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US High Production Volume Chemical Program

Category Summary

For

Pyrolysis C3+ and Pyrolysis C4+ Category

Prepared by:

Olefins Panel of the American Chemistry Council

May 16, 2005

EXECUTIVE SUMMARY

The Olefins Panel of the American Chemistry Council (ACC) hereby submits the category summary report for the Pyrolysis C3+ and Pyrolysis C4+ Category under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Chemical Challenge Program (Program). The purpose of this report is to:

- Present results of an assessment to determine whether two production streams from the Pyrolysis C3+ and Pyrolysis C4+ Category can be adequately characterized with existing data described in the Crude Butadiene C4 and High Benzene Naphthas Category summary reports.
- Summarize the SIDS (Screening Information Data Set) physicochemical, environmental fate and effects, and human health HPV Program endpoints for the Pyrolysis C3+ and Pyrolysis C4+ Categories.
- Provide a description of manufacturing processes, potential exposure sources, and uses for Pyrolysis C3+ and Pyrolysis C4+ streams.

The Pyrolysis C3+ and Pyrolysis C4+ streams were originally in the Crude Butadiene C4 Category, which contained four streams including the Pyrolysis C3+ and Pyrolysis C4+ streams (the Crude Butadiene C4 Category summary report has been submitted to the EPA). After all data were evaluated to determine whether the four streams formed a cohesive category, it was decided that the two streams, Pyrolysis C3+ and Pyrolysis C4+, should be considered as a separate category based on composition and potential effects of stream constituents, which were not shared by all four streams.

The Pyrolysis C3+ and Pyrolysis C4+ streams consist of a complex mixture of hydrocarbons. The typical carbon (C) number distribution for these streams ranges predominantly between C3 and C10, but can include beyond C12. Category streams can contain significant amounts of 1,3-butadiene and benzene, which form the basis for the human health toxicological review. Much of the data used to characterize this category are from 1,3-butadiene, which is a highly chemically reactive constituent, with a recognized hazard profile and hence presumed a major contributor to toxicological activity. Additionally, benzene can be present as a predominant component and is therefore, also considered an important factor in characterizing potential health effects. 1,3-Butadiene and benzene can be present in the two streams at concentrations between approximately 12 to 42% and 11 to 42% (by weight), respectively; thus, they can represent from 23 to 84% (by weight). The High Benzene Naphtha and Crude Butadiene C4 Categories include considerable toxicological data on streams with compositions that are encompassed by the Pyrolysis C3+ and Pyrolysis C4+ streams.

Exposure

The American Chemistry Council, Olefins Panel's Pyrolysis C3+ and Pyrolysis C4+ Category consists of two process intermediate streams of the ethylene manufacturing process. Although these two streams are common in-process streams of the ethylene manufacturing process, it is not routine for the streams to be isolated. The streams were included in the Olefins Panel HPV Program because two of the participants in the Panel's program isolate one or both of the streams during temporary shutdowns of their ethylene manufacturing processes. Two CAS RNs are used to represent the streams in this category.

When a category stream is isolated, it is stored on-site in pressure storage or tank cars, until it is returned to the ethylene manufacturing process. In the past seven years, these temporarily isolated streams were not transported off the manufacturing site where they were produced.

Inhalation is a likely route of exposure due to the volatility of the hydrocarbon components that make up the streams. Other possible exposure routes include dermal (from potential spills) and oral (in the event of contaminated ground water).

The most likely exposure potential occurs through inhalation of low-level concentrations in air of vapors that escape from the closed process, such as fugitive emissions from pump and valve packing seals. There is also a potential for exposure from storage or tank car loading emissions when tank cars are used for temporary on-site storage.

Occupational exposure and the potential for exposure to the neighboring public and environment are limited because the storage and loading of category streams, when loading occurs, is a closed process with vents routed to control systems. The OSHA (1997) 1,3-butadiene and benzene standards limit occupational exposures as well as do other OSHA PEL values or ACGIH TLVs. Management of the process streams is also controlled by other EPA and state environmental regulations that further limit potential exposure.

Human Health

The human health evaluation for streams in the Pyrolysis C3+ and Pyrolysis C4+ Category is based on data presented in the Crude Butadiene C4 and High Benzene Naphthas Categories whose summary reports have been submitted to EPA. Human health summaries for the two categories are described below, followed with an overall assessment describing potential implications for the Pyrolysis C3+ and Pyrolysis C4+ streams.

Crude Butadiene C4 Category

Crude Butadiene C4 streams have a low order of acute toxicity. The components of Crude Butadiene C4 streams are gaseous at normal temperature and pressure; thus, ingestion or dermal absorption of this material is unlikely. Minimal effects were observed at concentrations of 5,300 mg/m³.

A species difference in repeated dose toxicity of Crude Butadiene C4 was apparent between rats and mice. Minimal effects were reported in rat repeated dose toxicity tests exposed to several Crude Butadiene C4 streams (1,3-butadiene content ranging from 10 to 99.2%). The no observed adverse effect levels (NOAELs) were the highest concentrations tested or 17,679; 20,000; or 25,100 mg/m³ following 90, 36, or 9 days of exposure, respectively. In contrast, mortality was observed in mice exposed to 2,761 mg/m³ 1,3-butadiene (99.2%) for 90 days. Well-documented species differences in 1,3-butadiene metabolism are the likely reason for the noted differences in repeat dose toxicity. Mice produce greater amounts of toxic metabolites following 1,3-butadiene exposure than rats. Available data suggest human metabolism of 1,3-butadiene is similar to rats.

Test data demonstrate that Crude Butadiene C4 can produce genotoxicity. *In vitro*, Crude Butadiene C4 demonstrated little activity in reverse mutation assays conducted in *Salmonella typhimurium*, either in the presence or absence of metabolic activation. In addition, Crude Butadiene C4 did not increase the number of transformed foci in C3H/10T1/2 clone 8 mouse embryo fibroblast cells. In the mouse lymphoma assay, evidence of mutagenic activity in mouse lymphoma L5178Y cells in culture was observed in the absence metabolic activation, but not in the presence of metabolic activation. *In vivo*, several crude butadiene streams, containing 10 to 45% 1,3-butadiene, induced micronuclei formation in rats and mice following inhalation exposure.

No reproductive or developmental toxicity was observed in rats exposed to crude butadiene during the conduct of a repeat dose reproductive/developmental toxicity screen (OECD 422). Exposures to concentrations of 20,000 mg/m³ were without adverse effects. Further, in a prenatal developmental toxicity study, inhalation exposure of pregnant rats to 1,3-butadiene on days 5 to 16 (inclusive) of

gestation elicited no developmental toxicity at any tested concentration up to 2,210 mg/m³. Maternal toxicity was observed at levels of 442 mg/m³. As with observations of species differences in repeat dose toxicity, mice were more sensitive than rats to developmental and reproductive toxicity following exposure to 1,3-butadiene. This increased sensitivity was apparent in effects on male germ cells observed in a dominant lethal study and an assessment of sperm morphology in male mice and fetal effects observed in a prenatal developmental toxicity study.

High Benzene Naphthas Category

Evaluation of data on representative streams and read-across from chemical components indicates that High Benzene Naphthas streams are not acutely toxic by the oral, dermal, or inhalation routes of exposure. Streams of most interest for this category include a C5-C10 Fraction of Pyrolysis Gasoline (Rerun Tower Overhead) and a Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline).

It is unlikely that most streams in this category would cause significant genetic toxicity. Tested streams did not cause mutational events in bacteria, and a weak direct effect in mammalian cells from treatment with a C5-C10 fraction of Pyrolysis gasoline, was not confirmed *in vivo* by any expression of gene mutation in *Drosophila*. Although these streams contain substantial concentrations of benzene, a known clastogen, no cytogenetic damage was induced by oral administration of Hydrogenated C6-C8 stream (55% benzene) to rats, possibly demonstrating the inhibitory effects of other components in the stream, likely from competition for metabolic sites.

Benzene, as a predominant component in most streams included in this category is considered a key driver of potential health effects. Benzene-induced systemic toxicity therefore must be addressed; however, to provide a conservative evaluation of health hazard for this category, other individual components should also be considered. However, it should be noted that in the area of cytogenetic toxicology, for example, component mixtures can inhibit toxicity that is observed in individual components when tested alone.

Repeated dose studies from two representative streams in the High Benzene Naphthas Category reported skin irritation and concomitant effects on dermal tissue histology (NOAEL <0.10 ml/kg), but no other systemic toxicity in rabbits, and neuroleptic effects in rats from inhalation exposure at high doses (NOAEL <4,869 ppm). Results were similar to effects reported in the API Gasoline Blending Streams Test Plan, effects from which animals recovered after 4 weeks without exposure. Such data suggest that toxicity of the blended streams may be less severe than that of individual components, likely due to lower individual component concentrations, component interaction, and competitive inhibition.

No significant reproductive effects have been reported in multi-generation studies of stream components. Developmental effects from components present in High Benzene Naphthas streams occurred primarily at doses that were maternally toxic as well. A developmental study in rabbits with a representative High Benzene Naphthas stream did not result in adverse effects on any developmental parameter except for one high dose doe that aborted, and no malformations were induced (NOAEL = 50 mg/kg).

Pyrolysis C3+ and Pyrolysis C4+ Category

Based on data available for the two categories, Crude Butadiene C4 and High Benzene Naphthas, for which the combined composition encompasses the composition range of the Pyrolysis C3+ and Pyrolysis C4+ streams, the Pyrolysis C3+ and Pyrolysis C4+ Category is expected to:

- exhibit a low order of acute toxicity (based on results from the two read-across categories);

- cause minimal effects in repeated dose studies (based on effects reported in rats from exposure to several Crude Butadiene C4 streams with 1,3-butadiene content ranging from 10 to 99.2%, as well as the lack of systemic toxicity demonstrated by two streams in the High Benzene Naphthas Category);
- exhibit a potential to produce genotoxicity, although it is anticipated that the potential for expressing a genotoxic effect will decrease and possibly may be eliminated as concentrations of 1,3-butadiene and/or benzene decrease to minimal reported levels; and
- not produce significant reproductive or developmental effects (based on results from both read-across categories).

Environment

Results of distribution modeling show that chemical constituents of streams in the Crude Butadiene C4 Category will partition primarily to the air compartment, with a smaller amount partitioning to water. In the air, these constituents have the potential to rapidly degrade through indirect photolytic processes mediated primarily by hydroxyl radicals. This is expected to be the dominant route of loss and degradation process for constituents that comprise the bulk of these streams. Aqueous photolysis and hydrolysis will not contribute to the transformation of category constituents in aquatic environments because they are either poorly or not susceptible to these reactions.

The biodegradability of streams in this category has not been evaluated with standard testing procedures because of the gaseous state of a predominant fraction of category members. However, studies have demonstrated that several gaseous category constituents can be degraded by bacteria isolated from soil and surface water samples. Additionally, read-across data for substances that represent the composition of the C5 to C10 fraction of streams in this category show that these constituents can biodegrade to significant extents. Overall, biodegradation is likely to contribute to only a fraction of degradation of constituents from these streams because they tend to partition to the air compartment.

Due to the fact that streams in this category contain a predominant fraction of gaseous constituents that are expected to partition to the atmosphere at a very rapid rate from an aqueous phase, aquatic toxicity testing was not conducted. However, aquatic toxicity was assessed for select gaseous C4 constituents of this category with a model that is based on an equation developed for neutral organic chemicals, a reliable estimation method for the class of chemicals in streams from this category. Calculated toxicity values for two to four day exposures suggest that the C4 constituents have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates, based on LC₅₀ and EC₅₀ concentrations ranging from approximately 15 to 44 mg/L for selected stream constituents. Additionally, a similar moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates is expected from the C5 to C10 fraction of the streams in this category based on an effect range for constituents and hydrocarbon streams of similar composition between approximately 1 to 64 mg/L. Overall, members of this category are expected to exhibit at range of aquatic toxicity for the endpoints in the HPV Program equivalent to the range demonstrated by the C5 to C10 fraction. These constituents are liquid at environmentally relevant temperatures and could remain in solution during a standard test duration, whereas the gaseous fraction, under standard testing conditions, would not remain in solution for a significant duration, relevant to an acute exposure.

Conclusion

The extensive body of data available for mammalian and environmental endpoints on constituents of substances in this category and on streams used to assess two related categories are sufficient to fully characterize the potential toxicity of Pyrolysis C3+ and Pyrolysis C4+ Category members and

demonstrate the integrity of the category.

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Chemical Abstracts Service registration numbers in
the Pyrolysis C3+ and Pyrolysis C4+ Category

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1 CATEGORY DESCRIPTION AND JUSTIFICATION**1.1 Category Identification**

For purposes of the U.S. High Production Volume (HPV) Chemical Challenge Program (Program), the Pyrolysis C3+ and Pyrolysis C4+ Category developed from the Crude Butadiene C4 Category test plan submitted in May 2000 (Olefins Panel, HPV Implementation Task Group, 2000). The original Crude Butadiene C4 Category included four production streams and eleven Chemical Abstracts Service (CAS) registration numbers (RNs). However, after all data were evaluated to determine whether the four streams formed a cohesive category, it was decided that two of the streams, Pyrolysis C3+ and Pyrolysis C4+, should be considered as a separate category based on composition and potential effects of stream constituents, which were not shared by all four streams.

The following category report summarizes HPV Program data that characterize the Pyrolysis C3+ and Pyrolysis C4+ streams and category. Table 1 lists the two CAS RNs and names associated with the two streams in this category.

Table 1. Production Streams, CAS RNs, and CAS RN Names in the Pyrolysis C3+ and Pyrolysis C4+ Category

Process Stream	CAS RN	CAS RN Name
Pyrolysis C3+	64742-83-2	Naphtha, petroleum, light steam-cracked
	68513-68-8	Residues, petroleum, deethanizer tower
Pyrolysis C4+	64742-83-2	Naphtha, petroleum, light steam-cracked

Note: The definitions, found in the TSCA Chemical Substance Inventory, for the CAS RNs included in this category are very general and vague with respect to composition. It is not uncommon to find that the same CAS number is used to describe multiple streams or that two or more CAS numbers are used to describe a single stream. Multiple CAS RNs applying to the same streams arose as various companies supplied somewhat different compositional information when they registered similar substances.

The two commercial production streams, Pyrolysis C3+ and Pyrolysis C4+, are similar from a process and toxicology perspective. Each stream can vary in composition, not only between manufacturers but also for an individual manufacturer, depending on feedstock type and process operating conditions. Although the chemical composition of the streams can vary, the defining characteristic of the two streams is that each contains a mixture of chemicals from a reaction or separation activity in the Olefins Industry hydrocarbon processes and each contains 1,3-butadiene and benzene at a minimum concentration of approximately 12 and 11%, respectively.

The Pyrolysis C3+ and Pyrolysis C4+ streams consist of a complex mixture of hydrocarbons. The typical carbon (C) number distribution for these streams ranges predominantly between C3 and C10, but can include beyond C12. Category streams can contain significant amounts of 1,3-butadiene and benzene, which form the basis for the human health toxicological review. Much of the data used to characterize this category are from 1,3-butadiene, which is the most reactive constituent and hence presumed a more biologically active component and major contributor to toxicological activity. Additionally, benzene can be present as a predominant component and is therefore also considered a key driver in characterizing potential health effects. 1,3-Butadiene and benzene can be present in the two streams at concentrations between approximately 12 to 42% and 11 to 42% (by weight), respectively; thus, they can represent from 23 to 84% of total (by weight).

The TSCA Chemical Substance Inventory definitions for the CAS RNs in this and in other categories from the Olefins Panel's HPV Program can be vague with respect to composition.

Therefore, it is common that a single CAS RN is correctly used to describe different streams (different compositions) or that two or more CAS RNs are used to describe one stream (similar composition or process).

The Pyrolysis C3+ and Pyrolysis C4+ Category streams arise from production processes associated with ethylene manufacturing (see Appendix I for a description of the ethylene and associated processes). Pyrolysis C3+ and Pyrolysis C4+ are intermediate streams in the ethylene process and consist of the portions of the liquefied cracked gas remaining after removal of ethane and lighter components (for the C3+ stream) or removal of propane and lighter (in the case of the C4+ stream). These streams contain approximately 12 to 42% 1,3-butadiene and 11 to 42% benzene (Table 2). Other hydrocarbons in these streams can range from C3 to C12 or higher. Combined, these streams were referred to as the Full Range Butadiene Concentrate stream in the Crude Butadiene C4 Category summary report (Olefins Panel of the American Chemistry Council, 2004a).

Table 2. Typical Constituent (wt%) Range of Streams in the Pyrolysis C3+ and Pyrolysis C4+ Category

Constituent	Pyrolysis C3+ and Pyrolysis C4+ Streams (wt %)
Propylene	0 - 4.0
Other C3 & Lighter Hydrocarbons	0 - 1.0
Isobutane	0.0 - 1.1
Isobutylene	5.0 - 12
n-Butane	1.0 - 4.5
cis- & trans-Butene-2	1.5 - 6.4
Butene-1	5.0 - 11
1,3-Butadiene	12 - 42
1,2-Butadiene	0.0 - 1.0
1,4-Pentadiene	0.2 - 1.2
Pentene-1	0.5 - 2.3
2-Methyl-1,3-Butadiene (Isoprene)	0.6 - 3.2
cis- & trans-Pentene-2	0.1 - 2.0
1,3-Cyclopentadiene	1.0 - 9.5
cis- & trans-1,3-Pentadiene	1.0 - 7.2
Cyclopentene	0.5 - 2.6
Cyclopentane	2.0 - 4.0
C6-C8 Non-Aromatic Hydrocarbons	2.0 - 12
Benzene	11 - 42
Toluene	1.8 - 25
Xylenes	0.1 - 4.0
Ethylbenzene	0.1 - 1.3
Other C9+ Hydrocarbons	1.5 - 8.7
Dicyclopentadiene	2.0 - 10
Indene	0.3 - 1.9
Naphthalene	0.2 - 1.6

Note 1: The composition of category streams as listed in Table 2 do not represent all possible constituents, but rather those that were reported by the manufacturers. The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.

Note 2: The listed ranges should not be considered absolute values. They are instead the approximate highs and lows of the reported values, and are expected to be typical limit values.

1.2 Purity/Impurities/Additives

Additives are not added to Pyrolysis C3+ and Pyrolysis C4+ streams.

1.3 Physico-Chemical Properties

The two streams in this category are complex, containing many different hydrocarbons (Table 2), and can vary in composition not only between manufacturers but also for an individual manufacturer, depending on feedstock type and operating conditions. The 17 constituents listed in Tables 3 and 4 comprise significant proportions of the two streams, which is why they were selected to represent the potential range of physico-chemical (PC) properties of the streams in this category. Therefore, the data for these constituents can be used to adequately characterize the five PC endpoints of substances in this category for the HPV Program.

Table 3. Summary of Calculated Physico-Chemical Properties for Selected Chemicals Contained by Streams in the Pyrolysis C3+ and Pyrolysis C4+ Category

Chemical	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa@ 25°C)	Log P _{ow}	Water Solubility (mg/L)
Isobutane	-132.6	3.2	3.45 E3	2.23	496.4
n-Butane	-120.3	19.6	2.41 E3	2.31	424.1
Isobutylene	-130.9	10.2	2.97 E3	2.23	495.6
Cis-Butene-2	-120.4	27.8	2.31 E3	2.09	652.7
Trans-Butene-2	-120.4	27.8	2.31 E3	2.09	652.7
Butene-1	-121.7	17.6	2.48 E3	2.17	557.7
1,3-Butadiene	-123.2	15.6	2.73 E3	2.03	732.4
Isoprene	-118.9	35.0	7.35 E2	2.58	247.2
1,3-Cyclopentadiene	-91.8	69.2	5.69 E2	2.25	470.6
Isohexane	-105.8	56.3	2.48 E2	3.21	66.9
n-Hexane	-93.8	71.5	2.00 E2	3.29	57.4
Methylcyclopentane	-85.8	80.3	1.77 E2	3.10	84.0
Benzene	-77.9	102.2	1.16 E2	1.99	2634.0
Toluene	-59.2	125.7	31.60	2.54	832.7
m-Xylene	-40.7	148.3	8.83	3.09	258.4
Dicyclopentadiene	-16.8	176.8	2.20	3.16	51.9
Naphthalene	5.0	231.6	0.05	3.17	142.1

Calculated values derived by the EPIWIN program (EPIWIN, 1999)

Table 4. Summary of Measured Physico-Chemical Properties for Selected Chemicals Contained by Streams in the Pyrolysis C3+ and Pyrolysis C4+ Category

Chemical	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa@ 25°C)	Log P _{ow}	Water Solubility (mg/L)
Isobutane	-138.3	-11.7	3.08 E3	2.76	175.1
n-Butane	-138.2	-0.5	2.43 E3	2.89	135.6
Isobutylene	-140.4	-6.9	3.08 E3	2.34	399.2
cis-Butene-2	-105.5	0.8	2.33 E3	2.31	423.5
trans-Butene-2	-105.5	0.8	2.33 E3	2.33	407.1
Butene-1	-145.0	-1.3	3.00 E3	2.40	354.8
1,3-Butadiene	-108.9	-4.4	2.81 E3	1.99	792.3
Isoprene	-145.9	34.0	7.33 E2	2.42	338.6
1,3-cyclopentadiene	- 85.0	41.0	5.80 E2	na	na
Isohexane	-162.9	63.2	2.53 E2	3.60	31.1
n-hexane	- 95.3	68.7	2.01 E2	3.90	17.2
Methylcyclopentane	-142.5	71.8	1.84 E2	3.37	49.4
Benzene	5.5	80.0	1.26 E2	2.13	2000.0
Toluene	- 94.9	110.6	37.86	2.73	573.1
m-Xylene	- 47.8	139.1	11.05	3.20	207.2
Dicyclopentadiene	32.0	170.0	3.05	na	na
Naphthalene	80.2	217.9	0.11	3.30	142.1

Measured values from the EPIWIN experimental database (EPIWIN, 1999)

na not available

The following sections identify the values used to define the five PC endpoints of the two streams in this category.

1.3.1 Melting Point (Range)

Based on calculated values, the streams in this category can have a melting point range of -132.6 to 5.0°C. Based on measured values, the streams in this category can have a melting point range of -145.0 to 80.2°C. With the exception of two chemicals, the calculated data compare favorably with the measured data. The measured data are considered the appropriate primary data set to characterize the melting point range of category members.

1.3.2 Boiling Point (Range)

Based on calculated values, the streams in this category can have a boiling point range of 3.2 to 231.6°C. Based on measured values, the streams in this category can have a boiling point range of -11.7 to 217.9°C. The calculated data compare reasonably well with the measured data. The measured data are consistent with process knowledge and are considered the appropriate primary data set to characterize the boiling point range of category members.

1.3.3 Vapor Pressure (Range)

Based on calculated values, the streams in this category can have a vapor pressure range of 0.05 to 3.45 E3 hPa at 25°C. Based on measured values, the streams in this category can have a vapor pressure range of 0.11 to 3.08 E3 hPa at 25°C. The calculated data compare reasonably well with the measured data. The measured data are consistent with process knowledge and are considered the appropriate primary data set to characterize the vapor pressure range of category members.

1.3.4 Log P_{ow} (Range)

Based on calculated values, the streams in this category can have a log P_{ow} range of 2.03 to 3.29. Based on measured values, the streams in this category can have a log P_{ow} range of 1.99 to 3.90. The calculated data compare reasonably well with the measured data. The measured data are considered the appropriate primary data set to characterize the log P_{ow} range of category members.

1.3.5 Water Solubility (Range)

Based on calculated values, the streams in this category can have a water solubility range of 51.9 to 2634.0 mg/L. Based on measured values, the streams in this category can have a water solubility range of 17.2 to 2000.0 mg/L. The calculated data compare reasonably well with the measured data. The measured data are considered the appropriate primary data set to characterize the water solubility range of category members.

1.4 Category Justification

The data used to characterize human health endpoints of the two streams in the Pyrolysis C3+ and Pyrolysis C4+ Category include data for 1,3-butadiene and 1,3-butadiene-containing streams as presented in the C4 Crude Butadiene Category and for benzene and benzene-containing streams as identified in the High Benzene Naphthas Category (Olefins Panel of the American Chemistry Council; 2004a, 2004b). 1,3-Butadiene and benzene are considered the most biologically active of all the constituents in the Pyrolysis C3+ and Pyrolysis C4+ streams, and hence are the major contributors to toxicological activity. These chemicals can be present in the streams covered by this category at concentrations between approximately 11 to 42% (by weight). The presence of 1,3-butadiene at concentrations $\geq 11\%$ by weight presupposes that the stream would result in positive genotoxicity as the most sensitive endpoint. Supporting this presumption, two C4 Crude Butadiene stream samples, each with a different percentage of 1,3-butadiene (10 and 45%), have been shown to be genotoxic.

In conjunction with the C4 Crude Butadiene Category data, the information summarized in the High Benzene Naphthas Category provides data pertinent to the evaluation of these streams. Interestingly, data from the High Benzene Naphthas Category indicate that the complex nature of these benzene-containing streams may result in inhibition of the known genotoxic activity of benzene, likely due to interactions between components of similar structure. Thus, tested streams did not cause mutational events in bacteria, and a weak direct effect in mammalian cells from treatment with a C5-C10 fraction of pyrolysis gasoline was not confirmed *in vivo* by any expression of gene mutation in *Drosophila*. Although these streams contain substantial concentrations of benzene, a known clastogen, no cytogenetic damage was induced by oral treatment of rats with the Hydrogenated C6-C8 stream (55% benzene), demonstrating the inhibitory effects of other components in the stream, probably from competition for metabolic sites.

2 EXPOSURE AND USE

The Pyrolysis 3+ and Pyrolysis 4+ Category includes 2 CAS RNs (Table 1) that are associated with the following two process streams:

- Pyrolysis C3+
- Pyrolysis C4+

These streams are manufactured in ethylene production units (see Appendix I) and account for 100% of annual Pyrolysis C3+ and Pyrolysis C4+ production in the US. The total isolated volume for these two streams, as reported under the 1998 IUR, was less than 50 million pounds.

The American Chemistry Council Olefins Panel's Pyrolysis C3+ and Pyrolysis C4+ Category¹ consists of two intermediate process streams from the ethylene manufacturing process. Although they are common in-process streams, it is not routine for them to be isolated. The streams were included in the Olefins Panel's HPV program because two of the participants in the Panel's HPV program isolated one or both of the streams during temporary shutdowns of their ethylene manufacturing processes, as reported in their 1998 TSCA IUR. Some amounts of both streams are reported to have been isolated since 1997, and isolation could occur in the future. However, after these streams are isolated following a process shutdown, they are recycled back to the ethylene manufacturing process upon start-up.

High temperatures in the "Cracking" furnaces of the ethylene process are used to convert predominantly paraffinic hydrocarbon feedstock to ethylene. In addition to ethylene, other hydrocarbons are produced, including other olefins, aromatics and cyclics. In the typical process, the mixed gas stream from the cracking furnaces is cooled, compressed and then condensed in order to facilitate separation of the stream into the desired products or product streams, such as fuel gas (hydrogen and methane), ethylene, propylene, crude butadiene, and pyrolysis gasoline. The separation is accomplished in a series of unit operations including distillation operations. The Pyrolysis C3+ or deethanizer bottoms stream is a typical intermediate process stream produced in the distillation sequence. It consists of the liquefied portion of the cracking furnace outlet stream after removal of ethane and other components with boiling points lower than that of ethane (including ethylene, methane, and hydrogen). Similarly the C4+ or depropanizer bottoms stream is a typical intermediate process stream, consisting of the liquefied portion of the cracking furnace outlet after removal of propane and lower boiling components (including propane and propylene).

The individual components or hydrocarbon compounds that make up the streams in this category are also produced by other industrial processes and some are naturally occurring substances. Potential for exposure to the individual components from other manufacturing processes or from natural sources are considered to be out of scope of this assessment. This assessment is limited to potential exposures to the two streams in the category.

Storage and Transportation of the Category Streams

When either of the two streams is isolated, it is stored on-site in pressure storage tanks or tank cars, and then recycled to the ethylene process. The Pyrolysis C3+ stream was transported offsite in

¹ C3+ indicates that the stream is a mixed stream of hydrocarbon compounds that have 3 or more carbons in the molecule. A partial list or description of the components in the stream includes propylene, propane, 1,3-butadiene, butene isomers, butane, C5 dienes such as isoprene, C5 olefins & paraffins, benzene and other C6 compounds, toluene and other C7 compounds, styrene, ethylbenzene, xylenes, indene, dicyclopentadiene, naphthalene and methylnaphthalene and other cyclic hydrocarbons. The Pyrolysis C4+ is similarly defined, but does not contain significant amounts of propylene or propane (see Table 2 for compositional range information).

1997, but since that time both this stream and the Pyrolysis C4+ stream are stored on site and then returned to the ethylene manufacturing process.

Uses

The category streams are used in the ethylene manufacturing process, that is, further processed in the ethylene manufacturing process in essentially the same way that they would have been used if isolation had not occurred. There are no consumer uses of the streams.

Routes of Potential Human Exposure

Inhalation is a likely route of exposure due to the volatility of the hydrocarbon components that make up the streams. Other possible exposure routes include dermal (from potential spills) and oral (in event of contaminated ground water).

Sources of Potential Exposure

For industrial workers at facilities where these streams are isolated, the most likely exposure potential occurs through inhalation of low-level concentrations in air of vapors that escape from the closed process, such as fugitive emissions from pump and valve packing seals.

Emissions from the closed pressure storage tanks or resulting from loading the streams into pressure tank cars (in those cases where loading occurs) is another source of potential occupational exposure. At one site, the Pyrolysis C4+ stream was isolated in the same process vessel that contains the stream during normal process operation. Therefore, the exposure potentials for this stream are similar to the potentials that exist during the normal operation of the ethylene manufacturing process unit.

The above-described sources of emissions of the category streams may also present a potential for exposure to the public and to the environment adjacent to the industrial facilities.

Controls Limiting Exposure

The Pyrolysis C3+ and the Pyrolysis C4+ streams are complex mixtures that contain 1,3-butadiene and benzene. The OSHA Butadiene Standard² applies to these processes and thus limits exposure to the streams in this HPV Category. The Standard requires controls and work practices that limit 1,3-butadiene occupational exposure to less than 1 ppm, 8-hour time-weighted average (TWA), and a short-term level of 5 ppm (15 minute). In addition, the OSHA Standard establishes an Action Level of 0.5 ppm (8-hour TWA), which effectively limits occupational exposure to 1,3-butadiene.

Similarly the OSHA Benzene Standard³ applies to these processes and also limits exposures to the streams in the category. The standard requires controls and work practices that limit benzene occupational exposure to less than 1 ppm, 8-hour TWA, and a short-term level of 5 ppm (15 minute). In addition, the OSHA Standard establishes an Action Level of 0.5 ppm (8-hour TWA), which effectively limits occupational exposure to benzene.

OSHA PEL (personal exposure limit) values and ACGIH TLVs (threshold limit values) have been established for volatile organic chemicals (VOCs) present or possibly present in category streams in addition to 1,3-butadiene and benzene. Some of these values are listed in Table 5.

² OSHA Standard for 1,3-butadiene: 29 CFR 1910.1051

³ OSHA Standard for benzene: 29 CFR 1910.1028

Table 5. Constituents that can be Present in Streams of the Pyrolysis C3+ and Pyrolysis C4+ Category that have OSHA PEL Values or ACGIH TLVs

Component	OSHA PEL (ppm)	ACGIH TLV (ppm)	Component	OSHA PEL (ppm)	ACGIH TLV (ppm)
Xylene Isomers	100	100	Naphthalene	10	10
Isopropylbenzene	50	50	Octane Isomers	500	300
Cyclopentadiene	75	75	Indene	-	10
Cyclopentane	-	600	Heptane	500	400
Dicyclopentadiene	-	5	Toluene	200	50
Ethylbenzene	100	100	Vinyltoluene	100	50

Emission potentials for the Pyrolysis C3+ and Pyrolysis C4+ streams are minimized because the equipment and processes used to manage the streams are closed processes. Among other reasons, emissions of the streams are minimized because they are highly volatile and flammable hydrocarbons. When loaded into railcars, the vents from loading operations are controlled by routing to a flare. Potential exposures to loading operations personnel are limited by procedures that block in, depressurize, and clear the loading piping prior to disconnection.

Emissions of the category streams from the ethylene manufacturing process equipment are controlled under US EPA standards. The EPA National Emissions Standards for Hazardous Air Pollutants (NESHAP) 40 CFR Part 61 Subparts J and V, and the 40 CFR Part 63 NESHAP: Generic Maximum Achievable Control Technology (MACT) standards both limit fugitive emissions of the category streams. The MACT standard also limits emissions from loading and storage operations. In addition the ethylene manufacturing process is subject to various state environmental regulations and permits that further limit emissions of the category streams. These environmental controls also limit potential exposure.

Summary of Exposure Assessment

The American Chemistry Council, Olefins Panel's Pyrolysis C3+ and Pyrolysis C4+ Category consists of two process intermediate streams of the ethylene manufacturing process. Although these two streams are common in-process streams of the ethylene manufacturing process, it is not routine for the streams to be isolated. The streams were included in the Olefins Panel HPV Program because two of the participants in the Panel's program isolate one or both of the streams during temporary shutdowns of their ethylene manufacturing processes. Two CAS RNs are used to represent the streams in this category.

When a category stream is isolated, it is stored on-site in pressure storage tanks or tank cars, and then returned to the ethylene manufacturing process. In the past seven years, these temporarily isolated streams were not transported off the manufacturing site where they were produced.

Inhalation is a likely route of exposure due to the volatility of the hydrocarbon components that make up the streams. Other possible exposure routes include dermal (from potential spills) and oral (in the event of contaminated ground water).

The most likely exposure potential occurs through inhalation of low-level concentrations in air of vapors that escape from the closed process, such as fugitive emissions from pump and valve

packing seals. There is also a potential for exposure from storage tanks or tank car loading emissions when tank cars are used for temporary on-site storage.

Occupational exposure and the potential for exposure to the neighboring public and environment are limited because the storage and loading of category streams, when loading occurs, is a closed process with vents routed to control systems. The OSHA 1,3-butadiene and benzene standards limit occupational exposures as well as other OSHA PEL values or ACGIH TLVs. Management of the process streams is also controlled by other EPA and state environmental regulations that further limit potential exposure.

3 ENVIRONMENTAL FATE

3.1 Photodegradation

The atmosphere is the environmental compartment of interest when considering fate processes that can impact the persistence of streams in the Pyrolysis C3+ and Pyrolysis C4+ Category because they contain constituents that are gaseous as well as a range of hydrocarbons that are relatively volatile. Results from an environmental distribution model support the assessment that chemical constituents of these streams will partition predominantly to the air compartment. The modeling results can be largely explained by the high vapor pressure of the constituents evaluated. In spite of their water solubility, wet deposition of category constituents is not likely to play a significant role in their atmospheric fate. Constituents of streams in this category have the potential to degrade at a significant rate in the atmosphere through indirect photolytic process mediated primarily by hydroxyl radicals (OH). In comparison, direct photolysis is not expected to contribute to the degradative fate of these streams in the aqueous environment.

3.1.1 Direct Photodegradation

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982a). The reaction process is initiated when light energy at a specific wavelength elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110 to 750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982a). Higher wavelengths (e.g., infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the surface of the earth. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982a). Although the absorption of UV light in the 290 to 750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light at wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977). Saturated hydrocarbons do not absorb light above 200 nm. Characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ϵ) for several unsaturated hydrocarbons, including 1,3-butadiene, are listed in Table 5 (Harris, 1982a). Only

naphthalene, which is present only at small amounts in these category streams, demonstrated photochemical degradation at wavelengths above 290 nm.

Table 6. Characteristic Absorbance Maxima (λ_{\max}) and Associated Molar Absorptivities (ϵ) for Representative Unsaturated Hydrocarbons from Streams in the Pyrolysis C3+ and Pyrolysis C4+ Category

Hydrocarbon	λ below 290 nm		λ above 290 nm	
	λ_{\max}^*	ϵ	λ_{\max}^*	ϵ
1,3-Butadiene	217	20,900		
Benzene	255	215		
Naphthalene	221	100,000	311	250
	270	5,000		

* Values developed in organic solvents and regarded as approximate absorption maxima in aqueous solution.

Olefins with one double bond, two conjugated double bonds, or multiple un-conjugated bonds, which constitute the majority of the chemicals in the Pyrolysis C3+ and Pyrolysis C4+ Category, do not absorb appreciable light energy above 290 nm. Streams in this category do not contain significant concentrations of constituent molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical constituents in this category from the environment.

3.1.2 Indirect Photodegradation

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH^\cdot) radicals (Atkinson, 1988; Atkinson, 1989). The rate at which an organic compound reacts with OH^\cdot radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon an average atmospheric concentration of hydroxyl radicals.

Since the reactions necessary for this degradative process only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day. The nine chemicals selected to represent the atmospheric half-life range of streams in this category include one C4 and eight C5 hydrocarbons that are predominant among the two CAS RNs (Table 6).

Atmospheric oxidation because of hydroxyl radical attack can be a significant route of degradation for streams in this category. Based on calculated values, chemicals in streams from this category can have an atmospheric half-life range of 0.9 to 65.8 hours because of indirect photolysis by hydroxyl radical attack.

Table 7. Hydroxyl Radical Photodegradation Half-life of Selected Chemicals from Streams in the Pyrolysis C3+ and Pyrolysis C4+ Category

Chemical	Calculated Half-Life* (hrs)	OH ⁻ Rate Constant (cm ³ /molecule-sec)
Isobutane	52.6	2.4 E ⁻¹²
n-Butane	48.8	2.6 E ⁻¹²
Isobutylene	2.5	51.7 E ⁻¹²
Cis-Butene-2	2.3	56.7 E ⁻¹²
Trans-Butene-2	3.0	64.3 E ⁻¹²
Butene-1	4.7	27.4 E ⁻¹²
1,3-Butadiene	1.9	66.6 E ⁻¹²
1,3-Cyclopentadiene	0.9	142.6 E ⁻¹²
Isohexane	22.4	5.7 E ⁻¹²
n-Hexane	23.5	5.5 E ⁻¹²
Methylcyclopentane	22.7	5.7 E ⁻¹²
Benzene	65.8	1.9 E ⁻¹²
Toluene	24.6	5.2 E ⁻¹²
m-Xylene	9.5	13.6 E ⁻¹²
Dicyclopentadiene	1.1	28.1 E ⁻¹²
Naphthalene	5.9	21.6 E ⁻¹²

* Atmospheric half-life values are based on a 12-hr day and an OH⁻ concentration of 1.5E6, which is the default concentration used by the model.

Atmospheric oxidation because of hydroxyl radical attack can be a significant route of degradation for streams in this category. Based on calculated values, chemicals in streams from this category can have an atmospheric half-life range of 0.9 to 65.8 hours because of indirect photolysis by hydroxyl radical attack.

3.2 Stability in Water (Hydrolysis)

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H₂O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982b).

Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Pyrolysis C3+ and Pyrolysis C4+ Category, will react with water by an addition reaction mechanism (Gould, 1959). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (Harris, 1982b). This reaction differs from other reactions with water such as hydration of carbonyls that can lead to the formation of an alcohol beginning with the transfer of a proton from the water to an alkene. However, water by itself is too weak an acid to transfer a proton in the absence of a strong

acid, which could effect such an acid catalysed electrophilic addition. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis.

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The chemicals in this category are primarily olefins that contain at least one double bond (alkenes). The majority of the remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism described above. Therefore, chemicals in the Pyrolysis C3+ and Pyrolysis C4+ streams have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

3.3 Distribution in the Environment

Fugacity-based multimedia modeling provides basic information on the relative distribution of a chemical between selected environmental compartments, which can include air, soil, water, sediment, suspended sediment, and biota. A widely used fugacity model, the EQC (Equilibrium Criterion) Level I model (Mackay *et al.*, 1996; Mackay, 1998) calculates chemical distribution between these compartments based on the input of basic physicochemical parameters including molecular weight, water solubility, log P_{ow} , and melting point.

Results of the EQC Level I model (Table 7) for selected chemical constituents of streams from this category suggest that they will partition primarily to air, with a small percentage partitioning to water, soil, and sediment. These results can be explained by their high vapor pressure. Distribution of these chemicals to each remaining compartment (suspended sediment, biota) is calculated as less than 0.01%. In comparison to all the other representative chemicals, only naphthalene is calculated to partition to other compartments in addition to the air at significant percentages; naphthalene represents <2% by weight of the total components in these streams.

Table 8. Environmental Distribution as Calculated by the EQC Level I Fugacity Model for Selected Chemicals from Streams in the Pyrolysis C3+ and Pyrolysis C4+ Category

Chemical	Distribution Per Environmental Compartment (%)					
	Air	Water	Soil	Sediment	Suspended Sediment	Biota
Isobutane	99.99	0.01	<0.01	<0.01	<0.01	<0.01
n-Butane	99.99	0.01	<0.01	<0.01	<0.01	<0.01
Isobutylene	99.99	0.01	<0.01	<0.01	<0.01	<0.01
cis-Butene-2	99.98	0.02	<0.01	<0.01	<0.01	<0.01
trans-Butene-2	99.98	0.02	<0.01	<0.01	<0.01	<0.01
Butene-1	99.99	0.01	<0.01	<0.01	<0.01	<0.01
1,3-Butadiene	99.97	0.03	<0.01	<0.01	<0.01	<0.01
Isoprene	99.96	0.03	<0.01	<0.01	<0.01	<0.01
1,3-Cyclopentadiene	99.93	0.06	<0.01	<0.01	<0.01	<0.01
Isohexane	99.97	0.01	0.02	<0.01	<0.01	<0.01
n-Hexane	99.96	<0.01	0.04	<0.01	<0.01	<0.01
Methylcyclopentane	99.95	0.02	0.03	<0.01	<0.01	<0.01
Benzene	98.89	1.00	0.11	<0.01	<0.01	<0.01
Toluene	98.80	0.81	0.39	<0.01	<0.01	<0.01
m-Xylene	97.91	0.86	1.20	0.03	<0.01	<0.01
Dicyclopentadiene	98.55	0.63	0.80	0.02	<0.01	<0.01
Naphthalene	42.27	20.56	36.33	0.81	<0.01	<0.01

Note: The distribution values were determined using physical property data from the EPIWIN (1999) database.

The 17 chemicals selected to characterize the transport/distribution range include C4 to C10 hydrocarbons that are predominant across the streams in this category. Physical property data (Table 4) used in the model are from the EPIWIN (1999) database.

3.4 Biodegradation

Biodegradation is the use of an organic chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which can eventually be converted to inorganic forms such as carbon dioxide, nitrate, sulfate, and water, depending on the composition of the parent chemical.

The microbial metabolism of aliphatic alkenes can be initiated by attack at the double bond (Watkinson and Morgan, 1990). Four degradative processes have been identified:

- Oxygenase attack upon a terminal methyl group to the corresponding alcohol, aldehyde, and acid
- Subterminal carbon oxygenase attack to the corresponding alcohol and ketone
- Oxidation across the double bond to the corresponding epoxide

- Oxidation across the double bond to the corresponding diol

Streams in the Pyrolysis C3+ and Pyrolysis C4+ Category are composed predominantly of chemicals that range mainly from C4 to C10 (Table 2).

Constituent chemicals from the two process streams in this category are simple hydrocarbons, the majority of which are calculated to partition primarily to the air where physical processes will contribute to their rapid degradation (see Indirect Photodegradation above for specific degradation rates of selected chemicals from this category). This is especially true for the gaseous constituents. Consequently, their availability to microbial degraders can be significantly limited. Because of the partitioning behavior of chemicals in this category, biodegradative processes will be less likely to contribute to their loss from the environment.

Streams from the Pyrolysis C3+ and Pyrolysis C4+ Category do not lend themselves to being evaluated for biodegradability using standard experimental designs because a significant proportion of the streams is gaseous. However, there is microbial metabolism information for several of the unsaturated C4 constituents in this category, including 1,3-butadiene, that demonstrates the gaseous constituents have the potential to biodegrade. In comparison, there are sufficient data developed using standard testing procedures to characterize the potential biodegradability of the constituents in this category that have a carbon number greater than C4. Data for those constituents, as well as for some complex substances not in this category, but that contain chemicals found in the streams of this category and are also used as read-across data, suggest that the streams in this category have the potential to biodegrade to a great extent.

The sections immediately below summarize results of studies for selected gaseous constituents from this category. The data do not allow for an estimation of the extent of biodegradability relative to a standard 28-day test procedure using a microbial inoculum from a wastewater treatment facility. However, the gaseous constituents discussed below are predicted by BIOWIN, Biodegradation Probability Program (EPIWIN, 1999), as having the potential to biodegrade rapidly. BIOWIN is a model in EPIWIN that calculates the probability of an organic chemical to rapidly biodegrade by a mixed population of microorganisms. BIOWIN can also estimate the time required to meet primary and ultimate biodegradation criteria]. Lastly, there is also a section that describes the potential biodegradability of the constituents that are greater than C4.

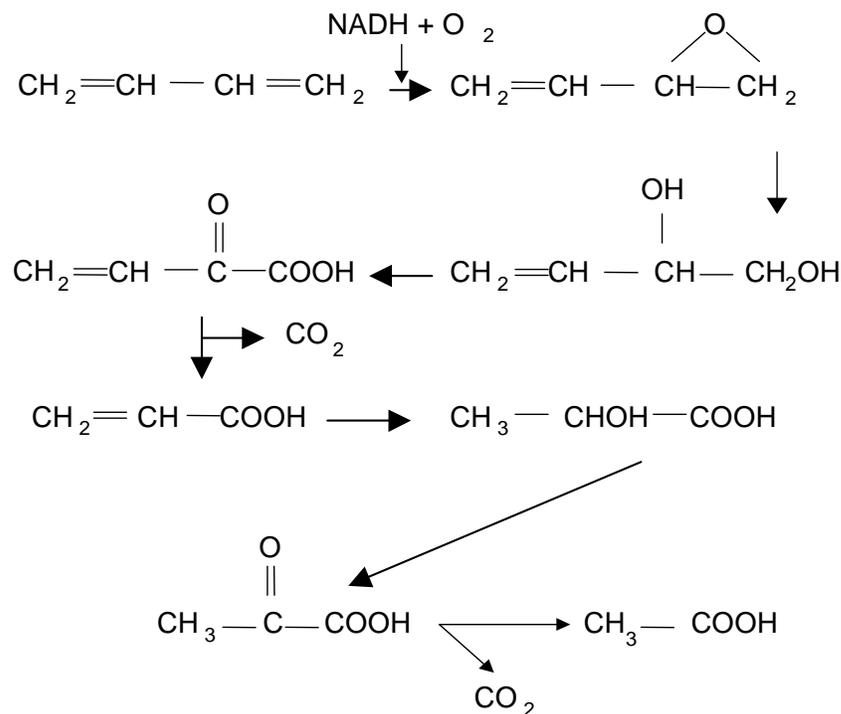
3.4.1 Propylene Biodegradation

Propylene (0 to 4% by weight) has been shown to be a growth substrate for several microorganisms. Isolated bacterial strains studied for their potential to biodegrade propylene under aerobic conditions were identified from the genus *Nocardia*, *Mycobacterium*, and *Xanthobacter* (de Bont *et al.*, 1980; de Bont *et al.*, 1982; de Bont *et al.*, 1983; van Ginkel and de Bont, 1986). Other species from the genus *Pseudomonas* and *Aerobacter* that were isolated from soil have also been associated with the ability to aerobically degrade propylene after they were shown to metabolize propylene oxide (Raja, 1991), an intermediate in the propylene metabolic pathway (van Agteren *et al.*, 1998).

Two pathways for the aerobic metabolism of propylene have been described (van Agteren *et al.*, 1998) that include the formation of either 1,2-propanediol or acetyl CoA prior to mineralization to CO₂.

3.4.2 1,3-Butadiene Biodegradation

Experimental studies to determine a catabolic pathway for 1,3-butadiene (12 to 42% by weight) as mediated by a *Nocardia sp.* (Watkinson and Somerville, 1976) resulted in the series of reactions shown in Figure 1.

Figure 1. Proposed Microbial Metabolic Pathway for the Degradation of 1,3-Butadiene by a *Nocardia sp.*

The intermediary metabolic steps depicted in Figure 1 result in the production of acetic acid (CH_3COOH) which can be further metabolized. In addition, 1,3-butadiene has been estimated to have an aerobic aquatic biodegradation half-life ranging from 1 to 4 weeks (Howard *et al.*, 1991).

3.4.3 1-Butene Biodegradation

Isolated bacterial strains have been evaluated for their potential to biodegrade 1-butene (5 to 11% by weight) under aerobic conditions. Bacteria from two genus, *Mycobacterium spp.* and *Xanthobacter spp.*, isolated from environmental samples have demonstrated the ability to degrade 1-butene (Hou *et al.*, 1983; Habets-Crützen *et al.*, 1984; van Ginkel and de Bont, 1986; Weijers *et al.*, 1995). Epoxybutane was shown to be converted to the corresponding ketone using a cell extract from a *Xanthobacter spp.* (Weijers *et al.*, 1995). These studies suggest that 1-butene can be biodegraded and that microbial metabolism can contribute to the overall loss of this chemical from the environment.

3.4.4 2-Butene Biodegradation

Although 2-butene (1.5 to 6.4% by weight) has not been reported as a microbial growth substrate, an isolated bacterial strain, *Xanthobacter spp.*, was evaluated for its potential to biodegrade various epoxyalkanes. Both diastereomeric forms of 2,3-epoxybutane were shown to degrade with degradation rates of 6 and 9 nmol/min/mg protein for trans- and cis- geometric isomers, respectively (Weijers *et al.*, 1988). These data suggest that a metabolic pathway is present in bacteria that will degrade these alkenes.

3.4.5 Isobutylene Biodegradation

Although isobutylene (5 to 12% by weight) has not been reported as a growth substrate for bacteria, isolated bacterial strains have been evaluated for their potential to biodegrade 1-butene under aerobic conditions. Epoxybutane was shown to be converted to the corresponding ketone using a cell extract from a *Xanthobacter spp.* (Weijers *et al.*, 1995). In the same study, 2-methyl-1,2-epoxypropane was not converted suggesting that isobutylene metabolism is not mediated in a manner similar to 1-butene by this organism. However, because of the structural similarity between 1-butene and isobutylene, isobutylene biodegradation may occur through a process not yet evaluated.

3.4.6 C5+ Fraction Biodegradation

The carbon number of constituents in this category that are not gaseous ranges primarily between C5 to C10 but can range up to C12. Results for several chemicals, including benzene, with carbon numbers in this range that are contained by the category streams have been shown to biodegrade from 63 to 100% after 14 or 28 days, while results for several comparable, complex products containing several components range from 21 to 96% after 28 days. Benzene itself was shown to be readily biodegradable (Olefins Panel of the American Chemistry Council, 2004b). As seen by the data in Table 9, there is a relatively large biodegradation database for single chemicals and complex substances that can be used to characterize this endpoint for streams in the Pyrolysis C3+ and Pyrolysis C4+ Category.

The data from the majority of tests in Table 9 were developed using a manometric respirometry test procedure. This procedure uses continuously stirred, closed systems, which is recommended when assessing the potential biodegradability of chemically complex, poorly water soluble, and volatile materials like those listed in the Table 9. Stirring is recommended when evaluating products containing several chemicals, some of which may have limited water solubility.

Table 9. Read-across Data for Chemical Constituents Greater than C4 that Contribute to Characterizing the Biodegradability of Streams in the Pyrolysis C3+ and Pyrolysis C4+ Category

CHEMICAL / SUBSTANCE	CARBON NUMBER	PERCENT BIODEGRADATION ^a (28 days)	REFERENCE
n-Pentane	5	87	IHSC ^e
Isopentane	5	71	IHSC ^e
Cyclohexane	6	77	IHSC ^e
Alkenes, C6 Rich	6 ^b	21	HOP ^f
1-Hexene (linear)	6	67-98 ^c	HOP ^f
Benzene	6	63	OP ^g
Alkenes, C7-C9, C8 Rich	7-9	29	HOP ^f
p-Xylene	8	89	XC ^h
Naphtha (Petroleum), light alkylate (gasoline stream)	5-8	42 ^d	API ⁱ
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8	74 ^d	API ⁱ
Naphtha (Petroleum), Light Catalytically Reformulated (gasoline stream)	5-9	96 ^d	API ⁱ
C8-C10 Aromatics, Predominantly C9 Alkylbenzenes	9 ^b	78	IHSC ^e
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 ^b	61	IHSC ^e

a Organization for Economic Co-ordination and Development (OECD) 301F, manometric respirometry test

b Predominant carbon number or range

c (Biological Oxygen Demand) BOD test

d Test method for determining the inherent aerobic biodegradability of oil products and modification of ISO/DIS 14593

e Covered by the International Hydrocarbon Solvents Consortium through the OECD Screening Information Data Set (SIDS) program

f Covered by the American Chemistry Council (ACC), Higher Olefins Panel: C6, C7, C8, C9, and C12 Internal Olefins and C16 and C18 Alpha Olefins Category test plan (submitted to EPA)

g Robust summary submitted with ACC, Olefins Panel, High Benzene Naphthas test plan; CEFIC APA/EU Risk Assessment Report for Benzene

h Covered by the Xylene Consortium and reviewed by OECD at SIDS Initial Assessment Meeting (SIAM) 16

i Robust summary submitted with American Petroleum Institute, Gasoline Blending Streams test plan (submitted to EPA)

3.4.7 Abiotic and Biotic Degradation Summary

The stream constituents from this category will partition primarily to the air where physical degradative processes will dominate their fate. Data show that these chemicals are subject to rapid physical degradation. Selected constituents of streams and complex substances containing chemicals similar to category streams have also been shown as biodegradable, some readily biodegradable. Overall, the constituent chemicals and consequently the streams from this category

are expected to degrade rapidly in the environment from physical and biological processes and not persist.

4 HUMAN HEALTH HAZARDS

4.1 Effects on Human Health

The two streams that comprise the Pyrolysis C3+ and Pyrolysis C4+ Category, which together contain two CAS RNs, vary in 1,3-butadiene content, ranging from 12 to 42% and in benzene content, ranging from 11 to 42%. Much of the data used to characterize this category are from 1,3-butadiene, which is the most biologically active of the constituents and hence major contributor to toxicological activity. These data were previously submitted with the Crude Butadiene C4 Category summary report. Additionally, benzene can be present as a predominant component and is therefore also considered a key driver in characterizing potential health effects. These data were previously submitted with the High Benzene Naphthas Category summary report (data are summarized in Appendix II; sources of data for the hazard evaluations are summarized in Appendix III). Data for pure 1,3-butadiene together with data from a mid 1,3-butadiene stream (approximately 45 to 67%), a low 1,3-butadiene stream (approximately 10%), along with data for benzene, benzene-containing streams, and additional select hydrocarbon substances adequately characterize the HPV Program human health effects endpoints for the streams in this category.

Chemical Component Interactions

- When tested as pure substances, some of the components in the Pyrolysis C3+ and Pyrolysis C4+ Category streams other than 1,3-butadiene and benzene have caused genetic damage and adverse target organ effects in repeated-dose animal studies. However, since the biologically active components of the Pyrolysis C3+ and Pyrolysis C4+ Category are metabolized through a common P450 metabolic pathway, it is anticipated that multiple components will compete for the same active enzyme sites. Component toxicities, which are dependent on the formation of biologically active metabolites, may be reduced, as less metabolite(s) will be produced through competition for these sites. Direct support for reduction or elimination of toxicities of individual components is provided by results of an existing mouse bone marrow micronucleus test with one of the High Benzene Naphtha streams, Hydrotreated C6-8 Fraction described in the summary of *in vivo* mutagenicity data below. This stream, containing approximately 55% benzene, was negative in a mouse bone marrow micronucleus test when administered by oral gavage at 2000 mg/kg to male and female CD-1 mice (see robust summary). Several studies have shown that benzene administered orally to CD-1 mice induces high frequencies of micronuclei in bone marrow erythrocytes for doses of 110 mg/kg (Ciranni *et al.*, 1988; Suzuki *et al.*, 1989; Hite *et al.*, 1980; Gad-El Karim *et al.*, 1986; Meyne and Legator, 1980). The presence in the Hydrotreated C6-8 Fraction of other components (approximately 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 3% cyclohexane, and 2% hexane) apparently inhibited the expected clastogenicity of benzene. Other similar interactions between components of the category also have been reported, in particular by Medinsky *et al.* (1994) and Bond *et al.* (1998), with reviews on the metabolism of benzene and the effects of interactions with other organic chemicals on benzene toxicity and metabolism. Reports of interactions between other components of the Pyrolysis C3+ and Pyrolysis C4+ Category have also been noted in the literature. Examples of these interactions and the effect on the formation of benzene metabolites and resultant hematotoxicity or genotoxicity are detailed in the following references: Gad-El-Karim *et al.*, 1984; Gad-El-Karim *et al.*, 1986; Andrews *et al.*, 1977; Bond *et al.*, 1998; Nylen, 1996; Nylen, 1989; ATSDR, 1999; Daughtrey *et al.*, 1999; Soiefer *et al.*, 1991.

4.1.1 Acute ToxicityCrude Butadiene C4 Category

Data are available to evaluate acute toxicity of streams in the Crude Butadiene C4 Category. As the streams are gaseous at room temperature, data are from inhalation toxicity studies (Table 10).

Table 10. Summary of Acute Inhalation Toxicity Data for Crude Butadiene C4 Streams

CAS RN and Stream/Chemical Name (% 1,3-Butadiene)	Test Organism	Exposure Duration (hr)	LC ₅₀ (mg/m ³)
68955-28-2 C4 Crude Butadiene (45)	Rat	4	5,300
106-99-0 1,3-Butadiene (>99)	Rat	4	285,000
106-99-0 1,3-Butadiene (>99)	Mouse	2	270,000

High Benzene Naphthas Category

Data are available to evaluate acute toxicity of streams in the High Benzene Naphthas Category. Data from the oral, dermal, or inhalation routes of exposure are presented in Table 11.

Table 11. Summary of Acute Toxicity Data for Representative High Benzene Naphtha Streams

Route	Dripolene	Hydrotreated C6-8 Stream (Hydrogenated Pyrolysis Gasoline)	C5-10 Fraction of Pyrolysis Gasoline (Rerun Tower Overheads)	Benzene ^a	Toluene ^a
Oral LD ₅₀	>2.0 g/kg	5.17 g/kg	>2.0 g/kg	0.81 to 1.0 g/kg	5.5 g/kg
Dermal LD ₅₀	>2.0 g/kg	---	>2.0 g/kg	---	12.4 g/kg
Inhalation LC ₅₀ [4-hr exposure]	---	>12,408 ppm	---	13,700 ppm	8000 to 8800 ppm

a data listed in Appendix II

Conclusion

Available data adequately address the acute toxicity of the Pyrolysis C3+ and Pyrolysis C4+ Category. Data from representative streams of the Crude Butadiene C4 and High Benzene Naphthas Categories demonstrate low acute toxicity by oral, dermal, or inhalation routes of exposure.

4.1.2 Repeated Dose ToxicityCrude Butadiene C4 Category

Repeated dose toxicity tests have been conducted on a variety of streams pertinent to this category (Table 12). These studies range from 9 to 98 days in duration and have been conducted in rats and mice.

Table 12. Summary of Repeated Dose Toxicity Data for Crude Butadiene C4 Streams

CAS RN and Stream Name (% 1,3-Butadiene)	Test Organism	Exposure Duration (days)	NOAEL (mg/m ³)
68476-52-8 C4 Crude Butadiene (10)	Crl:CD Rat	36	>20,000
106-99-0 1,3-Butadiene (>99)	CD Rat	91	>17,679
68955-28-2 C4 Crude Butadiene (45)	Fischer 344 Rat	9	>25,100
106-99-0 1,3-Butadiene (>99)	B6C3F1 Mouse	98	>2,760

Inhalation - Studies in Animals

Effects of repeated exposure to C4 Crude Butadiene (CAS# 68476-52-8: 10% 1,3-butadiene; 4% isobutane; 29% trans-2-butene; 29% 1-butene; 11% isobutylene; and 12% cis-2-butene) were evaluated as part of an Organization for Economic Co-ordination and Development (OECD) 422, Repeated Exposure Reproductive/Developmental Toxicity Screen in Crl:CD rats (Carney *et al.*, 2001). Twelve male and female rats were exposed to vapor concentrations 0; 2,000; 10,000; or 20,000 mg/m³ Crude Butadiene for 36 or 37 days, 6 hr/d, 7 d/wk (this study contained an additional group of twelve female rats for reproductive and developmental toxicity screening evaluation). Males and females were sacrificed at the end of exposure. Effects on general toxicity, neurobehavioral activity, clinical chemistry, and hematology were evaluated. At necropsy, organs were weighed, evaluated grossly and histopathological evaluation was conducted. No deaths or treatment related clinical observations were reported. No treatment related changes were observed in body weight, sensory evaluation, rectal temperature, fore/hindlimb grip performance, motor activity total counts, hematology, prothrombin time, clinical chemistry, organ weights, gross pathology, or histopathology. In evaluation of motor activity, the treatment-by-time-by-epoch interaction was significant. However, further evaluation indicated that this difference could be attributed to the time-by-epoch interaction rather than a treatment related effect. Females in the 2,000 mg/m³ dose group had an increased hematocrit and a decrease in serum protein. However, these effects did not demonstrate a dose response and were not observed in males at the same dose level. As such these findings were considered incidental and not indicative of a treatment related response. The NOAEL in this study was 20,000 mg/m³.

In a 90-day repeat dose study, groups of 40 male and 40 female CD rats were exposed to 0; 2,209; 4,417; 8,334; or 17,679 mg/m³ (0; 1,000; 2,000; 4,000; or 8,000 ppm, respectively) 1,3-butadiene (>99.2%, containing 120 ppm t-butyl catechol). Exposures were conducted for 6 hr/da, 5 da/wk for 13 weeks (Crouch *et al.*, 1979). Interim sacrifices of 10 rats/sex/group were conducted at 2 and 6 weeks, with blood being collected from all rats at these intervals and at terminal sacrifice. Body weights and food consumption were recorded weekly. Brain cholinesterase activity was determined in 5 rats/sex/group at the 2 and 6-week sacrifices and all rats at terminal sacrifice. Urine samples were collected from rats 1 to 2 weeks prior to sacrifice. Organ weights were determined for select organs with histopathology conducted on control and high exposure animals. Increased salivation was observed in female rats following 8 weeks of exposure. Decreased grooming was observed in male rats following ten weeks of exposure. Slight, non significant, reductions in body weight were observed in male rats. Organ weight and organ-to-brain weight ratios showed some scattered

statistically significant differences among the groups but did not follow any consistent dose response trend. The NOAEL in this study was determined to be 17,679 mg/m³.

No adverse effects were observed in rats following exposure to butadiene feedstock (CAS # 68955-28-2: 45% 1,3-butadiene; 20% butanes; and 30% butenes) in a well conducted short term repeated exposure study (Gulf Oil Chemicals Co., 1983a). Groups of five male and five female Fischer 344 rats were exposed to 0; 2,500; or 25,100 mg/m³ butadiene feedstock 6 hr/d, for a total of 9 days. Evaluations include body weight measurement, gross necropsy, organ weights, histopathology on selected organs, hematology, and clinical chemistry. With the exception of nasal discharge, no exposure related changes were observed. The NOAEL in this study was determined to be 25,100 mg/m³.

Groups of 10 B6C3F1 mice/sex/group were exposed to 0; 1,380; 2,761; 5,522; 11,040; or 17,670 mg/m³ (0; 625; 1,250; 2,500; 5,000; or 8,000 ppm, respectively) 1,3-butadiene (98.94% with 0.02% t-butyl catechol) 6 hr/d, 5 d/wk for 14 weeks (NTP, 1984). Limited observations were conducted and included mortality and morbidity, body weight changes, gross pathology, and histopathology on high dose and control animals. Mortality was observed in the 2,761 mg/m³ group (1/10 males) and higher concentrations. Body weights were decreased at 5,522 mg/m³ and higher concentrations. Despite mortality present at this concentration, the NOAEL was determined to be 2,761 mg/m³.

High Benzene Naphthas Category

Two streams were tested in repeat-dose studies. A 5-day rat inhalation study was conducted with a Hydrotreated C6-8 stream (Hydrogenated Pyrolysis Gasoline), and a 21-day rabbit dermal irritation study, which included evaluations for systemic effects, was conducted with a C5-C10 Fraction of Pyrolysis Gasoline (Rerun Tower Overheads).

Inhalation

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis gasoline; 55% benzene) was evaluated for toxicity in an 8-day inhalation study using F344 rats. Animals (5/sex/group) were exposed at concentrations of 0; 4,869; and 9,137 ppm daily for 5 days and sacrificed on day 8 after a 2-day post-exposure observation period (Rausina, 1984). Three rats (1M, 2F) from the high dose group died on days 1-2 of exposure. Rats were lethargic and showed labored respiration on days 1-5 of treatment; however, all but one high dose rat recovered fully by day 8. Group mean body weights were significantly decreased in a dose-related manner but no test material-related effects were reported at gross necropsy; a LOEL of <4,869 ppm was reported.

Dermal

C5-C10 Fraction of Pyrolysis Gasoline (Rerun Tower Overheads; 40% benzene) was evaluated for skin irritation and systemic toxicity in a 21-day dermal study using New Zealand White rabbits (Feiser *et al.*, 1980). Test material [undiluted] was applied to the shaved abraded backs of 4 male and 4 female rabbits per group at concentrations of 0, 0.1, 0.5, and 1.0 ml once a day for 21 consecutive days. Exposed sites were unoccluded and each rabbit wore a Plexiglas collar to retard ingestion of test material. Skin irritation and erythema were observed in a dose-related manner. No significant effects were seen on body or organ weight, feed consumption, hematology, or serum chemistries. No abnormal microscopic changes were observed in any organ system with the exception of damage to dermal layers consistent with gross observations of irritation. The authors concluded the following: NOAEL (irritation) <0.10 ml/kg; NOAEL (systemic) = 1.0 ml/kg.

Conclusion

Data are available to adequately characterize the repeated dose toxicity of the Pyrolysis C3+ and Pyrolysis C4+ Category for purposes of the HPV Program. Available studies from the C4 Crude Butadiene Category cover a wide range of 1,3-butadiene concentrations (10 to 99%). The data are

consistent in that they demonstrate minimal effects in rats with the exception of body weight changes, while mice demonstrate greater sensitivity following repeated inhalation exposures.

The effects reported for the High Benzene Naphthas category are similar to those observed for gasoline blending streams (API HPV Test Plan, 2003) in which dermal treatment induced primarily skin irritation and concomitant systemic effects, while inhalation exposure induced effects on lung, liver, kidney and blood at high doses, that were no longer observed after 4 weeks of recovery in most studies. Species and sex-specific light hydrocarbon nephropathy in male rat kidneys was observed when alkane content was high.

Repeated oral or inhalation exposures to many of the components of the Pyrolysis C3+ and Pyrolysis C4+ Category streams have been shown to cause adverse health effects in a variety of organs. Benzene demonstrated toxicity primarily in the hematopoietic system, toluene affected the central nervous system and light hydrocarbon nephropathy was seen with exposure to hexane isomers, to a 50/50 blend of n-butane, to n-pentane, or to dicyclopentadiene. However, existing data also show that antagonistic and synergistic interactions occur between some components comprising the streams, as noted above in the Chemical Component Interaction section of the Introduction to Section 4.1, which could alter the expression of toxicity of individual hydrocarbons. The target organs affected by exposure to the mixtures, and the severity of the effects, depend upon the relative concentrations of the components within each stream and the nature of the interactions between components.

4.1.3 Mutagenicity

Crude Butadiene C4 Category

Genetic toxicity of crude butadiene has been evaluated both *in vitro* and *in vivo*. *In vitro* assays include Ames *Salmonella* Reverse Mutation assay, unscheduled DNA synthesis in rat hepatocytes, mammalian cell transformation assay, and mouse lymphoma assay. Potential for the *in vivo* induction of micronuclei in bone marrow has been examined in rats and mice following inhalation exposure.

In Vitro Studies

Mutagenic activity of 1,3-butadiene (CAS # 106-99-0) was evaluated in the Ames *Salmonella* Reverse Mutation assay (Arce *et al.*, 1990). *Salmonella typhimurium* tester strains TA 97, TA 98, TA 100, and TA 1535 were overlaid on agar with or without mouse, rat, or human S9 activation systems in specially designed treatment chambers. 1,3-Butadiene gas was metered into the chambers at concentrations of 0, 30, 40, 50, and 60% for a 48-hour exposure period. An increase (just over 2-fold) in revertant colonies was observed only with the TA 1535 strain; all other strains demonstrated no increase. In this bacterial strain, mouse S9 had slightly higher activity than the uninduced rat or human S9 at 30% 1,3-butadiene in air. At concentrations greater than 30%, the number of revertants decreased in the presence of rat or human S9. Presence of human S9 did not substantially increase the number revertants compared to non S9 activated samples. Arochlor 1254 induced rat liver S9 fractions produced the same number of revertants as untreated mouse liver S9. Increasing the amount of rat S9 protein/plate slightly increased the number of revertants/plate without Arochlor 1254 induction, but did not produce an increase with Arochlor 1254 induction. In summary, 1,3-butadiene demonstrated weak mutagenic activity in this test system.

Butadiene concentrate (CAS # 68955-28-2: 67% 1,3-butadiene; 30% butenes; and 2% 1,2-butadiene) was evaluated for mutagenicity in the Ames *Salmonella* Reverse Mutation assay (Mobil Environmental and Health Sciences Laboratory, 1985b). Five strains of *Salmonella typhimurium* (TA 98, TA 100, TA 1535, TA 1537, and TA 1538) were incubated with 25, 50, 75, or 100 µl crude butadiene, with and without Arochlor 1254 rat liver S9 activating system. Reversion frequencies in

treated groups with and without S9 activation were similar to controls. The test stream was judged to be non-mutagenic in this assay.

Butadiene concentrate (CAS# 68955-28-2: 45% 1,3-butadiene; 20% butanes; and 30% butenes), did not induce cell transformations in BALB/3T3-A31-1-1 cells treated *in vitro* with up to 20,000,000 mg/m³ of the test stream (Gulf Oil Chemicals Co., 1983b). An increase in mutant frequency was observed in the mouse lymphoma cells following exposure to butadiene concentrate (CAS# 68955-28-2: 67% 1,3-butadiene; 30% butenes; and 1.2% 1,2-butadiene) in the absence of S9 activation. No increase was observed in the presence of S9 activating system (Mobil Environmental and Health Sciences Laboratory, 1985c). Unscheduled DNA synthesis (UDS) was observed in primary rat hepatocytes at 20,000,000 mg/m³ butadiene concentrate (CAS# 68955-28-2: 45% 1,3-butadiene; 20% butanes; and 30% butenes), a level where marked cytotoxicity was observed (Gulf Oil Chemicals Co., 1984a) potentially confounding the data. No UDS was observed at treatment levels less than or equal to 10,000,000 mg/m³.

In Vivo Studies

Six male and female B6C3F1 mice were exposed to concentration of 500; 10,000; or 20,000 mg/m³ C4 crude butadiene (CAS #, 68476-52-8: 10% 1,3-butadiene; 4% isobutane; 4% n-butane; 29% trans-2-butene; 29% 1-butene; 11% isobutylene; and 12% cis-2-butene) by inhalation for 2 days, 4 hr/d (Spencer *et al.*, 2001). Twenty-four hours following the final exposure, femoral bone marrow was collected to evaluate micronuclei formation in polychromatic erythrocytes. Cyclophosphamide was used as the positive control. Increases in the frequencies of micronuclei were observed in all groups treated with test material. Although a statistically significant dose response was indicated, the difference between the low and high dose groups was minimal. Crude butadiene was positive for induction of micronuclei in this test system.

Twenty female CB6F1 mice and ten male Wistar rats were exposed to 0, 50, 200, or 500 ppm 1,3-butadiene for 5 days, 6 h/d by inhalation (Autio *et al.*, 1994). One day following exposure, smears of blood and bone marrow erythrocytes were prepared and stained. In rats, toxicity in bone marrow cells was observed in the 500 ppm exposure group. In rats, no increase in micronuclei frequencies were observed in either peripheral blood or bone marrow erythrocytes. In mice, a clear dose-dependent increase in micronuclei formation was observed in blood and bone marrow at all exposure levels tested.

Male and female Crl:CD-1 BR Swiss mice were exposed to 0; 10,780; 20,671; or 35,430 ppm butadiene concentrate (CAS # 68955-28-2: 45% 1,3-butadiene; 20% butanes; and 30% butenes) *via* inhalation for 2 hr/d for 2 consecutive days (Gulf Oil Chemicals Co., 1984b). Five mice per sex per dose were sacrificed on day 3 and day 4 (24 and 48 hours post-exposure), and bone marrow smears prepared. Loss of consciousness was observed in mice during exposures; no other adverse effects were observed. An increased incidence of micronuclei formation was observed at all dose levels on day 3 and at the 2 highest dose levels on day 4. Male mice exhibited an increase in micronuclei formation at the highest dose on both days.

High Benzene Naphthas Category

In Vitro Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline; 55% benzene) did not induce mutagenic events in four strains of *Salmonella typhimurium* or one strain of *Escherichia coli* with or without metabolic activation from rat liver S9 (Ricchio and Stewart, 1991). This stream also did not induce unscheduled DNA synthesis in primary rat hepatocytes.

C5-C10 Fraction of Pyrolysis Gasoline (Rerun Tower Overheads; 40% benzene) did not induce mutagenic events in five strains of *Salmonella typhimurium*, with or without metabolic activation from rat liver S9. However, this stream did cause weak differential killing in DNA repair-deficient

strains of *E. coli* and *S. typhimurium* (Haworth, 1978). In mammalian cells, a weak positive response in mouse lymphoma cells without metabolic activation was induced but no increase in revertant colonies was seen with metabolic activation.

In Vivo Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline; 55% benzene) was evaluated for cytogenetic damage in the mammalian bone marrow erythrocyte micronucleus assay using male and female Swiss mice. Mice were given oral doses of 0, 0.5, 1.0, or 2.0 g/kg/d for 2 days or 1 dose of 2.0 g/kg for 1 day. Treatment did not increase the frequency of micronucleated polychromatic erythrocytes in mouse bone marrow (Khan, 1984).

C5-C10 Fraction of Pyrolysis Gasoline (Rerun Tower Overheads; 40% benzene) was tested in *Drosophila melanogaster* for gene (point) mutations and cytogenetic damage (chromosome loss or aberrations). This stream did not induce gene mutation or chromosome damage in this fruit fly system (Bowman, 1979).

Conclusion

Adequate data are available to evaluate the genotoxicity of the Pyrolysis C3+ and Pyrolysis C4+ Category. Data from the Crude Butadiene C4 category examined streams with a range of 1,3-butadiene content (10 to 99%). This range of 1,3-butadiene has been tested in both *in vitro* and *in vivo* test systems. *In vitro* studies indicate a weak mutagenic activity. *In vivo* studies in mice and rats demonstrated a genotoxic response in mice but not in rats from exposure to streams in this category with high 1,3-butadiene content. Studies of 1,3-butadiene metabolism in mice and rats have shown large inter-species differences, with mice 2- to 10-fold more efficient than rats in oxidizing 1,3-butadiene to electrophilic metabolites (Schmidt and Loeser, 1985; Csanady *et al.*, 1992). The existing metabolism data suggest that metabolism of 1,3-butadiene in humans appears to be more like metabolism in rats than in mice, therefore the relevance of the mouse genotoxicity studies to humans is questionable.

The representative streams tested from the High Benzene Naphthas category did not induce cytogenetic damage in animals. Streams from this category demonstrated how interaction and competition for metabolic sites can block toxicity of individual components. Although containing 55% benzene, presumably the presence of other components in the Hydrotreated C6-8 Fraction (approximately 25% toluene, 10% xylene, 7% pentane, 7% ethylbenzene, 3% cyclohexane, and 2% hexane) inhibited the expected clastogenicity of benzene. As discussed above and in the introduction to Section 4.1, coadministration of benzene with other hydrocarbons that are substrates for the same cytochrome P450 enzymes can reduce clastogenicity.

Although many of the category components did not induce mutation in bacteria and are not considered gene mutagens, clearly streams containing $\geq 10\%$ butadiene do result in mutagenicity and clastogenicity. Thus, based on composition and available data for representative streams, components and mixtures of components, it is likely that most streams in the Pyrolysis C3+ and Pyrolysis C4+ Category should be considered as gene mutagens and likely as clastogenic.

4.1.4 Carcinogenicity

Crude Butadiene C4 Category

Inhalation - In Vivo Studies

Male and female Sprague-Dawley rats were exposed to 0; 1,000; or 8,000 ppm 1,3-butadiene, 6 hr/d, 5 d/week for 111 weeks. Survival of both sexes was reduced at the high exposure level. An increase in incidence and number of animals with mammary tumors was observed in female rats at both the 1,000 and 8,000 ppm exposure levels. Increased incidences of thyroid gland adenomas and

carcinomas, uterine sarcomas and Zymbal gland tumors were observed in female rats. The incidence of uterine sarcomas and Zymbal gland tumors was within the historical control range for these tumor types and may not have been related to treatment. An increased incidence in exocrine pancreas adenomas was observed in male rats at 8,000 ppm. An exposure related increase in Leydig cell tumors was observed in male rats at both concentrations.

Two cancer bioassays have been conducted in B6C3F1 mice. In the first study, male and female mice were exposed to concentrations of 0; 625; or 1,250 ppm butadiene for 61 weeks, at which time the study was canceled due to poor survivability (NTP, 1984). Numerous tumor sites were observed in both sexes. A dose-related increase in lymphomas, cardiac hemangiosarcomas, and lung tumors was observed in both sexes. Increased incidence of papillomas or carcinomas of the forestomach, hepatocellular adenomas or carcinomas, ovarian granulosa cell tumors, acinar cell carcinomas of the mammary gland, brain gliomas, and Zymbal cell carcinomas were observed in one or both sexes.

Due to the poor survival rate in the initial study, a second study was conducted where B6C3F1 mice were exposed to 0, 6.25, 20, 62.5, 200 or 625 ppm 1,3-butadiene, 6 hrs/d, 5 d/week, for two years (NTP, 1993). Survival was reduced at exposure concentrations of 20 ppm and above. Tumors were observed at numerous sites including lymphocytic lymphomas, histiocytic sarcomas, cardiac hemangiosarcomas, Harderian gland adenomas and carcinomas, hepatocellular adenomas and carcinomas, alveolar/bronchiolar adenomas and carcinomas, mammary gland adenoacanthomas and carcinomas, ovarian granulosa cell tumors and forestomach squamous cell papillomas and carcinomas. Alveolar/bronchiolar tumors were observed at the lowest dose administered in females (6.25 ppm).

Studies in Humans

Two large cohort studies provide the most definitive assessment of the relationship between cancer and butadiene exposure. One study was conducted on butadiene exposed workers in the synthetic rubber industry. Butadiene exposed workers in the butadiene monomer industry were evaluated in the second.

Delzell *et al.* (1996) evaluated mortality in a cohort of over 13,000 men employed at eight different styrene-butadiene rubber (SBR) plants. The overall standardized mortality ratio (SMR) for leukemia was 1.31 (CI₉₅ = 0.97 to 1.74). Leukemia risks were concentrated among long-term workers with long latency working in jobs with the potential for high exposures to styrene and 1,3-butadiene. Greater than 2-fold increased leukemia risk occurred among hourly workers with more than 10 years employment and 20 years since hire and among workers in areas where there were potentially high exposures to 1,3-butadiene or styrene (*e.g.*, polymerization, maintenance labor, laboratories). Overall, about 75% of the cohort was exposed to 1,3-butadiene and 83% to styrene. In this same cohort of SBR workers, Delzell *et al.* (2001) evaluated the relationships between leukemia and exposure to 1,3-butadiene, styrene and dimethyldithiocarbamate (DMDTC). Past exposures to 1,3-butadiene, styrene and DMDTC were reconstructed through the use of exposure measurements and exposure modeling. In this analysis, leukemia mortality was significantly associated with cumulative 1,3-butadiene exposure, particularly for high ppm-years exposure levels. A stronger association was observed for cumulative 1,3-butadiene exposures with peak levels greater than 100 ppm. When concurrent exposure to styrene and DMDTC were considered, the effect of 1,3-butadiene exposure was reduced, but the exposure-response trend and apparent threshold remained. It was difficult to determine an independent effect of 1,3-butadiene exposure because of the high correlation of 1,3-butadiene exposure with styrene and DMDTC exposures. The strengths of this study are the large size, long follow-up, and quantitative estimate of exposure. The weakness of this study is the concomitant exposures to styrene and DMDTC and uncertainty in the effects of 1,3-butadiene alone.

Divine and Hartman (2001) evaluated a cohort of almost 2,800 men employed at a 1,3-butadiene monomer producing plant. There were 18 cases of leukemia with an overall SMR of 1.29 (CI₉₅ =

0.77 to 2.04) in 'all employed before 1950' (Divine and Hartman, 2001). The risk of leukemia decreased slightly among workers employed greater than 5 years compared to workers with less than 5 years employment in the high exposure group. This result was considered to be inconsistent with a dose-response effect. Over half the leukemia deaths occurred in subjects more than 40 years since hire, which is considered an unusually long latency for leukemia. Cumulative 1,3-butadiene exposure was based on job exposure class, calendar time and length of time in job, and was qualitative rather than quantitative as in the SBR study of Delzell *et al.* (2001). There was no suggestion of increasing risk with increasing 1,3-butadiene exposure. Because the exposure estimates were qualitative, it is not possible to determine the reasons for the apparent absence of risk associated with 1,3-butadiene exposure in the monomer compared to the SBR study. It has been suggested that the lack of risk among monomer workers could be due to the absence of concomitant styrene and DMDTC exposures, or that 1,3-butadiene exposures were lower than the apparent threshold observed in the SBR study. The absence of risk among monomer workers is consistent with the lack of genotoxic effects among a small group of monomer workers (25 cases and 25 controls) from Prague (Albertini *et al.*, 2003). Biomarkers of exposure were related to 1,3-butadiene exposure, in contrast to the lack of any genotoxic effects (despite clear exposure) which did not correlate with 1,3-butadiene. Albertini *et al.* (2003) suggested that the lack of a genotoxic effect was not supportive of a cancer classification.

High Benzene Naphthas Category

In Vivo Studies

No studies are available on High Benzene Naphtha streams. Of the significant components, benzene is a demonstrated leukemogen in humans (acute myelogenous leukemia) and also induces solid tumors in laboratory animals. However, toluene, also a major constituent of the High Benzene Naphthas Category streams and a competitor with benzene for metabolic sites, did not induce tumors at concentrations as high as 1200 ppm in a 2-year inhalation study in rats and mice (NTP, 1990). In a 2-year inhalation study of wholly vaporized gasoline, which has considerable benzene levels (MacFarland *et al.*, 1984), the principal tumorigenic effect occurred in kidneys of male rats and was later demonstrated to be a species- and sex-specific event unrelated to health hazards for humans (US EPA, 1991).

In Vitro Studies

Hydrotreated C6-C8 stream (Hydrogenated Pyrolysis Gasoline; 55% benzene) caused cell transformation in BALB-c/3T3 cells at a high concentration of 5000 µg/ml, a level that was too toxic for cells to recover and form colonies (Brecher, 1984).

C5-C10 Fraction of Pyrolysis Gasoline (Rerun Tower Overheads; 40% benzene) did not induce cell transformation in two test systems; the mouse embryo C3H 10T1/2 cell line or the BALB-c/3T3 cell line (Jensen and Thilager, 1978; Tu and Sivak, 1981).

Conclusion

The carcinogenic potential of the Pyrolysis C3+ and Pyrolysis C4+ Category streams will be driven largely by relative concentrations of two substances, 1,3-butadiene and benzene, which are either known or suspected human carcinogens under various regulatory classifications.

1,3-Butadiene is an animal carcinogen that demonstrates significant species differences in potency. 1,3-Butadiene is a potent, multi-site carcinogen in the mouse. Inhalation exposure to concentrations of 6.25 ppm produced lung tumors in B6C3F1 mice. Exposure to higher concentrations produced tumors at multiple sites. 1,3-Butadiene is a less potent carcinogen in rats. Although treatment-related tumors were observed in the rat study, the potency and total tumor incidence was markedly different when compared to the mouse bioassays. The differences observed are likely due to the differences in 1,3-butadiene metabolism described in section 4.1.3.

Carcinogenic effects of 1,3-butadiene are more difficult to discern for humans. Epidemiology studies of workers exposed to 1,3-butadiene in the monomer industry demonstrated no increase in carcinogenic risk. In the synthetic rubber industry, however, workers exposed to 1,3-butadiene demonstrated an increased risk of leukemia associated with long term exposure to high levels of 1,3-butadiene. The association was stronger when co-exposures to styrene and DMDTC were also considered. The difference in leukemia risk between these two groups could be related to differences in exposure to 1,3-butadiene, or the need for co-exposure to other agents in addition to 1,3-butadiene (styrene, DMDTC) for the expression of leukemia.

Benzene is a demonstrated leukemogen in humans (acute myelogenous leukemia) and also induces solid tumors in laboratory animals. However, toluene is also a major constituent of the category streams and a competitor of benzene for metabolic sites; toluene did not induce tumors at concentrations as high as 1200 ppm in a 2-year inhalation study in rats and mice (NTP, 1990). Cell transformation assays on representative streams in the High Benzene Naphthas Category demonstrated minimal if any carcinogenic potential. Transformation induced by the Hydrotreated C6-C8 stream (55% benzene) occurred at a high dose from which cells are unlikely to survive and produce potentially tumorigenic colonies, and the C5-C10 Fraction of Pyrolysis Gasoline (40% benzene) was not active.

Although no carcinogenesis studies were directly available on Pyrolysis C3+ and Pyrolysis C4+ Category streams, extrapolation from 2-year cancer bioassays on related components, in conjunction with the apparent competitive detoxifying effects of other components in the streams (*e.g.*, toluene when co-administered with benzene), the species-specific metabolism, and the *in vitro* data, suggest that carcinogenesis is unlikely to be a significant endpoint of toxicity for this category.

4.1.5 Toxicity for Reproduction

Crude Butadiene C4 Category

Several studies evaluated the reproductive and developmental toxicity of streams in the Crude Butadiene C4 Category (Tables 13 and 14). The streams evaluated ranged in 1,3-butadiene content from 10 to 100%. The majority of studies were conducted under standard protocols in compliance with GLP (good laboratory practices).

Table 13. Summary of Reproductive Toxicity Data for Crude Butadiene C4 Streams

CAS RN and Stream Name (% 1,3-Butadiene)	Test Organism	OECD Test Guideline	NOAEL (mg/m ³)
68476-52-8 C4 Crude Butadiene (10)	CrI:CD Rat	422	>20,000 (Systemic) >20,000 (Reproductive)
106-99-0 1,3-Butadiene (>99)	CrI:CD Rat	421	>663 (Systemic) >13,260 (Reproductive)

Table 14. Summary of Developmental Toxicity Data for Crude Butadiene C4 Streams

CAS RN and Stream Name (% 1,3-Butadiene)	Test Organism	OECD Test Guideline	NOAEL (mg/m ³)
68476-52-8 C4 Crude Butadiene (10)	Crl:CD Rat	422	>20,000 (Developmental) >20,000 (Maternal)
106-99-0 1,3-Butadiene (>99)	Crl:CD Rat	421	>13,260 (Developmental) >663 (Maternal)
106-99-0 1,3-Butadiene (>99)	CD Rat	414	>2,210 (Developmental) >442 (Maternal)
106-99-0 1,3-Butadiene (>99)	CD-1 Swiss Mice	414	>88.4 (Developmental) >88.4 (Maternal)

Effects on Fertility

Reproductive toxicity of C4 Crude Butadiene (CAS # 68476-52-8: 10% 1,3-butadiene; 4% isobutane; 4% n-butane; 29% trans-2-butene; 29% 1-butene; 11% isobutylene; and 12% cis-2-butene) was evaluated in an OECD 422 Repeat Dose Reproductive/Developmental Toxicity Screen (Carney *et al.*, 2001). Groups of 12 adult male and female Crl:CD Sprague-Dawley rats were exposed via inhalation to crude butadiene at concentrations of 0; 2,000; 10,000; or 20,000 mg/m³, 6 hr/d, 7 days per week two weeks prior to breeding, during breeding, continuing to gestation day 19. Male rats were exposed for 36 to 37 days. No differences were observed in parental body weights, body weight gains or feed consumption between the groups. No treatment related effects were observed on mating, conception, fertility, or time to mating. Evaluations of gonadal function revealed no difference between treated and control groups. The NOAEL for reproductive toxicity was determined to be 20,000 mg/m³.

Reproductive toxicity of 1,3-butadiene was evaluated in an OECD 421 inhalation reproduction and developmental toxicity screening test (WIL Research Laboratories, 2003). Adult male and female Crl:CD rats were exposed to concentrations of 0; 663; 3,313; or 13,260 mg/m³ 1,3-butadiene two week prior to breeding, during mating, gestation and lactation for a total of 83 to 84 consecutive days for F0 males, 60 to 70 total days for F0 females and 7 consecutive days for 2 groups of F1 offspring (one male and one female per litter on post natal days 21 to 27 or 28 to 34). In F0 and F1 animals, a reduction in body weight was observed at 3,313 and 13,260 mg/m³. Clinical signs of toxicity, chromodacryorrhea, chromorhinorrhea, and salivation in F0 animals as well as dried red material in the perioral and perinasal regions in the F1 pups, were observed at 13,260 mg/m³. No effect at any dose level was observed in any reproductive parameter examined including gonadal function, mating behavior, conception, gestation, parturition, and lactation. The systemic NOAEL for this study was 663 mg/m³. The reproductive NOAEL was >13,260 mg/m³.

The effect of 1,3-butadiene exposure on fertility in male mice was examined in a rodent dominant lethal test and sperm-head morphology assay (Morrissey, 1990). Male mice were exposed to 0; 442; 2,210; or 11,040 mg/m³ 1,3-butadiene *via* inhalation for 5 days, 6 hr/d. In the dominant lethal assay, CD-1 male mice were then mated to two unexposed female mice/week for eight consecutive weeks. In the two low dose groups slight differences were observed in ratio of dead to total implants, percentage of females with ≥2 dead implants and number of dead implants per pregnancy (also observed in the high dose group during week 1). No differences were observed in number of pregnant females, implantations per litter, number of live fetuses, dead implantations/total implantations, or number of resorptions during weeks 1 and 2. No differences were observed for

any endpoint during weeks 3 to 8. It was concluded, despite the lack of dose response, that 1,3-butadiene had an effect on mature germ cells. To assess sperm morphology, B6C3F1 mice were used and maintained for five weeks post exposure (Morrissey, 1990). At the end of the post exposure period, the reproductive tract was evaluated for gross lesions and sperm were obtained from the right cauda epididymus. A dose-dependent increase in percentage of abnormal sperm was observed, becoming significantly different from control at the two highest exposure concentrations.

Developmental Toxicity

As part of an OECD 422 Repeat Dose Reproductive/Developmental Toxicity Screen (Carney *et al.*, 2001), no developmental toxicity was observed in Crl:CD Sprague-Dawley rats following exposure to C4 Crude Butadiene (CAS # 68476-52-8: 10% 1,3-butadiene; 4% isobutane; 4% n-butane; 29% trans-2-butene; 29% 1-butene; 11% isobutylene; and 12% cis-2-butene). Groups of 12 adult male and female rats were exposed *via* inhalation to crude butadiene at concentrations of 2, 10, or 20 mg/L (2,000; 10,000; or 20,000 mg/m³), 6 hr/d, 7 days per week, 2 weeks prior to breeding, during breeding, and continuing to gestation day 19. No treatment related effects were observed in paternal body weights, body weight gains or feed consumption during the study. No difference was observed in number of viable litters, gestation length, litter size, pre implantation loss, pup body weight, or pup sex ratio. An increase was observed in post implantation loss in the low exposure group. This observation was considered spurious, given the lack of dose response. A single pup in the high dose group exhibited a hernia. This finding was considered spurious due to its low incidence. The NOAEL for this study was 20,000 mg/m³.

A guideline OECD 414 developmental toxicity study was conducted in pregnant CD rats exposed to 0, 40, 200, or 1,000 ppm 1,3-butadiene on gestation days 6 to 15, 6 hr/d (Morrissey, 1990). Dams were sacrificed on gestation day 20. Decreased weight gain was observed in dams at 2,210 mg/m³. There were no significant differences among the groups for number of live fetuses per litter, percent resorptions, malformations per litter, placental or fetal body weights or sex ratio. There was no evidence of developmental toxicity in any of the treated groups. The maternal NOAEL for this study was 442 mg/m³ and the fetal NOAEL was 2,210 mg/m³.

Developmental toxicity was evaluated in Crl:CD rats exposed to 0; 663; 3,313; or 13,260 mg/m³ (0; 301; 1,507; or 6,006 ppm, respectively) 1,3-butadiene during the conduct of an OECD 421 inhalation reproduction and developmental toxicity screening test (WIL Research Laboratories, 2003). Adult male and female Crl:CD rats were exposed to 1,3-butadiene two week prior to breeding, during mating, gestation and lactation for a total of 83 to 84 consecutive days for F0 males, 60 to 70 total days for F0 females and 7 consecutive days for two groups of F1 offspring (one male and one female per litter on post natal days 21 to 27 or 28 to 34). In F1 offspring, a reduction in weight gain was observed in the 3,313 and 13,260 mg/m³ groups during later stages of the lactation period. No indications of fetal toxicity or teratogenicity were observed. The systemic NOAEL for F0 and F1 animals was 663 mg/m³. The developmental NOAEL was 13,260 mg/m³.

Pregnant female CD-1 mice were exposed *via* inhalation to 0; 88.4; 442; or 2,210 mg/m³ (0; 40; 200; or 1,000 ppm, respectively) 1,3-butadiene on day 6 to 15 of gestation, 6 hr/d using the OECD 414 developmental toxicity guideline (Morrissey, 1990). On day 18 of gestation, dams were sacrificed and maternal and fetal evaluations were made. Decreased maternal body weight gain was observed at 442 and 2,210 mg/m³. Male and female fetal weights were reduced in the high dose groups. Placental weights were reduced for male fetuses at 200 ppm and for male and female fetuses at 2,210 mg/m³. Fetal variations (supernumary ribs and reduced sternbrae ossification) were increased in the 442 and 2,210 mg/m³ groups. The maternal and developmental NOAEL for this study was 88.4 mg/m³.

High Benzene Naphthas Category*Effects on Fertility*

No reproductive toxicity studies are available on High Benzene Naphtha streams. However, data are available on many components tested in reproductive studies and/or pathological evaluations of reproductive organs from systemic toxicity studies (see Table A3-1). In its review of benzene, ATSDR (1997) concluded that, although there are some data indicating adverse gonadal effects (*e.g.*, atrophy/degeneration, decrease in spermatozoa, moderate increases in abnormal sperm forms), data on reproductive outcomes are either inconclusive or conflicting. However, most studies indicate no effects on reproductive indices, even at high doses. Reproductive organ effects were seen after inhalation exposure to isoprene and hexane in subchronic toxicity studies but such effects may not affect reproductive capabilities in practice. However, for hydrocarbons tested in multi-generation reproductive studies, toluene, cyclohexane, pentane, commercial hexane (isomers), mixed xylenes, and styrene, no effects on fertility or other reproductive parameters were reported. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation two-generation reproductive toxicity study (Daughtrey *et al.*, 1994). Dicyclopentadiene demonstrated reproductive effects in a 3-generation reproductive study only at maternally toxic doses (Johnston and Belilies, 1979).

Developmental Toxicity

C5-C10 Fraction of Pyrolysis Gasoline (Rerun Tower Overheads; 40% benzene) was tested for developmental toxicity in New Zealand White rabbits at oral gavage doses of 0, 10, 25, and 50 mg/kg/d from day 6 to 28 of gestation. One rabbit given 50 mg/kg/d aborted on day 19 but all other animals completed gestation. Maternal body weights were comparable to controls throughout gestation. There were no biologically or statistically significant differences in pregnancy ratios, number of corpora lutea, total implantations, resorptions, postimplantation loss, viable fetuses, litter size, fetal sex index, or mean fetal body weights. No statistically significant differences in number of litters with malformations were reported. C5-C10 Fraction did not produce a teratogenic response in New Zealand White rabbits; the maternal NOAEL was 25 mg/kg/d the developmental NOAEL was 50 mg/kg/d (Schardein, 1981).

In addition to this study on a representative stream of the High Benzene Naphthas Category, developmental toxicity data exist for most components present in this category at concentrations greater than 5% (see Table A3-1). In these studies, no convincing evidence was seen for teratogenicity in the absence of maternal toxicity. Fetotoxicity has been reported for some components, but mostly in the presence of maternal toxicity (see Table A3-1). Only five components (pentenes, cyclopentene, 3-methylpentane, methylcyclopentane, 1,3-cyclopentadiene) lack developmental toxicity tests. However, data generated by other test plans within the HPV Program provide additional information about the potential of these substances to cause developmental effects. Three of the five materials are also components of the Pyrolysis C5s and Hydrotreated C5s streams (C5 Non-Cyclics Category) that were tested by the Olefins Panel using the OECD 422 combined repeated dose and reproduction/developmental rat toxicity test guideline. Those results, as well as results for 2-methyl-2-butene (a member of the C5 Non-Cyclics Category), produced no evidence of reproductive or developmental toxicity (Olefins Panel of the American Chemistry Council, 2004c). Pentenes are addressed by the International Hydrocarbon Solvents Consortium in their C5 Aliphatics Test Plan. In addition, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes. The American Chemistry Council's Higher Olefins Panel addressed hexenes as part of the HPV Program. 3-Methylpentane and methylcyclopentane were components (16.0% and 15.6%, respectively) of a commercial hexane stream that was negative in a rat inhalation developmental toxicity study (Keenan *et al.*, 1991).

Conclusion

Effects on fertility and developmental toxicity of Pyrolysis C3+ and Pyrolysis C4+ Category are adequately characterized with the available data. On the basis of available data, Pyrolysis C3+ and Pyrolysis C4+ Category streams seem unlikely to cause significant reproductive or developmental toxicity.

A stream with 1,3-butadiene concentration of approximately 10% produced no reproductive or developmental toxicity in rats exposed to concentrations as high as 20,000 mg/m³. No reproductive or developmental toxicity was observed in rats exposed to concentrations up to 13,260 mg/m³ 1,3-butadiene. No developmental toxicity was observed in rats exposed to 2,210 mg/m³ 1,3-butadiene in the presence of maternal toxicity. These two streams cover the range of C4 Crude Butadiene streams (10% to approximately 100% 1,3-butadiene). As observed with other endpoints, mice are more susceptible than rats to developmental and reproductive toxicity of 1,3-butadiene, most likely due to an increased metabolic capacity in mice to form reactive metabolites. This is evident by the observation of developmental toxicity in mice at 442 mg/m³ 1,3-butadiene exposure. There is some indication of male mediated toxicity in mice following 1,3-butadiene exposure; however, the effect appears to be weak. As humans metabolize 1,3-butadiene in a manner more consistent with rats than mice, reproductive and developmental toxicity data developed in rats is more appropriate to use in assessing human risk.

The ability of 1,3-butadiene to cause ovarian atrophy is dependent on the production of the diepoxide metabolite and this differs between species (US EPA, 2002). The mouse is the most sensitive species in terms of ovarian atrophy induction following 1,3-butadiene exposure while the rat is resistant to this effect. The observed species differences correlate with the production of the diepoxide metabolite of 1,3-butadiene, with the mouse producing higher levels of this toxic intermediate. Direct administration of the diepoxide metabolite of 1,3-butadiene can affect the rat ovary, albeit at higher dose levels than required for inducing similar effects in mice. Therefore, the mouse ovary is more sensitive to the toxic effects of both 1,3-butadiene and the diepoxide metabolite (US EPA, 2002).

Reproductive studies on High Benzene Naphthas streams or on components present in these streams overall gave negative results. The C5-C10 fraction of Pyrolysis gasoline, a representative High Benzene Naphtha stream, did not induce developmental effects in rabbits. Individual stream components, which induced developmental toxicity, did so primarily at doses that were also toxic to the dam.

Data generated through other test plans within the HPV Program provide additional information about the potential of these streams to cause reproductive and developmental effects. For example, some of these components are present in the Pyrolysis C5s and Hydrotreated C5s streams (members of the C5 Non-Cyclics Category) that were tested for reproductive toxicity by the Olefins Panel, as part of the HPV Program. Those results, as well as results for 2-methyl-2-butene (a member of the C5 Non-Cyclics Category), developed using the OECD 422 combined repeated dose and reproduction/developmental rat toxicity test guideline, produced no evidence of reproductive or developmental toxicity (Olefins Panel of the American Chemistry Council, 2004c). Also, based on structural similarity, pentenes are likely to have a developmental toxicity profile similar to hexenes, which will be addressed by the American Chemistry Council's Higher Olefins Panel as part of the HPV Program. Additional reproductive toxicity information is available from testing conducted by the Olefins Panel for the Resin Oils and Cyclodiene Dimer Concentrates Category (Olefins Panel of the American Chemistry Council, 2005) with streams distilled from Pyrolysis Gasoline. Overall, reproductive parameters were unaffected by exposure to representative resin oils and cyclodiene dimer concentrate streams; developmental effects were expressed primarily as low pup weight at birth and during lactation, and low pup weight gain. These developmental effects usually occurred when maternal weight was also affected. Differences in degree of toxic responses, which correlated

with chemical composition were evident, particularly for developmental effects, and appeared to be related to and predictable from DCPD and MCPD levels in the process streams.

4.2 Assessment Summary for Human Health

Pyrolysis C3+ and Pyrolysis C4+ Category streams appear to have a low order of acute toxicity. Representative streams from the compositionally similar Crude Butadiene C4 and High Benzene Naphthas Categories demonstrate minimal toxicity by oral, dermal or inhalation routes of exposure.

Data are available to adequately characterize the repeated dose toxicity of the Pyrolysis C3+ and Pyrolysis C4+ Category. Available studies from the C4 Crude Butadiene Category and the High Benzene Naphthas category cover a wide range of stream compositions. Repeated oral or inhalation exposures to many of the components of the Pyrolysis C3+ and Pyrolysis C4+ Category streams have been shown to cause adverse health effects in a variety of organs. Studies of streams with 1,3-butadiene concentrations ranging from 10 to 99% are consistent in that they demonstrate minimal effects in rats with the exception of body weight changes, while mice demonstrate greater sensitivity following repeated inhalation exposures. Benzene demonstrated toxicity primarily in the hematopoietic system, toluene affected the central nervous system and light hydrocarbon nephropathy was seen with exposure to hexane isomers, a 50/50 blend of n-butane and n-pentane, or with dicyclopentadiene. However, existing data also indicate that antagonistic and synergistic interactions occur between some components comprising the streams, as noted above in the Chemical Component Interaction section of the Introduction to Section 4.1, which apparently alter the expression of toxicity of the individual hydrocarbons. The target organs affected by exposure to the mixtures in this category, and the severity of the effects, depend upon the relative concentrations of the components within each stream and the nature of the interactions between components.

Adequate data are available to evaluate the genotoxicity of the Pyrolysis C3+ and Pyrolysis C4+ Category. Data from the Crude Butadiene C4 category examined streams with a range of 1,3-butadiene content (10 to 99%). *In vitro* studies indicate a weak mutagenic activity, while *in vivo* studies of 1,3-butadiene in mice and rats demonstrated a genotoxic response in mice but not in rats. The representative streams tested in the High Benzene Naphthas category did not induce genotoxicity. Streams from this category demonstrated how interaction and competition for metabolic sites may block toxicity of individual components. Most of the Pyrolysis C3+ and Pyrolysis C4+ category components, with the exception of 1,3-butadiene, did not induce mutation in bacteria and are not considered gene mutagens. However, based on butadiene content of 11 to 42%, and despite available data for representative streams, components and mixtures of components, it is likely that streams in this category should be considered as gene mutagens and likely clastogenic.

The carcinogenic potential of the Pyrolysis C3+ and Pyrolysis C4+ Category streams will be driven largely by relative concentrations of two substances, 1,3-butadiene and benzene, which are either known or suspected human carcinogens under various regulatory classifications. 1,3-Butadiene is an animal carcinogen that demonstrates significant species differences in potency. 1,3-Butadiene is a potent, multi-site carcinogen in the mouse. Carcinogenic effects of 1,3-butadiene are more difficult to discern for humans, with human epidemiology studies less certain. Benzene is a demonstrated leukemogen in humans (acute myelogenous leukemia) and induces solid tumors in laboratory animals. Thus, these streams are handled in accordance with regulations pertaining to 1,3-butadiene and benzene. However, although no carcinogenesis studies were directly available on Pyrolysis C3+ and Pyrolysis C4+ Category streams, extrapolation from 2-year cancer bioassays on related streams, and the apparent competitive detoxifying effects of other components in the streams (*e.g.*, toluene when co-administered with benzene), suggest that carcinogenesis is unlikely to be a significant endpoint of toxicity for this category.

Effects on fertility and developmental toxicity of Pyrolysis C3+ and Pyrolysis C4+ Category C4 are adequately characterized with the available data. On the basis of available data, Pyrolysis C3+ and Pyrolysis C4+ Category streams seem unlikely to cause significant reproductive or developmental toxicity. A stream with 1,3-butadiene concentration of approximately 10% produced no reproductive or developmental toxicity in rats exposed to concentrations as high as 20,000 mg/m³. No reproductive or developmental toxicity was observed in rats exposed to concentrations up to 13,260 mg/m³ 1,3-butadiene. No developmental toxicity was observed in rats exposed to 2,210 mg/m³ 1,3-butadiene in the presence of maternal toxicity. These two streams cover the range of C4 Crude Butadiene streams (10% to approximately 100% 1,3-butadiene). Reproductive studies on High Benzene Naphthas streams or on components present in these streams overall gave negative results.

5 HAZARDS TO THE ENVIRONMENT

5.1 Aquatic Toxicity

The aquatic toxicity of streams in this category is expected to fall within a relatively narrow range regardless of their composition. This is expected because the constituent chemicals of these streams are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis (Ramos *et al.*, 1998). The toxic mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (Van Wezel, 1995), and the differences between toxicities (i.e., LC/LL₅₀, EC/EL₅₀) can be explained by the differences between the target tissue-partitioning behavior of individual constituent chemicals (Verbruggen *et al.*, 2000).

The existing fish toxicity database for hydrophobic, neutral organic chemicals, which comprise the streams in this category, supports a critical body residue (CBR) for these chemicals between approximately 2 to 8 mmol/kg fish (wet weight) (McCarty *et al.*, 1991; McCarty and Mackay, 1993). The CBR is the internal concentration of a toxicant that causes mortality. When normalized to lipid content for most organisms, the CBR is approximately 50 µmol/g of lipid (Di Toro *et al.*, 2000). Therefore, only hydrocarbon streams with components of sufficient water solubility, such that their molar sum in solution is high enough to produce a total partitioning to the organism of approximately 50 µmol of hydrocarbon per gram of lipid, will demonstrate lethality.

The aquatic toxicity of streams in the Pyrolysis C3+ and Pyrolysis C4+ Category was characterized with data used to characterize the toxicity of the Crude Butadiene C4 and High Benzene Naphthas Categories (Olefins Panel, Implementation Task Group; 2004a, 2004b). The combined composition of these two categories, with regard to constituent chemicals, is similar to the composition of the Pyrolysis C3+ and Pyrolysis C4+ Category (see Table 2 for the composition of this category and Appendix IV for the composition of the Crude Butadiene C4 and High Benzene Naphthas Categories). Consequently, the aquatic toxicity of the two read-across categories is expected to be equivalent to the potential toxicity range of the Pyrolysis C3+ and Pyrolysis C4+ Category. Category summary reports for the two read-across categories and their robust summaries have previously been submitted to EPA under the HPV Program. The robust summaries, which contain data used to support the Pyrolysis C3+ and Pyrolysis C4+ Category are not submitted with this report, but can be obtained with the Crude Butadiene C4 and High Benzene Naphthas Category summary reports through the EPA HPV database.

The Pyrolysis C3+ and Pyrolysis C4+ Category contains both gaseous constituents (primarily C3 and C4 hydrocarbons) and hydrocarbons that range largely between C5 and C10. Therefore, application of the toxicity data from the two read-across categories is justified to characterize the toxicity of this category for the following reasons:

- The read-across data are from chemicals or combinations of chemical classes (*i.e.*, olefins, aromatics, paraffins) that are found in streams from this category.
- The chemicals and complex substances used for read-across purposes have a carbon number or carbon number range that falls within the range of carbon numbers found in streams from this category.
- Chemicals and complex substances used for read-across purposes as well as the substances in this category are composed of chemicals that all act by a similar mode of action.

Although measured data were not available to assess the aquatic toxicity of the gaseous constituents, structure-activity relationship (SAR) data developed with the ECOSAR model (Cash and Nabholz, 1999) were used to characterize the aquatic toxicity of these constituents for three trophic levels [the ECOSAR model used was from EPIWIN (1999)]. The ECOSAR model is a reliable and valid SAR model to apply to constituent chemicals from this category because it is based on a related chemical dataset that calculates the toxicity of neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis as discussed above. The calculated aquatic toxicity values were determined using measured log P_{ow} values (see Table 4; ECOSAR requires selected physicochemical data and chemical structure to calculate effect concentrations).

Calculated aquatic toxicity values for the C3 and C4 gaseous chemicals in streams from this category fall within a relatively narrow range. The effect range is a function of the range of log P_{ow} values identified for the chemicals. The selected components are expected to demonstrate 96-hour LC_{50} fish toxicity values in the range of 6.28 to 40.98 mg/L, 48-hour LC_{50} invertebrate toxicity values in the range of 7.15 to 43.88 mg/L, and 96-hour EC_{50} alga toxicity values in the range of 4.71 to 27.42 mg/L (Table 15).

Table 15. Summary of Aquatic Toxicity Data for Gaseous Chemical Constituents in the Pyrolysis C3+ and Pyrolysis C4+ Category

Chemical Constituent (Log P_{ow} *)	Fish Toxicity 96-hour LC_{50} (mg/L)	Invertebrate Toxicity 48-hour EC_{50} (mg/L)	Alga Toxicity 96-hour EC_{50} (mg/L)
Isobutane (2.76)	8.32	9.39	6.13
n-Butane (2.89)	6.28	7.15	4.71
Isobutylene (2.34)	19.93	21.86	13.94
cis-Butene-2 (2.31)	21.26	23.28	14.81
trans-Butene-2 (2.33)	20.36	22.32	14.22
Butene-1 (2.40)	17.50	19.28	12.33
1,3-Butadiene (1.99)	40.98	43.88	27.42

* The log P_{ow} values used in the ECOSAR model are from the EPIWIN experimental database.

The aquatic toxicity of streams in the High Benzene Naphthas Category was characterized using read-across data from constituent chemicals of those streams and comparably complex substances and streams (including gasoline blending streams). These data are used to assess the C5 to C10+ fraction of the Pyrolysis C3+ and Pyrolysis C4+ Category. Study specifics and robust summaries for the gasoline blending streams can be found in the American Petroleum Institute, HPV Program Gasoline Blending Streams test plan available through the US EPA HPV Program.

The data in Table 16 provides a comparison of the range of compositions (*i.e.*, carbon number, chemical class, weight percent) for substances in the High Benzene Naphthas Category that have been used to characterize the aquatic toxicity of this category. This comparison illustrates the

similarity in carbon number range between the High Benzene Naphthas Category and the selected substances with read-across data.

Table 16. Approximate Weight (wt) Percent and Carbon Number Comparison of Hydrocarbons in the High Benzene Naphthas Category and Substances¹ with Aquatic Toxicity Data

Substance/ Stream Name	Olefins		Aromatics		Paraffins	
	wt %	C # ^a	wt %	C # ^a	wt %	C # ^a
Substances in High Benzene Naphtha Category	1 - 34	5 - 9	>40 - 100	6 - 11	>4 - 75	5 - 10
Alkenes, C6 Rich	100	5 - 7	0	-	0	-
Alkenes, C7-9, C8 Rich	100	7 - 9	0	-	0	-
C8-C10 Aromatics, Predominantly C9 Aromatics	0	-	>97	8 - 10	<3	-
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	0	-	>94	10 - 14	<6	-
Naphtha (petroleum), Light Alkylate (gasoline stream)	0	-	0	-	92	5 - 8
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	24	5 - 6	16	6 - 8	21	5 - 7
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	0	-	38	6 - 7	50	5 - 7

1 Approximate weight percent and carbon number ranges of the predominant chemical components by chemical class [olefins/aromatics/paraffins] for selected products contained by the High Benzene Naphtha Category and for comparable substances and streams not in this category that have aquatic toxicity data that can be used as read-across data for the Pyrolysis C3+ and Pyrolysis C4+ Category (% compositions may not total 100%).

a Predominant carbon number range.

The data in Tables 17, 18, and 19 establish the range of aquatic toxicity for the C5 to C10+ constituents in the Pyrolysis C3+ and Pyrolysis C4+ Category. Generally, the fish, invertebrate, and alga studies followed the OECD Guidelines 203, 202, and 201, respectively. For complex substances, the test procedures used to develop the test material exposure solutions also applied the OECD guidance described in Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures (OECD, 1999). For these studies, the results are represented as lethal loading (LL) endpoints, a designation used to define results for multi-hydrocarbon mixtures, tested as water accommodated fractions (WAFs), compared to the data developed for pure chemicals, which represent results as lethal concentration endpoints where test material is analytically verified.

Table 17. Fish Acute Toxicity Data for Chemicals and Complex Substances used to Support a Characterization of Pyrolysis C3+ and Pyrolysis C4+ Streams Toxicity

Chemical / Substance	Carbon Number	Organism	Aquatic Toxicity ^a (96-hr, mg/L)	Data Source
n-Pentane	5	<i>Oncorhynchus mykiss</i>	LC ₅₀ = 4.3	IHSC ^b
n-Hexane	6	<i>Pimephales promelas</i>	LC ₅₀ = 2.5	IHSC ^b
Benzene	6	<i>Oncorhynchus mykiss</i>	LC ₅₀ = 5.9	^c
Alkenes, C6 Rich	5-7 ^d	<i>Oncorhynchus mykiss</i>	LL ₅₀ = 12.8	HOP ^e
C7-8 Cycloparaffins, C7 Rich	7	<i>Oncorhynchus mykiss</i>	LC ₅₀ = 5.4 ^e	IHSC ^b
Toluene	7	<i>Pimephales promelas</i>	LC ₅₀ = 14.6	IHSC ^b
C7-9Alkenes, C8 Rich	7-9 ^d	<i>Oncorhynchus mykiss</i>	LL ₅₀ = 8.9	HOP ^f
o-Xylene	8	<i>Pimephales promelas</i>	LC ₅₀ = 16.4	XIC ^g
p-Xylene	8	<i>Oncorhynchus mykiss</i>	LC ₅₀ = 2.6	XIC ^g
p-Xylene	8	<i>Pimephales promelas</i>	LC ₅₀ = 8.9	XIC ^g
Ethylbenzene	8	<i>Pimephales promelas</i>	LC ₅₀ = 12.1	^h
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 ^d	<i>Pimephales promelas</i>	LL ₅₀ = 8.2	API ⁱ
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	5-8 ^d	<i>Pimephales promelas</i>	LL ₅₀ = 46	API ⁱ
Naphtha (petroleum), Light Catalytically Reformulated (gasoline stream)	5-7 ^d	<i>Pimephales promelas</i>	LL ₅₀ = 34	API ⁱ
1,2,4-Trimethylbenzene	9	<i>Pimephales promelas</i>	LC ₅₀ = 7.7	IHSC ^b
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 ^d	<i>Oncorhynchus mykiss</i>	LL ₅₀ = 18.0	IHSC ^b
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 ^d	<i>Oncorhynchus mykiss</i>	LL ₅₀ = 3.0	IHSC ^d

a Endpoint is mortality; LC = Lethal Concentration; LL = Lethal Loading; values cited as “concentration” are based on measured values

b Covered by the International Hydrocarbon Solvents Consortium

c Galassi S, Mingazzini M, Viagano L, Cesareo D, and Tosato M (1988). Benzene is in the OECD SIDS program.

d Predominant carbon number or range

e 93-hour value

f Robust summary from the Higher Olefins Panel HPV Test Plan (submitted to EPA under the HPV Program)

g Xylenes were covered by the Xylene ICCA Consortium and were reviewed by OECD (Organization for Economic Co-ordination and Development) as part of SIAM (SIDS Initial Assessment Meeting) 16

h Ethylbenzene was reviewed by OECD as part of SIAM 15

i Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted to EPA under the HPV Program)

Table 18. Invertebrate Acute Toxicity Data for Chemicals and Complex Substances used to Support a Characterization of Pyrolysis C3+ and Pyrolysis C4+ Streams Toxicity

Chemical / Substance	Carbon Number	Organism	Aquatic Toxicity ^a (48-hr, mg/L)	Data Source
n-Pentane	5	<i>Daphnia magna</i>	EC ₅₀ = 2.7	IHSC ^e
n-Hexane	6	<i>Daphnia magna</i>	EC ₅₀ = 2.1	IHSC ^e
Cyclohexane	6	<i>Daphnia magna</i>	EC ₅₀ = 0.9	IHSC ^e
Benzene	6	<i>Daphnia magna</i>	EC ₅₀ = 18 ^b	f
Toluene	7	<i>Daphnia magna</i>	EC ₅₀ = 14.9	g
o-Xylene	8	<i>Daphnia magna</i>	EC ₅₀ = 1.0	XIC ^h
m-Xylene	8	<i>Daphnia magna</i>	EC ₅₀ = 4.7	XIC ^h
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-7 ^c	<i>Daphnia magna</i>	EL ₅₀ = 10	API ⁱ
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8 ^c	<i>Daphnia magna</i>	EL ₅₀ = 32	API ⁱ
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 ^c	<i>Daphnia magna</i>	EL ₅₀ = 18	API ⁱ
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 ^c	<i>Daphnia magna</i>	EL ₅₀ = 21.3	IHSC ^e
Naphthalene	10	<i>Daphnia magna</i>	EL ₅₀ = 16.7 ^d	j
C8-C10 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 ^c	<i>Daphnia magna</i>	EL ₅₀ = 3.0	IHSC ^e

a Endpoint is immobility; EC = Effect Concentration; EL = Effect Loading; values cited as “concentration” are based on measured values

b Covered by the International Hydrocarbon Solvents Consortium

c 24-hour study

d Benzene was reviewed by OECD (Organization for Economic Co-ordination and Development) as part of SIAM (SIDS Initial Assessment Meeting) 15

e Hermens J, Canton H, Janssen P and deJong R (1984). Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anesthetic potency: acute lethal and sublethal toxicity to *Daphnia magna*. *Aquat. Toxicol.* **5**, 143–154 [In EU Toluene SIAR (SIDS Initial Assessment Report) 10888].

f Xylenes were covered by the Xylene ICCA Consortium and were reviewed by OECD as part of SIAM 16

g Predominant carbon number or range

h Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted to EPA under the HPV Program)

i Based on nominal values

j Naphthalene was reviewed by OECD as part of SIAM 13

Table 19. Alga Toxicity Data for Chemicals and Complex Substances used to Support a Characterization of Pyrolysis C3+ and Pyrolysis C4+ Streams Toxicity

Chemical / Substance	Carbon Number	Organism	Aquatic Toxicity ^a (72-hr, mg/L)	Data Source
n-Pentane	5	<i>Pseudokirchneriella subcapitata</i> ^b	EbC ₅₀ = 10.7 ErC ₅₀ = 7.5 NOECb = 1.3 NOECr = 2.0	IHSC ^c
Benzene	6	<i>Pseudokirchneriella subcapitata</i>	EbL ₅₀ = 29	^d
Naphtha (Petroleum), Light Catalytically reformed (gasoline stream)	5-7 ^e	<i>Pseudokirchneriella subcapitata</i>	EbL ₅₀ = 8.5 NOELRb = 5.0	API ^f
Naphtha (Petroleum), Light alkylate (gasoline stream)	5-8 ^e	<i>Pseudokirchneriella subcapitata</i>	EbL ₅₀ = 45 NOELRb = 18	API ^f
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8 ^e	<i>Pseudokirchneriella subcapitata</i>	EbL ₅₀ = 64 NOELRb = 51	API ^f
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10 ^e	<i>Pseudokirchneriella subcapitata</i>	EbL ₅₀ = 2.6 ErL ₅₀ = 2.9 NOELRb = 1.0 NOELRr = 1.0	IHSC ^c
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12 ^e	<i>Pseudokirchneriella subcapitata</i>	EbL ₅₀ = 1 to 3 ErL ₅₀ = 1 to 3 NOELRb = 1.0 NOELRr = 1.0	IHSC ^c

a Endpoint is growth inhibition; EbC = Effect Concentration for biomass; ErC = Effect Concentration for growth rate; EbL = Effect Loading for biomass; ErL = Effect Loading for growth rate; NOECb = No Observed Effect Concentration for biomass; NOECr = No Observed Effect Concentration for growth rate; NOELRb = No Observed Effect Loading Rate for biomass; NOELRr = No Observed Effect Loading Rate for growth rate; values cited as “concentration” are based on measured values

b Formally known as *Selenastrum capricornutum*

c Covered by the International Hydrocarbon Solvents Consortium

d Benzene was reviewed by OECD (Organization for Economic Co-ordination and Development) as part of SIAM (SIDS Initial Assessment Meeting) 15

e Predominant carbon number or range

f Robust summary from the American Petroleum Institute: Gasoline Blending Streams Test Plan (submitted to EPA under the HPV Program)

The Pyrolysis C3+ and Pyrolysis C4+ streams are likely to exhibit a moderate range of acute toxicity in freshwater fish and invertebrates and a moderate level of toxicity in freshwater algae based on an overall range of toxicity defined by the two read-across categories. Acute fish toxicity values would be expected to range between 2.5 to 46.0 mg/L, while acute invertebrate toxicity values would be expected to range between 0.9 to 43.9 mg/L. In comparison, alga toxicity values would be expected to range between 1.0 to 64 mg/L (for biomass or growth rate endpoints), while

alga loading rate NOELR values would be expected to range between 1.0 to 51 mg/L (for biomass and growth rate endpoints).

5.2 Assessment Summary for the Environment

Results of distribution modeling show that streams in the Pyrolysis C3+ and Pyrolysis C4+ Category will partition primarily to the air compartment, with a small percentage partitioning to water, soil, and sediment. Although constituents have a moderate degree of water solubility, wet deposition of category constituents is not likely to play a significant role in their atmospheric fate because they rapidly photodegrade. Volatilization to the air will contribute to the rapid loss of category constituents from aqueous and terrestrial habitats. In the air, these constituents have the potential to rapidly degrade through indirect photolytic processes mediated primarily by hydroxyl radicals with calculated degradation half-lives ranging from 0.9 to 65.8 hours, depending on hydroxyl radical concentration. Aqueous photolysis and hydrolysis will not contribute to the transformation of category constituents in aquatic environments because they are either poorly or not susceptible to these reactions.

Although the biodegradability of streams in this category has not been evaluated with standard testing procedures, studies have demonstrated that several gaseous constituents can be degraded by bacteria isolated from soil and surface water samples. Additionally, read-across data to characterize the non-gaseous constituents of category streams show that this fraction is also subject to biodegradation and that many constituents can be rapidly biodegraded.

Extensive calculated and measured read-across data show that streams in this category have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates.

In summary, based on biological and physical degradation processes, and aquatic toxicity data, streams in the Pyrolysis C3+ and Pyrolysis C4+ Category, although moderately toxic, are not expected to persist in the environment.

6 DATA SUMMARY

Physico-chemical, environmental fate and effects, and human health data that characterize the two streams in the Pyrolysis C3+ and Pyrolysis C4+ Category are summarized in Tables 20 and 21. CAS RNs are associated with streams as follows:

- **Pyrolysis C3+ Stream**
 - 64742-83-2
 - 68513-68-8
- **Pyrolysis C4+ Stream**
 - 64742-83-2

Table 20. Physico-Chemical and Environmental Data Used to Characterize Streams and CAS RNs in the Pyrolysis C3+ and Pyrolysis C4+ Category

Endpoint	Pyrolysis C3+ and Pyrolysis C4+ Category Streams and CAS RNs	
	Pyrolysis C3+ Stream	
	Pyrolysis C4+ Stream	
	64742-83-2	68513-68-8
Melting Point*/ Range (°C)	-145.0 to 80.2 (m)	
Boiling Point*/ Range (°C)	-11.7 to 217.9 (m)	
Vapor Pressure*/ Range (hPa)	0.11 to 3.08 E3 (m)	
Log P _{ow} */ Range	1.99 to 3.90 (m)	
Water Solubility*/ Range (mg/L)	17.2 to 2000.0 (m)	
Direct Photodegradation	Direct photolysis will not contribute to degradation	
Indirect (OH-) Photodegradation* (half-life, hrs) (c)	0.9 to 65.8 (a)	
Hydrolysis	Hydrolysis will not contribute to degradation	
Distribution*	Partitions primarily to air A small fraction is estimated to partition to water, soil, and sediment	
Biodegradation	Potential to biodegrade	
96-hr Fish Acute LL/LC ₅₀ * (mg/L)	2.5 to 46.0 (c)	
48-hr Invert Acute EL/EC ₅₀ * (mg/L)	0.9 to 43.9 (c)	
96-hr Alga EL/EC ₅₀ * (mg/L)	1.0 to 64 (c)	

* Constituent chemicals used to define selected endpoints include: isobutane; n-butane; isobutylene; cis-butene-2; trans-butene-2; butene-1; 1,3-butadiene; isoprene; n-pentane; 1,3-cyclopentadiene; isohexane; n-hexane; methylcyclopentane; benzene; toluene; m-xylene; styrene; dicyclopentadiene; naphthalene

(m) Measured values

(c) Includes calculated and measured values.

(a) Atmospheric half-life values are based on a 12-hr day.

Table 21. Human Health Data Summary Used to Characterize Streams and CAS RNs in the Pyrolysis C3+ and Pyrolysis C4+ Category

Endpoint	Pyrolysis C3+ and Pyrolysis C4+ Category Streams and CAS RNs	
	Pyrolysis C3+ Stream	
	Pyrolysis C4+ Stream	
	64742-83-2	68513-68-8
Acute Toxicity (rat)	LC ₅₀ >5,300 mg/m ³	
Repeat Dose Toxicity (rat)	NOAEL >17,679 mg/m ³	
Mutagenicity Ames Assay	Weakly Positive	
Mutagenicity Mouse Micronucleus	Positive	
Reproductive Toxicity (rat)	NOAEL >13,260 mg/m ³	
Developmental Toxicity (rat)	NOAEL (M) >663 mg/m ³ NOAEL (F) >13,260 mg/m ³	

M Male

F Female

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APPENDIX I**Ethylene Process Description****A. Ethylene Process****1. Steam Cracking**

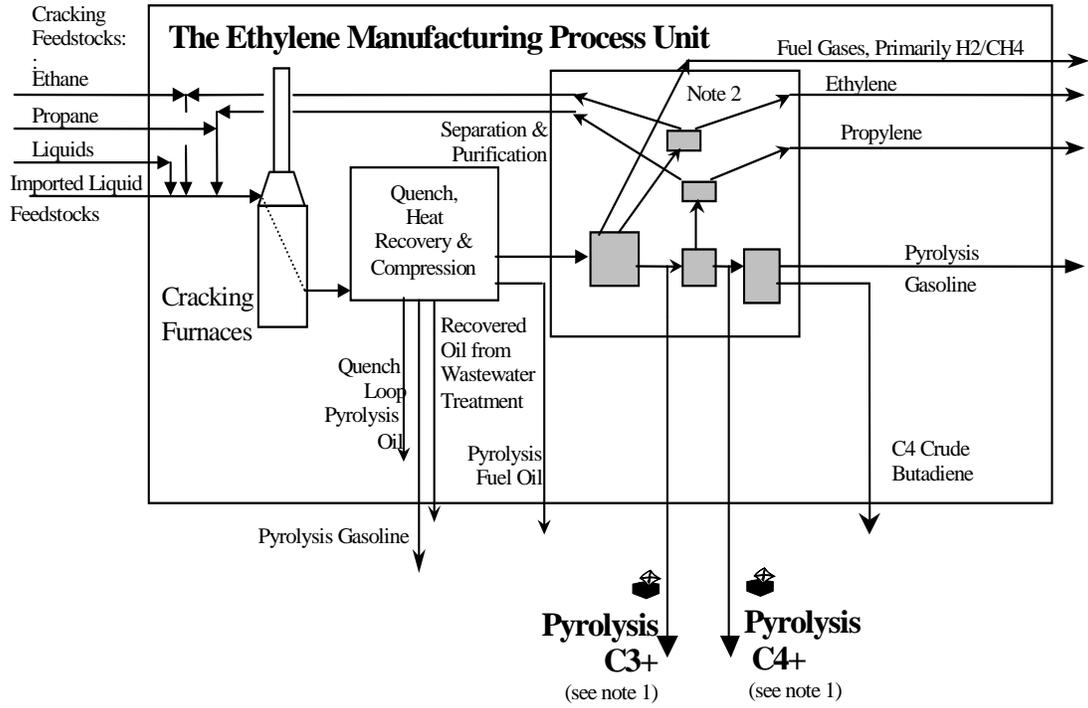
Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturates. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired streams. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as “steam cracking” or simply “cracking” and the furnaces are frequently referred to as “crackers”.

Subjecting the feedstocks to high temperatures in this manner results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the hydrocarbon compounds that are associated with the liquid feedstocks are also converted to ethylene. Other valuable hydrocarbons are also formed, including other olefins, diolefins, aromatics, paraffins, and lesser amounts of acetylenes. These other hydrocarbon streams include compounds with two or more carbon (C) atoms per molecule, i.e., C₂, C₃, C₄, etc. Propane and propylene are examples of C₃ hydrocarbons and benzene, hexene, and cyclohexane are a few examples of the C₆ hydrocarbons.

The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as “cracked gas” and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two or more carbon atoms per molecule (C₂₊). The relative amount of each constituent in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes, a liquid fuel oil stream is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the streams are contained in pressurized systems (see Figure 2 for a pictorial representation of the ethylene manufacturing process). The final streams from the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity chemicals, ethylene and propylene. Other streams from the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges. C₄ Crude Butadiene and Pyrolysis Gasoline are the two most common of these mixed streams.

Figure 2. Process Streams Flow Diagram from the Ethylene Manufacturing Process Unit for the Pyrolysis C3+ and Pyrolysis C4+ Streams

The Pyrolysis C3+ and Pyrolysis C4+ Category streams are shown in bold in the diagram below and marked with a diamond icon. Other streams are shown for clarity.



Note 1: Pyrolysis C3+ & C4+ are typically in-process streams; the streams have been reported as isolated (rare) during process unit shutdowns.
Note 2: Separation sequence shown is typical. Other sequences are used.

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefin streams, such as from the light ends product of a catalytic cracking process. This separation is similar to that used in steam crackers, and in some cases, both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus, the finishing of these refinery gas streams yields primary ethylene and ethane, and/or propylene and propane.

B. Pyrolysis C3+ and Pyrolysis C4+ Category Streams

The cracked gas from the ethylene process furnaces is cooled, compressed, and then separated into the desired product streams by a series of unit operations, primarily distillation. Pyrolysis C3+ is an intermediate stream in the separation sequence that results after removal of the C2 and lighter components from condensed cracked gas. The Pyrolysis C3+ is typically produced at the deethanizer tower bottoms. Similarly, Pyrolysis C4+ is the intermediate stream that is produced after removal of the C3 and lighter components, and is produced at the debutanizer tower bottoms. Infrequently, these two streams are temporarily isolated during ethylene process unit shutdowns. During normal operation, the Pyrolysis C4+ stream is separated by distillation into two streams, the butadiene containing C4 Crude Butadiene stream and pyrolysis gasoline (C5+). The Pyrolysis C3+ stream is separated into these two streams plus a C3 stream. The C3 stream (Propylene Streams Category) and pyrolysis gasoline (High Benzene Naphthas Category) are covered by separate categories sponsored by the Olefins Panel of the American Chemistry Council (Table 22). There are only two examples where these broad-range streams are reported to be isolated. The 1,3-butadiene content of Pyrolysis C3+ and Pyrolysis C4+ streams can range from 12 to 42% (Table 2).

Table 22. HPV Program Categories Sponsored by the Olefins Panel of the American Chemistry Council

Category Number	Category Name
1	Crude Butadiene C4
2	Low 1,3-Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams
5	High Benzene Naphthas
6	Low Benzene Naphthas
7,8,9	Resin Oils & Cyclodiene Dimer Concentrates
10	Fuel Oils
11	Pyrolysis C3+ and Pyrolysis C4+

APPENDIX II

**Summary Results from Existing Human Health Effects Data for
Chemical Components and Streams of High Benzene Naphthas Category**

[Note: This table is the product of a good faith effort to briefly summarize results of toxicity studies that were available to the reviewer for SIDS endpoints. Results from non-SIDS endpoints are not included. Since all information for a particular chemical may not have been available to the reviewer, the results presented should not be considered as final assessments of the hazards of the listed chemicals. Component data were not reviewed for data adequacy. Robust summaries for the listed components will not be submitted with the Test Plan.]

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Vinyl Acetate	Oral LD50 = 2.9 g/kg; inhalation LC50 = 3680 ppm [4h]	Negative in Ames Test	Positive in mouse bone marrow micronucleus test by i.p. but negative in rats and mice by inhalation and oral; positive in <i>in vitro</i> chrom ab	4 and 13-wk rat and mouse inhalation study: decrease in BW gain, respiratory tract effects; no clearly treatment related effects in 4- and 13-wk rat and mouse oral	In rat inhalation study, no embryolethality or teratogenicity seen; fetal growth retardation seen at maternally toxic doses. In rat oral study, no effects.	In an oral rat 2-gen repro study, no effects were seen except for reduction in BW gain in high-dose F1 pups.		Reviews: IRIS ⁴ , 1990; HSDB ⁵ ; ATSDR, 1992 ⁴

⁴ IRIS: EPA Integrated Risk Information System

⁵ HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc.]

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
1,3-Butadiene	Rat inhalation LC50[4h] = 129,000 ppm	Negative in UDS in mouse and rat, and <i>Drosophila</i> ; negative and positive in mouse lymphoma; positive in Ames, CHO and <i>in vivo</i> mouse spleenocyte HPRT tests and mouse spot test	Positive in mouse dominant lethal but negative in rat; positive in mouse bone marrow micronucleus and chrom. ab.; negative in rat bone marrow micronucleus	Many studies: Toxicity to blood cells in mice; no effects in rats [inhalation]	Effects seen at maternally toxic doses	No effect at any dose level was observed in any reproductive parameter examined including gonadal function, mating behavior, conception, gestation, parturition, and lactation.. The reproductive NOAEL was >13,260 mg/m ³ . in (OECD 421 inhalation reproduction / developmental toxicity screening test).	Olefins Panel's Crude Butadiene C4 Category, OECD SIDS	Reviews: ECETOC Special Report No. 12 - 1997 ⁶ ; ATSDR ⁷ , 1993

⁶ ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

⁷ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Isoprene (2-methylbutadiene-1,3)	Rat oral LD50= 2.1 g/kg; inhalation LC50 [4h] = 64,500 ppm	Negative in Ames Test	Negative in in-vitro CHO chrom. ab., mouse bone marrow chrom. ab. and rat lung cell micronucleus [inhalation]; positive in mouse bone marrow micronucleus [inhalation]	Many studies: Effect on testes in rats seen at 26 wks but not at 13 wks; effects on blood cells, nasal epithelium, liver, stomach, and testes in mice [inhalation]	No effects in rats; fetotoxicity in mice	Limited repro tox data [sperm motility, vaginal cytology, histopath of repro organs]obtained as part of 13-wk inhalation study: [slight effect on testis in rats; effects on testes, epididymus, sperm, estrus cycle in mice]	Olefins Panel's C5 Non-Cyclics Category/ICCA OECD SIDS/ICCA	Review: IARC ⁸ 1999
Pentenes				2-pentene: 4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 2 g/kg/d w/60% mortality			International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; also, pentenes are likely to have a toxicity profile similar to hexenes which will be addressed by the Higher Olefins Panel	Review: Halder <i>et al.</i> , 1985

⁸ IARC: International Agency for Research on Cancer

HPV CHEMICAL CATEGORY SUMMARY:

PYROLYSIS C3+ AND

PYROLYSIS C4+ CATEGORY

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Pentane	Rat oral: LD50>2 g/kg; inhalation LC50[4h] >7000 ppm	Negative in Ames Test	Negative in rat bone marrow micronucleus [inhalation] and dominant lethal [i.p.]; positive [not reproducible] in in-vitro CHO chrom. ab.	90-day rat inhalation: no effect at ~ 7000ppm. 16 wk and 7-30 wk rat inhalation neurotox evaluations : negative With 50/50 blend of n-butane and n-pentane, in a 90-day rat inhalation study with scope limited to evaluation of nephrotoxicity: decrease in BW and male hydrocarbon nephropathy.	No effect in rat oral	No effect on repro organs in 90-day rat inhalation	API [addressed in Petroleum Gases Test Plan]; International Hydrocarbon Solvents Consortium [C5 Aliphatics Category Test Plan]; OECD SIDS	Reviews: McKee <i>et al.</i> , 1998; Galvin and Marashi, 1999

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
1,3-Cyclopentadiene	Rat oral: 4/5 died at 1 g/kg; inhalation LC50 [4h] = 39 mg/L			Mild liver and kidney effects in rats after 35 exp. of 500 ppm ; no effects in guinea pigs, rabbits, dogs after 135 exp. of 250 ppm, or in dogs after 39 additional exp of 400 ppm and 16 additional exp of 800 ppm [inhalation]				Reviews: ACGIH ⁹ ; RTECS ¹⁰ ; EPA Documents [86960000024, 86960000121S]
Cyclopentene	Rat oral LD50 = 1.66 g/kg; inhalation LCLo [4h] = 16,000 ppm							Review: RTECS
3-Methylpentane (Isohexane)				16 wk and 7-30 wk rat inhalation neurotox evaluations : negative				Review: Frontali <i>et al.</i> , 1981

⁹ ACGIH: American Conference of Governmental Industrial Hygienists

¹⁰ RTECS: Registry of Toxic Effects of Chemical Substances

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Hexane isomers [commercial hexane tested: 52.2% n-hexane, 16.0% 3-methylpentane, 15.6% methylcyclopentane, 11.6% 2-methylpentane, 3.2% cyclohexane]		Negative in Ames Test, CHO HPRT	Negative in in-vitro CHO chrom. ab. and rat bone marrow chrom. ab. [inhalation]	No neurotoxicity; male rat hydrocarbon nephropathy [inhalation]	No effects in rats via inhalation	No effect in rat 2-gen study via inhalation except decrease in weight gain in high dose offspring		Daughtrey <i>et al.</i> , 1994 a,b; 1999; Kirwin <i>et al.</i> , 1991
Hexane	Rat oral LD50=28.7 g/kg; inhalation LC50[4h] = 48,000 ppm	Negative in Ames Test and in vitro UDS	Negative in in-vitro CHO chrom. ab. , inhalation dominant lethal and mouse micronucleus [inhalation and IP]; positive in rat oral bone marrow chrom. ab.	Several studies: Effects on peripheral nervous system and testes	Negative in inhalation and oral developmental studies	No repro tox studies found; testicular atrophy seen in subchronic inhalation studies	OECD SIDS - Reviews: ICCA	Reviews: ATSDR ¹¹ 1999; HSDB ¹² [rat chrom. Ab. report]
Methylcyclopentane				4 wk rat oral evaluating nephrotoxicity showed no kidney lesions at 0.5 g/kg/d but lesions at 2g/kg w/40% mortality				Review: Halder <i>et al.</i> , 1985

¹¹ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

¹² HSDB: Hazardous Substances Data Bank [TOMES, MICROMEDEX, Inc]

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Benzene	Rat oral LD50=810 mg/kg: Rat oral LD50=1000mg/kg [Smyth et al., 1962] Inhalation LC50 [4h] = 13,700 ppm	Negative in Ames Test, mouse lymphoma, CHO HPRT, in-vitro UDS, Drosophila; positive in mouse spleen HPRT	Positive in vitro/in vivo in numerous studies and species [oral, inhalation]; in-vitro human lymphocytes; chrom. ab. and micronucleus in mouse bone marrow and spleen lymphocytes; rat bone marrow chrom. ab. and micronucleus	Many studies: Primary effect toxicity to blood cells	Several studies: fetotoxic at maternally toxic doses; not tetratogenic	No standard repro studies; most inhalation studies with repro parameters indicate no effect on reproductive indices, even at high doses	OECD SIDS	Reviews: ATSDR, 1997; EU Risk Assessment, 2001 [Draft]

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Cyclohexane	Rat oral LD50 > 5 g/kg; inhalation LC50[4h] = 4044 ppm	Negative in Ames Test, mouse lymphoma, human lymphocyte UDS	Negative in rat bone marrow chrom. ab. [inhalation]	Effects on liver in mice and rats; on liver and kidney in rabbits [inhalation]	No effects seen in rats or rabbits [inhalation]	No effects in rat 2-gen inhalationrepro at doses not maternally toxic	OECD SIDS	Reviews: SRC Technical Support Document #TR-86-030 [Beals <i>et al.</i> , 1986, draft] ¹³ ; EU Risk Assessment, 2000 [Draft]; Bamberger, 1996; Kreckman, 1997; Malley, 1996 a,b

¹³ SRC: Syracuse Research Corporation Center for Chemical Hazard Assessment, prepared for Test Rules Development Branch, Existing Chemical Assessment Division, Office of Toxic Substances; Smyth, H.F. Carpenter, C.P., Weil, C.S. et al., 1962. Range-finding toxicity data. List VI. Ind. Hyg. J 23: 95-107.

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Toluene	Rat oral LD50 = 5.5 – 7.53 g/kg; inhalation LC50[4h] = 8000 - 8800 ppm	Negative in Ames Test, SHE transformation, and Drosophila SLRL; equivocal in mouse lymphoma	Negative in in-vitro human lymphocyte and CHO chrom. ab., dominant lethal [oral], chrom. ab. in mice [oral] and rats [inhalation], and mouse micronucleus [oral]	Many studies: Effects on central nervous system; hearing loss in rats	In rats and mice: lower birth weight, delayed postnatal development and behavioral effects [inhalation]	No effects in mouse 2-gen inhalation repro study; in rats, effect on sperm count and epididymal weight at 2000 ppm, but no effect on fertility	OECD SIDS	Reviews: ATSDR ¹⁴ , 2000; IARC ¹⁵ , 1999; EU Risk Assessment, 2001; Genetic toxicity review: McGregor, 1994
Ethylbenzene	Rat oral LD50> 3.5 g/kg; inhalation LC50[4h] LC50 = 4000 ppm	Negative in Ames Test, Drosophila SLRL, and in-vivo UDS in mouse hepatocytes; equivocal in mouse lymphoma	Negative in in-vitro CHO and RL4 cells chrom. ab. and in inhalation/i.p. mouse micronucleus	Several studies: Effects seen in liver, kidney, and lung in rats and mice; hearing loss in rats via inhalation	No effects in rabbits; only supernumerary ribs seen in rats	No repro study; in subchronic rat and mouse studies, no effects seen in gonads sperm, extrus cycle	OECD SIDS	Reviews: ATSDR ¹⁶ , 1999

¹⁴ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

¹⁵ IARC: International Agency for Research on Cancer

¹⁶ ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Xylenes, mixed	Rat oral LD50 = 3.5-8.6 g/kg; Rat inhalation [4h]LC50 = 6,350 - 6,700 ppm	Negative Ames Test and mouse lymphoma	Negative in human lymphocytes [only w/o S9 tested] and CHO chrom. ab.	Many studies: liver, and nervous system effects via inhalation; hearing loss in rats via inhalation; nervous system effects via oral exposure	Fetotoxic effects seen in rat and mouse [oral, inhalation], mostly secondary to maternal toxicity	Negative in rat repro [exposed by inhalation 131 days prior to mating, during mating, gestation, day 5-20 of lactation]; no effect on repro organs in rat and mouse	ACC Toluene Xylene Panel/OECD SIDS/ICCA	Reviews: ATSDR, 1995; WHO EHC, 1997 ¹⁷ ; ECETOC, 1986
Styrene	Rat oral LD50 ≥ 5 g/kg; inhalation LC50 [4h] = 4940 ppm	Inconsistent results in Ames Test	Inconsistent results in in-vitro chrom. ab. tests; negative in chrom. ab. and micronucleus tests in mice and rats by oral and inhalation exposure	Many studies: Effects on liver in rats [oral, inhalation] and mice [inhalation]; hearing loss in rats [inhalation]; respiratory tract in rats [inhalation]; lungs in mice [oral]	No birth defects in rats [oral, inhalation] or in mice, rabbits and hamsters [inhalation]; other effects seen only at maternally toxic doses	Negative in rat 3 gen repro study [oral]	OECD SIDS	Reviews: ATSDR, 1992; IARC ¹⁸ , 1994; Brown, 1991, 1993 [repro/devel]

¹⁷ WHO EHC: World Health Organization, International Programme on Chemical Safety. Environmental Health Criteria

¹⁸ IARC: International Agency for Research on Cancer

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Dicyclopentadiene	Rat oral LD50 ranged from 347 – 820 mg/kg; inhalation LC50[4h] ranged from 359 to 500-1000 ppm	Negative in Ames Test	Negative in in-vitro CHO and CHL chrom. ab.	Many studies: Most studies showed no effects in rats or mice in dietary or inhalation studies except male rat hydrocarbon nephropathy in inhalation studies	No effect in rats in oral [diet] studies	Effects only at maternally toxic doses in rat 3-gen repro study [in diet]	OECD SIDS	Reviews: ECETOC ¹⁹ , 1991; JETOC ²⁰ Issue 3 No. 32, 1998 [CHL chrom. ab and OECD 422 studies]; NTP ²¹ [CHO chrom. ab.]

¹⁹ ECETOC: European Centre for Ecotoxicology and Toxicology of Chemicals

²⁰ JETOC: Japanese Chemical Industry Ecology – Toxicology and Information Center

²¹ NTP: National Toxicology Program – personal communication

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
Naphthalene	Rat oral LD50 ranged from 2200 to 2600 mg/kg; no effect at 78 ppm [4h] inhalation	Negative in Ames Test, cell transformation assay, in-vivo UDS in rat liver	Negative in mouse micronucleus; positive in in-vitro CHO chrom. ab.	Many studies: Toxicity to blood cells in dogs [hemolytic anemia][oral]but not rats or mice; cataracts in rabbits, rats, mice, guinea pigs [oral]; local irritative effects after inhalation in rats and mice	No birth defects in rabbits, rats, and mice [oral]; reduced litter size in mice at maternally toxic doses [oral on gestation day 7-14]; no effect in rabbits exposed orally on gestation days 6-18		OECD SIDS	Reviews: ATSDR ²² , 1995; EU Risk Assessment Document Draft, 2001
STREAMS								
Rerun Tower Overheads [approx. 40% benzene, 13% toluene, 26% C5s, 20% other] [HPV stream: C5-10 Fraction of Pyrolysis Gasoline]	Rat oral LD50 > 2 g/kg; rabbit dermal LD50>2g/kg	Negative Ames Test, Drosophila (point mutation), and cell transformation assay (BALB-c/3T3 and C3H 10T ^{1/2}); weakly positive in mouse lymphoma and bacterial DNA repair	Negative in Drosophila chromosome loss and chromosome aberration studies	Rabbit 21-day dermal irritation: NOAEL (systemic) = 1.0 ml/kg/d (top dose); NOAEL (irritation) = <0.10 ml/kg/d	No effects in rabbits in oral teratology pilot and main studies		American Petroleum Institute	Robust Summaries in: API Petroleum HPV Gasoline Blending Streams Test Plan

²² ATSDR: U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

HPV CHEMICAL CATEGORY SUMMARY:

PYROLYSIS C3+ AND

PYROLYSIS C4+ CATEGORY

Components Identified in Streams at Concentrations >5%	Acute Toxicity [only rat oral and inhalation data shown; data for other species and routes available for most components]	Genetic Point Mutation/Other Genetic Effects	Genetic Chromosome Aberration	Subchronic	Developmental	Reproduction	Other Panel Category or Other Program Addressing this Chemical	Toxicity Reviews/References
STREAMS								
Dripolene [HPV stream: Pyrolysis Gasoline]	Rat oral and dermal LD50 > 2 g/kg						American Petroleum Institute	Robust Summaries in: API Petroleum HPV Gasoline Blending Streams Test Plan
Hydrogenated Pyrolysis Gasoline [55% benzene 25% toluene 10% xylene 7% pentane 7% ethylbenzene 2% hexane 3% cyclohexane] [HPV stream: Hydrotreated C6-8 Fraction]	Rat Oral LD50 = 5.17 g/kg; inhalation 4h LC50>12,408 ppm	Negative in Ames Test, in-vitro UDS; positive in cell transformation assay	Negative in micronucleus [mouse oral]	Rat 5 day inhalation: NOAEL <4869 ppm [deaths, bodyweight]			American Petroleum Institute	Robust Summaries in: API Petroleum HPV Gasoline Blending Streams Test Plan

APPENDIX III**Sources of Data for Hazard Evaluations for Mammalian Toxicity**

[Note: All streams are subject to the OSHA 1,3-Butadiene and the Benzene Standards. For hazard communication, the final hazard characterization for each stream will include the hazards of benzene (cancer, genetic toxicity, hematotoxicity) plus any reproductive or developmental toxicity or target organ effects of the other components, unless there is clear evidence that specific component interactions eliminate toxicity.]

Stream	Sources of Data for Hazard Evaluation [These data will be evaluated using scientific judgment and complying with the requirements of the OSHA benzene, 1,3-butadiene, and hazard communication standards]
Pyrolysis Gasoline	<ul style="list-style-type: none"> • Available data for components [benzene, 1,3-butadiene, cyclohexane, cyclopentadiene, cyclopentene, 3-methylpentane, dicyclopentadiene, ethylbenzene, hexane, isoprene, methylcyclopentane, naphthalene, pentadiene, pentane, pentenes, styrene, toluene, vinyl acetate, xylene] • Data for streams containing Pyrolysis Gasoline or fractions thereof [Pyrolysis Gasoline Fractions, Dripolene, Hydrogenated Pyrolysis Gasoline (robust summaries provided)] • Data for streams distilled out of Pyrolysis Gasoline that are being tested in other Panel HPV Test Plans [C5 Non-Cyclics and Resin Oils and Cycloidiene Dimer Concentrates categories] • Data for gasoline blending streams referenced in the API Petroleum HPV Gasoline Blending Streams Test Plan • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Data for hexenes being developed by the ACC Higher Olefins Panel, for C5 aliphatic components being addressed by the ACC Hydrocarbon Solvents Panel in its C5 Aliphatics Category, and for pentane which is addressed in the API Petroleum Gases Test Plan • Literature data regarding interactions between components present in these streams
Pyrolysis C6 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, 1,3-butadiene, cyclopentadiene, ethylbenzene, isoprene, pentenes, pentadiene, toluene] • Data for streams distilled out of Pyrolysis Gasoline that are being tested in other Panel HPV Test Plans [C5 Non-Cyclics Category] • Data for hexenes being developed by the ACC Higher Olefins Panel (as structurally similar to pentenes), for C5 aliphatic components being addressed by the ACC Hydrocarbon Solvents Panel in its C5 Aliphatics Category • Literature data regarding interactions between components present in these streams

Stream	Sources of Data for Hazard Evaluation [These data will be evaluated using scientific judgment and complying with the requirements of the OSHA benzene, 1,3-butadiene, and hazard communication standards]
Pyrolysis C6-C8 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, dicyclopentadiene, ethylbenzene, hexane, styrene, toluene, xylene] • Literature data regarding interactions between components present in these streams
Pyrolysis C5-C6 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, cyclopentene, isoprene, pentenes, toluene] • Data for hexenes being developed by the ACC Higher Olefins Panel (as structurally similar to pentenes) • Literature data regarding interactions between components present in these streams
Hydrotreated C6 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, cyclohexane, hexane, 3-methylpentane] • Data for commercial hexane, which contains n-hexane, 3-methylpentane, methylcyclopentane, 2-methylpentane, cyclohexane • Literature data regarding interactions between components present in these streams
Hydrotreated C6-C8 Fraction	<ul style="list-style-type: none"> • Available data for components [benzene, toluene and other identified components] • Data for Hydrogenated Pyrolysis Gasoline (robust summaries provided) • Literature data regarding interactions between components present in these streams
Quench Loop Pyrolysis Oil and Compressor Oil	<ul style="list-style-type: none"> • Available data for components [benzene, dicyclopentadiene, ethylbenzene, naphthalene, styrene, toluene, xylene and other identified components] • Literature data regarding interactions between components present in these streams
Recovered Oil from Waste Water Treatment	<ul style="list-style-type: none"> • Available data for components, on a case-by-case basis
Extract from Benzene Extraction Unit	<ul style="list-style-type: none"> • Available data for components [benzene, toluene] • Literature data regarding interactions between components present in these streams

APPENDIX IV**Composition of the Crude Butadiene C4 and High Benzene Naphthas Categories**
(Olefins Panel, Implementation Task Group; 2004a, 2004b)**Typical Stream Compositions (wt %) for the Crude Butadiene C4 Category** (*see notes at end of table*)

Constituent	C4 Crude Butadiene Stream (wt %)	Butadiene Unit Heavy Ends Stream (wt %)
tert-Butyl Catechol	0 - 0.01	
Methanol	0.0 - 0.3	
Methylacetylene & Propadiene	0.0 - 2.3	
Ethyl- & Vinylacetylene	0.7 - 3.0	
Propylene	0.0 - 1.9	
Other C3 & Lighter Hydrocarbons	0.5 - 1.7	
Isobutane	0.4 - 22	
Isobutylene	0.5 - 29	
n-Butane	1.5 - 30	0.0 - 6.0
cis- & trans-Butene-2	3.5 - 54	5 - 50
Butene-1	2.5 - 25	0.0 - 4.0
1,3-Butadiene	10 - 82	13 - 92
1,2-Butadiene	0.0 - 1.4	0.0 - 2.0
Other C5 & Higher	0.0 - 8.0	
Vinylcyclohexene	0.0 - 1.0	
Isopentane		0.0 - 3.0
Other C8 Hydrocarbons		0.0 - 4.0

Note 1: The balance of these streams is expected to be other hydrocarbons that have boiling points in the ranges of the listed constituents.

Note 2: The ranges should not be considered to represent absolute limits for these streams. They represent the high and low reported values, and are industry typical limit values.

Typical Stream Compositions (wt %) for the High Benzene Naphthas Category (see notes at end of table)

Component Name	Pyrolysis Gasoline	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydro-treated C6 Fraction	Hydro-treated C6-C7 Fraction	Hydro-treated C6-C8 Fraction	Quench Loop Pyrolysis Oil	Waste Water Treatment [see note 4]	Extract From Benzene Unit
Vinyl Acetate	9.9									
1,3-Butadiene	6.7	0.1 - 2.0								
C4's	0.5 - 5.0	0.1 - 1.5								
1,4-Pentadiene	0.3 - 0.9	0.1 - 2.0								
Isopentane (2-methylbutane)	2.0	0.1 - 1.0								
1-Pentene (Amylene)	0.6 - 4.0	1.0 - 3.0								
2-Methyl-1-Butene	1.0									
Pentene-2 (isomer mix)	0.2 - 1.8	0.1 - 5.0								
Isoprene (2-methylbutadiene-1,3)	0.6 - 10.0	2.0 - 6.0		6.0						
Pentenenes				10.0						
Pentane	10.0					1.0				
2-Methyl-2-Butene	1.2	2.0								
Other C5's	0.3						2.0			
3-methyl-1,2-butadiene		1.0 - 3.0								
1,3-Cyclopentadiene	1.0 - 20.0	0.1 - 5.0	1.0							
1,3-Pentadiene (isomer mix)	0.7 - 4.4	0.3 - 4.0								
Cyclopentene	0.6 - 5.0			8.0						
Cyclopentane	2.3				4.0	1.0 - 5.0				
1,5-Hexadiene	0.6									
2-Methylpentane	4.0				4.0					
2-Methyl-1-Pentene	0.0 - 2.2									
3-Methylpentane (Isohexane)	1.3				4.0	10.0 - 20.0				
Hexene-1	0.0 - 2.2									

Typical Stream Compositions (wt %) for the High Benzene Naphthas Category (continued)

Component Name	Pyrolysis Gasoline	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydro-treated C6 Fraction	Hydro-treated C6-C7 Fraction	Hydro-treated C6-C8 Fraction	Quench Loop Pyrolysis Oil	Waste Water Treatment [see note 4]	Extract From Benzene Unit
Hexenes						2.0				
Methylcyclopentadiene	5.0		1.0							
Hexane Isomers			1.0 - 3.0			5.0 - 20.0				
Ethyltoluenes	0.1 - 2.0									
C9 Paraffins & Naphthenes	0.3 - 1.3									
1,3,5-Trimethylbenzene (mesitylene)	3.0									
C10+								40.6		
1,2,4-Trimethylbenzene (Pseudocumene)	0.0 - 3.3		1.0							
4-Methylstyrene	0.0 - 3.3									
Cyclopentadiene/Methylcyclopentadiene Codimers	0.9 - 4.4		1.0 - 3.0							
Dicyclopentadiene	20.0		1.0 - 5.0					3.7		
1-Decene	1.5									
Vinyl Toluene	0.1 - 1.1									
Dihydro-dicyclopentadiene	2.0									
Decane	0.1 - 5.0									
C10 Aromatics	1.6									
C10's								1.6 - 27.0		
Indene	0.6 - 5.0									
C11+								38.8 - 50.0		
Naphthalene	15.0							4.3 - 10.0		
Methylnaphthalene	2.9									
1-Methylnaphthalene	1.0									

Typical Stream Compositions (wt %) for the High Benzene Naphthas Category (continued)

Component Name	Pyrolysis Gasoline	Pyrolysis C6 Fraction	Pyrolysis C6-C8 Fraction	Pyrolysis C5-C6 Fraction	Hydro-treated C6 Fraction	Hydro-treated C6-C7 Fraction	Hydro-treated C6-C8 Fraction	Quench Loop Pyrolysis Oil	Waste Water Treatment [see note 4]	Extract From Benzene Unit
1,1"-Biphenyl	0.1 - 0.9									
C10 Olefins	1.2									

Note 1: The composition data shown above are composites of reported values.

Note 2: The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.

Note 3: The listed highs and lows should not be considered absolute values for these limits. They are instead highs and lows of reported values.

Note 4: No specific composition data are available. This stream is expected to contain components of Pyrolysis Gasoline.