HIGH PRODUCTION VOLUME (HPV) CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For The

Low 1,3-Butadiene C4 Category

Prepared by:

American Chemistry Council
Olefins Panel
HPV Implementation Task Group

July 9, 2001

PLAIN ENGLISH SUMMARY

This test plan addresses streams that are products of the ethylene process, associated butadiene purification process and other related C4 processes. The category includes CAS numbers that represent streams with a carbon number distribution that is predominantly C4 and that contain relatively low 1,3-butadiene content (less than 5%). Also included in this category are high purity C4 hydrocarbons that are components of some of the mixed streams. The plan addresses the category by evaluating the major C4 components including butene-1 (testing will be conducted), butene-2 (SIDS listed material), isobutylene (SIDS listed material), isobutane (Petroleum HPV Test Group), and butane (Petroleum HPV Test Group), and by evaluating data from mixed C4 streams (some testing in progress). Supporting data will be reviewed on many of the components as part of other test plans under the HPV Challenge Program, the ICCA program, or from chemicals already sponsored in the OECD SIDS program.

EXECUTIVE SUMMARY

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies hereby submit for review and public comment the Low 1,3-Butadiene C4 Category test plan under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of the Panel and its member companies to use new information in conjunction with a variety of existing data and scientific judgment/analysis to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this category.

This test plan addresses streams that are products of the ethylene process and associated C4 processes and that contain predominantly isobutane, isobutylene, butane, 1-butene, and 2-butene. The plan addresses the category by evaluating some mixed C4 process streams and most of the major C4 components.

- Butane

  Butane will be evaluated by the Petroleum HPV Testing group as part of the petroleum gases category.

- Isobutane

  Isobutane will be evaluated by the Petroleum HPV Testing group as part of the petroleum gases category.

- Isobutylene

  Isobutylene is in the OECD SIDS program.

- 1-Butene

  This is a high purity 1-butene stream. Some data for HPV endpoints already exist for 1-butene. A rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screening study (OECD Guideline 422) will be conducted. 1-Butene is sponsored by the Olefins Panel through the International Council of Chemical Associations (ICCA) HPV program.

- 2-Butene

  2-Butene is in the OECD SIDS program.

The basic strategy for this test plan category is to evaluate data on most of the C4 components and on some mixed C4 streams. Evaluation of a mixed C4 stream (containing approximately 10 % 1,3-butadiene) was included as part of the strategy for the Crude 1,3-Butadiene C4 Category test plan, previously submitted. Results from studies on this stream will be used to read across, when possible, to evaluate the members of the Low 1,3-Butadiene C4 Category. Additional supporting data will be collected on many of the components of the streams in this category as part of other test plans under the HPV program, the ICCA program, or from chemicals already sponsored in the OECD SIDS program.

Predictive computer models will be used to develop relevant environmental fate and physicochemical data for substances in the Low 1,3-Butadiene C4 Category. Environmental fate information will be summarized either through the use of computer models when meaningful projections can be developed or in technical discussions when computer modeling is not applicable. For mixed streams, physicochemical properties will be represented as a range of values according to component composition. These data will be calculated using a computer model cited in an EPA guidance document prepared for the HPV Challenge Program.

LIST OF MEMBER COMPANIES
THE OLEFINS PANEL

The Olefins Panel includes the following member companies:

BP Amoco Chemical Company
Chevron Phillips Chemical Company
CONDEA Vista Company*
The Dow Chemical Company*
E.I.du Pont de Nemours and Company*
Eastman Chemical Company*
Equistar Chemicals, LP
ExxonMobil Chemical Company
Fina Oil and Chemical Company*
Formosa Plastics Corporation, U.S.A.*
The B.F. Goodrich Company*
The Goodyear Tire & Rubber Company*
Huntsman Corporation
Koch Industries*
NOVA Chemicals Inc.*
Shell Chemical Company
Sunoco, Inc.*
Texas Petrochemicals Corporation
Westlake Chemical Corporation*
Williams Olefins, LLC*

*These companies are part of the Olefins Panel but do not produce streams in the Low 1,3-butadiene C4 Category.

TABLE OF CONTENTS

TEST PLAN FOR THE LOW 1,3-BUTAIDENE C4 CATEGORY

TEST PLAN FOR THE LOW 1,3-BUTADIENE C4 CATEGORY

I. INTRODUCTION

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies have committed to develop screening level human health effects, environmental effects and fate, and physicochemical data for the Low 1,3-Butadiene C4 Category under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program (Program).

In preparing this test plan, the Panel has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As directed by EPA in that letter, the Panel has sought to maximize the use of scientifically appropriate categories of related chemicals and structure activity relationships. Additionally, and also as directed in EPA's letter, in analyzing the adequacy of existing data, the Panel has conducted a thoughtful, qualitative analysis rather than use a rote checklist approach. The Panel has taken the same thoughtful approach when developing its test plan. The Panel believes its test plan conforms to the principles articulated in EPA's letter.

This plan identifies CAS numbers used to describe process streams in the category, identifies existing data of adequate quality for substances included in the category, and outlines testing needed to develop screening level data for this category under the Program. This document also provides the testing rationale for the Low 1,3-Butadiene C4 Category. The objective of this effort is to identify and develop sufficient test data and/or other information to adequately characterize the human and environmental health and environmental fate for the category in compliance with the EPA HPV Program. Physicochemical data that are requested in this program will be calculated as described in the EPA guidance documents.

II. DESCRIPTION FOR THE LOW 1,3-BUTADIENE C4 CATEGORY

A. The Category

The Low 1,3-Butadiene C4 Category was developed by grouping ethylene manufacturing streams that the Panel believes are similar from both a process and a toxicology perspective, which is why this group is considered a category for purposes of the HPV Program. Eight CAS numbers (Table 1) are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The CAS numbers used to represent the four mixed streams are generally vague with respect to the specifics that distinguish the streams within the category. Therefore, more than one CAS number may correctly represent a single stream and a CAS number may be applicable to more than one stream. A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. A description of the ethylene processes is included in Appendix 1.

The streams in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these streams contain significant levels of olefins. The typical compositions of the streams in this category are shown in Table 2.

The CAS numbers in the Low 1,3-Butadiene C4 Category are associated with seven streams, which are commercial products, or isolated intermediates:

1. C4 Raffinate 1
2. C4 Raffinate 2
3. Isobutylene
4. Butene-1
5. C4 Raffinate 3
6. Butane
7. Catalytic butylenes

Descriptions of the seven streams associated with the Low 1,3-Butadiene C4 Category are presented below.

1. C4 Raffinate 1

C4 Raffinate 1 (raff 1) is a co-product of the butadiene extraction process unit. Raff 1 is the balance of the C4 butadiene concentrate after separation of butadiene by a solvent process, either extraction or more typically extractive distillation. Raff 1 consists predominantly of C4 mono-olefins and C4 paraffins. The stream is sometimes referred to as mixed butylenes because the composition is often about 75% C4 mono-olefins. The saturated hydrocarbons in Raff 1 are mostly iso- and normal-butane. The mono-olefin content varies depending on the feedstock of the ethylene process unit that produced the C4 butadiene concentrate.

2. C4 Raffinate 2

C4 Raffinate 1 may be further processed to remove the isobutylene. This can be accomplished in a two-step process by reaction with water to make tertiary-butyl alcohol or with methanol to produce methyl-tertiary-butyl-ether, which can then be re-cracked to high purity isobutylene. Raffinate 1, after removal of the isobutylene, is referred to as C4-raffinate 2. This stream consists predominantly of butene-1, butene-2 and butanes.

3. Isobutylene

As discussed above, the isobutylene can be obtained from C4 Raffinate 1 by reaction with water or methanol and then re-cracking the product to high purity isobutylene.

Alternatively, isobutylene is obtained by isomerization of Raffinate 2 or by dehydrogenation of isobutane. Typically, commercial isobutylene is 95% pure.

4. Butene-1

High purity butene-1 is produced by distillation from isobutylene plant raffinate.

5. C4 Raffinate 3

This is the stream that remains after removal of butene-1 from C4 Raffinate 2. It is a mixed butenes product, containing the mixed isomers cis- and trans-butene-2 and sometimes n-butane.

6. Butane

Butane is sometimes used as a feedstock for the ethylene process. An ethylene producer who operates an isobutylene alkylation process (typically a petroleum refinery process used to produce alkylates for gasoline formulations) lists butane from this source as a co-product. Butane is also sometimes separated by distillation from C4 Raffinate 3.

7. Catalytic Butylenes

Catalytic Butylenes refers to the C4 cut from a catalytic cracker (a petroleum refinery process). A typical composition is about 55% butenes and 45% butanes with a carbon number distribution of C3 to C5. The stream is relatively low in 1,3-butadiene and diolefins (e.g. a few tenths of a percent). In some cases the stream is a combination of catalytic cracker C4 butylenes and ethylene process C4 Raffinate 1 from the butadiene unit.

III. TEST PLAN RATIONALE

A. Overview

Mammalian/Human Health Effects and Test Strategy

The Low 1,3-Butadiene C4 Category consists of mixed hydrocarbon streams with a carbon number distribution that is predominantly C4 or of relatively pure C4 materials. A number of the components of the streams listed in this category are already SIDS (Screening Information Data Set) listed materials including isobutylene and butene-2. Some of the remaining components will be tested by the American Chemistry Council Olefins Panel as part of this or other test categories or by other groups within the HPV or ICCA program.

Existing toxicology data suggests that the most biologically active C4 hydrocarbon is likely to be 1,3-butadiene and that positive genotoxicity is the most sensitive health effect endpoint. The Low 1,3-Butadiene C4 Category consists of C4 process streams that have had most of the 1,3-butadiene content removed. The 1,3-butadiene concentration is typically less than one percent but may range from zero to five percent. 1,3-butadiene must be biotransformed prior to causing toxicity and other C4 alkenes are biotransformed through a common metabolic pathway. It is anticipated that mixed components will compete for the same active enzyme sites. It is therefore likely that the positive genotoxicity of 1,3-butadiene will be reduced or eliminated by the greater presence (greater than or equal to 95 percent) of the other components. It should be noted that a mixed C4 stream containing approximately ten percent 1,3-butadiene is being evaluated for potential genotoxicity and other relevant SIDS endpoints as part of the Crude Butadiene C4 category that was previously submitted by the Olefins panel. Preliminary results from the rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screening study on this stream have not identified any treatment-related adverse effects. Early results also suggest that the presence of 10% 1,3-butadiene in a mixed C4 stream causes a slight increase in micronuclei in the mouse. On the other hand, existing studies on relatively pure 1-butene and isobutylene indicate that both are negative in the mouse micronucleus test.

The strategy for characterizing the hazards of this category includes the evaluation of data on the major C4 components including butene-1, butene-2, isobutylene, isobutane and butane. Isobutylene and butene-2 are already sponsored in the OECD SIDS program and as such, data are or will become available for these materials. Butane and isobutane will be evaluated as part of the Petroleum HPV Test Group program. Mutagenicity studies including a bacterial gene mutation assay and a mouse micronucleus assay already exist for butene-1. A rat inhalation combined repeated dose/ reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422) will be completed on butene-1. Results from the combined repeat-dose reproductive/developmental screen on the mixed C4 stream containing approximately ten percent 1,3-butadiene in the Crude Butadiene C4 Category will be used to evaluate the effect of C4 mixtures. The Olefins Panel believes that conducting an OECD 422 study on a C4 stream with less 1,3-butadiene (less than 10%) would not contribute significantly to our current understanding of the toxicology of these process streams, especially when one considers that data evaluating reproductive/developmental endpoints are or will become available for isobutylene, butene-1, butene-2, isobutane and n-butane. Results from the OECD 422 study on the crude 1,3-Butadiene C4 stream containing approximately ten percent 1,3-butadiene along with data on individual components will be used to read across to the mixed C4 streams in this category for the developmental and reproductive toxicity end points.

The inhalation route of exposure was chosen for the health effects testing because inhalation is the most relevant route of exposure for the Low 1,3-Butadiene C4 Category streams. The rat will be used in the repeated dose/reproductive and developmental effects/neurotoxicity screen because this test was designed for the rat and there is a more substantial historical database for the rat. The rat is also the standard species for reproductive toxicity tests.

The recommended testing, together with existing data and data for the components under development by the American Chemistry Council Olefins Panel for other categories under the HPV program, by other HPV consortia, and by the OECD SIDS program, will be sufficient to adequately characterize the toxicity of the range of substances included in this category.

Physicochemical Properties

Physicochemical data for each of the streams in the Low 1,3-Butadiene C4 Category will be developed using the EPIWIN model[1], as discussed in the EPA document titled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program." In addition, measured data will also be provided for selected products in this category where readily available.

Ecotoxicity

There are three aquatic endpoints in the HPV Program

- Acute Toxicity to Fish
- Acute Toxicity to Aquatic Invertebrates
- Toxicity to Algae (Growth Inhibition)

EPA identifies the following test methods to determine these endpoints: OECD Guideline 203, Fish Acute Toxicity Test; Guideline 202,Daphnia sp., Acute Immobilization Test; and Guideline 201, Alga Growth Inhibition Test.

The OECD aquatic toxicity test methods were not designed to assess the acute toxicity of gaseous substances like those in the Low 1,3-Butadiene C4 Category. Therefore, the Panel will develop a Robust Summary Statement that addresses the physical nature of these substances and the fact that their primary route of loss will be to the air. This discussion will include calculated toxicity data for selected chemical components. The calculated data will be developed using ECOSAR, a SAR program found in EPIWIN[1].

Environmental Fate

Predictive models will be used to develop meaningful data for chemicals that are gaseous at relevant environmental temperatures and pressures. The environmental fate data include:

- Photodegradation
- Stability in Water (Hydrolysis)
- Transport and Distribution (Fugacity)
- Biodegradation

1. Photodegradation

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough then the resultant excited state of the chemical may undergo a transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline [2]. UV light absorption of selected chemicals representative of this category will be evaluated to identify those having the potential to degrade in solution. First-order reaction rates will be calculated, for those chemicals with a potential for direct photolysis in water.

Photodegradation can also be measured [3] (EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the EPA [4]. An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Chemicals that are gases will be available for atmospheric oxidation reactions with photochemically generated hydroxyl radicals. This will be the most significant route of degradation in the environment for category members.

The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) [1] is used by OPPTS. This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hr day, and a given OH- concentration. This calculation will be performed for representative chemical components identified in the Low 1,3-Butadiene C4 Category.

2. Stability in Water (Hydrolysis Testing and Modeling)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters [5]. Stability in water can be measured [3] (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA [4]. An estimation method accepted by the EPA includes a model that can calculate hydrolysis rate constants for esters, carbamates, epoxides, halomethanes, and selected alkylhalides. The computer program HYDROWIN (aqueous hydrolysis rate program for Microsoft windows) [1] is used by OPPTS.

All of the chemical structures included in the Low 1,3-Butadiene C4 Category are simple hydrocarbons. That is, they consist entirely of carbon and hydrogen. As such, they are not expected to hydrolyze at a measurable rate. A technical document will be prepared describing the potential hydrolysis rates of these substances, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water

3. Chemical Transport and Distribution In The Environment (Fugacity Modeling)

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model [6]. EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data* [3], which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent partitioned to 6 compartments within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model will be used to calculate distribution values for representative chemical components identified in streams in this category. A computer model, EPIWIN - version 3.04 [1], will be used to calculate the properties needed to run the Level I EQC model.

4. Biodegradation Testing

Biodegradation is the utilization of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which are ultimately converted to an inorganic form such as carbon dioxide, nitrate, sulfate, and water. Assessing the biodegradability of organic chemicals using a standard testing guideline can provide useful information for evaluating chemical hazard.

Substances in this category are gaseous at room temperature. Standard OECD biodegradation test methods were not designed to assess the relative biodegradability of gaseous materials. To provide relevant information for this endpoint, a discussion will be developed on the physical nature of these substances and the fact that their primary route of loss will be to the air compartment where they will degrade through hydroxyl radical attack, which is briefly described under *photodegradation* above.

B. Stream Specific Rationales

The rationales for the test plan strategy specific to each stream in the Low 1,3-Butadiene C4 Category are presented below.

1. C4 Raffinate 1

   This stream represents the balance of C4 components after removal of the 1,3-butadiene. The toxicity profile of this stream is expected to be represented by the toxicity of the major C4 components excluding 1,3-butadiene. No testing of this stream is currently proposed.

2. C4 Raffinate 2

   This stream consists predominantly of butene-1, butene-2 and butanes. The toxicity of this stream is expected to be similar to that of pure butene-1, butene-2 and butanes. No testing of this stream is currently proposed.

3. Isobutylene

   Isobutylene is in the OECD SIDS program. Therefore, data addressing each of the endpoints is or will become available for this material under the OECD SIDS program.

4. Butene-1

   Butene-1 is a major component in most of the streams in this category and is itself a high production volume chemical. An OECD 422 study will be performed on butene-1 to complete the SIDS battery on this material. Data from this test material will be used to read across to other streams that contain butene-1 as a component. Butene-1 is sponsored by the Olefins Panel in the ICCA program.

5. C4 Raffinate 3

   This stream typically consists predominantly of cis- and trans-butene-2, and in some cases butane. The toxicity of this material will be characterized based on the toxicity studies from each of the components. No testing of this stream is currently proposed.

6. Butane

   The Petroleum HPV Testing Group is evaluating Butane under the HPV program.

7. Catalytic butylenes

   Catalytic butylenes consists predominantly of butenes and butanes with less than one percent 1,3-butadiene. Test data from components of this stream will be used to characterize the toxicity of this stream. No testing of this stream is currently proposed.

IV. TEST PLAN SUMMARY

The following testing, modeling, and technical discussions will be developed for the Low 1,3-Butadiene C4 Category.

- Conduct a rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422) on a high purity butene-1 stream. Butene-1 is sponsored through the ICCA HPV Program.
- Prepare a technical discussion on the potential of chemical components comprising streams in this category to photodegrade.
- Prepare a technical discussion on the potential of chemical components comprising streams in this category to hydrolyze.
- Prepare a technical discussion on the potential of chemical components comprising streams in this category to biodegrade.
- Calculate fugacity data for selected chemical components of streams in this category.
- Calculate physiochemical data as described in the EPA document titled, *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* and identify readily available data.

Summaries of the results will be developed once the data and analyses are available. This test plan is expected to provide adequate data to characterize the human health effects and environmental fate and effects endpoints for the category under the Program.

V. OTHER SUPPORTING DATA

Additional data for components of the low 1,3-butadiene C4 streams that will provide support for this category will be collected by other test plans within the Olefins Panel's HPV program (see Table 4), by other consortia participating in the HPV or ICCA programs, or from chemicals sponsored in the OECD SIDS program.

- n-Butane: Will be evaluated by the Petroleum HPV Test Group.
- Isobutane: Will be evaluated by the Petroleum HPV Test Group.
- Isobutylene: OECD SIDS
- Butene-2: OECD SIDS
- Crude Butadiene (Mixed C4s): Will be characterized as part of the Olefins Panel Crude 1,3-Butadiene C4 Category.

REFERENCES

1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04**.** Syracuse Research Corporation, Syracuse, NY, USA.

2. Zepp, R. G., and D. M. Cline, 1977. Rates of Direct Photolysis in the Aqueous Environment. Environ. Sci. Technol. 11:359.366.

3. US EPA. 1999. Determining the Adequacy of Existing Data. OPPT, EPA.

4. US EPA. 1999. The Use of Structure Activity Relationship (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA.

5. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, Florida, USA.

6. Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15:1627-1637.

TABLES AND FIGURES

Table 1. CAS Numbers And Descriptions.

CAS Numbers	CAS Number Description
106-97-8	Butane
106-98-9	1-Butene
115-11-7	1-Propene, 2-methyl
25167-67-3	Butenes
68477-42-9	Gases, petroleum, extractive, C3-5, butene-isobutylene-rich
68477-83-8	Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed
68527-19-5	Hydrocarbons, C1-4, debutanizer fraction
68606-31-5	Hydrocarbons, C3-5, butadiene purification by-product

Table 2. Typical Composition Ranges (Percent) For Low 1,3-Butadiene C4 Streams

Components	C4 Raffinate 1	C4 Raffinate 2	C4 Raffinate 3	Isobutylene	Butene-1	Butane	Catalytic Butylenes
Acetonitrile, ppm	0-50						
Carbonyl ppm	0-50						
Propylene		0-1					
Propane	1-5						1.2-1.3
Propadiene	0-1	0-1					
Isobutane	0-65	1-7.5				3.5	
Isobutylene (Isobutene)	30-55	1-5		99.4			5
C5 Olefins				1.1			
1-Butene	7-50	2.5-65	0.2		99.2		
1,3-Butadiene	0-5	0.1-0.5		0.1	0.005		0.5
Other C4s					1.4		
Butanes							40-46
Butane	1-26	10-39	55.2			88.2	
Butenes							48-58
Butene-2 (isomer mix)	1-50	11-55	45.2				
Isopentane (2-methylbutane)						5.3	

Table 3. Assessment Plan for Low 1,3-Butadiene C4 Category Under the Program

	Human Health Effects						Ecotoxicity				Environmental Fate			
Stream Description/Stream Component	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Reproduc-tion	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photo-deg.	Hydro-lysis	Fugacity	Biodeg.
Low 1,3-Butadiene C4														
n-Butane[1]	A	A	T	T	T	T	NA	NA	NA	SAR	TD	TD	CM	TD
Isobutane[1]	A	A	T	T	T	T	NA	NA	NA	SAR	TD	TD	CM	TD
Isobutylene[2]	A	A	A	A	A[4]	A[4]	NA	NA	NA	SAR	TD	TD	CM	TD
Butene-1[3]	A	A	A	T	T	T	NA	NA	NA	SAR	TD	TD	CM	TD
Butene-2[2]	A	A	A	A	A	A	NA	NA	NA	SAR	TD	TD	CM	TD
C4 Raffinate 1	RA	RA	RA	RA	RA	RA	NA	NA	NA	SAR	TD	TD	CM	TD
C4 Raffinate 2	RA	RA	RA	RA	RA	RA	NA	NA	NA	SAR	TD	TD	CM	TD
C4 Raffinate 3	RA	RA	RA	RA	RA	RA	NA	NA	NA	SAR	TD	TD	CM	TD
Catalytic Butylenes	RA	RA	RA	RA	RA	RA	NA	NA	NA	SAR	TD	TD	CM	TD

A Adequate existing data available
CM Computer modeling proposed
NA Not applicable
TD Technical discussion proposed
T Testing proposed
RA Read-Across
SAR Structure-Activity-Relationship modeling and readily available data

[1] Testing to be conducted and/or robust summaries provided by the Petroleum HPV Testing Group.
[2] Addressed as part of the OECD SIDS program.
[3] Sponsored through ICCA.
[4] Data not yet available but should be addressed as part of the SIDS program

Table 4. American Chemistry Council Olefins Panel Sponsored HPV Test Categories

Category Number	Category Description
1	Crude 1,3-Butadiene C4
2	Low 1,3-Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams (3) – Propylene sponsored through ICCA
5	High Benzene Naphthas
6	Low Benzene Naphthas
7	Resin Oils – High Dicyclopentadiene
8	Resin Oils – Low Dicyclopentadiene
9	Cyclodiene Concentrate
10	Fuel Oils

APPENDIX 1

ETHYLENE PROCESS DESCRIPTION

A. The Ethylene Production Process

1. <u>Steam Cracking</u>

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 products. 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 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 liquid feedstocks are also converted to ethylene. While the predominant products produced are ethylene and propylene, a wide range of additional products are also formed. These products range from methane (C1) through fuel oil (C12 and higher) and include other olefins, diolefins, aromatics and saturates (naphthenes and paraffins).

2. <u>Refinery Gas Separation</u>

Ethylene and propylene are also produced by separation of these olefins from refinery gas streams, such as from the light ends product of a catalytic cracking process or from coker off-gas. 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. Products of the Ethylene Process

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 component 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 product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges. Further processing of one of these mixed streams, the Crude Butadiene C4 stream, results in additional mixed streams and high purity products that make up the main constituents of the Low Butadiene C4 category.

The chemical process operations that are associated with the process streams in the Low Butadiene C4 category are shown in Figure 1.

Olefins Industry Flowsheet for the HPV
C4 Low 1,3-ButadieneTest Category
Figure 1

July 9, 2001

HPV C4 Low 1,3-Butadiene Category Streams are shown in Bold with "*" following the name.