentrations at ambient conditions, even before atmospheric dilution. Potentially hazardous components in this group were therefore removed from the list. All carcinogens regardless of boiling points were, however, included on the list.

Base case conditions for fugitive emissions were set considering vapor pressure effects at ambient temperatures in excess of 90°F. All fugitive emissions with adequate vapor pressures were considered to be converted to atmospheric emissions; in other words, collection and removal of liquid drips and spills in an organic liquid recovery system was not assumed to be utilized in reducing fugitive losses.

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The fugitive emission sources are shown on Figure 2.2-1 for a typical atmospheric crude still. Pumps, major valves and piping and the major streams are identified on the figure. Fugitive emissions have been quantified by applying published mass emission factors to each potential fugitive emission source (DA-069). The emission factors and rates are presented in Table 2.2-2 for each stream at the atmospheric tower and for the total tower emissions.

Emission factors were not available for flanges and fittings. Also, no attempt was made to estimate the number and location of vent, sample, and drain valves, nor were emissions from blowdowns, turnarounds, and maintenance estimated. For these reasons, fugitive emissions calculated from sources shown on the schematic flow sheet will tend to be conservative. To compensate for these emissions, the calculated emission rate was scaled up by a factor of three to give a total fugitive emission rate of approximately 86 kg/day for a 15,900 m³/day refinery.

TABLE 2.2-2
FUGITIVE EMISSION FACTORS AND RATES
FOR THE ATMOSPHERIC CRUDE TOWER

<u>Source</u>	<u>Emission Factor</u> <u>kg/day/valve or seal</u>	<u>Emission Rates</u> <u>kg/day</u>
4 Hand Valves (Gas)	0.222	0.888
66 Hand Valves (Liquid)	0.049	3.234
7 Pump Seals	1.915	13.405
7 Relief Valves	1.596	11.172
	TOTAL	28.699

Selected product streams from the atmospheric tower (light ends, naphtha, distillate, gas oil, and the topped crude) were characterized as to temperatures and pressures at sampling point and by major component categories. They were also characterized

as to the concentrations and TLV's of components known to be present in concentrations considered hazardous. This information is listed in Tables 2.2-3A through 2.2-3E.

The worst case of exposure to hazardous materials assumes no ambient air dilution. This case could be represented by an operator working directly over a leaking pump or a purged vessel in the immediate area. Table 2.2-3 includes potentially hazardous compounds which may have concentrations lower than TLV concentrations, but which under special circumstances may reach hazardous levels.

In crude distillation, separations are seldom so sharp that a particular component will exist entirely in one stream. Instead, a component will be distributed among several product streams. However, components tend to concentrate in products with boiling ranges closest to the component boiling point. For this study, it was assumed for simplification that each component will be found only in the particular product stream whose boiling range includes the boiling point of the component.

The information on trace elements is limited. Most trace element analyses in the literature did not attempt to determine the form in which the elements were found. Trace elements could conceivably exist either in the elemental form or as organics or organometallic (such as porphyrin) compounds. In addition, the TLV information on metals is often for the elemental form in a particular physical state, such as dust or fumes. For this reason all trace elements that have a hazardous rating are listed as potentially hazardous regardless of their physical form. TLV's for trace elements are not reported in selected streams since specific data as to the form of the compounds are not given in the literature.

TABLE 2.2-3A
FUGITIVE LIGHT ENDS EMISSIONS
FROM ATMOSPHERIC DISTILLATION COLUMN

A. Major Components (Non-Pollutants)

<u>Component</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
Methane	0.2	10,000	RO-188
Isobutane	31.0	-	WA-074

B. Known to be hazardous and known to be present

<u>Compound</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
n-Butane	48.6	500	WA-074
Propane	19.6	500	WA-074
Ethane	1.5	500	WA-074
H ₂ S	1.0	10	PE-140, HA-316
HCl	0.7	5	PE-140
Methanethiol	0.2	0.5	BE-147, GR-123

C. Potentially hazardous if present

<u>Compound</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
Ammonia		25	ME-107, KL-032

D. Sampling Conditions

Temperature - 30°C

Pressure - 2.44-3.14 kg/cm² (20-30 psig)

TABLE 2.2-3B
FUGITIVE NAPHTHA EMISSIONS FROM
ATMOSPHERIC DISTILLATION COLUMN

A. Major Components

<u>Components</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
C ₅ to C ₁₀ Paraffins	40.0		GR-123
C ₅ to C ₁₀ Cyclo- paraffins	40.0		GR-123
Aromatics	20.0		GR-123

B. Known to be hazardous and known to be present

<u>Compound</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
C ₅ to C ₈ n-Alkanes	16.9-25.7	100-600	RO-189, CA-227
Cyclopentane	0.14-1.3	-1	RO-189
Cyclohexane	1.83-10.7	300	RO-189
Methylcyclo- hexane	0.35-17.5	400	RO-188, RO-189
Benzene	0.2 -1.23	10	CA-227, RO-189
Toluene	1.0 -7.4	100	CA-227, RO-189
Xylenes	3.51-9.92	100	RO-189
Ethylbenzene	0.19-0.93	100	RO-188, RO-189
Isopropyl- benzene	0.12-0.33	50	RO-189
1,2,3-Trimethyl- benzene	0.56	25	RO-188
1,3,5-Trimethyl- benzene	0.32-1.34	35	RO-189
Ethanethiol	0.03	0.5	GR-123
2-Butanethiol	0.02	0.5	GR-123
Mercaptans	~0.10	-2	GR-123

C. Potentially hazardous if present

<u>Compound</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
C ₁ to C ₄ Alka- noic Acids		5-10	LO-112
Cyclohexane		300	RO-189
2,2,4-Trimethyl- pentane		-1	RO-189
Pyridine		5	PE-140
Alkyl Pyridines		-3	BA-325
Pyrrole		-1	PE-140

TABLE 2.2-3B - FUGITIVE NAPHTHA EMISSIONS FROM ATMOSPHERIC DISTILLATION COLUMN (Cont.)

D. Potentially hazardous trace elements

<u>Element</u>	<u>Concentration⁴ ($\mu\text{g}/\text{ml}$)</u>	<u>TLV⁵ (ppm)</u>	<u>Reference</u>
Antimony	0.005-<0.5	-	VO-027
Arsenic	<1.0-<10.0	-	VO-027
Cadmium	0.009-<0.028	-	VO-027
Chromium	<0.1-<0.5	-	VO-027
Copper	0.096-4.0	-	VO-027
Lead	-	-	VO-027
Magnesium	0.5-250	-	VO-027
Mercury	0.01-0.1	-	VO-027
Nickel	<0.5	-	VO-027
Phosphorus	15	-	VO-027
Selenium	<0.07-<0.1	-	VO-027
Vanadium	0.035-<10	-	VO-027

E. Sampling Conditions

Temperature - 30°C

Pressure - 3.14-5.25 kg/cm² (30-60 psig)

1. Rated as moderately toxic (SA-175).
2. All mercaptans are considered toxic.
3. No TLV data, but assumed as hazardous as pyridine.
4. Reported concentrations for low lead blended gasoline.
5. Refer to Table A, Appendix B, for toxicity data concerning trace elements.

TABLE 2.2-3C
FUGITIVE DISTILLATE EMISSIONS FROM
ATMOSPHERIC DISTILLATION COLUMN

A. Major Components

Components	Vol. %	TLV (ppm)	Reference
C ₁₁ to C ₁₅ Paraffins	40.0		GR-123
C ₁₁ to C ₁₅ Cycloparaffins	45.0		GR-123
C ₁₁ to C ₁₅ Aromatics	15.0		GR-123

B. Known to be hazardous and known to be present

Compound	Vol. %	TLV (ppm)	Reference
1,2,3-Trimethyl- benzene	.44	25	RO-188
1,2,3,4-Tetrahydro- naphthalene	.11	25	RO-189
Naphthalene	.06	10	RO-188

C. Potentially hazardous if present

Compound	Vol. %	TLV (ppm)	Reference
1-Methyl-4-iso- propylbenzene		50	NA-231
2-Methylnaphtha- lene		-1	RO-188
Indoles		carcinogens	PE-140
Phenol		5	BE-147
Cresols		5	FI-083
Naphthol		-2	LO-112
Biphenyl		0,2	RO-188
Quinoline		-3	BA-325
Alkyl Quino- lines		-4	BA-325
Alkyl Pyridines		-5	BA-325
Octanethiol		-3	GR-123

D. Potentially hazardous trace elements

Element	Concentration (µg/ml)	TLV (ppm) ⁶	Reference
Antimony	0.7		VO-027
Arsenic	0.0545		AN-104
Cadmium	<0.015		AN-104
Chromium	0.045		AN-104
Cobalt	0.33		AN-104

TABLE 2.2-3C - FUGITIVE DISTILLATE EMISSIONS FROM ATMOSPHERIC DISTILLATION COLUMN (Cont.)D. Potentially hazardous trace elements (Cont.)

<u>Element</u>	<u>Concentration</u> <u>($\mu\text{g/ml}$)</u>	<u>TLV (ppm)</u> ⁶	<u>Reference</u>
Copper	0.25		AN-104
Iron	4.96		AN-104
Lead	0.88		AN-104
Manganese	0.08		AN-104
Molybdenum	0.155		AN-104
Nickel	16.1		AN-104
Silver	0.0023		AN-104
Vanadium	49.0		AN-104

E. Sampling Conditions

Temperature - 57°C

Pressure - 3.14-5.25 kg/cm² (30-60 psig)

-
1. Limited experiments suggest high toxicity.
 2. Rated as moderately toxic (SA-175).
 3. Rated as severely toxic (SA-175).
 4. Assumed similar in toxicity to quinoline.
 5. Some alkyl pyridines have been described as highly toxic.
 6. Refer to Table A, Appendix B, for toxicity data concerning trace elements.

TABLE 2.2-3D
FUGITIVE GAS OIL EMISSIONS FROM
ATMOSPHERIC DISTILLATION COLUMN

A. Major Components

<u>Components</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
C ₁₅ to C ₂₅ Paraffins	30.0		GR-123
C ₁₅ to C ₂₅ Cyclo- paraffins	50.0		GR-123
C ₁₅ to C ₂₅ Aromatics	20.0		GR-123

B. Known to be hazardous and known to be present

<u>Compound</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
Phenanthrenes	-1	carcinogens	CA-228
Perylenes	-1	carcinogens	CA-228
Benzanthracenes	-1	carcinogens	TY-008
Chrysenes	-1	carcinogens	TH-086
Pyrenes	-1	carcinogens	DO-074

C. Potentially hazardous if present

<u>Compound</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
Anthracene		0.01 mg/m ³	DO-074

D. Potentially hazardous trace elements

<u>Element</u>	<u>Concentration (µg/ml)</u>	<u>TLV (ppm)²</u>	<u>Reference</u>
Arsenic	0.021		AN-104
Cadmium	<0.01		AN-104
Chromium	0.025		AN-104
Cobalt	<0.02		AN-104
Copper	0.10		AN-104
Iron	0.76		AN-104
Lead	0.12		AN-104
Manganese	<0.02		AN-104
Mercury	0.0034		AN-104
Molybdenum	<0.10		AN-104
Nickel	<0.04		AN-104
Vanadium	0.10		AN-104
Zinc	0.09		AN-104

TABLE 2.2-3D - FUGITIVE GAS OIL EMISSIONS FROM ATMOSPHERIC DISTILLATION
COLUMN (Cont.)

E. Sampling Conditions

Temperature - 52°C

Pressure - 3.14-5.25 kg/cm² (30-60 psig)

-
1. Cited in literature as being present, and therefore it is deemed a hazard.
 2. Refer to Table A, Appendix B, for toxicity data concerning trace elements.

TABLE 2.2-3E
FUGITIVE TOPPED CRUDE EMISSIONS FROM
ATMOSPHERIC DISTILLATION COLUMN

A. Major Components

<u>Components</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
>C ₂₅ Paraffins	20.0		GR-123
>C ₂₅ Cyclo- paraffins	45.0		GR-123
>C ₂₅ Aromatics	30.0		GR-123
Residue	5.0		GR-123

B. Known to be present and known to be hazardous

<u>Compound</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
Benzopyrenes	-1	carcinogens	TH-086
Benzfluorenes	-1	carcinogens	TY-008
Benzantracenes	-1	carcinogens	TY-008
Fluoranthenes	-1	carcinogens	TY-008
Alkyl Pyrenes	-1	carcinogens	DO-074

C. Potentially hazardous if present

<u>Compound</u>	<u>Vol. %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
-----------------	---------------	------------------	------------------

None; only the carcinogens mentioned above are believed to be hazardous mainly due to the very low vapor pressure of the topped crude components.

D. Sampling Conditions

Temperature - 250°C

Pressure - 3.14-5.25 kg/cm² (30-60 psig)

1. Cited in literature as being present, and therefore, it is deemed a hazard.

Sampling Conditions

The product streams from a crude distillation unit can conveniently be sampled and analyzed for hazardous materials. Because of this, the natural separation of components in the column can be used as an aid in simulating the composition of the fugitive emissions from the general tower area. The hazardous components in these "simulated" fugitive emissions can in effect be identified as components in discrete streams before these streams are emitted from equipment and fittings.

The light ends may be sampled at the compressor from the overhead accumulator at about 30°C and 2.09-3.14 kg/cm² (20-30 psig) using a suitable gas phase sampling apparatus. The liquid naphtha, distillate, and gas oil streams may be sampled at their product pumps at about 30°C, 57°C, and 52°C, respectively, and 3.14-5.25 kg/cm² (30-60 psig). The hot topped crude may be sampled at the bottoms pumps at about 250°C and 3.14-5.25 kg/cm² (30-60 psig). The sampling points will generally be at ground level and are shown in Figure 2.2-1.

2.2.2 Atmospheric Still Condensate

Process Analysis

The atmospheric still condensate includes all steam used or generated within the atmospheric still. The sources are steam used in heavy resid steam distillation, stripping steam from the side product strippers, and steam produced from the brine in the incoming refinery crude.

Steam condensed from the tower is collected in an overhead accumulator drum as shown in Figure 2.2-2. In the drum the aqueous condensate separates from the organic liquids (naphtha) and the light ends. The condensate either is pumped or flows by gravity from the accumulator to the API sewer. The wastewater is collected in the sewer and later steam stripped.

Definition of Effluent Emissions Basis

The accumulator drum of the atmospheric still contains aqueous condensate which is in direct contact with the straight run naphtha. The drum conditions are approximately 30°C and atmospheric pressure. Water soluble components in the straight run naphtha are dispersed in the aqueous condensate. Table 2.2-4 lists hazardous components (and their solubilities) which are potentially found in the straight run naphtha. The TLV's listed are hazardous concentrations in air and are not directly applicable to liquid phase systems. They are used in this case to indicate degree of hazard involved in handling the components in either the organic or aqueous liquid phases.

Other components found in the overhead condensate stream include light organics from the crude, ammonia, hydrogen chloride, salts, trace metals, and hydrogen sulfide.

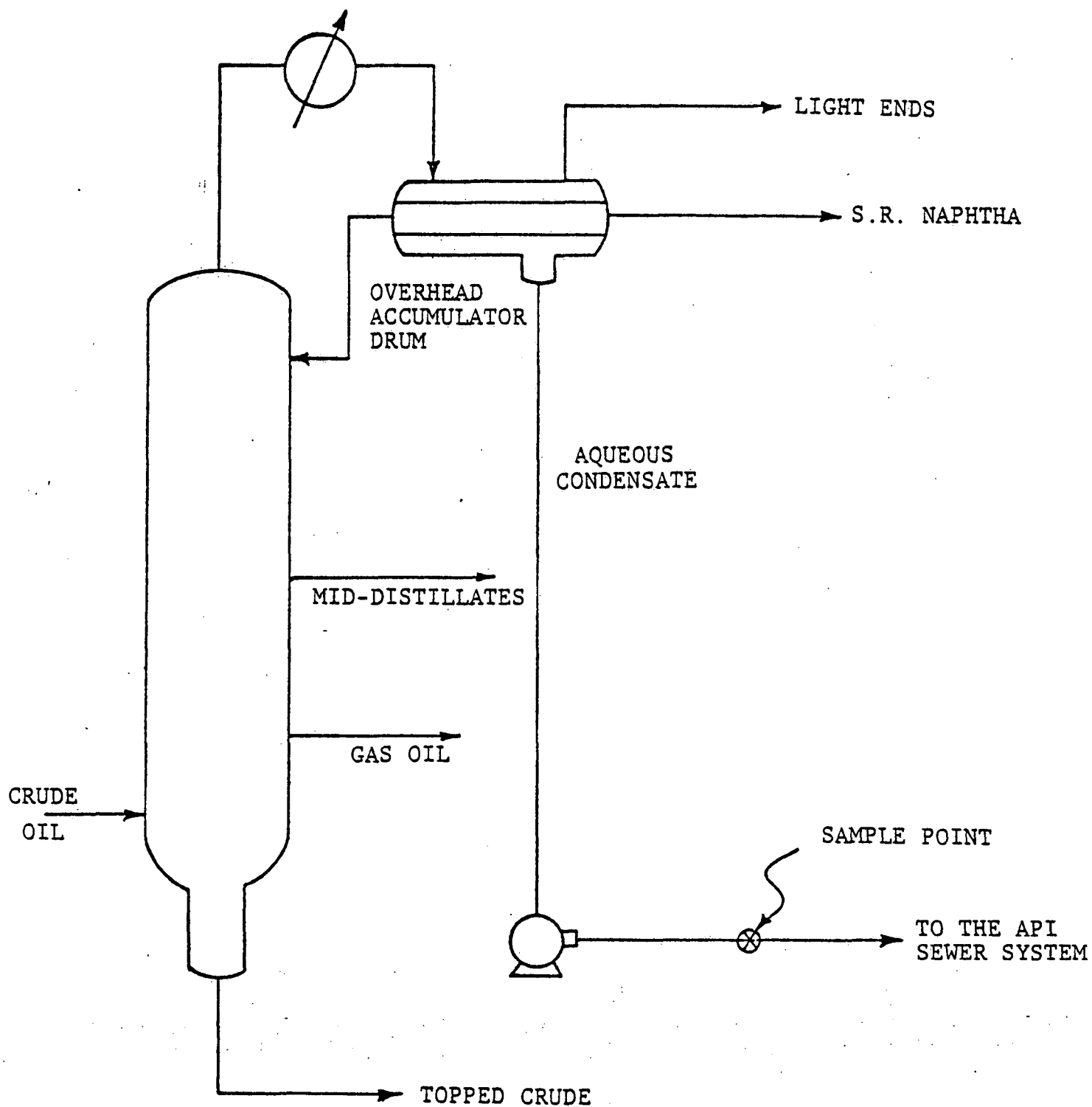


FIGURE 2.2-2 ATMOSPHERIC DISTILLATION COLUMN

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TABLE 2.2-4
ATMOSPHERIC STILL CONDENSATE
Potentially Hazardous Pollutants

A. Potentially hazardous if present

Compound	Solubility ¹ mg/liter	TLV (ppm)	Reference
Acetic Acid	Miscible @ 15.6°C	10	LO-112
Formic Acid	Miscible	5	LO-112
Pyridine	Miscible @ 15.5°C	5	LO-112
Alkyl Pyridines	Very Soluble	-	LO-112
Phenol	82,000 @ 15°C	5	BE-147
m-Cresol	5,000 @ 30°C	5	BE-147
o-Cresol	25,000 @ 30°C	5	BE-147
p-Cresol	18,000 @ 36°C	5	BE-147
Methanethiol ²	Soluble	0.5	GR-123
Ethanethiol ³	15,000 @ 20°C	0.5	GR-123
Butanethiol ³	590 @ 30°C	0.5	GR-123
C ₄ -C ₆ n-Alkanes ³	approx. 250-300 @ 30°C	100-600	CA-227, SM-094
Benzene ³	1,730 @ 30°C	10	SM-094
Isopropylbenzene ³	80 @ 30°C	50	SM-094
Xylenes ³	189 @ 30°C	100	SM-094
Ethylbenzene ³	200 @ 30°C	100	SM-094
Toluene ³	665 @ 30°C	100	SM-094
1-Pentene	900 @ 15.5°C	1,000	CA-227
1, 3, 5-Trimethylbenzene ³	20 @ 15.5°C	35	RO-189
1, 2, 3-Trimethylbenzene ³	Insoluble	25	RO-189
Cyclohexane ³	63 @ 30°C	300	SM-094
Methylcyclohexane ³	Insoluble	400	SM-094
1-Methyl-4-isopropylbenzene	-	50	RO-189

B. Potentially hazardous trace elements

Element ⁴	Solubility mg/liter	TLV (ppm)	Reference
Antimony	-	-	VO-027
Arsenic	-	-	VO-027
Cadmium	-	-	VO-027
Chromium	-	-	VO-027
Copper	-	-	VO-027
Lead	-	-	VO-027
Magnesium	-	-	VO-027
Mercury	-	-	VO-027
Nickel	-	-	VO-027
Phosphorus	-	-	VO-027
Selenium	-	-	VO-027
Vanadium	-	-	VO-027

1. The values which are given here are for solubility in water only and will be affected by pH and temperature.
2. Cited literature values for the concentration of the components in the light ends stream given in Table 2.2-3A.
3. Cited literature values for the concentration of the compounds in the naphtha stream given in Table 2.2-3B.
4. No solubility or toxicity (TLV) data given due to the lack of information on the state of the trace elements.

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The light organics include low boiling point materials, generally C_4 and lighter. Methane, ethane, and propane are assumed to be non-hazardous in the aqueous phase due to their high TLV's and low solubilities.

Ammonia is sometimes injected into the distillation column to neutralize the HCl and H_2S acids (BE-147, PE-140). Some ammonia is also generated within the column by slight hydrogenation of nitrogen in the crude feedstock (BE-147).

Hydrogen chloride evolves from the salt brine in the incoming feedstock. Although the chloride ion exhibits a low vapor pressure and should theoretically end up in the heavy ends, it actually appears in all the product streams because of carry-over in the tower. This carry-over is in the form of a spray or a foam, and is caused either by excess charging rates to the fractionator or by fouling of the trays with solids (PE-140).

Other salts in the brine are also carried over in a similar manner. These salts include sodium, magnesium, calcium, aluminum, and iron salts of chlorides, bromides, sulfates, and bicarbonates (PE-140, VE-021).

Carry-over is also a cause of trace metals in side products streams. Some are also distributed among the various product streams due to their volatile nature. Table 2.2-4 lists metals which have been shown to be present in naphtha products which can potentially exist as organometallic or inorganic metallic compounds.

Hydrogen sulfide is a potential aqueous contaminant found in distillation light ends. The H_2S is present in the distillation column and is primarily removed from the column as part of the light ends stream. The H_2S is in contact with the

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aqueous condensate while leaving the overhead condenser and entering the accumulator drum. Sulfides in the condensate have been measured at 100 to 5,000 ppm (BE-147). The sulfides concentration will depend greatly on the pH of the condensate.

Conditions in the aqueous condensate may permit the formation of an emulsion of the water and hydrocarbon phases. The emulsion will mean a higher average concentration of potentially hazardous organic compounds in the aqueous layer.

Sampling Conditions

If the condensate is pumped to the API sewer system from the accumulator drum, the conditions at the point of sampling are approximately 30°C and 3.15-5.25 kg/cm² (30-60 psig). However, if no pump is required, the point of sampling will be at approximately atmospheric pressure and the same temperature. The condensate is over 99 percent water.

2.2.3 API Separator Effluent

Process Analysis

• API separators are used throughout refineries for the primary treatment of oil wastewaters. Oil separated from the wastewater is returned to the refinery for reprocessing. The effluent waters normally require secondary water treating before release from the plant. Suspended solids are also removed in these separators. Figure 2.2-3 shows a typical API separator used in a refinery.

In the API separator, separations are achieved using simple gravity settling. The separation efficiency can vary between 50 and 100 percent, depending on the physical characteristics of the oil. Therefore, considerable oil can still be released to receiving waters when separation efficiencies are low.

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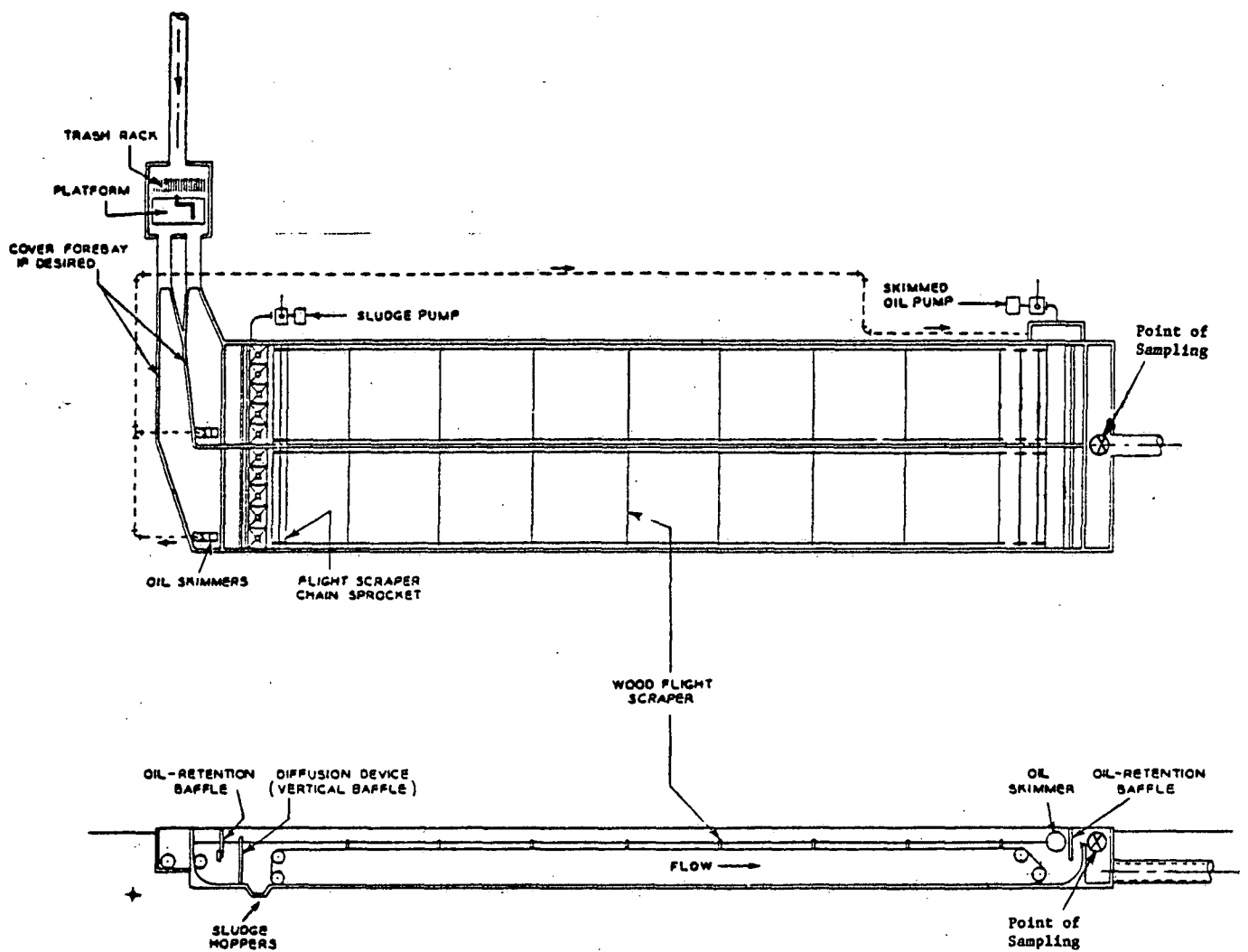


FIGURE 2.2-3 API OIL-WATER SEPARATOR INCLUDING
POINT OF SAMPLING

Source: (AM-062)

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Data on the efficiency of removing suspended solids are scarce, but it has been estimated that suspended solids content in the effluent may be twice the oil content (BL-038).

The following process sources represent the main contributors of water to the API separators:

- tank drawoffs
- desalters
- steam strippers
- barometric condensers

A brief discussion of each follows.

Incoming crude to a refinery contains small quantities of water. The crude is generally pumped to storage tanks where the water settles out. Approximately one-half gallon of water per barrel of crude is collected and sent to the API separators (NA-182). This water contains both oil and salts.

Desalting is generally the first unit operation the raw crude undergoes. Water is mixed with the crude and heated. Water, along with dissolved impurities, is separated from the crude by physical decanting or electrostatic coalescing. Approximately two gallons of water per gallon of crude charge is drawn from this unit. The main contaminants are dissolved solids and inorganic metal salts, although oils, sulfides, and phenols are also found in the water in lesser concentrations.

Steam stripping is used throughout refineries as an economical distillation method. Condensate from steam stripping is a major contributor to API separators.

Processing units included on the flow diagram in Section 2.1 which typically employ steam strippers are atmospheric distillation, naphtha HDS, fluid catalytic cracking, catalytic hydrocracking, residual HDS, coking, and deasphalting. The steam used for stripping in these processes is condensed and discharged as an oily (often sour) aqueous effluent.

Many process units employing steam strippers produce a sour aqueous effluent which is routed to a sour water stripper. In this unit most of the sulfides, ammonia, and phenols are removed from the water prior to sending it to the API separator.

Barometric condensers present the largest and most offensive source of aqueous hydrocarbon emissions. In modern refineries, barometric condensers are generally replaced by surface condensers. For purposes of this report, however, it is assumed that barometric condensers are in use.

Oily water effluent rates of about 310 liters per cubic meter of charge have been reported (TH-038) with oil and oil emulsion concentrations up to 1.5 kilograms per cubic meter of charge (DI-044). Based on this data, an API separator influent of about 7.95 million liters/day, (or 500 liters per cubic meter of crude charged) was calculated for the refinery. Separator operations were calculated to be about 85% efficient for an effluent oil concentration of 140 ppm.

Definition of Effluent Emission Basis

A threefold approach was taken to assess potentially hazardous pollutants in the water effluent from the API separators. Investigative stages were: (1) a definition of API separator feed sources, (2) an evaluation of the hazardous materials present

in the feed, and (3) an evaluation of the hazardous materials present in the API separator effluent. A discussion of each stage of investigation follows.

A review of all processes listed on the refinery flow sheet was conducted to determine which processes produced an oily aqueous effluent that would be routed to the API separator for oil-water separation. The major process contributors of water to the API separator were found to be tank drawoffs, desalters, barometric condensers, and stream strippers.

Published data on hazardous materials in aqueous streams were sparse. Data were obtained, however, which characterized these streams as to the major contaminants, i.e., sulfides, oil content, ammonia, BOD, etc. (BE-147, AM-041, WI-071).

The hydrocarbon streams from the various processes which come into direct contact with the oily water were studied to determine which hazardous materials could be present. Special emphasis was placed on identifying the properties of the hazardous compounds that might be present in the hydrocarbon stream. Engineering judgement was then applied to determine the likelihood of these compounds being present in the aqueous effluent.

The EPA research laboratories in Ada, Oklahoma, and Athens, Georgia, are currently involved in programs for defining the composition of API separator effluent wastes. These programs are to characterize both organic and inorganic trace compounds within the streams. Presently the study has been devoted to identification of phenolic and acidic organic compounds and also trace inorganic elements and metals (KE-151, BU-159).

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The results of these individual evaluations were combined to provide the estimated composition of the API separator effluent shown in Tables 2.2-5, 2.2-6, and 2.2-7. Table 2.2-5 contains a characterization of water quality and Table 2.2-6 lists hazardous pollutants potentially present. The compounds given are representative of the hazardous chemicals believed to be present in the API separator effluent. Trace elements which are potentially present are shown in Table 2.2-7.

Solubilities of these compounds, to a certain extent, indicate the likelihood of their presence. The threshold limit values (TLV) listed are for atmospheric emissions and are intended for use only as references to show relative degrees of toxicity. Trace elements listed in Table 2.2-7 deserve a special note. As a class, they are insoluble in their elemental state. They may, however, form salts in wastewater systems which, as a rule, are soluble. Organometallics, such as tetraethyl lead, may also be present in this stream. No solubility or TLV data is given for trace elements because the forms in which they may be present are uncertain.

Sampling Conditions

The point of sampling as shown in Figure 2.2-3 will be the effluent channel through which the separated water passes on its route toward further processing. Typical water conditions are approximately 37.8°C and atmospheric pressure (AM-062). The sampling will be conducted at ground level, and the effluent rate expected is 500 liters per cubic meter of crude charged to the refinery.

TABLE 2.2-5
API SEPARATOR EFFLUENT
Water Quality Characterization

Water is greater than 98 volume percent of the total flow.

	<u>Expected Concentrations (ppm)</u>		
	<u>min.</u>	<u>max.</u>	<u>avg.</u>
BOD	1	1,180	413
COD	69	3,080	1,170
Oil	3	870	140
Phenols	0.5	335	76
Solids			
Suspended	-	1,950	480
Dissolved	83	15,180	2,630
Alkalinity	14	2,620	600
Sulfide	0.2	240	30
Phosphorus	0.5	6	3
NH ₃ (N)	21	1,000	480
pH	6.8	9.5	8.2

Sources: (BE-147, DI-044, PE-066, AM-041)

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TABLE 2.2-6
API SEPARATOR EFFLUENT
Potentially Hazardous Pollutants

<u>Compounds</u>	<u>Solubilities¹</u> <u>mg/liter</u>	<u>TLV (ppm)</u>	<u>Reference²</u>
Formic acid	Miscible	5	-
Hydrochloric acid	Miscible @ 15.6°C	10	BE-147
Acetic acid	Miscible	5	-
Naphthanoic acid	Slightly Soluble	- ³	BU-159
Pyridine	Miscible @ 15.5°C	5	-
Ammonia	74,000 @ 96°C	25	BE-147
Methanethiol	Soluble	0.5	-
Ethanethiol	15,000 @ 20°C	0.5	-
Butanethiol	590 @ 30°C	0.5	-
H ₂ S	Slightly soluble	10	BE-147
o-Cresol	5,000 @ 30°C	5	KE-151
m-Cresol	25,000 @ 30°C	5	KE-151
p-Cresol	18,000 @ 36°C	5	KE-151
Phenol	82,000 @ 15°C	5	KE-151
HCN	Soluble	10	-
Formaldehyde	Very soluble	2	-
Benzene	1,730 @ 30°C	10	-
Anthracene	0.75 @ 15.5°C	0.1 mg/m ³	-
Biphenyl	7.5 @ 25°C	0.2	-
Naphthalene	30 @ 15.5°C	10	-
1,2,3,4-Tetrahydro- naphthalene	Insoluble	25	-
Trimethylbenzene	20 @ 25°C	25	-
1-Methyl-4-isopropyl- benzene	Insoluble	50	-
Isopropylbenzene	80 @ 30°C	50	-

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TABLE 2.2-6 API SEPARATOR EFFLUENT (Cont.)

Compounds	Solubilities mg/liter	TLV (ppm)	Reference ²
Decahydronaphthalene	Insoluble	50	-
Xylene	189 @ 30°C	100	-
Ethylbenzene	200 @ 30°C	100	-
Toluene	665 @ 20°C	100	-
C ₂ -C ₈ n-Alkanes	approx. 250-300 @30°C	100-600	-
Cyclohexane	900 @ 15.5°C	300	BU-159
3-Methyl-2-butene	Insoluble	- ³	-
2-Methyl-2-butene	Insoluble	- ³	-
1-Hexene	Insoluble	- ³	-
Pyrenes	0.16 @ 26.7°C	Carcinogens	-
Benzo(a)pyrene	.004 @ 15.5°C	Carcinogens	-
Phenanthrenes	1.6 @ 15.5°C	Carcinogens	-
Benzanthracenes	-	Carcinogens	-
Chrysenes	.0015 @ 15.5°C	Carcinogens	-
Fluoroanthrenes	Insoluble	Carcinogens	-

¹Solubilities will vary with effects of temperature and pH.

²If a reference source is given, then the compound has been identified as being present. If no reference is given, then the compound is suspected of being present because it was in contact with API separator wastewater within the refinery.

³Deemed moderately hazardous (see Table A of this appendix).

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TABLE 2.2-7
API SEPARATOR EFFLUENT
Potentially Hazardous Trace Elements

Trace elements which have been identified in API effluents
(KE-151):

Barium	Fluorine	Potassium
Boron	Iron	Selenium
Chlorine	Magnesium	Sulfur
Chromium	Manganese	Vanadium
Cobalt	Nickel	Zinc
Copper	Phosphorus	

Trace elements suspected of being present in API effluents:

Antimony	Lead	Tin
Arsenic	Mercury	Uranium
Beryllium	Molybdenum	Zirconium
Cadmium	Silver	

2.2.4 Incinerator Tail Gas from the Sulfur Recovery Unit

Process Analysis

Sulfur recovery units convert hydrogen sulfide in gas streams to elemental sulfur. This is accomplished through a process of controlled combustion and reactions occurring in a series of catalytic beds. The feed to the Claus converter is acid gas removed from light ends in the acid gas removal unit and some acid gas from the sour water stripper. Most of the hydrogen sulfide in these streams has been produced from various types of hydrotreating or cracking units throughout the refinery. Not all the sulfur will be removed in the Claus plant. Unconverted sulfur compounds (primarily hydrogen sulfide) escaping from the Claus plant can be oxidized to sulfur dioxide in tail gas incinerators (GR-145, BE-150).

Estimates of potentially hazardous emissions in the incinerated tail gas must necessarily include the contributions of all the Claus feeds. The units feeding the Claus unit are off-gases from the acid gas removal unit and the sour water stripper.

Acid Gas Sources

The major source of feed to the sulfur recovery unit is the acid gas removal unit. The acid gas is contained in light ends from atmospheric distillation of the crude. This mixture includes low boiling hydrocarbons, hydrogen sulfide, and ammonia. Additional hydrogen sulfide is scrubbed from the light ends produced by various process units in the refinery. These sources are listed in Table 2.2-8.

TABLE 2.2-8
SOURCES OF H₂S GASES TO THE CLAUS UNIT*

<u>Process Unit</u>	<u>Light Ends Produced (kg/day)</u>	<u>H₂S Produced (kg/day)</u>	<u>References</u>
Acid Gas Removal			
Atmospheric	230,000	1,450	MC-078
Distillation			
Naphtha HDS	750	480	HY-013
Distillate HDS	8,650	7,140	HY-013
Gas Oil HDS	10,500	5,960	HY-013
Residual Oil HDS	19,500	13,590	HY-013
Hydrocracker	96,850	7,250	HY-006
FCCU	1,064,000	36,500	WO-025
Delayed Coker	144,600	11,130	NE-044
Sour Water Stripper		4,500-10,000	BE-147

*Basis: 15,900 m³/day (100,000 bpcd) refinery

A typical acid gas removal process involves amine scrubbing to separate the acid gas from the hydrocarbons (DI-090). The major sorbents used are alkanolamines, of which monoethanolamine (MEA) is the most common (LO-113). In the regenerator, hydrogen sulfide is released from the amine solution by heating in a reboiler. The liberated acid gas is sent to the Claus unit. The flow scheme of a typical acid gas removal process is shown in Figure 2.2-4.

The hydrodesulfurizing units listed in Table 2.2-8 produce not only light ends for the acid gas removal unit, but also water which is treated in a sour water stripper. Other units which contribute to the sour water stripper are the atmospheric distillation column, the catalytic cracker, the hydrocracker, and the coker. Sour water is taken from these sources in the form of steam stripper condensate (BE-147).

A typical sour water stripper consists of a column and a reboiler which are used to separate acid gas into an overhead hydrogen sulfide stream and a bottoms product containing ammonia and water. Hydrogen sulfide is routed to the Claus unit. The bottoms stream may be further refined with an ammonia stripper to produce ammonia. The flow scheme for a typical sour water stripper is shown in Figure 2.2-5.

The acid gas contribution to the Claus unit from the sour water stripper is much less than the feedstock from the acid gas removal unit, as indicated in Table 2.2-8.

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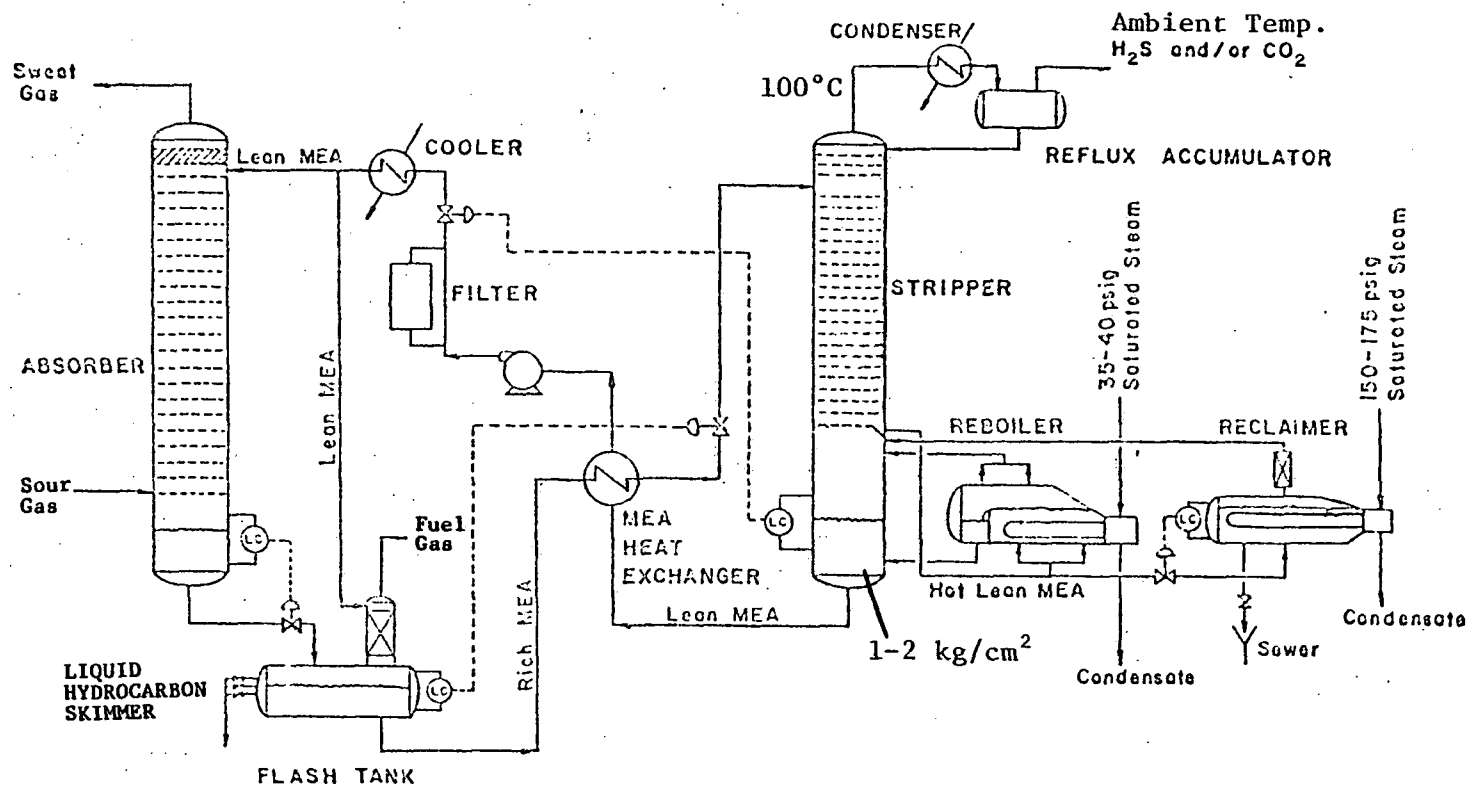


FIGURE 2.2-4 A TYPICAL MEA ACID GAS REMOVAL UNIT

Source: (DI-091)

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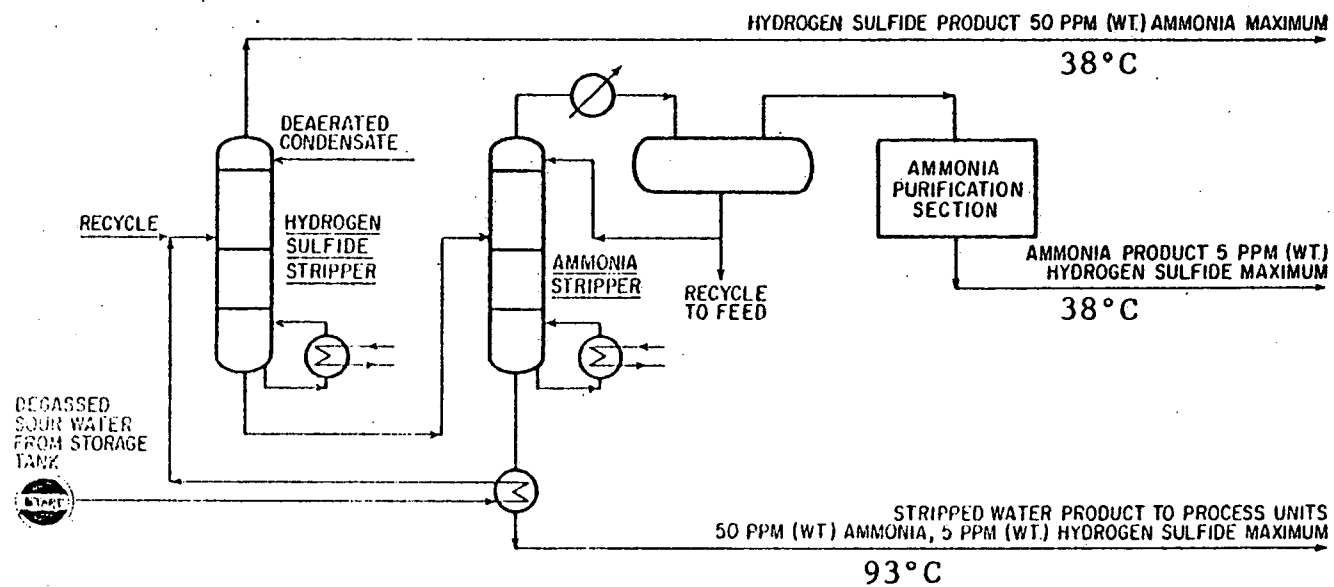


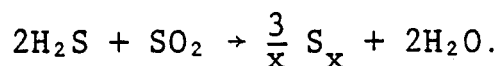
FIGURE 2.2-5 SOUR WATER STRIPPER WITH AMMONIA SEPARATION PROCESS

Source: (KL-032)

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Sulfur Recovery Process

The process involves first combusting the acid gas from the acid gas removal unit and the sour water stripper with a substoichiometric amount of air. About one-third volume percent of the hydrogen sulfide is oxidized. The sulfur dioxide formed reacts with the remaining hydrogen sulfide to form elemental sulfur (PE-142). The main reaction is as follows:



Sulfur recovered by this process in the furnace accounts for 50-70% of the total plant conversion (BR-110). The elemental sulfur is condensed and recovered as a liquid.

The remaining acid gas passes through a series of reactors and condensers to convert the remaining sulfur compounds to elemental sulfur. Two, three, or four reactors are used to achieve total sulfur conversions between 94 and 97 percent (BA-166, BE-150). Each reactor consists of a reheater and a catalytic converter, followed by a condenser. Typical operating conditions for all the processes in a Claus unit are given in Table 2.2-9. A diagram of a two-reactor Claus unit is shown in Figure 2.2-6.

Incinerator Tail Gas

The purpose of the incinerator is to convert all remaining sulfur compounds in the Claus tail gas to sulfur dioxide. This is usually accomplished by burning the tail gas at 540-650°C (BE-150). Light ends produced in the refinery are normally used for fuel gas in the process. The actual burning takes place in a fire box at the base of the incinerator stack.

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TABLE 2.2-9
CLAUS UNIT OPERATING CONDITIONS

<u>Stream or Unit</u>	<u>Operating Conditions</u>	<u>References</u>
Feed		
temperature	40°C	GR-145
pressure	1.5 kg/cm ²	GR-145
flow rate	86,200-95,300 kg/day	*
Furnace		
temperature	1000°C	PE-142
H ₂ S conversion	50-70%	BR-110
Reactor (reheater and catalytic converter)		
temperature	245-260°C	BE-150
pressure	1-2 kg/cm ²	BE-150
H ₂ S conversion	25-45%	*
catalysts	bauxite, cobalt molybdate on alumina	PE-142 BR-110
Condenser		
temperature	127-140°C	BE-150, GR-145
pressure	1 kg/cm ²	GR-145
Incinerator		
temperature	540-650°C	BE-150
Tail Gas		
temperature	400°C	GR-145
pressure	1 kg/cm ²	GR-145
flow rate	82,000-91,000 kg/day	*
Product		
elemental sulfur	3,600-4,500 kg/day	DI-090

*Calculated for a typical (15,900 m³/day) refinery.

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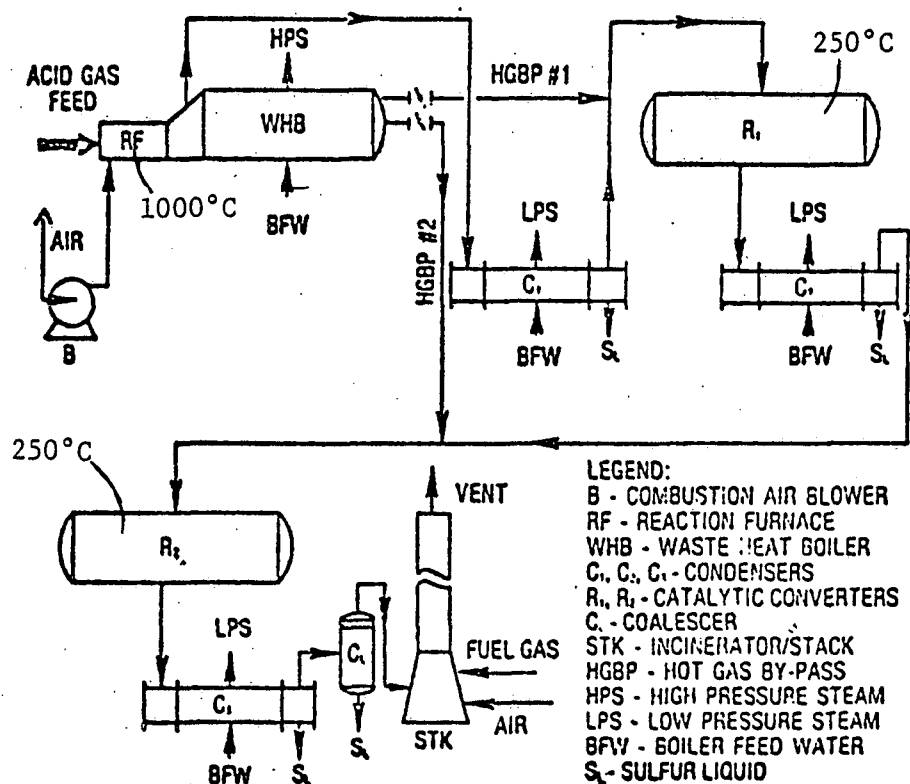


FIGURE 2.2-6 A TYPICAL CLAU S SULFUR RECOVERY PLANT

Source: (GO-107)

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Definition of Effluent Emissions Basis

Factors which determine the characteristic components and their concentrations in the incinerator tail gas are the following: (1) feed streams and process conditions in the acid gas removal unit, (2) feed streams and process conditions in the sour water stripper, and (3) acid gas processing in the Claus unit. Claus unit processes involve reactions in the furnace, reactors (reheaters and catalytic converters), condensers, and finally, the incinerator. A discussion of the contributions of these processes to the estimated incinerator tail gas composition follows.

Acid Gas Removal Unit

Refinery streams which are treated in acid gas removal units include light end streams from the atmospheric distillation column, the hydrocracker, fluidized catalytic cracker, delayed coker, and the various desulfurizing units.

Desulfurizing units in refineries typically process naphtha, distillate, gas oil, and residual oil streams. The major components in streams from these units are light hydrocarbons, hydrogen sulfide, and ammonia (DI-090). Hydrogen sulfide and ammonia are hydrogenation products of the desulfurization and denitrification processes. Light hydrocarbons are first scrubbed to remove hydrogen sulfide and ammonia, and then pass to the fuel gas system. Hydrogen sulfide acid gas and ammonia are then separated in a steam stripper. The acid gas is sent to the Claus unit and the ammonia is further processed in an ammonia recovery unit. Some carbon dioxide is also potentially present in the acid gas stream (DI-091).

The amine absorption and regeneration process determine to an extent the feed stream to the Claus unit. The major component of the product stream is hydrogen sulfide which has been removed from the hydrocarbons using the amine sorbent. The amine sorbent is then recovered in a stripping column which removes the H_2S . Some amine misting occurs which accounts for significant amounts of ammonia in the feed to the Claus unit (ME-107). Light hydrocarbons are never completely separated from the acid gas. Therefore, small amounts can be expected to be in the Claus plant feed (BR-110).

Additional procedures are usually used to limit the quantities of amines and hydrocarbons present in the acid gas. An entrainment-separation mesh pad or equivalent device reduces amine carry-over, but does not eliminate ammonia (GO-107). The best procedure for reducing hydrocarbons is a flash tank used to separate both liquid and gaseous hydrocarbons prior to stripping (BR-110). Nevertheless, significant quantities of hydrocarbons escape in the Claus plant feed (GR-145).

Sour Water Stripper

Refinery streams typically treated in a sour water stripper include water streams from the fluidized catalytic crackers, hydrocrackers, delayed cokers, and hydrodesulfurization units. The major contributions to refinery sour water are the condensates from steam stripping of light ends from these units.

The major pollutants in sour water are hydrogen sulfide and ammonia. They are products of hydrotreating and dissolution in the steam condensate. Ammonia, which is highly water soluble, tends to concentrate in the sour water stream, while most of the hydrogen sulfide, which is less soluble, tends to leave in the

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acid gas. Most of the ammonia present has been produced from nitrogen compounds in catalytic cracking and hydrocracking units (BR-110, KL-032).

Claus Unit

A combination of the acid gas and the sour water stripper gas is fed to the Claus unit. Ammonia is removed from the Claus unit feed by steam stripping. A list of components potentially present in the sour water and acid gas feed is given in Table 2.2-10.

The exit stream going into the tail gas incinerator is affected by performance of the furnace, the catalytic converters, and condensers within the Claus unit. Each of these is discussed in the following pages.

Furnace. The major purpose of the furnace is to convert about one-third of the hydrogen sulfide to sulfur dioxide (DI-090). Sulfur dioxide then reacts with the remaining hydrogen sulfide to give elemental sulfur. At the same time ammonia is converted to nitrogen and water vapor along with small amounts of nitrogen oxides (BR-110, GO-107).

In furnace side reactions, light hydrocarbons react with sulfur to form toxic carbonyl sulfide and carbon disulfide (PE-142, BR-110). These compounds are also produced by the reaction of carbon monoxide with sulfur. Carbon monoxide is formed in the furnace by carbon dioxide dissociation at high temperatures (ME-107). It is generally assumed that the heavier organics, such as the phenols and cresols, are converted to carbonaceous matter (GO-107). Water as steam vapor passes through the furnace unchanged.

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TABLE 2.2-10
COMPONENTS POTENTIALLY PRESENT IN CLAUS UNIT FEEDS

<u>Component</u>	<u>TLV (ppm)</u>	<u>Reference</u>
Methane	10,000	GR-145, BR-110
Ethane	500	GR-145, BR-110
Propane	500	GR-145, BR-110
Isobutane	-	GR-145, BR-110
Butane	500	GR-145, BR-110
H ₂ S	10	KL-032
CO ₂	5,000	KL-032
H ₂ O	-	GR-145
NH ₃	50	ME-107, KL-032
HCN	10	BR-110
HCl	5	PE-140
Phenols	5	GO-107, BR-110, BE-147
Cresols	5	GO-107, BR-110
Methanethiol	0.5	BE-147
Ethanethiol	0.5	BE-147
Other Mercaptans	-	BE-147, DI-090
Monoethanolamine	3	ME-107

Reactors. The reactors convert the remaining sulfur compounds to elemental sulfur by passing the hot acid gas over a bauxite or cobalt molybdate catalyst (PE-142). Reheaters are used to maintain the acid gas temperature of about 250°C (BE-150). This prevents condensation of sulfur in the reactors (GO-107). Additional carbonyl sulfide and carbon disulfide are formed during reheating. These compounds are unusually difficult to convert to elemental sulfur and thus constitute a source of potentially hazardous compounds in the gas passing to the incinerator (BA-166, GO-107).

Catalyst deactivation results from both aging and poisoning. Specific catalyst poisons are ammonia, nitrogen oxides, and carbonaceous matter (PE-142, GO-107).

Condensers. Liquid sulfur is separated from the acid gas in the condensers. Virtually no reactions occur in the condensers. It is assumed that virtually all elemental sulfur is removed from the feed stream to the incinerator (GR-145).

Claus Unit Tail Gas Incinerator

Remaining hydrogen sulfide is converted to sulfur dioxide in the incinerator. However, since the combustion process is not complete, the incinerator tail gas contains traces of hydrogen sulfide in addition to carbon monoxide and nitrogen oxides (GR-145, DA-069). Entrained catalyst particles, which are potentially hazardous, have been identified in the tail gas, also. Potentially hazardous components in the tail gas are significant during incinerator flame-out periods.

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Major components (non-pollutants), hazardous compounds known to be present, and those hazardous if present are given in Table 2.2-11.

Sampling Conditions

The point of sampling is defined as eight diameters above the flame at the base of the incinerator stack. Typical conditions are 400°C and 1 kg/cm² (GR-145). Calculated tail gas flow rate for a 15,900 cubic meter per day refinery with a sulfur content in the crude of 0.851 wt% is 84,000 kg/day. This value was determined by totaling estimated feeds to the Claus unit and then subtracting the amount of sulfur recovered. Factors which easily affect this rate are: (1) the sulfur concentration in the crude, (2) the operating conditions of the desulfurizing units in the refinery, (3) the sulfur conversion rate of the Claus unit, and (4) the fuel gas flow rate in the incinerator.

2.2.5 Fluidized Catalytic Cracking Regenerator Off-Gas

Process Analysis

Fluidized catalytic cracking (FCC) is used to convert distillate oils to: (a) high octane gasoline and raw materials for alkylate production, (b) petrochemical raw materials, (c) heating oils and diesel oils, and (d) LPG. A flow diagram of the typical fluid cat cracking operation is shown in Figure 2.2-7. The operating conditions for the FCC unit reactor, regenerator, and waste heat boiler are given in Table 2.2-12.

The distillate oils are preheated before introduction into the reactor portion of the FCC unit. Upon injection the oil is vaporized and contacted with the fluidized catalyst bed, where the heavy gas oil is cracked into lighter fractions.

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TABLE 2.2-11
INCINERATOR TAIL GAS FROM
SULFUR RECOVERY UNITS

A. Major Components (Non-Pollutants)

<u>Compound</u>	<u>Vol %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
N ₂	71.07		GR-145
H ₂ O	18.57		GR-145
O ₂	7.39		GR-145
CO ₂	1.45		GR-145
H ₂	0.50		GR-145

B. Known to be hazardous and known to be present

<u>Compound</u>	<u>Vol %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
SO ₂	0.89	5	GR-145
CO	0.10	50	GR-145
COS	0.02		GR-145
CS ₂	0.01	20	GR-145
H ₂ S	<0.001	10	GR-145

C. Potentially hazardous if present

<u>Compound</u>	<u>Vol %</u>	<u>TLV (ppm)</u>	<u>Reference</u>
C ₁ -C ₄ n-alkanes	-	500 - 10,000	GR-145, BR-110
Methanethiol	-	0.5	BE-147
Ethanethiol	-	0.5	BE-147
Other Mercaptans	-	-	BE-147
Phenol		5	GO-107, BR-110, BE-147
Cresols		5	GO-107, BE-147
NO		25	DA-069
NO ₂		5	DA-069
NH ₃		50	ME-107, KL-032
HCN		10	BR-110
HCl		5	PE-140
Monoethanolamine		3	ME-107
Bauxite or Cobalt Molybdate cata- lyst particulates		5 x 10 ⁷ particles/ ft ³ (Al ₂ O ₃)	BR-110

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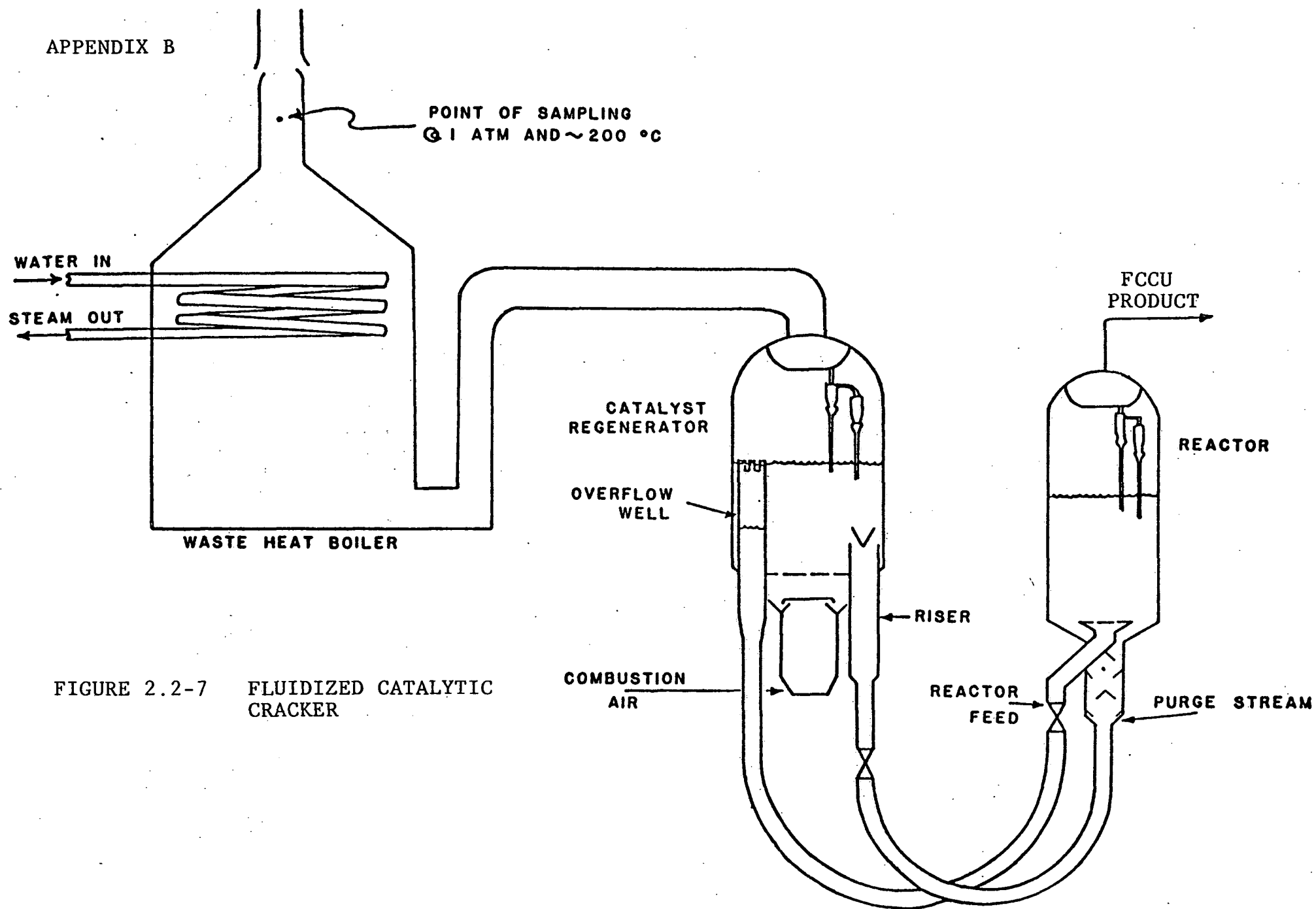


FIGURE 2.2-7 FLUIDIZED CATALYTIC CRACKER

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TABLE 2.2-12
FLUIDIZED CATALYTIC CRACKING UNIT
OPERATING CONDITIONS

<u>Unit</u>	<u>Operating Conditions</u>	<u>References</u>
Reactor		
Temperature	470-540°C	WO-025, BL-078
Pressure	23.8-29.7 kg/cm ²	BL-078
Catalyst-to-oil ratio ¹	3.0-12.0:1.0	BL-078, WO-025
Space Velocity ²	3.0-100:1.0	WO-025
Regenerator		
Temperature	565-675°C	BL-078, CO-111
Catalyst Surface Temperatures	650-700°C	GR-123
Pressure	21.9-23.8 kg/cm ³	BL-078
Residence time	Approx. 40 min.	CO-111
Wt% coke on catalyst:		
Hydrotreated feed	2.0-7.1, avg. 3.6	
Unhydrotreated feed	4.9-12.6, avg. 6.6	
Wt% coke remaining on catalyst	0.2-0.5	CO-111
Waste Heat Boiler		
Inlet temperature	565-675°C	BL-078, CO-111
Outlet temperature	176-204°C	-
Outlet pressure	atmospheric	-

¹ Defined as the ratio of the weight of catalyst circulated per hour to the weight of oil charged (fresh and recycle) per hour.

² Defined as the ratio of the weight of oil charged (fresh and recycle) per hour to the weight of catalyst in the reactor zone.

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Also formed during the cracking process is a coke residue. The coke can be attributed to four sources: (1) catalytic cracking products, (2) metal contamination, (3) residue in the feed material, and (4) hydrocarbons remaining in the catalyst pores (CO-111). Much of the volatile hydrocarbon material held within the catalyst pores is removed in the steam stripping section under the reactor. The volatile material is not actually stripped but rather is displaced by the steam within the pores. The heavy hydrocarbon residues from catalytic cracking products, metal contamination, and residue in the feedstock account for 80-85 wt% of the coke after steam stripping. The remaining coke is from the volatile hydrocarbons entrained within the catalyst.

The steam purged catalyst is transferred into the fluidized catalyst regenerator. Within the regenerator the heavy coke residue is removed from the catalyst as completely as possible by combustion. Complete combustion cannot be attained because of resulting high temperatures which will sinter the catalyst. At lower regeneration temperatures the excess oxygen level is kept low. This operating procedure enhances the formation of CO. The regenerator off-gas consists of volatile material and steam released from the catalyst pores combined with the combustion gases. The major components of off-gas are listed in Table 2.2-13. The hot flue gases are routed through a waste heat boiler to recover the sensible heat, then vented to the atmosphere through a stack.

Definition of Effluent Emissions Basis

The four major factors to consider in the determination of the composition and character of the regenerator off-gas stream are: (1) the gas oil feed composition, (2) the coke formation during reactor operations, (3) steam stripping of the

TABLE 2.2-13
THE FCCU REGENERATOR OFF-GAS
Major Components

<u>Major Components</u>	<u>Reported Concentration Values</u> <u>Vol. %</u>		
	<u>Min.</u>	<u>Max.</u>	<u>Avg.</u>
CO ₂ (dry basis)	7.8	13.4	8.5
O ₂ (dry basis)	2.0	5.1	3.5
N ₂ (dry basis)	80.2	84.6	82.5
CO (dry basis)	0	7.8	5.4
H ₂ O	18.7	26.3	20.0
Particulates	0.0174 ⁺	0.262 ⁺	-

⁺lb/ton of catalyst recirculated.

Source: (DA-069)

catalyst before regeneration, and (4) coke burn-off in the regenerator. The following analysis of these factors is made in consideration of the potentially hazardous emissions from the FCCU regenerator.

Feed Composition. The gas oil used as feed material is typically a hydrocarbon fraction with a distillation range of approximately 300°C to 450°C (HY-013). Salts, nitrogen compounds, sulfur compounds, and metallic compounds are also present in the gas oil stocks.

The salts typically found in the gas oil are sodium chloride, sodium sulfate, sodium bicarbonate, calcium chloride, and magnesium chloride, with sodium chloride the most common (PE-140). Aluminum, iron, bromine, and other bicarbonate salts may also exist (PE-140). The salts appear in the gas oil due to carry over of residual brine material in the crude distillation unit. These trace chlorides in the gas oil can be converted to HCl which is emitted in the regenerator off-gas. These salt concentrations can be maintained at very low levels through use of modern crude desalting techniques.

About 25 to 30 weight percent of the nitrogen compounds found in the gas oil feed are nitrogen bases, and include such compounds as quinolines and pyridines (PE-140). These nitrogen bases reduce cracking catalyst activity by occupying the active acid sites on the catalyst (BR-229). The loss in activity causes a decrease in conversion, an increase in coke formation, and an increase in required coke burn-off in the regenerator. The nitrogen compounds in the feed can be reduced by hydrotreating the FCCU feed (GU-058). A specific method for reducing the nitrogen bases is acid treatment of the gas oil feed. This acid pretreatment will also reduce organometallics in the feed (PE-140).

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Sulfur is present in the gas oil as sulfate salts, thiophenes, and thiols. Most of the hydrogen sulfide formed during the cracking operations comes from the thiols (WO-025). Most of the remaining sulfur ends up in the cycle oil, with small amounts distributed between the gasoline and coke-on-catalyst. Approximately 95% of the sulfur in the cracked cycle oil is in the form of thiophenes and multiringed thiophenes. The cycle oil is sometimes recycled back into the FCC unit which tends to cause an increase in the amount of sulfur going to coke-on-catalyst (WO-025).

Most of the metals entering with the gas oil feed are in the form of organometallics such as porphyrin complexes (PE-140). The main organometallics are heavy metals, nickel, vanadium, chromium, iron, magnesium, manganese, arsenic, and zinc. The heavy metals include molybdenum, lead, and mercury (PE-140). Other metals potentially present include cadmium and cobalt (VO-027). About 5% of the metals contained in the crude distillation feed end up in the side product streams other than the resid (PE-140). The metals in the gas oil deposit on the FCCU catalyst and reduce activity. The metal contamination will cause an increase in coke formation and also an increase in gas production (especially hydrogen). The coke produced due to the effects of contaminant metals is on the order of 15 to 30 weight percent of the total coke formed (CI-011).

Recycling gas oils will affect the ultimate products from the catalytic cracker. The cycle stock is generally richer in aromatic hydrocarbons, has a lower hydrogen-carbon ratio, has a higher concentration of thiophenes, and has a lower end point than the fresh FCCU charge stock (GR-123). Mixing the recycle oil with the fresh feed increases the overall conversion, but it also increases coke laydown on the catalyst (BU-079). The coke also has a somewhat higher sulfur content because of high concentrations of hard-to-crack thiophenes (WO-025). Modern designs include dual reactors

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(riser type); one reactor for fresh feed, the other for recycle feed. The net result of this operation is a decrease in the coke production at equivalent conversions.

Coke Formed During Reactor Operations. The coke formation in the reactor can be divided into four categories: catalytic, cat-to-oil, carbon residue, and contaminant coke (CI-011). Catalytic coke results directly from the cracking of hydrocarbons on the acidic catalyst. Cat-to-oil coke is a measure of hydrocarbons retained by the pores in the catalyst. This coke can be reduced through use of an efficient steam stripping section.

Carbon residue is formed from heavy material in the gas oil feed. Included in the residue are asphaltenes, which are colloiddally dispersed amorphous molecules made up of carbon, hydrogen, oxygen, nitrogen, sulfur, vanadium and nickel. The asphaltenes have a molecular weight on the order of 3,000 to 5,000 (RE-141). Contaminant coke is coke resulting from catalyst poisoning by nitrogen bases and metals.

Coke formation in the reactor is dependent on the operating conditions, catalyst used, and feed materials. Coke formation is enhanced at elevated temperatures and pressures (GR-123). Other operating variables affecting the rate of coke formation are catalyst-to-oil ratios, space velocity, and process time.

Generally speaking, the more active catalysts will have less coke formation. This is mainly attributed to the higher conversion rates required for active catalysts which allow for greater space velocities. Feed materials containing heavy residues tend to promote coke formation. Heavier feeds also generally have more trace metals which deactivate catalysts and result in greater coke production.

Steam Stripping of Catalyst. After passing through the FCCU reactor section, the catalyst enters the steam stripping section for removal of entrained hydrocarbons. This is actually a displacement-type operation in which hydrocarbons retained in the porous catalyst are displaced by the steam. Steam stripping rates are carefully regulated to minimize dilution of the reactor products and to achieve maximum displacement of hydrocarbons (BU-079).

Hydrocarbons remaining after steam stripping are believed to be a major source of potentially hazardous air pollutants. The regenerator is operated at a higher temperature than the reactor-stripper and thus can potentially release many of the entrained hydrocarbons. Also, combustion gases release hydrocarbons in much the same manner as the stripping steam in displacing hydrocarbons from spaces in the catalyst bed.

Coke Burn-Off. Three basic mechanisms operating to release hazardous compounds from the coke into the regenerator off-gas are: (1) displacement, (2) volatilization, and (3) combustion. Specific hazardous compounds found in the off-gas because of these mechanisms can be predicted.

The displacement of hydrocarbons trapped in the catalyst pores is accomplished in much the same manner as in the stripping section of the reactor. The hydrocarbons are stripped or displaced by the upward flowing combustion gases. The elevated temperatures within the regenerator tend to enhance the stripping action. Table 2.2-14 lists hazardous compounds which could potentially be displaced. These compounds are representative of cracked products carried over in the catalyst from the reactor.

TABLE 2.2-14
THE FCCU REGENERATOR OFF-GAS
Potentially Hazardous Pollutants
Released by Displacement

<u>Pollutant</u>	<u>TLV (ppm)</u>	<u>Reference</u>
<u>Saturates</u>		
C ₂ -C ₈ n-Alkanes	100-600	HY-013, ME-108
Cyclopentane	-	ME-108
Cyclohexane	300	ME-108
Methylcyclohexane	400	ME-108
<u>Olefins</u>		
2-Methyl-1-butene	-	ME-108
3-Methyl-1-butene	-	ME-108
2-Methyl-2-butene	-	ME-108
1-Hexene	-	ME-108
<u>Monocyclic Aromatics</u>		
Benzene	10	ME-108
Toluene	100	ME-108
Ethylbenzene	100	ME-108
o-Xylene	100	ME-108
m-Xylene	100	ME-108
p-Xylene	100	ME-108
Isopropylbenzene	50	ME-108
1,3,5-Trimethylbenzene	35	ME-108
1,2,3-Trimethylbenzene	25	ME-108
<u>Polycyclic Aromatics</u>		
Naphthalene	10	HU-114
Biphenyl	0	HU-114
Anthracene	0.1 mg/m ³	HU-114
Phenanthrenes*	carcinogens	TY-008

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TABLE 2.2-14 THE FCCU REGENERATOR OFF-GAS (Cont.)

<u>Pollutant</u>	<u>TLV (ppm)</u>	<u>Reference</u>
<u>Polycyclic Aromatics</u> <u>(Cont.)</u>		
Benzofluorenes	carcinogens	TY-008
Benzanthracenes	carcinogens	TY-008
Pyrenes* (Benzo- phenanthrenes)	carcinogens	TY-008
<u>Heterocyclics</u>		
Thiophene	-	WO-025
Alkyl pyridines	-	LO-112
Quinoline	-	LO-112
Alkyl Quinoline	-	LO-112
<u>Phenols</u>		
Phenol	5	ME-108
o-Cresol	5	ME-108
m-Cresol	5	ME-108
p-Cresol	5	ME-108
<u>Trace Metals</u>		
Arsenic	-	PE-140
Cadmium	-	AN-104
Chromium	-	AN-104
Cobalt	-	AN-104
Copper	-	PE-140
Iron	-	PE-140
Lead	-	AN-104
Manganese	-	AN-104
Mercury	-	AN-104
Molybdenum	-	AN-104
Nickel	-	PE-140
Vanadium	-	PE-140
Zinc	-	PE-140

*Found in the gas oil feed and therefore potentially present in the regenerator.

The FCCU regenerator is operated typically some 85° to 110°C hotter than the reactor. At the increased temperatures, some of the heavy components layed down on the catalyst in the reactor are volatilized. Among the components identified in this stream are polycyclic aromatic hydrocarbons. Table 2.2-15 lists the hazardous components potentially released by volatilization.

The combustion of the coke-on-catalyst within the regenerator is a very complicated reaction. Not only are the usual combustion gases formed, but additional heavier hydrocarbons and nitrogen and sulfur compounds are released due to cracking of the agglomerated, amorphous coke structure. These heavier components may also combust after cracking from the coke. This afterburning, which may occur if excess oxygen is present, enhances the formation of CO₂, NO₂, and SO₃ over CO, NO, and SO₂. Afterburning is promoted by metal contaminants such as vanadium and nickel. Table 2.2-16 lists hazardous chemicals potentially formed during combustion in the regenerator.

The high temperature and excess oxygen in the regenerator provide a favorable oxidizing environment. As a result of this most of the trace metals which are listed in Table 2.2-14 will probably exit the regenerator in a simple, oxidized, inorganic form.

Sampling Point and Conditions

Sensible heat is recovered from the off-gases from the regenerator by means of a waste heat boiler. High boiling point materials in the off-gas can condense in the boiler. Some of this condensate is re-entrained in the gases and eventually emitted with the stack gases. The sample to be used in analyzing the gas composition is taken from the waste heat boiler stack as shown in Figure 2.2-7. The conditions in the stack are approximately 200°C and atmospheric pressure.

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TABLE 2.2-15
THE FCCU REGENERATOR OFF-GAS
Potentially Hazardous Pollutants
Released By Volatilization

<u>Pollutant</u>	<u>TLV (ppm)</u>	<u>Reference</u>
Perylenes	Carcinogens	HA-011
Benzo(a)pyrene	Carcinogen	TY-008
Benzo(e)pyrene	Carcinogen	TY-008
Benzo(ghi)perylene	Carcinogens	HA-011

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TABLE 2.2-16
THE FCCU REGENERATOR OFF-GAS
Potentially Hazardous Pollutants

Released from Combustion			
Pollutants	Flue Gas Concentration Cited in Literature (ppm)	TLV (ppm)	Reference
CO	0 - 78,000	50	DA-069
CO ₂	78,000 - 134,000	5,000	DA-069
SO ₂	308 - 2,190	5	DA-069
SO ₃ ¹	25.6	-	DA-069
COS	9 - 190	-	RE-142
CS ₂	0 - 2	2	RE-142
H ₂ S	0 - 12	10	RE-142
Mercaptans ²	60 - 169	0.5	RE-142
Aldehydes (as formaldehyde) ³	3 - 130	5	DA-069
Cyanides (as HCN) ⁴	0.19 - 0.94	10	DA-069
NO _x as NO ₂	8 - 394	5	DA-069
NO	11 - 310	25	DA-069
NH ₃	67 - 675	50	DA-069
HCl	Not Cited	5	PE-140
Formic Acid	Not Cited	5	DA-069
Acetic Acid	~12 ⁵	10	DA-069

Also various hydrocarbons and nitrogen and sulfur compounds resulting from cracking of the amorphous coke.

-
1. 1.0 mg/m³ as H₂SO₄
 2. Potentially methanethiol, ethanethiol, and 1- and 2-butanethiol
 3. Potentially formaldehyde and acetaldehyde
 4. Potentially HCN and methylcyanide
 5. Cited as organic acids in the effluent from a CO boiler

3.0 FUGITIVE EMISSIONS

Fugitive emissions are unique among the five refinery effluents selected for study in this program. By definition, fugitive emissions are not characteristic of any one emission source, but rather are representative of many, perhaps hundreds, of small leaks from process equipment. The extent of these emissions and the degree of hazard associated with a specific emitting area are determined in part by the process operating temperatures and pressure, the nature of compounds being processed (toxic, non-toxic, carcinogenic, etc.), and the general housekeeping in the process area. Good housekeeping comes down to the number of leaks the operator will allow in his process plant. Obviously, this is a highly variable, but very significant factor.

In this program, two sampling techniques were considered. One method is to sample the emission source in the process piping before the fugitive losses occur. The other method is to sample the emissions from the work environment or unit area after the emissions have been leaked into the atmosphere. There are advantages and disadvantages to each method. The process analysis was performed so that either of the two sampling methods could be considered in developing the sampling and analytical strategy.

3.1 Line Sampling

The first approach is based on drawing five samples from product lines leaving the atmospheric crude tower. These samples are representative of the heaviest (topped crude) to the lightest (off-gas) products leaving the tower. The rationale behind selecting these four liquid streams and the one gas stream is that all such material leaked from the operating equipment

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through pump seals, valves, etc. will ultimately vaporize, thus generating a "composite" fugitive emission characteristic of that area occupied by the atmospheric crude still. It was assumed, however, that a portion of the heaviest (highest boiling) hydrocarbons would not vaporize and thus would not contribute to fugitive air emissions.

The advantages of the line sampling method are as follows:

- 1) Sampling is simple and inexpensive.
- 2) Samples can be held for relatively long periods without degradation or reaction of components before analysis.
- 3) The sample contains potential pollutants in much higher concentration than do unit area samples which have been highly diluted with air.
- 4) Because of the fractionation that occurs in the crude tower, a certain amount of sample "pre-separation" is performed which benefits the analyst.

A disadvantage of line sampling is that it does not directly represent the hazardous components emitted at any given time. It is also necessary to apply emission factors to the process in question in order to determine the rough quantity of emissions expected.

3.2 Direct Fugitive Emission Sampling

The advantage of the fugitive emission sample is that samples are taken directly from the atmosphere in the emission area as the emissions are occurring. There are strong overriding disadvantages to this approach, however. These disadvantages are summarized as follows:

- 1) A network of relatively complicated unit area sampling stations must be set up, calibrated, and operated.
- 2) It is an expensive method.
- 3) It is unpredictable because of the strong effects of changing wind currents.
- 4) Long sampling periods are required because of the highly dilute samples being collected.
- 5) Reactions of sample components are likely because of long exposure in the air stream.
- 6) Background interference from other process units is highly likely.

Conclusion. The line sampling technique appears to be the more feasible approach for characterizing fugitive emissions from crude still process areas.

4.0 CRUDE OIL ANALYSIS

Crude oil is the primary source of chemicals in refinery products and by-products. The methods of characterizing crudes typically used in domestic refineries are outlined in this section.

4.1 General Characteristics

As a means of typifying domestic refinery crudes, average feedstock characteristics were determined based on both foreign and domestic crude production. The foreign crudes analyzed came from the seven leading exporting nations. Quantities of crudes from these sources in 1974 are shown in Table 4.1-1. These countries accounted for 91.2% of all U.S. oil imports. The average characteristics of the foreign crudes are based on the analyses of the major producing fields within the countries and also on their respective production rates. These fields and their yearly productions are given in Table 4.1-2.

The domestic fields used in the development of an average domestic crude are listed in Table 4.1-3. These fields were chosen on the basis of both production and location. The largest producing fields were selected as were fields from every major producing area. The total production from the fields chosen represents approximately 27% of the total U.S. production. The average domestic crude characteristics are based on the properties and production rates of this representative mix of crude oils.

The average characteristics of the domestic and foreign crudes and a combination of the averages are given in Table 4.1-4. The distillation data for these crudes is given

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TABLE 4.1-1
U.S. CRUDE OIL IMPORTS
FROM SELECTED COUNTRIES

<u>Country</u>	<u>1974 Crude Oil Imports</u> <u>(1,000 bbl)</u>	<u>% of Crude Imports</u>
Algeria	65,764	5.18
Canada	288,763	22.75
Indonesia	103,482	8.15
Iran	168,956	13.31
Nigeria	254,358	20.04
Saudi Arabia	159,827	12.59
Venezuela	116,437	9.17
Total	1,157,587	91.19
All Countries	1,269,155	100

Source: (US-209).

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TABLE 4.1-2
FOREIGN FIELDS USED TO DEFINE
AN AVERAGE FOREIGN CRUDE

<u>Country</u>	<u>Field</u>	<u>1970 Production</u> <u>(1,000 bbl)</u>
Algeria	Hassi Messaoud	144,185
Canada	Golden Spike	14,819*
	Swan Hills	10,437*
Indonesia	Minas	138,113
Iran	Agaha Jari	315,459
	Gach Saran	292,090
Nigeria	Meren	19,919
Saudi Arabia	Abquaiq	266,275
	Ghawar	553,845
	Safaniya	213,173
Venezuela	Bachaquero	282,552
	LaGunilles	322,639
	Lama	141,591
	Tia Juana	132,598

Source: (FE-100)

* 1969 production rates.

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TABLE 4 .1-3
DOMESTIC FIELDS USED TO DEFINE
AN AVERAGE UNITED STATES CRUDE

<u>State</u>	<u>Field</u>	<u>1974 Production (1,000 bbl)</u>	<u>% of Total U.S. Production</u>
Alaska	Swanson River	9,741	0.3186
California	Huntington Beach	19,035	0.6228
	Kern River	26,765	0.8757
	Wilmington	65,382	2.1394
Colorado	Rangely	20,284	0.6635
Louisiana	Calliou Island	18,023	0.5898
	Bay Marchano (Block 2)	32,632	1.0677
	Eugene Island (Block 330)	19,747	0.6461
	Grand Isle (Block 43)	20,999	0.6871
	West Delta (Block 30)	22,586	0.7392
Oklahoma	Sho-vel-tum	34,250	1.1208
Texas	Tom O'Connor (Dist. 2)	25,667	0.8397
	Hastings East and West (Dist. 3)	27,912	0.9132
	Conroe (Dist. 3)	21,737	0.7113
	Webster (Dist. 3)	24,762	0.8102
	Van and Van Shallow (Dist. 5)	16,264	0.5321
	East Texas (Dist. 6)	72,312	2.366
	Hawkins (Dist. 6)	39,630	1.2967
	Kelly-Snyder (dist. 8-9)	76,433	2.5010
	Seminole (Dist. 8-9)	20,102	0.6579
	Slaughter (Dist. 8-9)	47,033	1.5389
	Wasson (Dist. 8-9)	86,784	2.8397
	Yates (Dist. 8-9)	18,192	0.5954
	Spraberry Trend (Dist 8-9)	18,190	0.5951
Utah	Greater Altamont	21,898	0.7166
Wyoming	Salt Creek	13,284	0.4348
Source: (HE-119)		819,644	26.82

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TABLE 4.1-4
AVERAGE CRUDE OIL CHARACTERISTICS

	<u>United States Crude</u>	<u>Foreign Crude</u>	<u>Average Crude*</u>
Specific Gravity	0.8728	0.8552	0.8702
Wt% Sulfur	0.8625	0.8151	0.8511
Wt% Nitrogen	0.0840	0.0918	0.0866
Wt% Conradson Carbon			
- Residuum	8.268	8.168	8.263
- Crude	2.877	2.523	2.780

*Based on 70.65% United States crude and 29.35 % foreign crude.

Source: (FE-100, MC-154)

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in Table 4.1-5. The data used for determining the characteristics came from Bureau of Mines laboratories (FE-100, MC-154). Based on 1974 statistics the United States crudes accounted for 70.65% of the total refinery crudes used in the U.S. (US-209). This percentage was used to obtain weighted averages shown in Table 4.1-4. The calculated typical United States refinery crude feed distillation curve is plotted along with API° gravity and weight percent sulfur in Figure 4.1-1. This data was used in determining product flows in the representative refinery described in Section 1.0 of this appendix.

4.2 Specific Components

The specific components of the refinery crude and components formed during refinery operations were defined as completely as possible through literature data. Sources such as API Project No. 6, Project No. 48, and Project No. 52 were used in the definition. The general categories of the components included: (1) straight chain paraffins and olefins, (2) cyclic paraffins and olefins, (3) monoaromatics, (4) polyaromatics, (5) sulfur compounds, (6) nitrogen compounds, (7) phenols, (8) organic acids, (9) organic bases, (10) trace metals, and (11) salts. A complete list of the specific compounds and elements and their reference sources is given in Table B of this appendix.

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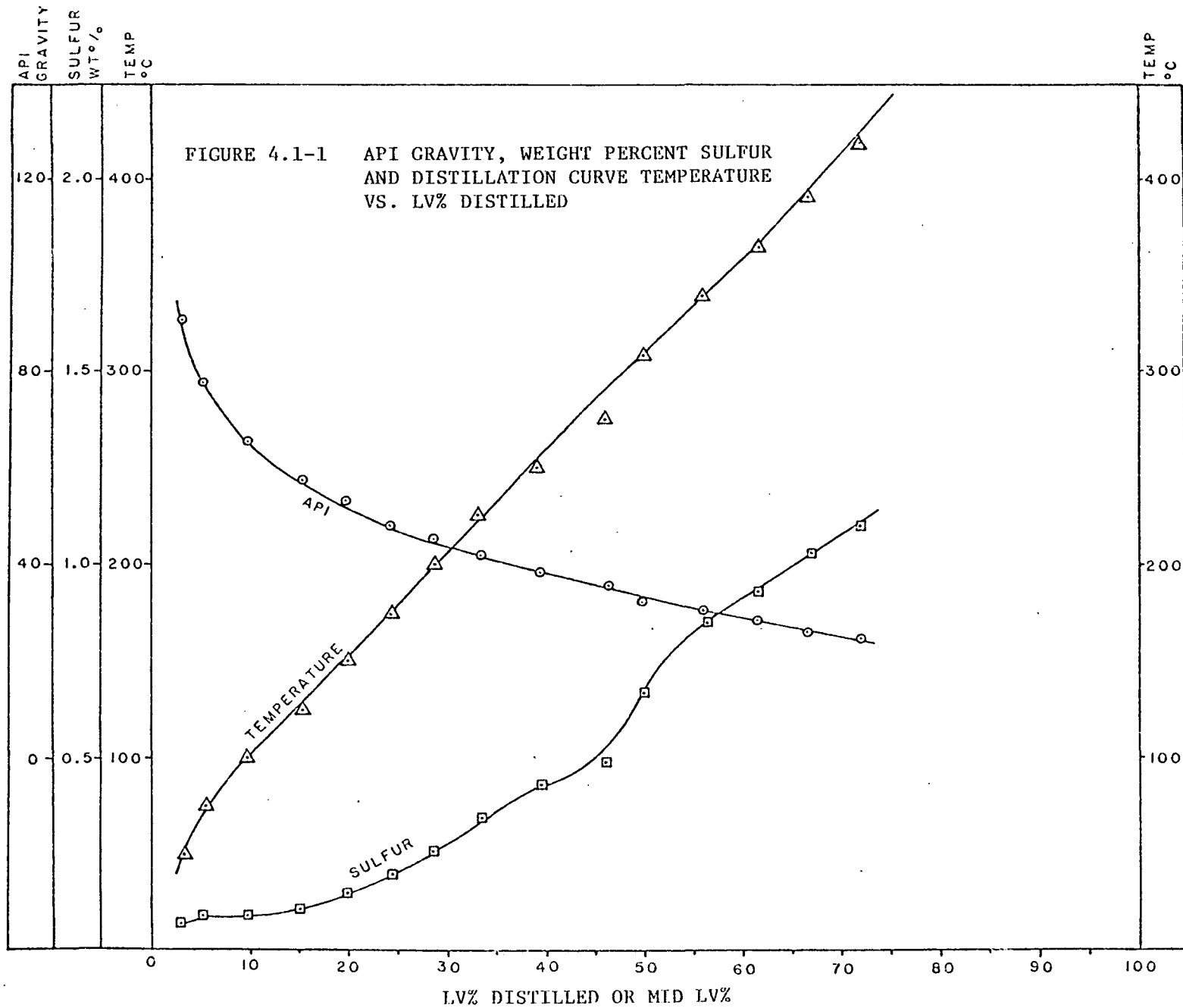
TABLE 4.1-5
DISTILLATION OF A
TYPICAL REFINERY CRUDE
(at 760 mm Hg)

Fraction No.	Cut Temp. °C	United States Crude		Foreign Crude		Average Crude*	
		Vol%	Sp.Gr.	Vol%	Sp.Gr.	Vol%	Sp.Gr.
1	50	1.164	0.6357	1.873	0.6402	1.372	0.6370
2	75	2.191	0.6812	2.611	0.6693	2.314	0.6777
3	100	4.321	0.7216	4.624	0.7158	4.410	0.7199
4	125	5.007	0.7492	5.731	0.7426	5.219	0.7473
5	150	4.528	0.7684	5.360	0.7631	4.772	0.7669
6	175	4.199	0.7919	5.165	0.7814	4.482	0.7888
7	200	4.107	0.8013	4.648	0.7956	4.265	0.7996
8	225	4.766	0.8186	4.844	0.8089	4.789	0.8157
9	250	5.866	0.8338	5.579	0.8244	5.782	0.8311
10	275	7.258	0.8507	5.810	0.8368	6.833	0.8466
11	308	3.460	0.8654	4.090	0.8553	3.645	0.8624
12	336	6.451	0.8753	5.883	0.8636	6.284	0.8719
13	364	5.846	0.8878	5.244	0.8767	5.669	0.8845
14	392	5.287	0.9028	5.799	0.8886	5.144	0.8986
15	419	5.589	0.9121	3.518	0.8976	4.981	0.9078
Residuum		28.785	0.9756	27.042	0.9743	28.274	0.9753

*Based on 70.65% United States Crude and 29.35% foreign crude.

Source: (FE-100, MC-154)

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5.0 CHEMICALS IDENTIFICATION AND CLASSIFICATION

This section includes the hazardous chemicals identified in this study and a complete listing of the components identified in the refinery streams. The components are listed in tabular form. Appropriate information concerning toxicity is included in Table A, Section 5.1.1. The complete component listing along with selected physical properties is given in Table B, Section 5.2.

5.1 Toxicity of Refinery Stream Compounds

The amount of data published on the toxicity of the specific components found in the refinery effluent streams is very large. This data is also sometimes hard to relate in terms which describe their specific degree of hazard to man. Due to these facts and the limited scope of this project, it is relatively impossible for this report to describe all known adverse biological effects of the components on man. A preliminary attempt was made, however, in defining the relative hazard of the known refinery chemicals resulting in the toxicity data and references given in Table A. The references listed in Section 5.3 are to be used if additional work is desired to determine more completely the toxicity along with the mutagenicity, teragenicity, or tumoricity of the refinery effluent components. Specific toxicity data was found for relatively few of the many compounds identified.

The toxicity data given in Table A is for airborne emissions only. The toxic chemicals are assumed absorbed into the body by inhalation or through the skin. No convenient method was found for classifying the relative hazard of the chemicals by ingestion. Generally, however, chemicals are less toxic by ingestion than by inhalation. Good examples of this are the

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carcinogens such as pyrene and benzo(a)pyrene. If additional research is desired, many references in Tables C, D, and E give information on the relative hazards of chemicals which are found in aqueous streams such as in the refinery.

5.1.1 Clasification Techniques

The primary toxicity indicator used in this report is the Threshold Limit Value (TLV). The American Conference of Governmental Industrial Hygienists (ACGIH) defines the TLV as "conditions under which it is believed that nearly all workers may be repeatedly exposed day after day, without adverse affect" (SA-175). For gases the TLV is given in parts per million (ppm). For fumes and mists and for some dusts the TLV is usually given as milligrams per cubic meter (mg/m^3).

N. Irving Sax in his book entitled Dangerous Properties of Industrial Materials rates hazardous compounds on a scale of zero to three (and U for material for which there is no known toxicology data) (SA-175). A explanation of the toxicity ratings is given in the following paragraphs:

U = Unknown. This designation is given to substances falling into one of the following categories:

No toxicity information could be found in the literature and none was known to the authors (Sax et al.).

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- Limited information based on animal experiments was available but in the opinion of the authors this information could not be applied to human exposures. In some cases this information is mentioned so that the reader may know that some experimental work has been done.
- Published toxicity data were felt by Sax to be of questionable validity.

0 = No Toxicity. This designation is given to materials which fall into one of the following categories:

- Materials which cause no harm under any conditions of use.
- Materials which produce toxic effects on humans only under the most unusual conditions or by overwhelming dosage.

1 = Slight Toxicity. This designation applies to the materials producing the following effects:

- Acute Local. Materials which on single exposures lasting seconds, minutes or hours cause only slight effects on the skin or mucous membranes regardless of the extent of the exposure.

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- Acute Systemic. Materials which can be absorbed into the body by inhalation or through the skin and which produce only slight effects following single exposures lasting seconds, minutes, or hours regardless of the quantity absorbed or the extent of exposure.

In general, those substances classified as having "slight toxicity" produce changes in the human body which are readily reversible and which will disappear following termination of exposure, either with or without medical treatment.

2 = Moderate Toxicity. This designation applies to materials producing the following effects:

- Acute Local. Materials which on single exposure lasting seconds, minutes or hours cause moderate effects on the skin or mucous membranes. These effects may be the result of intense exposure for a matter of seconds or moderate exposure for a matter of hours.
- Acute Systemic. Materials which can be absorbed into the body by inhalation or through the skin and which produce moderate effects following single exposures lasting seconds, minutes or hours.

Those substances classified as having "moderate toxicity" may produce irreversible as well as reversible changes in the human body. These changes are not of such severity as to threaten life or produce serious permanent physical impairment.

3 = Severe Toxicity. This designation applies to materials producing the following effects:

- Acute Local. Materials which on single exposures lasting seconds or minutes cause injury to skin or mucous membranes of sufficient severity to threaten life or to cause permanent physical impairment or disfigurement.

- Acute Systemic. Materials which can be absorbed into the body by inhalation or through the skin and which can cause injury of sufficient severity to threaten life following a single exposure lasting seconds, minutes or hours.

5.1.2 Criteria For Table A Compounds

For the purposes of the study the following criteria were used to define a compound as hazardous. First, any compound with a Threshold Limit Value will be hazardous. Secondly, all carcinogenic compounds in concentrations above ten ppb are considered hazardous. And finally, compounds which have a rating of two or three for either the acute local inhalation rating or the acute systemic inhalation rating or both will be hazardous in concentrations above one ppm.

Along with the TLV and Sax's rating system, additional comments are given in Table A. These comments are to aid the reader in drawing conclusions as to the relative toxicity of various components. This information includes data on the carcinogenic compounds, nature of the biological effect of the compound to man, and mention of the lack of toxicity data for certain compounds.

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TABLE A - TOXICITY OF REFINERY STREAM COMPOUNDS

Page 1 Compounds	TLV (ppm)	Acute Local Inhalation Rating	Acute Systemic Inhalation Rating	Comments	References
ALIPHATIC HYDROCARBONS					
Methane	10,000 ¹	0	1	An asphyxiant	PL-033, SA-175
Ethane	500	0	2	An asphyxiant	AM-030, SA-175
Propane	500	0	1	Hazardous to the eye	DR-039, SA-175, AM-131
Isobutane		0	1	An asphyxiant	SA-175
2,2-Dimethyl- propane		U	U	Probably irritant and narcotic in high concentrations	SA-175
n-Butane	500 (600 ²)	0	2	Simple asphyxiant, L.C. (rat) ¹³ = 658 mg/m ³	SA-175, DR-039, CH-217
2-Methylbutane				Same as n-pentane	SA-175
n-Pentane	600 ²	U	1	Narcotic in high concentrations, L.C. (mice) ¹³ = 13%	SA-175
Cyclopentane		U	2	High concentrations have narcotic action	SA-175
2,2-Dimethyl- butane		U	U	Probably is irritant and narcotic in high conc.	SA-175
2,3-Dimethyl- butane		U	U	Probably is irritant and narcotic in high conc.	SA-175
2-Methyl- pentane		U	U	May have narcotic or anesthetic properties	SA-175
3-Methyl- pentane		U	U	May have narcotic or anesthetic properties	SA-175
n-Hexane	100	1	1	Toxic concentration for man is 1,400 ppm	SA-175, CH-217
Cyclohexane	300		2	Can cause skin irritation	SA-175
2,4-Dimethyl- pentane		U	U	Probably irritant and narcotic in high concentrations	SA-175
2,3-Dimethyl- pentane		U	U	Probably irritant and narcotic in high concentrations	SA-175
n-Heptane	400			Toxic concentration for man is 1,000 ppm	SA-175, CH-217
Methylcyclo- hexane	400 ²	U	2	L.C. ¹³ (rabbit) = 15,000 ppm	SA-175
2,4-Dimethyl- hexane		U	U	Probably irritant and narcotic in high concentrations	SA-175
2,3-Dimethyl- hexane		U	U	Probably irritant and narcotic in high concentrations	SA-175
2,2,4-Trimethyl- pentane		1	2	High concentrations can cause narcosis	SA-175
2-Methyl- heptane				Same as 2,2,4-Trimethylpentane	SA-175
Cycloheptane		U	U	May be narcotic, moderate toxicity	SA-175

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)
Page 2

Compounds	TLV (ppm)	Acute Local Inhalation Rating	Acute Systemic Inhalation Rating	Comments	References
ALIPHATIC HYDRO- CARBONS (Cont.)					
2,2,5-Trimethyl- hexane		U	U		SA-175
n-Octane	360 ²	0	2	May act as an asphyxiant, narcotic in high concentrations	SA-175
trans-Decahydro- naphthalene	50	2	2	Irritating to skin and eyes, may cause kidney damage	SA-175
n-Undecane		U	U		SA-034
n-Dodecane		U	U	Probably irritant and narcotic in high concentrations	HA-264
n-Tridecane				Low Toxicity	HA-264
n-Hexadecane		U	U		SA-175
OLEFINS					
Ethene		0	2	High concentrations cause anesthesia, L.C. (mice) 13 = 95% in air	SA-175
Propene		0	2	A simple asphyxiant	SA-175
Isobutene				A simple asphyxiant	SA-175
1-Butene				An asphyxiant	SA-175
cis & trans- 2-Butene		U	U	May act as a simple asphyxiant	SA-175
3-Methyl-1- Butene		2	2	Narcotic in high concentrations, an asphyxiant	SA-175
1-Pentene	1,000 ¹	2	2	Narcotic in high concentrations, an asphyxiant	SA-175, SA-034
2-Methyl- 1-Butene		2	2	Narcotic in high concentrations, an asphyxiant	SA-175
cis & trans- 2-Pentene		U	U	Probably narcotic in high concentra- tions	SA-175
2-Methyl- 2-Butene		2	3	Narcotic in high concentrations, an asphyxiant	SA-175
1,3-Butadiene		2	2	Inhalation in high concentrations can cause unconsciousness and death	SA-175
4-Methyl- 2-Pentene		U	U	Probably irritant and narcotic in high concentrations	SA-175
2-Methyl- 2-Pentene		U	U		SA-175
2-Methyl- 1-Pentene		U	U	Probably irritant and narcotic in high concentrations	SA-175
1-Hexene		2	2		SA-175
2-Hexene		U	U	Animal experiments show low toxicity	SA-175

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)
Page 3

Compounds	TLV (ppm)	Acute Local Inhalation Rating	Acute Systemic Inhalation Rating	Comments	References
OLEFINS (Cont.)					
n-Heptene		U	U		SA-175
3-Ethylhexene				2-Ethyl C ₆ * has an acute systemic inhalation rating of 2	SA-175
n-Octene		U	U		SA-175
Cyclohexene	300	2	2	Extreme fire hazard, 50 mg/l is toxic for animals	SA-175, FA-092
Cyclopentene				Cyclopentadiene has a TLV = 75 ppm	SA-175
Methylcyclohexene		U	U	Probably irritant and narcotic in high conc.	SA-175
C ₃ +dicycloolefins				Dicyclo pentadiene has a TLV = 5 ppm	SA-175
MONOAROMATICS					
Benzene	10 ²	1	2	Eye irritant, L.D. (rat) ¹⁴ = 4080 mg/kg	SA-175, AM-131, CH-217
Toluene	100	1	2	Eye irritant, narcotic in high concentrations	SA-175, AM-131
Ethylbenzene	100	1	2	Eye irritant, L.D. (rat) ¹³ = 4,000 ppm, 0.2% causes dizziness to humans.	SA-175, AM-131, CH-217
o,m,p-Xylene	100	1	2	Eye irritant, L.D. (rat) ¹⁴ = 4 g/kg	SA-175, AM-131
Isopropylbenzene	50	1	3	L.C. (mice) = 2,000 ppm, nerve depressant	SA-175, CH-217, SA-034
n-Propylbenzene				Limited animal experiments show moderate acute vapor toxicity, L.C. (mice) ¹³ = 0.4%	SA-175
1,3,5-Trimethylbenzene	35	U	3	Narcotic and causes disturbances in the blood	SA-175, PL-033, DR-039
1,2,3-Trimethylbenzene	25				SA-175, AM-030
1,2,4-Trimethylbenzene	25	1	2	Can cause CNS depression, anemia, or bronchitis	SA-175
1-Methyl-4-Isopropylbenzene	50 ¹			L.D. (rat) = 5,000 mg/kg	CH-217, GE-066
1,2,3,4-Tetrahydronaphthalene	25 ¹	2	2	An irritant, narcotic in high concentrations	SA-175, PL-033, GE-066
t-Butylbenzene		U	U	May be similar to ethylbenzene	SA-175
Isobutylbenzene		U	U	Probably irritant and narcotic in high concentrations	SA-175

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)

Page 4

Compounds	TLV (ppm)	Acute Local Inhalation Rating	Acute Local Inhalation Rating	Comments	References
MONOAROMATICS (Cont.)					
sec-Butylbenzene		U	U	May be similar to ethylbenzene	SA-175
1-Methyl-4-Isobutylbenzene				1-Methyl-4-t-Butylbenzene has a TLV = 10 ppm	SA-175
PHENOLS					
Phenol	5	3	3	Eye irritant, affects mainly the central nervous system	SA-175, AM-131
o,m,p-Cresol	5	2	2	Eye irritant, less severe than phenol	SA-175, AM-131
1,3,5,-Xylenol				Eye irritant, L.D. (rat) ¹⁴ = 444 mg/kg	CH-217, AM-131
Naphthol		2	2	Eye irritant, L.D. (rabbit) ¹⁴ = 9 g/kg	SA-175
m-Ethylphenol				Similar toxicity to phenol	SA-175
o-Ethylphenol		1		A chemical preservative food additive	SA-175
2,6-Di-tert-butyl-p-cresol				Limited animal experiments suggest low toxicity	SA-175
POLYNUCLEAR AROMATICS					
Naphthalene	10	2	2	Eye irritant, may cause many types of systemic disorders	SA-175, AM-131
Anthracene	0.1 mg/m ³	1	U	A recognized carcinogen of the skin, eye irritant	SA-175, PL-033, AM-131
Phenanthrene		1	U	Causes skin photosensitization and is a carcinogen	SA-175
Biphenyl	0.2	U	2	Experimentally in animals causes paralysis and convulsions	SA-175
1-Methylnaphthalene				Details unknown, see 2-Methylnaphthalene	SA-175
2-Methylnaphthalene				Limited animal experiments suggest high toxicity	SA-175
Perylene				Highly toxic, a suspected carcinogen	SA-175
Benzo(a)-pyrene				A strong carcinogen	KO-059
Benzo(e)-pyrene				A carcinogen	HA-011
Methylcholanthrene				A carcinogen	TY-008
Benzanthracenes				A carcinogen	KO-059
Chrysene				A carcinogen	KO-059
Indole				A carcinogen	HA-264

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)

Compounds	TLV (ppm)	Acute Local Inhalation Rating	Acute Systemic Inhalation Rating	Comments	References
POLYNUCLEAR AROMATICS (Cont.)					
Pyrene (Benzo-phenanthrene)				A carcinogen	SA-175
Fluoranthene				Limited animal experiments suggest moderate toxicity, a carcinogen	SA-175, TY-008
Benzo(a)fluorenes				A carcinogen	TY-008
Benzo(g,h,i)-perylene				A carcinogen	SA-168
SULFUR COMPOUNDS					
H ₂ S	10	3	3	An irritant and an asphyxiant	SA-175
Methanethiol	0.5	2	2	In air L.C. (rats) ¹³ = 12	SA-175
Ethanethiol	0.5	2	2	L.D. (mouse) ¹⁴ = 25 mg/kg	CH-217, SA-175
1-Propanethiol		U	U	Probably toxic	SA-175
2-Propanethiol		U	U	Probably toxic	SA-175
1-Butanethiol	0.5	2	2		SA-175
2-Butanethiol	0.5	2	2		SA-175
3-Methyl-2-Thiobutane				(Isopropyl mercaptan) Toxic	SA-175
Thiophene				Animal experiments suggest moderate toxicity, L.D. (rabbits) = 830 mg/kg	SA-175
2-Methylthiophene				L.D. (mouse) ¹⁴ = 500 mg/kg	CH-217
3-Methylthiophene				L.D. (mouse) ¹⁴ = 500 mg/kg	CH-217
Mercaptans (in general)		3	3	High concentrations can produce unconsciousness	SA-175
CYANIDES					
HCN	10	2	3	Trace protoplasmic poisons	SA-175, AM-030
Methylcyanide				Highly toxic, L.D. (rats) ¹⁴ = 3.8 g/kg	SA-175
Cyanides (in general)	5 mg/m ³ ¹⁰	1	3	Inhibits tissue oxidation and caused death through asphyxia	SA-175, AM-030
ACIDS AND ANHYDRIDES					
Acids:					
Formic	5	2	2	Irritant to the mucous membrane	SA-175, AM-030
Acetic	10	2	U	Caustic, irritating, can cause burns, dermatitis, and ulcers	SA-175, HA-264

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)

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Compound	TLV (ppm)	Acute Local Inhalation Rating	Acute Systemic Inhalation Rating	Comments	References
ACIDS AND ANHYDRIDES (Cont.)					
Propionic		2		Data based on animals show low toxicity	SA-175
Isobutyric		2		Data based on limited animal experiments	SA-175
n-Butyric		1	1	A synthetic flavoring substance and adjuvant	SA-175
n-Pentanoic		U	U	Animal experiments suggest low toxicity and high irritation	SA-175
2-Methylpentanoic		U	U		SA-175
n-Hexanoic		3	1	Data based on animal experiments	SA-175
n-Heptanoic		U	U	Limited animal experiments suggest low toxicity	SA-175
n-Octanoic		U	U	Experimental data suggest low toxicity	SA-175
n-Nonanoic		U	U	Limited data suggest low toxicity and high skin irritation	SA-175
n-Decanoic				Limited animal experimentation suggest moderate toxicity and irritation	SA-175
Benzoic Acid		1		A chemical preservative food additive	SA-175
Naphthoic		2	2		SA-175
Hydrochloric	5	3	3	Irritant to mucous membranes of the eye and respiratory tract	SA-175
Anhydrides: Dimethylmaleic				Maleic anhydride has a TLV = 0.25	SA-175
Amines					
Ammonia	25	3	U	Irritating to eyes and mucous membranes of the respiratory tract	SA-175
Monocethylamine	3	2	2	L.D. (rat) ¹⁴ = 2 g/kg	SA-175
CARBONYL COMPOUNDS					
Formaldehyde	2	3	3	Irritant, suspected carcinogen of the lung	SA-175
Aldehydes (in general)		3	2	Possesses anaesthetic properties, irritants, low molecular weights are most toxic	SA-175

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)

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Compound	TLV (ppm)	Acute Local Inhalation Rating	Acute Systemic Inhalation Rating	Comments	References
COMBUSTION GASES					
CO ₂	5,000	0	1	A simple asphyxiant	SA-175
CO	50	0	3	Inhibits the blood from carrying oxygen	SA-175
COS		1	3	Narcotic in high concentrations	SA-175
NO	25	3	3	Irritant, may cause pulmonary edema	SA-175
NO ₂	5			Highly toxic, see NO above	SA-175
SO ₂	5	3	U	Eye irritant, can cause edema of the lungs	SA-175
SO ₃		3	U	Sulfuric acid (H ₂ SO ₄) has a TLV of 1.0 mg/m ³	SA-175
CS ₂	20	1	3	Mainly toxic to the central nervous system	SA-175
H ₂ S	10	3	3	Both an irritant and an asphyxiant	SA-175
Mercaptans				See SULFUR COMPOUNDS in this table	
Aldehydes				See CARBONYL COMPOUNDS in this table	
Cyanides				See CYANIDES in this table	
HETEROCYCLICS					
Thiophene				Animal experiments suggest moderate toxicity, L.D. (rabbits) ¹⁴ = 830 mg/kg	SA-175
2-Methyl-thiophene				L.D. (mouse) ¹⁴ = 500 mg/kg	CH-217
3-Methyl-thiophene				L.D. (mouse) ¹⁴ = 500 mg/kg	CH-217
2-Methyl-pyridine ¹²				A respiratory irritant, L.D. (rats) ¹⁴ = 1.4 g/kg	SA-175
3-Methyl-pyridine ¹²		U	U	See 2-Methylpyridine	SA-175
4-Methyl-pyridine ¹²		U	U	See 2-Methylpyridine	SA-175
2,6-Dimethyl-pyridine ¹²		U	U	See 2-Methylpyridine	SA-175
4-Ethyl-pyridine ¹²		U	U	See 2-Methylpyridine	SA-175
Methyl-ethyl-pyridine ¹²				Variable, some isomers highly toxic, some not	SA-175
Quinoline		U	3	May produce retinitis, L.D. (rats) ¹⁴ = 460 mg/kg	SA-175
2-Methyl-quinoline		3	3	Data based on animal experiments	SA-175
Pyrrole		U	2	L.D. (mice) ¹⁴ = 60.5 g/kg	SA-175

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)
Page 8

Compound	TLV ³ (mg/m ³)	Acute Local Inhalation Rating ⁴	Acute Systemic Inhalation Rating ⁴	Comments	References
TRACE ELEMENTS					
Ag	0.01			Can cause argyria ⁶ , irritant to skin and mucous membrane	SA-175, DR-039
Al		0	0	Generally not regarded as an industrial poison	SA-175
As	0.5	3	3	Causes systemic irritation	SA-175, AM-030
Au				Low toxicity	SA-175
B	10 ⁷	2	U	Not highly toxic and therefore not considered an industrial poison	SA-175
Ba	0.5	1	3	Barium salts are somewhat caustic, BaO is toxic	SA-175, AM-030
Be	0.002	3	3	Leads to lung deterioration	SA-175, PL-033, DR-039
Ca		1	U	Generally toxic when combined with a toxic anion	SA-175
Cd	0.1	3	3	Highly irritant, can degenerate kidneys, suspected carcinogen	SA-175, TH-080, PL-033
Co	0.1		1	TLV based on metal dust and fumes, suspected carcinogen	SA-175, AM-030
Cr	0.1	3	U	Corrosive action on the skin and mucuous membranes	SA-175, PL-033, DR-039
Cu	0.1	1	2	Metal oxide fumes in animals have caused extensive systemic damage	SA-175, DR-039
Fe	10			Harmful to certain body tissues, some compounds are suspected carcinogens	SA-175, HA-264
Ga				Low toxicity	SA-175
Hg (organic)	0.01	3	3	Alkyl mercury is highly toxic, aryl mercury is less toxic	SA-175, AM-030
K		3	U	Toxicity is almost always that of the anion	SA-175
La		U	1	Leads to hemorrhages and liver damage	SA-175
Mg	15	1	2	The toxicity of Mg compounds is usually dependent on the anion	SA-175, AM-130
Mn	5	U	2	Damages central nervous system	SA-175, PL-033
Mo	5	1	U	May be somewhat toxic, but no known fatalities	SA-175, AM-130
Na				Variable, sodium ion is practically non-toxic	SA-175
Nd				Probably moderately toxic	SA-175
Ni	0.5	1	3	Generally not a cause of systemic poisoning, a recognized carcinogen	SA-175
P	0.1			Most toxic by ingestion, less toxic by inhalation	SA-175, DR-039
Pb	0.15	0	3	Common industrial poison, suspected carcinogen	SA-175, AM-030

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)

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Compound	TLV ³ (mg/m ³)	Acute Local Inhalation Rating ⁴	Acute Systemic Inhalation Rating ⁴	Comments	References
TRACE ELEMENTS (Cont.)					
Rb				Toxicity of rubidium compounds is almost always that of the anion.	SA-175, AM-030
S				Variable, depends on the specific material	SA-175
Sb	0.5		3	Causes deterioration of the liver in animals, an irritant	SA-175, TH-080
Se	0.1	2	2-3	Some organoselenium compounds have high toxicity	SA-175, AM-130, TH-080
Si		2 ⁹	0 ⁹	Chief cause of pulmonary dust disease	SA-175
Sn	2			Alkyl tin compounds may be highly toxic and produce skin rashes	SA-175, AM-030
Sr				Has a low order of toxicity	SA-175
Ti		1	U	Considered physiologically inert	SA-175
U	0.05			A recognized carcinogen and highly toxic on an acute basis	SA-175, PL-033, DR-039
V	0.05 ^b	0	1	Variable toxicity but mainly irritants	SA-175
Zn	5 ⁵			Zinc compounds generally have low toxicity	SA-175, AM-030
Zr	5			Most compounds are insoluble and considered inert	SA-175, AM-130
INORGANIC SALTS					
Al ⁺⁺⁺				Generally not considered an industrial poison	SA-175
Ba ⁺⁺		1	3	Barium salts are somewhat toxic, irritant to eyes, nose and throat	SA-175
Bc ⁺⁺		3	3	Causes dermatitis and skin ulcers	SA-175
Ca ⁺⁺		1	U	Generally toxic when combined with a toxic anion	SA-175
Cd ⁺⁺				See toxicity data for Cd as a trace element	SA-175

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TABLE A-TOXICITY OF REFINERY STREAM COMPOUNDS (Cont.)

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Compound	TLV mg/m ³	Acute Local Inhalation Rating ⁴	Acute Systemic Inhalation Rating ⁴	Comments	References
Inorganic Salts (Cont.)					
Br ⁻		2		Produce depression and in severe cases mental deterioration	SA-175
Cl ⁻				Varies widely, some have low toxicity, some high	SA-175
CN ⁻	5	1	3	Inhibits tissue oxidation and causes death through asphyxia	SA-175, AM-030
F ⁻	2.5	3	3	Generally highly irritant and toxic	SA-175
SO ₄ ⁼				Variable, toxicity generally determined by cation	SA-175
S ⁼		2	2	Irritant, is rapidly oxidized to sulfate L.D. (fish) ¹⁴ = 1-6 ppm in water	SA-175, BE-147
Fe ⁺⁺				Irritant, L.D. (rat) ¹⁴ = 900 mg/kg estimated L.D. (man) ¹⁴ = 400 mg/kg	SA-175
K ⁺		3	0	Toxicity is almost always that of the anion	SA-175
Li ⁺		2	2	High central nervous system toxicity	SA-175
Hg ⁺⁺		1	2	Toxicity is usually determined by the anion	SA-175
Na ⁺				Variable, sodium ion is practically non-toxic	SA-175
Ni ⁺⁺	0.1 ⁴			Many nickel compounds are recognized carcinogens	SA-175

¹ Approximate value

² New proposed TLV values which should be considered trial limits that will remain in the listing for a period of at least two years (from 1974).

³ TLV for pure metal elements unless otherwise stated.

⁴ Based on metal compounds not pure metals.

⁵ As ZnO

⁶ As V₂O₅ fumes. V₂O₅ dust has a TLV of 0.5 mg/m³.

⁷ As boron oxide.

⁸ Argyria is a general greying of the skin pigment due to long exposures (2 to 25 years) of silver compounds.

⁹ For silica dioxide.

¹⁰ 5 mg/m³ as - CN.

¹¹ Given as the ions which are potentially present.

¹² Pyridine has a TLV = 5 ppm (SA-175).

¹³ L.C. (Lethal Concentration) is the statistical concentration of the particular compound which is required to kill 50% of an infinite population of the test animal stated.

¹⁴ L.D. (Lethal Dose) is a statistical estimate of the oral dosage necessary to kill 50% of an infinite population of the test animal stated.

APPENDIX B

5.2 Components in Refinery Streams

Table B is a collection of specific compounds reported to be present in various refinery streams. Physical properties and concentrations of these compounds, where such data are known, are also listed. Literature sources for the table entries are provided.

Explanations of the table headings are given in the following paragraphs:

Component. All individual compounds are listed under class headings in the order of increasing boiling points. The two exceptions to this rule are the combustion gases and the trace elements. In these cases the components are listed alphabetically according to their symbols or formulas.

Molecular weight. Molecular weights were obtained from standard references (CH-134, HA-264).

Boiling points. Atmospheric boiling points were found in the standard references (CH-134, HA-264) or from references citing component concentration data. All temperatures are listed in degrees centigrade.

Solubility. Water solubilities for the components were also found in the same references (CH-134, HA-264). The varying degrees of solubility are indicated by the following symbols: insoluble (IS), slightly soluble (SS), soluble (S), very soluble (VS), miscible (M), decomposes (D). The temperature is assumed to be room temperature unless it is noted as cold water (CW) or hot water (HW). Solubilities of many components will be affected by temperature and pH.

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Concentration. Literature values for concentrations are listed usually as volume per cent of the stream in which they are found. In many cases a concentration range is given because of different literature sources or because different processes affect the stream. The ranges always include the maximum and minimum values found. Some other terms used to describe the concentration are weight per cent (wt), parts per million (ppm), micrograms per milliliter ($\mu\text{g/ml}$) or per gram ($\mu\text{g/g}$) and nanograms per gram (ng/g). Where the concentrations of components were not available, the following designations are used: probably present (p), identified (i), and trace amounts (t).

Stream. The streams in which the components were identified were grouped into major refinery streams and numerically identified as follows:

1. Crude
2. Naphtha
3. Distillate
4. Gas Oil
5. Resid
6. Catalytically Cracked Naphtha
7. Blended Gasoline
8. Cracked Still Gasoline
9. Reformate
10. Deasphalted Oil
11. Claus Plant Feed
12. Catalytic Cracker Off-gas
13. API Separator Wastewater

Reference. The reference number identifies the data source from which concentration data was obtained.

APPENDIX B

TABLE B
IDENTIFIED COMPONENTS OF REFINERY STREAMS

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Acids and Anhydrides</u>						
Hydrochloric	36	-85	VS	0.0009-0.022 wt. %	3	PE-140
Formic	46	101	M	i	1	LO-112
Acetic	60	118	M	i	1	LO-112
Propanoic	74	141	M	i	1	LO-112
2-Methylpropanoic	88	153	VS	i	1	LO-112
n-Butanoic	88	163	M	i	1	LO-112
2,2-Dimethylpropanoic	102	164	SS	i	1	LO-112
2-Methylbutanoic	102	176	SS	i	1	LO-112
				i	13	BU-159
3-Methylbutanoic	102	177	S	i	1	LO-112
				i	13	BU-159
Methylethylacetic	102			p	1	LO-112
Trimethylacetic	102			p	1	LO-112
n-Pentanoic	102	186	S	i	1	LO-112
				i	13	BU-159
2-Methylpentanoic	116		SS	i	1	LO-112
				i	13	BU-159
3-Methylpentanoic	116	199		i	1	LO-112
				i	13	BU-159
4-Methylpentanoic	116	200	SS	i	1	LO-112
				i	13	BU-159
n-Hexanoic	116	205	IS	i	1	LO-112
				i	13	BU-159
3-Ethylpentanoic	130	212		i	1	LO-112
Cyclopentanecarboxylic	114	214	SS	i	1	LO-112
2-Methylhexanoic	130	215	M	i	1	LO-112
3-Methylhexanoic	130			i	1	LO-112
5-Methylhexanoic	130	216	SS	i	1	LO-112
4-Methylhexanoic	130	217	SS	i	1	LO-112
2-Methylcyclopentane- carboxylic	114			i	1	LO-112
3-Methylcyclopentane- carboxylic	114			i	1	LO-112
Cyclohexanecarboxylic	114	232	SS	i	1	LO-112
n-Heptanoic	130	233	SS	i	1	LO-112
				i	13	BU-159

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Acids and Anhydrides (cont)</u>						
Cyclopentaneacetic	128			i	1	LO-112
3-Methylcyclopentane- acetic	142			i	1	LO-112
1,2,2-Trimethylcyclo- pentanecarboxylic	142			i	1	LO-112
n-Octanoic	144	239	SS-HW	i	1	LO-112
				i	13	BU-159
2,3-Dimethylcyclo- pentaneacetic	156			i	1	LO-112
Chaulmoogric	280	247	IS	p	1	LO-112
Benzoic	122	249	SS	i	13	BU-159
n-Nonanoic	158	255	IS	i	1	LO-112
6-Methyloctanoic	158	(250-260)		i	13	BU-159
p-Hexahydrotoluic	128			i	1	LO-112
2-Methylbenzoic	136	258-9	IS	i	13	BU-159
n-Decanoic	172	270	SS	i	1	LO-112
1,2,2-Trimethylcyclopentane-1,3-dicarboxylic	172			i	1	HU-114
2,4-Dimethylbenzoic	150	Sublimes @ 267	SS	i	13	BU-159
3-Methylbenzoic	136	Sublimes @ 275	SS	i	13	BU-159
2,6-Dimethylbenzoic	150	275	SS	i	13	BU-159
2,4,5-Trimethylbenzoic	164		SS-HW	i	13	BU-159
2,4,6-Trimethylbenzoic	164		SS	i	13	BU-159
3,4,5-Trimethylbenzoic	164		SS-HW	i	13	BU-159
Naphthoic	172	>300	SS-HW	i	13	BU-159
Methylnaphthoic	186			i	13	BU-159
Dimethylnaphthoic	200			i	13	BU-159
Dimethylmaleic	144			i	1	HU-114
Hydronocarpic				p	1	LO-112
Bicyclic acids				p	1	LO-112
Dimethylmaleic anhydride	126	223	SS	i	1	LO-112

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Amines</u>						
Ammonia	17	-33	VS	i	11	ME-107
				67-675 ppm	12	DA-069
Monoethanolamine	61	170	M	i	11	ME-107
<u>Inorganic Salts</u>						
Sulfates (as Na ₂ SO ₄)				<0.0031 wt. %	1	PE-140
Chlorides (as NaCl)				0.043 wt. %	1	PE-140
				<0.068 wt. %	3	PE-140
Other Salts ¹ (Ca+Mg)				0.026 wt. %	1	PE-140
<u>Carbonyl Compounds</u>						
<u>Ketones and Aldehydes</u>						
Acetyl-1-isopropyl- methylcyclopentane	168			0.0005 wt. %	1	BR-217
Alkylfluorenones		320-330		i	1	LA-162
Formaldehyde	30	-21	S	i	12	DA-069
<u>Combustion Gases</u>						
CO	28	-190	SS	0.01	11	GR-145
				0-78,000 ppm	12	DA-069
CO ₂	44	Sublimes @ 78	S	1.45	11	GR-145
				78,000-134,000 ppm	12	DA-069
COS	60	-50	S	0.02	11	GR-145
				9-140 ppm	12	RE-142
CS ₂	76	46	SS	0.01	11	GR-145
				0-2 ppm	12	RE-142
H ₂	2	-252	SS	0.50	11	GR-145
H ₂ O	18	100	M	18.57	11	GR-145
N ₂	28	-196	SS	0.08-0.66	1	DU-082
NO	30	-88	SS	i	11	DA-069
				11-310 ppm	12	DA-069
NO ₂	48	21	S-CW	i	11	DA-069
NO _x (as NO ₂)				8-394 ppm	12	DA-069

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Carbonyl Compounds (cont)</u>						
<u>Combustion Gases (cont)</u>						
O ₂	32	-183	S	7.39	11	GR-145
SO ₂	64	-10	S	0.89	11	GR-145
				308-2190 ppm	12	DA-069
SO ₃	80	45	D	25.6 ppm	12	DA-069
<u>Heterocyclic</u>						
<u>Pyridines</u>						
Pyridine(s) ²	79	115	M	i	1,3,6	PE-140, BA-325
2-Methylpyridine	93	129	VS	i	6	BA-325
3-Methylpyridine	93	144	M	i	3,6	BA-325
4-Methylpyridine	93	145	M	i	6	BA-325
2,6-Dimethylpyridine	107	146	M	i	3,6	BA-325
2,5-Dimethylpyridine	107	157	VS-HW	i	3,6	BA-325
2,4-Dimethylpyridine	107	159	VS	i	3,6	BA-325
2,3-Dimethylpyridine	107	163	S	i	3,6	BA-325
3,4-Dimethylpyridine	107	164	SS	i	6	BA-325
4-Ethylpyridine	107	168	S	i	6	BA-325
2,3,4-Trimethylpyridine	121			i	3	BA-325
2,4,6-Trimethylpyridine	121	170	S	i	6	BA-325
3,5-Dimethylpyridine	107	172	S	i	6	BA-325
2,3,6-Trimethylpyridine	121	177	S-HW	i	6	BA-325
2-Methyl-5-ethylpyridine	121	178	SS-HW	i	6	BA-325
2-Methyl-4-ethylpyridine	121	179	S	i	6	BA-325
2-Methyl-6-ethylpyridine	121			i	6	BA-325
3-Methyl-5-ethylpyridine	121			i	3	BA-325
2,3,5-Trimethylpyridine	121	187	SS	i	3	BA-325
3-Cyclopentylpyridine	147			i	3	BA-325
4-Cyclopentylpyridine	147			i	3	BA-325
5,6,7,8-Tetrahydroquino- line	133	222	SS	i	3	BA-325
2,3-Dimethyl-6-isopropyl- pyridine	147			i	3	BA-325
dl-2-sec-Butyl-4,5- dimethylpyridine	163			i	3	BA-325

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Heterocyclic (cont)</u>						
<u>Pyridines (cont)</u>						
2,4-Dimethyl-6-(2,2,6-Trimethylcyclohexyl)-pyridine	231			i	3	BA-325
<u>Pyrroles</u>						
Pyrrole(s) ²	67	130	SS	i	1	PE-140
<u>Cyclic Sulfides</u>						
Thiacyclopentane	88	121		0.000077 wt. %	1	GR-123
				8	2	BA-324
2-Methylthiacyclopentane	102	133		0.0023 wt. %	1	GR-123
				i	2	BA-324
3-Methylthiacyclopentane	102	139		0.191 wt. %	3	BI-057
				0.00046 wt. %	1	GR-123
				i	2	BA-324
Thiacyclohexane	102	142		0.504 wt. %	3	BI-057
				0.00032 wt. %	1	GR-123
				i	2	BA-324
trans-2.5-Dimethylthiacyclopentane	116	142		0.122 wt. %	3	BI-057
				0.0025 wt. %	1	GR-123
cis-2,5-Dimethylthiacyclopentane	116	142		i	2	BA-324
				0.0024 wt. %	1	GR-123
				i	2	BA-324
2,4-Dimethylthiacyclopentane	116	148		0.344 wt. %	3	BI-057
2,3-Dimethylthiacyclopentane	116	148		0.516 wt. %	3	BI-057
2,5-Dimethylthiacyclopentane	116			i	1	HA-317
2-Methylthiacyclohexane	116	153		0.0029 wt. %	1	GR-123
				i	2	BA-324
				i	3	BI-057
2-Ethylthiacyclopentane	116	156		0.055-0.29 wt. %	3	BI-057
2,3,5-Trimethylthiacyclopentane	130	156		i	1	HA-317
				0.49-1.24 wt. %	3	BI-057
3-Methylthiacyclohexane	116	158		0.000024 wt. %	1	GR-123
				i	2	BA-324
				0.069 wt. %	3	BI-057

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Heterocyclic (cont)</u>						
<u>Cyclic Sulfides (cont)</u>						
4-Methylthiacyclohexane	116	159		0.000048 wt. % i	1 2	GR-123 BA-324
3,4-Dimethylthiacyclohexane and/or	130	164		0.014-0.4 wt. % i	3 1	BI-057 HA-317
2,3,4-Trimethylthiacyclopentane	130	164		0.73 wt. % i	3 1	BI-057 HA-317
2,6-Dimethylthiacyclohexane and/or	130	164		i	1	HA-317
2-Methyl-5-ethylthiacyclopentane	130	164		0.52 wt. % i	3 1	BI-057 HA-317
3-Methyl-4-ethylthiacyclopentane and/or	130	180		i	1	HA-317
3-Isopropylthiacyclopentane	130	180		0.60 wt. % i	3 1	BI-057 HA-317
2,3-Dimethyl-5-ethylthiacyclopentane and/or	144	180		i	1	HA-317
2,4-Diethylthiacyclopentane and/or	144	180		0.30 wt. % i	3 1	BI-057 HA-317
2,3,6-Trimethylthiacyclopentane	130	180				
2,5-Dimethyl-3-ethylthiacyclopentane and/or	144	180		i	1	HA-317
2,3-Diethylthiacyclopentane	144	180		0.18 wt. % i	3 1	BI-057 HA-317

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Heterocyclic (cont)</u>						
<u>Bicyclic Sulfides</u>						
2-Thia[3.3.0]bicyclo- octane	128			i	1	HA-317
8-Thia[3.2.1]bicyclo- octane	128	187-91		i	3	BI-057
cis-1-Thiahydrindane	142			i	3	BI-057
trans-1-Thiahydrindane	142			i	3	BI-057
3-Methyl-2-thia[3.3.0]- bicyclooctane	142			i	1	HA-317
or						
6-Thia[4.3.0]bicyclo- nonane	142			i	1	HA-317
4-Methyl-2-thia[3.3.0]- bicyclooctane	142			i	1	HA-317
2-Thia[4.3.0]bicyclo- nonane	142			i	1	HA-317
3,4-Dimethyl-2-thia [3.3.0]bicyclooctane	156			i	1	HA-317
4-Ethyl-2-thia[3.3.0]- bicyclooctane	156			i	1	HA-317
or						
9-Methyl-6-thia[4.3.0]- bicyclononane	156			i	1	HA-317
Thiadamantane				0.034 wt. %	3	BI-057
<u>Thiophenes</u>						
Thiophene	84	84		i	1	HA-317
2-Methylthiophene	98	112	IS	i	1,6	HA-317, MC-157
3-Methylthiophene	98	115	IS	i	1,6	HA-317, MC-157
2-Ethylthiophene	112	134	IS	i	6	MC-157
3-Ethylthiophene	112	136	IS	i	6	MC-157
2,3-Dimethylthiophene	112	141	IS	i	6	MC-157
3,4-Dimethylthiophene	112			i	6	MC-157
2,3,4-Trimethylthiophene	126	175-8		i	1,3	HA-317 BI-057

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Heterocyclic (cont)</u>						
<u>Thiophenes (cont)</u>						
2,4-Dimethyl-3-ethyl- thiophene	140	187-91		i	3	BI-057
3,4-Dimethyl-2-ethyl- thiophene	140	187-91		i	3	BI-057
2,3-Dimethyl-4-ethyl- thiophene	140	193		0.03-0.05 wt. %	1,3	HA-317, BI-057
2,3,4,5-Tetramethyl- thiophene	140	193		0.4 wt. %	1,3	HA-317, BI-057
2,3,4-Trimethyl-5-ethyl- thiophene	154			i	1	HA-317
3,4,5-Trimethyl-2-ethyl- thiophene	154	205		i	3	BI-057
<u>Others</u>						
Tricyclic sulfides				p	1	DO-074
Tetracyclic sulfides				p	1	DO-074
Pentacyclic sulfides				p	1	DO-074
Hexacyclic sulfides				p	1	DO-074
Thienobicyclic sulfides				p	1	DO-074
Thienotricyclic sulfides				p	1	DO-074
Thienotetracyclic sul- fides				p	1	DO-074
Thienopentacyclic sul- fides				p	1	DO-074
Thienohexacyclic sul- fides				p	1	DO-074
<u>Hydrocarbons</u>						
<u>Aliphatic</u>						
Methane	16	-161	S	i	1	RO-188
				39.2-44.8	8	GR-123
Ethane	30	-89	IS	i	1	RO-188
				16.2-21	8	GR-123
Propane	44	-42	S	i	1	RO-188
				0.13	6	ME-108

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aliphatic (cont)</u>						
Propane				7.4-16.2	8	GR-123
2-Methylpropane	58	-12	IS	i	1	RO-188
				0.2	2	CA-227
				0.08-0.81	6	CA-227, ME-108
n-Butane	58	-1	S	i	1	RO-188
				2.1	2	CA-227
				0.77-3.1	6	CA-227
2,2-Dimethylpropane	72	9	IS	0.045	6	CA-227
2-Methylbutane	72	28	IS	i	1	RO-188
				4.29	2	CA-227
				19.9	6	CA-227
n-Pentane	72	36	IS	i	1	RO-188
				5.41	2	CA-227
				1.14-16.0	6	ME-108, CA-227
Cyclopentane	70	49	IS	0.05	1	RO-188
				0.14-1.3	2	RO-189
				0.2-1.09	6	RO-189, CA-227
2,2-Dimethylbutane	86	50	IS	0.04	1	RO-188
				0.11-0.8	2	RO-189
				0.2	6	RO-189
2,3-Dimethylbutane	86	58	IS	0.08-0.1	1	RO-188, TO-039
				0.08-1.5	2	SM-094, RO-189
				0.28-3.2	6	CA-227
2-Methylpentane	86	60	IS	0.37-0.65	1	RO-188, TO-039
				1.1-5.9	2	RO-189
				1.71-10.2	6	ME-108, CA-227

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aliphatic (cont)</u>						
3-Methylpentane	86	63	IS	0.2-0.35	1	TO-039,
				1.04-3.6	2	RO-188
				1.31-6.5	6	RO-189
						ME-108,
						CA-227
n-Hexane	86	69	SS	1.8	1	RO-188
				2.4-7.7	2	RO-189,
						CA-227
				0.43-5.95	6	ME-108,
						CA-227
Methylcyclopentane	84	72	IS	0.87	1	RO-188
				2.6-3.7	2	RO-189,
						CA-227
				1.3-3.9	6	CA-227,
						RO-189
2,2-Dimethylpentane	100	79	IS	0.02	1	RO-188
				0.06-1.4	2	RO-189
				0.35-0.9	6	CA-227,
						RO-189
2,4-Dimethylpentane	100	80	IS	0.08	1	RO-188
				0.11-14	2	CA-227,
						RO-189
				0.22-0.9	6	ME-108,
						RO-189
2,2,3-Trimethylbutane	100	81	IS	t	2	RO-189
Cyclohexane	84	81	IS	0.71	1	RO-188
				1.83-10.7	2	RO-189
				0.25	6	CA-227
3,3-Dimethylpentane	100	86	IS	t	2	RO-189
				0.13	6	CA-227
1,1-Dimethylcyclo-	98	88		0.16	1	RO-188
pentane				0.43-7.0	2	RO-189
				0.04-0.2	6	CA-227,
						RO-189

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aliphatic (cont)</u>						
2,3-Dimethylpentane	100	90	IS	0.15	1	RO-188
				0.21-9.2	2	RO-189
				0.088-3.6	6	ME-108, RO-189
2-Methylhexane	100	90	IS	0.73	1	RO-188
				2.18-9.2	2	RO-189
				<0.77-3.6	6	ME-108, RO-189
1,trans-3-Dimethylcyclopentane	98	91		0.87	1	RO-188
				1.09-7.0	2	CA-227, RO-189
				0.13-3.7	6	CA-227, RO-189
1,cis-3-Dimethylcyclopentane	98	92		0.21	1	RO-188
				0.63-7.0	2	RO-189
				<0.36-3.7	6	ME-108, RO-189
3-Methylhexane	100	92	IS	0.51	1	RO-188
				<0.45-9.2	2	RO-189
				0.77-2.5	6	ME-108, RO-189
1,trans-2-Dimethylcyclopentane	98	92		0.48	1	RO-188
				1.44-7.0	2	RO-189
				1.45-3.7	6	CA-227, RO-189
3-Ethylpentane	100	93	IS	0.06	1	RO-188
n-Heptane	100	98	IS	0.18-1.5	2	RO-189
				2.3	1	RO-188
				3.3-7.0	2	RO-189, CA-227
2,2,4-Trimethylpentane	114	99	IS	0.46-1.3	6	ME-108, RO-189
				t	2	RC-189
				1.65 wt. %	6	PU-033

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APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aliphatic (cont)</u>						
1, cis-2-Dimethylcyclopentane	98	99		t	1	RO-189
				t	2	RO-189
				0.11-0.33	6	ME-108, CA-227
Methylcyclohexane	98	101	IS	1.6	1	RO-188
				0.35-17.5	2	RO-188, RO-189
				1.3-2.6	6	CA-227, RO-189
Ethylcyclopentane	98	103	IS	0.16	1	RO-188
				0.06-2.2	2	SM-094, RO-189
				0.26-0.6	6	CA-227, RO-189
1,1,3-Trimethylcyclopentane	112	105		0.30	1	RO-188
				1.6-2.2	2	CA-277, RO-189
				0.061-0.4	6	ME-108, RO-189
2,2-Dimethylhexane	114	107	IS	0.01	1	RO-188
				0.03-2.4	2	RO-189
				0.1	6	RO-189
2,5-Dimethylhexane	114	109	IS	0.06	1	RO-188
				0.165-2.4	2	RO-189
				0.2-0.6	6	ME-108, RO-189
1, trans-2, cis-4-Tri- methylcyclopentane	112	109		0.22	1	RO-188
				0.66	2	RO-189
				0.072	6	ME-108
2,4-Dimethylhexane	114	109	IS	0.06	1	RO-188
				0.16-2.4	2	RO-189
				0.11-0.6	6	ME-108, RO-189

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aliphatic (cont)</u>						
2,2,3 Trimethylpentane	114	110	IS	0.004	1	RO-188
				0.012	2	RO-189
				1.15 wt. %	6	PU-033
1,trans-2,cis-3-Tri- methylcyclopentane	112	110		0.26	1	RO-188
				0.78	2	RO-189
				0.057	6	ME-108
3,3-Dimethylhexane	114	112	IS	0.03	1	RO-188
				0.09	2	RO-189
				<0.8	6	RO-189
2,3,4-Trimethylpentane	114	113	IS	0.005	1	RO-188
				0.015	2	RO-189
1,1,2-Trimethylcyclo- pentane	112	114		0.06	1	RO-188
				0.18	2	RO-189
				0.01	6	ME-108
2,3,3-Trimethylpentane	114	115	IS	0.006	1	RO-188
				0.018	2	RO-189
2,3-Dimethylhexane	114	116	IS	0.07	1	RO-188
				4.0	2	RO-189
				0.10-0.8	6	ME-108, RO-189
2-Methyl-3-ethylpen- tane	114	116	IS	0.06	1	RO-188
				0.18	2	RO-189
				<0.8	6	RO-189
1,cis-2,trans-4-Tri- methylcyclopentane	112	117		0.01	1	RO-188
				0.03-0.096	2	RO-189, ME-108
1,cis-2,trans-3-Tri- ethylcyclopentane	112	117		0.07	1	RO-188
				0.21	2	RO-189
				0.019	6	ME-108
1,cis-2,cis-4-Trimeth- ylcyclopentane	112	117		t	1	RO-189
				t	2	RO-189
				0.035	6	ME-108

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APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aliphatic (cont)</u>						
B-111	1-Methyl-cis-3-ethyl- cyclopentane	112	121	<0.12	1	RO-188
				<0.36	2	RO-189
				<0.28	6	ME-108
	1-Methyl-trans-2-ethyl- cyclopentane	112	121	0.14	1	RO-188
				0.42	2	RO-189
				0.021	6	ME-108
	1-Methyl-1-ethylcyclo- pentane	112	122	0.03	1	RO-188
				0.09	2	RO-189
	1,1,cis-3,trans-4-tetra- methylcyclopentane	126	122	0.04	1	RO-188
				0.12	2	RO-189
	2,2,4,4-Tetramethyl- pentane	128	123	t	1	RO-189
				t	2	RO-189
	1,cis-2,cis-3-trimethyl- cyclopentane	112	123	t	1	RO-189
				t	2	RO-189
	1,trans-2-Dimethylcyclo- hexane	112	123	IS	1	RO-188
				0.93-1.2	2	RO-189,
				0.05-3.15	6	CA-227 ME-108,
	2,2,5-Trimethylhexane	128	124	IS	1	RO-188
				0.002	2	RO-189
				0.006	6	PU-033
	1,cis-4-Dimethylcyclo- hexane	112	124	IS	1	RO-188
				0.09	2	RO-189
				0.27	6	ME-108
	1,trans-3-Dimethylcy- clohexane	112	124	IS	1	RO-188
				0.07	2	RO-189
				0.21	6	ME-108
	n-Octane	114	126	IS	1	RO-188
				1.9	2	RO-189
				5.7	6	ME-108,
	Isopropylcyclopentane	112	126	0.22	6	PU-033
				0.01	1	RO-188
				0.03	2	RO-189
				0.022	6	ME-108

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aliphatic (cont)</u>						
2,2,4-Trimethylhexane	128	127		t	1	RO-189
				t	2	RO-189
1,trans-2,cis-3,trans-4-Tetramethylcyclopentane	126	127		0.11	1	RO-188
				0.33	2	RO-189
1-Methyl-cis-2-ethylcyclopentane	112	128		0.04	1	RO-188
				0.12	2	RO-189
				0.031	6	ME-108
1,cis-2-Dimethylcyclohexane	112	130	IS	0.06	1	RO-188
				0.18	2	RO-189
				0.004	6	ME-108
n-Propylcyclopentane	112	131		0.06	1	RO-188
				0.18	2	RO-189
2,3,5-Trimethylhexane	128	131		0.03	1	RO-188
				0.09	2	RO-189
				0.09 wt. %	6	PU-033
Ethylcyclohexane	112	132	IS	0.37	1	RO-188
				1.1-2.3	2	RO-189, CA-227
2,6-Dimethylheptane	128	135		0.05	1	RO-188
				0.15	2	RO-189
1,1,3-Trimethylcyclohexane	126	137		0.2	1	RO-188
				0.6	2	RO-189
2,3-Dimethylheptane	128	140		0.05	1	RO-188
				0.15	2	RO-189
4-Methyloctane	128	142	IS	0.1	1	RO-188
				0.3	2	RO-189
2-Methyloctane	128	143	IS	0.4	1	RO-188
				1.2	2	RO-189
3-Methyloctane	128	144		0.1	1	RO-188
				0.3	2	RO-189
n-Nonane	128	151	IS	1.8	1	RO-188
				5.4	2	RO-189
				0.7	6	RO-189

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aliphatic (cont)</u>						
4-Methylnonane	142	166		0.1	1	RO-188
				0.3	2	RO-189
2-Methylnonane	142	167		0.3	1	RO-188
				0.9	2	RO-189
3-Methylnonane	142	168		0.1	1	RO-188
				0.3	2	RO-189
n-Decane	142	174	IS	1.8	1	RO-188
				5.4	2	RO-189
trans-Decahydro- naphthalene	138	187		i	1	RO-188
n-Undecane	156	196	IS	1.6	1	RO-188
n-Dodecane	170	216	IS	1.4	1	RO-188
n-Tridecane	184	235	IS	1.2	1	RO-188
				i	4	RO-189
n-Tetradecane	198			1.0	1	RO-188
				i	4	RO-189
n-Pentadecane	212			0.8	1	RO-188
				i	4	RO-189
n-Hexadecane	226	287	IS	0.7	1	RO-188
				i	4	RO-189
n-Heptadecane	240	302	IS	0.6	1	RO-188
				i	4	RO-189
n-Octadecane	254	316	IS	i	1	RO-188
n-Nonadecane	268	330	IS	i	1	RO-188
n-Eicosane	282	343	IS	i	1	RO-188
n-Heneicosane	296	357	IS	0.32	1	GR-123
n-Docosane	310	369	IS	0.28	1	GR-123
n-Tricosane	324	380	IS	0.24	1	GR-123
n-Tetracosane	338	391	IS	0.21	1	GR-123

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Olefins</u>						
Ethene	28	-104	IS	4.0	8	GR-123
Propene	42	-47	IS	7.4-14.2	8	GR-123
2-Methyl-1-propene	56	-7		0.05-0.91	6	CA-227, ME-108
1-Butene	56	-6	IS	0.14-0.64	6	CA-227, ME-108
1,3-Butadiene	54	-4	IS	<1.3	8	GR-123
trans-2-Butene	56	1	IS	0.77-1.35	6	CA-227, ME-108
cis-2-Butene	56	4	IS	1.05	6	ME-108
1,2-Butadiene	54	10	IS	<1.3	8	GR-123
3-Methyl-1-butene	70	20	IS	0.23	6	CA-227, PU-033
1-Pentene	70	30	IS	0.81-1.20	6	CA-227, ME-108
2-Methyl-1-butene	70	31	IS	0.71-2.93	6	ME-108, CA-227
trans-2-Pentene	70	36	IS	0.43-3.54	6	ME-108, CA-227
cis-2-Pentene	70	37	IS	3.97	6	ME-108, PU-033
2-Methyl-2-butene	70	39	IS	4.61-6.66	6	ME-108, CA-227
3,3-Dimethyl-1-butene	84	41	IS	0.21	6	ME-108
1,3-Pentadiene	68	42		0.05 wt. %	6	PU-033
Cyclopentene	68	44	IS	0.4-0.69	6	ME-108, CA-227
3-Methyl-1-pentene	84	41	IS	<0.53	6	CA-227
4-Methyl-1-pentene	84	54	IS	0.27-0.53	6	ME-108, CA-227
2,3-Dimethyl-1-butene	84	56		0.53-0.98	6	CA-227; ME-108
4-Methyl-2-pentene	84	56	IS	0.91	6	CA-227, PU-033

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Olefins (cont)</u>						
2-Methyl-1-pentene	84	61	IS	0.61-1.76	6	ME-108, CA-227
1-Hexene	84	63	IS	0.14-0.57	6	CA-227, ME-108
Methylcyclopentenenes	82	64-76		0.75	6	ME-108
2-Ethyl-2-butene	84			0.51 wt. %	6	PU-033
2-Ethyl-1-butene	84	65	IS	0.25-0.99	6	ME-108, CA-227
3-Methyl-1-cyclopentene	82	65		0.67	6	CA-227
4-Methyl-1-cyclopentene	82	66		<0.53	6	CA-227
3-Hexene	84	66-67	IS	<1.79	6	ME-108
3-Methyl-2-pentene	84	67-70	IS	0.49-2.55	6	CA-227, ME-108
2-Methyl-2-pentene	84	67		0.85-1.97	6	ME-108, CA-227
2-Hexene	84	68-69	IS	<1.79	6	ME-108
4,4-Dimethyl-1-pentene	98	72		0.18 wt. %	6	PU-033
2,3-Dimethyl-2-butene	84	73-77		0.08	2	CA-227
				0.40	6	ME-108, PU-033
2,2-Dimethylpentenes	98	73-77		0.006	6	ME-108
1-Methyl-1-cyclopentene	82	75		<0.53	6	CA-227
2,4-Dimethylpentenes	98	81-83	IS	0.11	6	ME-108, PU-033
Cyclohexene	82	83	IS	0.015-0.11	6	ME-108, CA-227
2,3-Dimethylpentenes	98	84-97	IS	0.48	6	ME-108, PU-033
3-Methylhexenes	98	84-94		<1.42	6	ME-108
3-Ethylpentenes	98	85-95		0.13	6	ME-108
2-Methylhexenes	98	86-95		1.24	6	ME-108

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Olefins (cont)</u>						
1,3-Dimethylcyclopentenes	96	92	IS	<1.58	6	ME-108
n-Heptenes	98	93-98		1.2	6	ME-108
2-Ethylpentenes	98	94		<1.42	6	ME-108
Ethylcyclopentenes	96	98-107		0.26	6	ME-108
3-and 4-Methyl-1-cyclohexene	96	102		0.44	6	CA-227
Trimethylpentenes	112	102-116		<0.41	6	ME-108
Dimethylhexenes	112	102-122		<0.41	6	ME-108
Methylcyclohexenes	96			0.42	6	ME-108
1,2-Dimethylcyclopentenes	94	106		<1.58	6	ME-108
1,1-Dimethylcyclopentenes	96			0.012	6	ME-108
1-Methyl-1-cyclohexene	96	110		0.13	6	CA-227
3-Ethylhexenes	112	110-121		0.088	6	ME-108
3-Methylheptenes	112	111-122		0.73	6	ME-108
2-Methylheptenes	112	112-122		0.45	6	ME-108
4-Methylheptenes	112	112-122		0.40	6	ME-108
n-Octenes	112	122-126		0.23	6	ME-108
1,3-Dimethylcyclohexenes	110	127		<0.15	6	ME-108
1,4-Dimethylcyclohexenes	110	128		<0.15	6	ME-108
1,2-Dimethylcyclohexenes	110	138		<0.15	6	ME-108
1,1-Dimethylcyclohexenes	110			0.051	6	ME-108
Trimethylcyclopentenes	110			0.48	6	ME-108
1-Methyl-1-ethylcyclopentenes	110			0.047	6	ME-108
1-Methyl-2-ethylcyclopentenes	110			0.14	6	ME-108
<u>Aromatics</u>						
Benzene	78	80	SS	0.15	1	RO-188
				0.20-1.23	2	CA-227,
						RO-189
				0.21-1.8	6	ME-108,
						RO-189
				0.536 wt. %	9	NA-231

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aromatics (cont)</u>						
Toluene	92	111	IS	0.51 0.988-7.37	1 2	RO-188 CA-227, RO-189
				1.26-8.5	6	CA-227, RO-189
Ethylbenzene	106	136	IS	7.77 wt. % 0.19 0.19-0.93	9 1 2	NA-231 RO-188 RO-188, RO-189
				1.07	6	ME-108
p-Xylene (1,4-Dimethylbenzene)	106	138	IS	3.35 wt. % 0.10 0.50-1.78 0.84-3.4	9 1 2 6	NA-231 RO-188 RO-189 ME-108, RO-189
m-Xylene (1,3-Dimethylbenzene)	106	139	IS	3.69 wt. % 0.51 1.93-6.1 2.30-8.8	9 1 2 6	NA-231 RO-188 RO-189 ME-108, RO-189
o-Xylene (1,2-Dimethylbenzene)	106	144	IS	8.58 wt. % 0.27 0.88-2.04 1.20-4.0	9 1 2 6	NA-231 RO-188 RO-189 ME-108, RO-189
Isopropylbenzene	120	152	IS	4.82 wt. % 0.07 0.12-0.33 0.18-0.4	9 1 2 6	NA-231 RO-188 RO-189 ME-108, RO-189
n-Propylbenzene	120	159	IS	0.335 wt. % 0.09 0.28-0.46 0.16-0.4	9 1 2 6	NA-231 RO-188 RO-189 ME-108, RO-189
				1.34 wt. %	9	NA-231

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aromatics (cont)</u>						
1-Methyl-3-ethylbenzene	120	161	IS	0.17	1	RO-188
				0.57-1.47	2	RO-189
				<3.6	6	RO-189
1-Methyl-4-ethylbenzene	120	162	IS	3.6 wt. %	9	NA-231
				0.06	1	RO-188
				0.26-0.49	2	RO-189
				<3.6	6	RO-189
1,3,5-Trimethylbenzene	120	165	IS	1.74 wt. %	9	NA-231
				0.12	1	RO-188
				0.32-1.34	2	RO-189
				<2.5	6	RO-189
				1.94 wt. %	9	NA-231
1-Methyl-2-ethylbenzene	120	165	IS	0.09	1	RO-188
				0.24-0.32	2	RO-189
				<2.5	6	RO-189
tert-Butylbenzene	134	169	IS	1.41 wt. %	9	NA-231
				0.01	1	RO-188
				0.02-0.05	2	RO-189
				<3.6	6	RO-189
1,2,4-Trimethylbenzene	120	169	IS	0.51	1	RO-188
				1.18-2.56	2	RO-189
				3.6	6	RO-189
				6.97 wt. %	9	NA-231
Isobutylbenzene	134	173	IS	i	1	RO-188
				0.20 wt. %	9	NA-231
sec-Butylbenzene	134	173	IS	i	1	RO-188
				0.20 wt. %	9	NA-231
1-Methyl-3-isopropylbenzene	134	175	IS	i	1	RO-188
				0.27 wt. %	9	NA-231
1,2,3-Trimethylbenzene	120	176	IS	0.12	1	RO-188
				1.47 wt. %	9	NA-231
1-Methyl-4-isopropylbenzene	134	177	IS	0.067 wt. %	9	NA-231
1-Methyl-2-isopropylbenzene	134	178	IS	t	9	NA-231

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aromatics (cont)</u>						
Indan	118	178	IS	0.003	1	RO-188
				0.60 wt. %	9	NA-231
1,3-Diethylbenzene	134	181	IS	0.47 wt. %	9	NA-231
1-Methyl-3-n-propylben- zene	134	181		i	1	RO-188
				1.27 wt. %	9	NA-231
n-Butylbenzene	134	183	IS	i	3	RO-189
				0.47 wt. %	9	NA-231
1-Methyl-4-n-propyl- benzene	134	183		i	3	RO-189
				<0.74 wt. %	9	NA-231
1,2-Diethylbenzene	134	183	IS	i	1	RO-188
				i	3	RO-189
				0.067 wt. %	9	NA-231
1,3-Dimethyl-5-ethylben- zene	134	184		i	3	RO-189
				1.14 wt. %	9	NA-231
1,4-Diethylbenzene	134	184	IS	i	3	RO-189
				<0.74 wt. %	9	NA-231
1-Methyl-2-propyl- benzene	134	185		i	1	RO-188
				i	3	RO-189
				0.47 wt. %	9	NA-231
1-Phenyl-2,2-dimethyl- propane	148	186		i	3	RO-189
1,4-Dimethyl-2-ethyl- benzene	134	187		i	1	RO-188
				i	3	RO-189
				0.80 wt. %	9	NA-231
2-Methylindan	132	187		<0.067 wt. %	9	NA-231
1-Methylindan	132	188-190		<0.067 wt. %	9	NA-231
1,3-Dimethyl-4-ethyl- benzene	134	188		i	1	RO-188
				i	3	RO-189
				0.74 wt. %	9	NA-231

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aromatics (cont)</u>						
1-Phenyl-3-methylbutane	148	188		i	3	RO-189
1-Methyl-3-tert-butyl- benzene	148	189		i	3	RO-189
1,2-Dimethyl-4-ethyl- benzene	134	190		i	1	RO-188
				i	3	RO-189
				1.34 wt. %	9	NA-231
1,3-Dimethyl-2-ethyl- benzene	134	190		i	1	RO-188
				i	3	RO-189
				t	0	NA-231
3-Phenylpentane	148	191		i	3	RO-189
2-Phenyl-2-methylbutane	148	192		i	3	RO-189
1-Ethyl-3-isopropylben- zene	148	192		i	3	RO-189
				0.064 wt. %	9	NA-231
2-Phenyl-3-methylbutane	148			i	3	RO-189
1-Ethyl-2-isopropylben- zene	148	193		i	3	RO-189
				0.17 wt. %	9	NA-231
B-120 1-Methyl-4-tert-butyl- benzene	148	193	IS	i	3	RO-189
2-Phenylpentane	148	193		i	3	RO-189
1,2-Dimethyl-3-ethyl- benzene	134	194		i	1	RO-188
				i	3	RO-189
				0.268 wt. %	9	NA-231
1-Methyl-3-isobutyl- benzene	148	194		i	3	RO-189
1-Methyl-3-sec-butyl- benzene	148	194	IS	i	3	RO-189
				0.16 wt. %	9	NA-231
1,3-Dimethyl-5-isopro- pylbenzene	148	194		i	3	RO-189
				0.085 wt. %	9	NA-231
1-Methyl-4-sec-butyl- benzene	148	195		i	3	RO-189
1-Methyl-4-isobutyl- benzene	148	196		i	3	RO-189

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aromatics (cont)</u>						
1-Methyl-2-sec-butyl- benzene	148	196	IS	i 0.06 wt. %	3 9	RO-189 NA-231
1-Methyl-2-isobutyl- benzene	148	196		i	3	RO-189
1,4-Dimethyl-2-isopro- pylbenzene	148	196		i t	3 9	RO-189 NA-231
1-Ethyl-4-isopropyl- benzene	148	196		i 0.007 wt. %	3 9	RO-189 NA-231
1-Methyl-4-sec-butyl- benzene	148	197	IS	i 0.039 wt. %	3 9	RO-189 NA-231
1-Phenyl-2-methyl- butane	148	197		i	3	RO-189
1,3-Dimethyl-2-isopro- pylbenzene	148	197		i	3	RO-189
1,3-Dimethyl-4-isopro- pylbenzene	148	197		i 0.01 wt. %	3 9	RO-189 NA-231
1,2,4,5-Tetramethyl- benzene	134	197	IS	i i	1 3	RO-188 RO-189
				0.74 wt. %	9	NA-231
1,2,3,5-Tetramethyl- benzene	134	198	IS	i i	1 3	RO-188 RO-189
				1.07 wt. %	9	NA-231
1-Phenyl-3-methylbutane	148	199		i	3	RO-189
1-Methyl-2-tert-butyl- benzene	148	200		i	3	RO-189
1-Methyl-3,5-diethylben- zene	148	200		i	3	RO-189
				0.21 wt. %	9	NA-231
1-Ethyl-3-n-propylben- zene	148	201		i	3	RO-189
				0.27 wt. %	9	NA-231
1,3-Dimethyl-5-n-propyl- benzene	148	202		i	3	RO-189
1,2,-Dimethyl-4-isopro- pylbenzene	148	202		i	3	RO-189
5-Methylindan	132	202		0.40 wt. %	9	NA-231
1-Methyl-2,3-diethyl- benzene	134	202		i	3	RO-189

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aromatics (cont)</u>						
1,2-Dimethyl-3-isopropylbenzene	148	203		i	3	RO-189
1-Methyl-3,4-diethylbenzene	148	203		i	3	RO-189
1-Ethyl-2-n-propylbenzene	148	203		i	3	RO-189
1-Methyl-3-n-butylbenzene	148	204	IS	0.06 i	; 3	RO-188 RO-189
1,4-Dimethyl-2-propylbenzene	148	204	IS	i	3	RO-189
4-Methylindan	132	204		i	1	BA-325
1,2,3,4-Tetramethylbenzene	134	205	IS	0.87 wt. % 0.2 i	9 1 3	NA-231 RO-188 RO-189
1-Ethyl-4-n-propylbenzene	148	205	IS	0.34 wt. % i	9 3	NA-231 RO-189
1-Methyl-2,4-diethylbenzene	148	205		i	3	RO-189
n-Pentylbenzene	148	205		i	3	RO-189
1,3-Dimethyl-4-n-propylbenzene	148	207		0.03 i	1 3	RO-188 RO-189
1-Methyl-4-n-butylbenzene	148	207		i	3	RO-189
1,2,3,4-Tetrahydronaphthalene	132	208		0.03 i	1 3	RO-188 RO-189
1,2-Dimethyl-4-n-propylbenzene	148	209		0.067 wt. % 0.03	9 1	NA-231 RO-188
Trimethylethylbenzene	148	212		0.04	1	RO-188
6-Methyl-[1,2,3,4-tetrahydronaphthalene]	146	229		0.09	1	RO-188

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Hydrocarbons (cont)</u>						
<u>Aromatics (cont)</u>						
5-Methyl-[1,2,3,4-tetrahydronaphthalene]	146	234		0.08	1	RO-188
2-Methyl-[1,2,3,4-tetrahydronaphthalene]	146	234		0.04	1	RO-188
Biphenyl(s)	154	255	IS	i	1	RO-188, DO-074
Naphthenobiphenyls				p	1	DO-074
Dinaphthenobiphenyls				p	1	DO-074
Trinaphthenobiphenyls				p	1	DO-074
Tetranaphthenobiphenyls				p	1	DO-074
Pentanaphthenobiphenyls				p	1	DO-074
Hexanaphthenobiphenyls				p	1	DO-074
Heptanaphthenobiphenyls				p	1	DO-074
Triphenylenes				p	1	DO-074
Naphthenotriphenylenes				p	1	DO-074
Dinaphthenotriphenylenes				p	1	DO-074
Indanes				p	1	DO-074
Tetralins				p	1	DO-074
Dinaphthenobenzenes				p	1	DO-074
Trinaphthenobenzenes				p	1	DO-074
Tetranaphthenobenzenes				p	1	DO-074
Pentanaphthenobenzenes				p	1	DO-074
Hexanaphthenobenzenes				p	1	DO-074
Heptanaphthenobenzenes				p	1	DO-074
Octanaphthenobenzenes				p	1	DO-074
Nonaphthenobenzenes				p	1	DO-074
<u>Lactones</u>						
Oxyallobetul-2-ene	438			i	3	BA-313

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Phenols</u>						
Thiophenol	110	169	IS	i	6	GA-141
Phenol	94	182	S	0.0006 wt. %	6	ME-108
				i	13	KE-151
Methylpropylphenol	134	182-185		i	13	KE-151
o-Cresol	108	191	S-HW	i	6	FI-083
				i	13	KE-151
o-Thiocresol	126	194	IS	i	1	LO-112
p-Cresol	108	202	S-HW	i	6	FI-083
m-Cresol	108	203	S	i	6	FI-083
				i	13	KE-151
o-Ethylphenol	122	207	SS	i	13	KE-151
2,5-Xylenol	122	210	SS	i	6	FI-083
Dimethylphenol	122	210-225		i	13	KE-151
m-Ethylphenol	122	214	SS	i	1	LO-112
2,3-Xylenol	122	218	SS	i	6	FI-083
3,5-Xylenol	122	220	S	i	6	FI-083
3,4-Xylenol	122	225		i	6	FI-083
2,4-Xylenol	122	225	SS	i	6	FI-083
Isopsuedocuminol	136	233		i	6	FI-083
2-Ethyl-4-methylphenol	138			i	1	LO-112
Methylethylphenol	136			i	13	KE-151
Trimethylphenol	136	Sublimes @ ~221,232		i	13	KE-151
2,6-Di-tert-butyl-p-cresol	206			i	13	KE-151
<u>Polynuclear</u>						
<u>Aromatic Hydrocarbons</u>						
Naphthalene	128	218	IS	0.06	1	RO-188
				0.74 wt. %	9	NA-231
2-Methylnaphthalene	142	241	IS	0.2	1	RO-188
1-Methylnaphthalene	142	245	IS	0.1	1	RO-188
2,6-Dimethylnaphthalene	156	262		i	1	RO-188
Dimethylnaphthalenes	156	262-70	IS	i	1	RO-188
Trimethylnaphthalenes	170	285-88	IS	i	1	RO-188
Anthracene(s) ^b	178	340	IS	i	1	DO-074

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Aromatic Hydrocarbons (cont)</u>						
Phenanthrene	178	340	IS	i	1	CA-228
Perylene	252	Sublimes @ 350-400	IS	i	1	CA-228
2,6-Dimethylanthracene	206	350-357		i	1	CA-228
2,7-Dimethylanthracene	206	350-360		i	1	CA-228
1,3,5,7-Tetramethyl- anthracene	234	380-382		i	1	CA-228
1,3,6,7-Tetramethyl- anthracene	234	385-387		i	1	CA-228
2,3,6,7-Tetramethyl- anthracene	234	385-387		i	1	CA-228
3-Methylchrysene	242			i	1	CA-228
Naphthalenes				p	1	DO-074
Naphthenophthalenes				p	1	DO-074
Dinaphthenonaphthalenes				p	1	DO-074
Trinaphthenonaphthalenes				p	1	DO-074
Tetranaphthenonaphtha- lenes				p	1	DO-074
Pentanaphthenonaphtha- lenes				p	1	DO-074
Hexanaphthenonaphtha- lenes				p	1	DO-074
Hepthanaphthenonaphtha- lenes				p	1	DO-074
Octanaphthenonaphtha- lenes				p	1	DO-074
Phenanthrenes				p	1	DO-074
Acenaphthalene				p	1	TH-086
Naphthenoacenaphtha- lenes or naphtheno- fluorenes				p	1	DO-074
Dinaphthenoacenaphtha- lenes or dinaphtheno- fluorenes				p	1	DO-074
Trinaphthenoacenaphtha- lenes or trinaphtheno- fluorenes				p	1	DO-074

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Aromatic Hydrocarbons (cont)</u>						
Trinaphthenoacenaphthalenes or phenylbenzoin- danes or indanylnaphthalenes				p	1	DO-074
Tetranaphthenoacenaphthalenes or naphtheno- phenylbenzoin- danes or naphthenoindanylnaphthalenes				p	1	DO-074
Pentanaphthenoacenaphthalenes or dinaphtheno- phenylbenzoin- danes or dinaphthenoindanylnaphthalenes				p	1	DO-074
Hexanaphthenoacenaphthalenes or trinaphtheno- phenylbenzoin- danes or trinaphthenoindanylnaphthalenes				p	1	DO-074
Tetranaphthenophenylbenzoin- danes or tetra- naphthenoindanylnaphthalenes				p	1	DO-074
Pentanaphthenophenylbenzoin- danes or pentanaphthenoindanylnaphthalenes				p	1	DO-074
Hexanaphthenophenylbenzoin- danes or hexanaphthenoindanylnaphthalenes				p	1	DO-074
Phenanthrenes/anthracenes				p	1	DO-074
Naphthenophenanthrenes/anthracenes				p	1	DO-074
Dinaphthenophenanthrenes/anthracenes				p	1	DO-074

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Aromatic Hydrocarbons (cont)</u>						
Trinaphthenophenan- threnes/anthracenes				p	1	DO-074
Tetranaphthenophenan- threnes/anthracenes				p	1	DO-074
Pentanaphthenophenan- threnes/anthracenes				p	1	DO-074
Diacenaphthalenes				p	1	DO-074
Naphthenodiacenaphtha- lenes				p	1	DO-074
Dinaphthenodiacenaphtha- lenes				p	1	DO-074
Pyrenes				p	1	DO-074
Naphthenopyrenes or chry- senes				p	1	TH-086
Naphthenochrysenes				p	1	TH-086
Dinaphthenochrysenes				p	1	TH-086
Benzopyrene				p	1	TH-086
Benzofluorenes				i	5	TY-008
Benzanthracenes				i	5	TY-008
Benzophenanthrenes				i	5	TY-008
Fluoranthenes				i	5	TY-008
<u>Aza Arenes</u>						
Quinoline	129	238	S-HW	i	6	BA-325
Isoquinoline(s) ²	129	243	IS	i	1	PE-140
				i	6	BA-325
3-Methylisoquinoline	143	246	SS	i	6	BA-325
2-Methylisoquinoline	143			i	6	BA-325
1-Methylisoquinoline	143	248	SS	i	6	LO-112
2-Methylquinoline	143	248	SS	i	6	BA-325
8-Methylquinoline	143	249	SS	i	6	BA-325
Indole(s) ²	117	254	S-HW	i	1	PE-140
2,8-Dimethylquino- line	157	255	SS	i	3,6	BA-325
7-Methylquinoline	143	258	SS	i	6	BA-325
3-Methylquinoline	143	260	SS	i	6	BA-325

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Aza Arenes (cont)</u>						
4-Methylquinoline	143	264	SS	i	6	BA-325
Methylindole	131	265-272	SS	i	5	RO-188
2,4-Dimethylquinoline	157	266	SS	i	3	BA-325
2,3-Dimethylquinoline	157		IS	i	3	BA-325
2,4,8-Trimethylquinoline	171	288		i	3	BA-325
2,3,8-Trimethylquinoline	171			i	3	BA-325
2-Methyl-8-ethylquinoline	171			i	3	BA-325
2,3-Dimethyl-8-ethyl- quinoline	185			i	3	BA-325
2,4-Dimethyl-8-ethyl- quinoline	185			i	3	BA-325
2,3,4,8-Tetramethyl- quinoline	185			i	3	BA-325
2,3-Dimethyl-8-n-propyl- quinoline	199			i	3	BA-325
2,4-Dimethyl-8-n-propyl- quinoline	199			i	3	BA-325
2,3,4-Trimethyl-8-ethyl- quinoline	199			i	3	BA-325
2,3,8-Trimethyl-4-ethyl- quinoline	199			i	3	BA-325
2,3,4-Trimethyl-8-n- propylquinoline	213			i	3	BA-325
2,3,4-Trimethyl-8- isopropylquinoline	213			i	3	BA-325
2,3-Dimethyl-4,8- diethylquinoline	213			i	3	BA-325
2,4-Dimethyl-8-sec- butylquinoline	213			i	3	BA-325
2,3-Dimethyl-4-ethyl- 8-n-propylquinoline	227			i	3	BA-325
2,3-Dimethylbenzo(h)- quinoline	207			i	3	BA-325
Carbazole(s) ²	167	355	IS	i	1	PE-140
2-Methylcarbazole	181					
Porphyrin				12-380 ppm 9 ppm	1 4	DU-082 DU-070

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Thio Arenes</u>						
Monocyclic sulfides				p	1	DO-074
Bicyclic sulfides				p	1	DO-074
Tricyclic sulfides				p	1	DO-074
Tetracyclic sulfides				p	1	DO-074
Pentacyclic sulfides				p	1	DO-074
Hexacyclic sulfides				p	1	DO-074
Heptacyclic sulfides				p	1	DO-074
Thiaindanes/thiatetra- lins				p	1	DO-074
Naphthenothiaindanes/ thiatetralins				p	1	DO-074
Dinaphthenothiaindanes/ thiatetralins				p	1	DO-074
Trinaphthenothiaindanes/ thiatetralins				p	1	DO-074
Benzothiophenes				p	1	DO-074
Naphthenobenzothiophenes				p	1	DO-074
Dinaphthenobenzothio- phenes				p	1	DO-074
Trinaphthenobenzothio- phenes				p	1	DO-074
Tetranaphthenobenzothio- phenes				p	1	DO-074
Pentanaphthenobenzothio- phenes				p	1	DO-074
Dibenzothiophenes				p	1	DO-074
Naphthenodibenzothio- phenes				p	1	DO-074
Dinaphthenodibenzothio- phenes				p	1	DO-074
Trinaphthenodibenzothio- phenes				p	1	DO-074
Diphenyl disulfides				p	1	TH-086
Naphthenodiphenyl disulfides				p	1	TH-086
Dinaphenodiphenyl disulfides				p	1	TH-086

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Thio Arenes (cont)</u>						
Trinaphthenodiphenyl disulfides				p	1	TH-086
Tetranaphthenodiphenyl disulfides				p	1	TH-086
Thienocyclic sulfides				p	1	DO-074
Naphthenothienocyclic sulfides				p	1	DO-074
Dinaphthenothienocyclic sulfides				p	1	DO-074
Thienoindenes				p	1	TH-086
Dibenzothiophenes				p	1	DO-074
Naphthenodibenzothio- phenes				p	1	DO-074
Dinaphthenodibenzo- thiophenes				p	1	DO-074
Thienoacenaphthalenes				p	1	DO-074
Thienonaphthenoacenaphtha- lenes or thienophenan- threnes/anthracenes				p	1	DO-074
Thienodinaphthenoace- naphthalenes or thieno- naphthenophenanthrenes/ anthracenes				p	1	DO-074
Thienotrinaphthenoace- naphthalenes or thienodinaph- thenophenanthrenes/an- thracenes				p	1	DO-074
Thienotetranaphthenoace- naphthalenes or thieno- trinaphthenophenan- threnes/anthracenes				p	1	DO-074
Naphthalene cyclic sulfides				p	1	TH-086
Naphthalene dicyclic sulfides				p	1	TH-086
Naphthalene tricyclic sulfides				p	1	TH-086

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Thio Arenes (cont)</u>						
Naphthalenotetracyclic sulfides				p	1	DO-074
Naphthalenopentacyclic sulfides				p	1	DO-074
Naphthalenohexacyclic sulfides				p	1	DO-074
Naphthalenoheptacyclic sulfides				p	1	DO-074
Naphthalenooctacyclic sulfides				p	1	DO-074
Thienodiacenaphthalenes				p	1	DO-074
Thienopyrenes				p	1	DO-074
Thienonaphthenodiace- naphthalenes				p	1	DO-074
Thienonaphthenopyrenes				p	1	DO-074
Thienochrysenes				p	1	DO-074
Thienotriphenylenes				p	1	TH-086
Thienonaphthenochrysenes				p	1	DO-074
Thienobenzopyrenes				p	1	DO-074
Thienodibenzothio- phenes				p	1	DO-074
Thienonaphthenodibenzo- thiophenes				p	1	DO-074
Thienodinaphthenodibenzo- thiophenes				p	1	DO-074
Dithienoacenaphthalenes				p	1	DO-074
Dithienonaphthenoace- naphthalenes or di- thienophenanthrenes/ anthracenes				p	1	DO-074
Dithienodinaphtheno- acenaphthalenes or dithienonaphtheno- phenanthrenes/antra- cenes				p	1	DO-074
Dithienotrinaphthenoace- naphthalenes or dithieno- dinaphthenophenanthrenes/ anthracenes				p	1	DO-074

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Thio Arenes (cont)</u>						
Dithienotetranaphtheno- acenaphthalenes or di- thienotrinaphthenophenan- threnes/anthracenes				p	1	DO-074
Thienonaphthalene cyclic sulfides				p	1	TH-086
Thienonaphthalene bi- cyclic sulfides				p	1	TH-086
Thienonaphthalene tri- cyclic sulfides				p	1	TH-086
Thienonaphthalenotetra- cyclic sulfides				p	1	DO-074
Thienonaphthalenopen- tacyclic sulfides				p	1	DO-074
Thienonaphthalenohexa- cyclic sulfides				p	1	DO-074
Thienonaphthalenohepta- cyclic sulfides				p	1	DO-074
Dithienopyrenes				p	1	DO-074
Dithienonaphthenopyrenes				p	1	DO-074
Dithienochrysenes				p	1	DO-074
Dithienodibenzothiophenes				p	1	DO-074
Dithienonaphthenodiben- zothiophenes				p	1	DO-074
Dithienodinaphthenodibenzo- thiophenes				p	1	DO-074
Trithienoacenaphtha- lenes				p	1	DO-074
Dibenzodithiophenes				p	1	TH-086
Dinaphthenodibenzodi- thiophenes				p	1	TH-086
Dithienonaphthelene cy- clic sulfides				p	1	TH-086
Dibenzotrithiophenes				p	1	TH-086
Naphthenodibenzotri- thiophenes				p	1	TH-086
Dinaphthenodibenzotri- thiophenes				p	1	TH-086

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Polynuclear (cont)</u>						
<u>Thio Arenes (cont)</u>						
Trithienoacenaphthalene				p	1	TH-086
<u>Oxa Arenes</u>						
Naphthol	144	288	SS-HW	p	1	LO-112
Alkyl Fluorenones		320-330		i	1	LA-162
<u>Sulfur Compounds</u>						
<u>H₂S, Mercaptans</u>						
H ₂ S	34	-60	S	0.49 wt. % <0.018 wt. % <0.001 <12 ppm	2 3 11 12	HA-316 PE-140 GR-123 RE-142
B-133 Methanethiol	48	6	SS-HW	0.0024 wt. %	1	GR-123
Ethanethiol	62	35	SS	0.0053 wt. %	1	GR-123
2-Propanethiol	76	53	SS	0.00199 wt. %	1	GR-123
2-Methyl-2-propane- thiol	90	64	IS	0.00055 wt. %	1	GR-123
1-Propanethiol	76	68	SS	0.0041 wt. %	1	GR-123
2-Butanethiol	90	85		0.00386 wt. %	1	GR-123
2-Methyl-1-pro- panethiol	90	89	SS	0.00003 wt. %	1	GR-123
1-Butanethiol	90	98	SS	t	1	GR-123
3-Methyl-1-butane- thiol	104		IS	i	1	HA-317
2,2-Dimethyl-1-pro- panethiol	104			i	1	HA-317
2-Methyl-2-butane- thiol	104	99		0.00064 wt. %	1	GR-123
3-Methyl-2-butane- thiol	104	110		i	1	GR-123
2-Pentanethiol	104	113		0.0014 wt. % i	1 2	GR-123 BA-324
3-Pentanethiol	104	114		0.00057 wt. % i	1 2	GR-123 BA-324
1-Pentanethiol	104	127	IS	i	1	HA-317

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Sulfur Compounds (cont)</u>						
<u>H₂S, Mercaptans (cont)</u>						
2-Methyl-1-pentane-thiol	118			i	1	HA-317
2-Methyl-3-pentane-thiol	118			i	1	HA-317
3-Methyl-3-pentane-thiol	118			i	1,2	BA-324
4-Methyl-2-pentane-thiol	118			i	1,2	BA-324
Cyclopentanethiol	102	132		i	1,2	BA-324
2-Hexanethiol	118	142	IS	0.0028 wt. %	1	GR-123
				i	2	BA-324
1-Hexanethiol	118	151	IS	i	1	HA-317
3-Hexanethiol	118			i	1,2	BA-324
Cyclohexanethiol	116	159		0.0012 wt. %	1	GR-123
				i	2	BA-324
2-Methylcyclopentane-thiol	116			i	1,2	BA-324
2-Octanethiol	146	186		i	1	GR-123
Isoamylthiol	104			i	1	HA-317
Amylthiol	104			i	1	HA-317
Hexylthiol	118			i	1	HA-317
<u>Sulfides</u>						
2-Thiapropane	62	37	IS	0.00088 wt. %	1	GR-123
2-Thiabutane	76	67	IS	0.00222 wt. %	1	GR-123
3-Methyl-2-thiabutane	90	85		0.00064 wt. %	1	GR-123
3-Thiapentane	90	92	SS	0.00075 wt. %	1	GR-123
				i	2	BA-324
2-Thiapentane	90	96	S	0.0003 wt. %	1	GR-123
				i	2	BA-324
3,3-Dimethyl-2-thiabutane	104	99		i	1	GR-123
2-Methyl-3-thiapentane	104	107		i	1	GR-123
3-Thiahexane	104	118		0.00012 wt. %	1	GR-123

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Sulfur Compounds (cont)</u>						
<u>Sulfides (cont)</u>						
2,2-Dimethyl-3-thia- pentane	118	120		0.000058 wt. %	1	GR-123
2,4-Dimethyl-3-thia- pentane	118	120	IS	0.00053 wt. %	1	GR-123
2-Thiahexane	104	123		0.000077 wt. %	1	GR-123
2,4-Dimethyl-3-thia- hexane	132			i	1	HA-317
2-Methyl-3-thiahexane	118	132		0.000078 wt. %	1	GR-123
				i	2	BA-324
4-Methyl-3-thiahexane	118	134		0.0005 wt. %	1	GR-123
				i	2	BA-324
2,3-Dithiapentane	108			i	1	HA-317
4-Thiaheptane	118	142	IS	i	1	HA-317
3-Thiaheptane	118	144		0.000078 wt. %	1	GR-123
				i	2	BA-324
3-Thiaoctane	132			i	1	HA-317
5-Thianonane	146	189	IS	i	1	HA-317
2,6-Dimethyl-4-thia- heptane	146			i	1	HA-317
5-Thiadecane	160			i	1	HA-317
6-Thiaundecane	174	230	IS	i	1	HA-317
7-Thiatridecane	198	230		i	1	HA-317
Diphenyldisulfide				p	1	TH-086
<u>Trace Elements</u>						
<u>Metals³</u>						
Ag	108			0.0006-0.1 ppm	5	VO-027
				<0.001-0.3 µg/ml	7	VO-027
Al	27			i	1	GR-123
				0.140 µg/ml	13	KE-151
As	75			0.005-0.142 ppm	1	VE-021
				54.5 ng/g	3	AN-104
				21 ng/g	4	AN-104
				0.2-1.0 ppm	5	VO-027
				<0.02-200 µg/ml	7	VO-027

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Trace Elements (cont)</u>						
<u>Metals³(cont)</u>						
Au	197			i	1	KA-167
B	11			<0.002-0.2 ppm	5	VO-027
				<0.02-2.0 µg/ml	7	VO-027
				0.020 µg/ml	13	KE-151
Ba	137			1-3.6 ppm	1	MA-279
				0.3-5 ppm	5	VO-027
				0.001-10 µg/ml	7	VO-027
				0.300 µg/ml	13	KE-151
Be	9			0.005-0.5 ppm	5	VO-027
				0.0001-0.02	7	VO-027
				µg/ml		
Ca	40			7-400 ppm	5	VO-027
				<0.05-20 µg/ml	7	VO-027
				2.6 µg/ml	13	KE-151
B-136 Cd	112			<15 ng/g	3	AN-104
				10 ng/g	4	AN-104
				0.003-1 ppm	5	VO-027
				0.001-20 g/g	7	VO-027
Co	60			0.28 ppm	1	VE-021
				0.37 µg/g	3	AN-104
				<0.02 µg/g	4	AN-104
				0.015 µg/ml	13	KE-151
Cr	52			0.08-01	1	MA-279
				0.045 µg/g	3	AN-104
				0.025 µg/g	4	AN-104
				0.7-4 ppm	5	VO-027
				0.001-0.5 µg/g	7	VO-027
				0.170 µg/ml	13	KE-151
Cu	63			<0.1-2.3 ppm	1	VE-021
				0.25 µg/g	3	AN-104
				0.10 µg/g	4	AN-104
				41 ppm	5	BA-161
				0.2-1 ppm	5	VO-027
				0.005-10 µg/ml	7	VO-027
				0.4 ppm	10	BA-161
				0.030 µg/ml	13	KE-151

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Trace Elements (cont)</u>						
<u>Metals³(cont)</u>						
Fe	56			0.11-32 ppm	1	MA-279
				4.96 µg/g	3	AN-104
				0.76 µg/g	4	AN-104
				10-20 ppm	5	VO-027
				<0.1-0.6 µg/ml	7	VO-027
				0.300 µg/ml	13	KE-151
Ga	70			i	1	KA-167
				0.015 µg/ml	13	KE-151
Ge	73			i	1	KA-167
Hg	200			2.3 ng/g	3	AN-104
				3.4 ng/g	4	AN-104
				0.002-0.4 ppm	5	VO-027
				0.008-0.1 µg/ml	7	VO-027
K	39			0.8-5 ppm	5	VO-027
				0.1-75 µg/ml	7	VO-027
				0.800 µg/ml	13	KE-151
La	139			i	1	GR-123
Li	7			0.02-3 ppm	5	VO-027
				0.001-0.6 g/g	7	VO-027
Mg	24			2-3 ppm	5	VO-027
				0.01-250 µg/ml	7	VO-027
				3.6 µg/ml	13	KE-151
Mn	55			<1 ppm	1	MA-279
				0.08 µg/g	3	AN-104
				<0.02 µg/g	4	AN-104
				0.21-1 ppm	5	VO-027
				0.005-1 µg/g	7	VO-027
				0.020 µg/ml	13	KE-151
Mo	96			1 ppm	1	MA-279
				0.155 µg/g	3	AN-104
				<0.10 µg/g	4	AN-104
Na	23			0.42-36.2 ppm	1	VE-021
				<0.4-30 ppm	5	VO-027
				0.1-500 µg/g	7	VO-027

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Trace Elements (cont)</u>						
<u>Metals³ (cont)</u>						
Nd	144			i	1	GR-123
Ni				<1-109 ppm	1	MA-279, VE-021
				16.1 µg/g	3	AN-104
				<0.04 µg/g	4	AN-104
				300 ppm	5	BA-161
				20-90 ppm	5	VO-027
				<0.01-6 µg/g	7	VO-027
				18 ppm	10	BA-161
				0.003 µg/ml	13	KE-151
P	31			0.2-15 µg/g	7	VO-027
				0.200 µg/ml	13	KE-151
Pb	207			0.88 µg/g	3	AN-104
				0.12 µg/g	4	AN-104
				1-4 ppm	5	VO-027
				2-650 µg/ml	7	VO-027
Rb	85			0.080 µg/ml	13	KE-151
Sb	122			0.003-0.5 ppm	5	VO-027
				0.0004-1 µg/g	7	VO-027
Se	79			0.02-0.15 ppm	5	VO-027
				0.001-0.2 µg/g	7	VO-027
				0.001 µg/ml	13	KE-151
Si	28			8-30 ppm	5	VO-027
				0.5-50 µg/g	7	VO-027
Sn	119			<1 ppm	1	MA-279
				0.01-5 ppm	5	VO-027
				0.003-7 µg/ml	7	VO-027
Sr	88			<0.4-0.5 ppm	5	VO-027
				<0.001-75 µg/g	7	VO-027
				0.480 µg/ml	13	KE-151
Ti	48			i	1	GR-123
U	238			0.0009 ppm	1	BA-161
				0.008 ppm	5	BA-161
				0.002 ppm	10	BA-161

APPENDIX B
TABLE B (cont)

Component	MW	Boiling Point (°C)	Solubility	Conc. (Vol. %)	Stream	Ref.
<u>Trace Elements (cont)</u>						
<u>Metals³(cont)</u>						
V	51			0.008-430 ppm	1	MA-279, VE-021
				49 µg/g	3	AN-104
				0.10 µg/g	4	AN-104
				330 ppm	5	BA-161
				2.3-855 ppm	5	NE-042
				0.0001-10 µg/g	7	VO-027
				18 ppm	10	BA-161
				0.010 µg/ml	13	KE-151
Zn	65			0.6-2 ppm	1	VE-021
				0.7 µg/g	3	AN-104
				0.09 µg/g	4	AN-104
				0.4-2 ppm	5	VO-027
				0.1-4 µg/ml	7	VO-027
				0.017 µg/ml	13	KE-151
Zr	91			i	1	GR-123
<u>Nonmetals³</u>						
Br	35			<0.01-0.32 ppm	1	VE-021
Cl	35			2.3-8.3 ppm	9	CA-226
				0.080 µg/ml	13	KE-151
F	19			0.004 ppm	5	VO-027
				<0.0003 µg/ml	7	VO-027
				0.160 µg/ml	13	KE-151
S _{elemental}	32			<0.49 wt. %	2	HA-318
				33 µg/ml	13	KE-151
<u>Cyanides</u>						
Hydrogen cyanide	27	26	M	i	11	BR-110
				i	12	DA-069
Methyl cyanide	41			i	12	DA-069
<u>Other</u>						
Water	18	100	M	0.05-0.97	1	PE-140

APPENDIX B

APPENDIX B TABLE B (cont)

FOOTNOTES

¹ Other elements that can potentially occur as salts are listed as trace elements. They include Al, Ba, Be, Br, Ca, Cd, Cl, F, Fe, K, Li, Mg, Na, and Ni. The cyanide ion can also occur as a salt. Others mentioned include Al, Ca, Fe, Mg, and Na salts (PE-140).

² These compounds are assumed to be present since their groups are cited as being present.

³ Boiling points and solubilities are not given because the physical form of the trace metals or elements is not known.

APPENDIX B

5.3 Additional References for Toxicity and Mutagenicity

A literature search was conducted by the Toxicology Information Response Center located at Oak Ridge National Laboratory, Oak Ridge, Tennessee, for select references on mutagenicity and other mammalian toxicological information. The references found were divided into two groups: (1) Mutagenic references and (2) General toxicological references. The general toxicological information was obtained from secondary sources including books, monographs, reviews, and government reports. The TOXLINE computer system was also searched.

Sources Searched: EMIC¹ file; TIRC² files and
library; TOXLINE

Terms Searched: Mutagenicity; Metals; Petroleum
wastes; Hydrocarbons

Tables C, D, and E list the information found in the EMIC file, the TIRC files and library and the TOXLINE file, respectively.

¹Environmental Mutagen Information Center

²Toxicology Information Response Center

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TABLE C

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