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HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

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TEST PLAN

For The

Propylene Streams Category

Prepared by:

American Chemistry Council Olefins Panel
HPV Implementation Task Group

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PLAIN ENGLISH SUMMARY

This test plan addresses four streams that are products of the ethylene process. The category includes two CAS numbers that represent two grades of propylene and two propylene-containing streams that are predominantly C3 hydrocarbons. The basic strategy for this test plan is to use data on propylene to characterize streams that are predominantly propylene and to use data on propylene and propane to characterize the mixed streams. Propylene is already sponsored in the ICCA (International Council of Chemical Associations) program by the CEFIC (European Chemical Industry Council) Lower Olefins Sector Group. Robust summaries for existing and new studies will become available as part of that program. Propane is sponsored in the EPA HPV Chemical Challenge Program by the API Petroleum HPV Testing Group as part of the Petroleum Gases Test Plan and robust summaries on existing and new studies for propane will become available as part of the this program.

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TEST PLAN FOR THE PROPYLENE STREAMS

I. INTRODUCTION

The Olefin 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 Propylene Streams 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 requested 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 requested 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. The objective of this effort is to identify and develop sufficient test data and/or other information to adequately characterize human health, environmental effects and environmental fate for the category in compliance with the EPA HPV Program. Data for the physicochemical endpoints in this program will be developed using a computer model described in the EPA HPV guidance documents. Measured physicochemical data will also be identified where readily available and provided with the calculated data.

II. DESCRIPTION OF THE PROPYLENE STREAMS CATEGORY

A. The Category

Two CAS numbers are used to describe the streams in the Propylene Streams category (Table 1). In addition to polymer grade and chemical grade propylene, the category includes two propylene-containing streams. This category represents hydrocarbon streams with a carbon number distribution that is predominantly C3. The Panel believes these streams are similar from a toxicology perspective. Existing data and new data being generated as part of the ICCA and EPA HPV program on propylene and propane will be used to characterize the streams.

Table 1. CAS Numbers and Descriptions of Propylene Streams Category

CAS Number	CAS Number Description
115-07-1	1-Propene
68606-26-8	Hydrocarbons, C3

The CAS numbers in the Propylene Streams category are associated with four streams that are commercial products or isolated intermediates (Table 2). The four streams arise from production processes associated with ethylene manufacturing. Composition data is provided in Table 3. A description of the ethylene and associated processes is included in Appendix 1.

Table 2. Process Streams in the Propylene Streams Category

Stream (Industry Description)
1. Propylene, polymer grade
2. Propylene, chemical grade
3. Propylene Stream
4. Light Ends from Butadiene Plant

1. Propylene, polymer grade: Polymer grade propylene is a high purity (99%+) product of the ethylene unit. It is obtained by fractionation of a portion of the condensed cracking furnace effluent and other processing steps (e.g. C3 acetylene removal). The final polymer grade propylene is produced as the distillate from the C3 splitter. The main impurities in the stream are typically ethane and propane.

2. Propylene, chemical grade: Chemical grade propylene is a C3 product with typical propylene content of 93 to 95%. Propane accounts for most of the balance of the composition. An ethylene process using a scheme similar to that used for polymer grade propylene, but with fewer or less rigorous purification steps, produces this grade.

3. Propylene Stream: This is the C3 stream prior to separation into propylene and propane. Typically, this stream is produced as the overhead from the depropanizer in an ethylene unit. It is a narrow boiling-range mixture that consists predominantly of C3 hydrocarbons. A typical composition is 85% propylene, 12% propane and 3% C3 acetylenes.

4. Light ends from Butadiene Plant: This hydrocarbon stream is produced by fractionation of the C4 Crude Butadiene to remove relatively low levels of propane and propylene that may be contained in the stream. The carbon number distribution for the stream is predominantly C3.

III. TEST PLAN RATIONALE

A. Overview

The components of the Propylene Streams category, primarily propylene and propane, are commercially produced gases, highly volatile and practically insoluble in water. They are anesthetics of comparatively low toxicity.[1,2,3] The basic strategy for this assessment plan is to use data on propylene to characterize streams that are predominantly propylene and to use data on propylene and propane to characterize the mixed streams. Propylene is a major chemical intermediate produced by catalytic or thermal cracking of hydrocarbons or as a by-product of petroleum refining. Propylene is in the ICCA (International Council of Chemical Associations)

program and the assessment is expected to be completed by the end of 2002. The strength of the propylene toxicological data includes the availability of a long-term (lifetime), controlled exposure study in rats and mice. [3,4,5] No increase in tumors was seen at any tested dose level. The only effects reported were low-grade irritation to the nasal cavity in rats and mice and a questionable inflammatory change in the mouse kidney.

In order to complete the OECD SIDS screening level toxicity data set for the ICCA program, propylene will be tested in a developmental toxicity test and a micronucleus test *in vivo*. Data of adequate quality exist for other SIDS end points to sufficiently address the toxicity of propylene and the potential human health effects under the HPV Program. The toxicity of the other major component - propane - will be evaluated by the Petroleum HPV Testing Group associated with the American Petroleum Institute.

Environmental effects and biodegradation test data do not exist for products in this category. This is not unexpected because standard testing guidelines are not designed to evaluate gaseous products. In addition, because these substances are gases, it is highly unlikely that they will pose a hazard to aquatic or terrestrial environments. As a result, aquatic toxicity and biodegradation testing will not be conducted based on the physical state of these substances and their physicochemical parameters (i.e., low boiling point, high volatility and high Henry's Law constants). However, the environmental fate endpoints, photodegradation, and fugacity, will either be calculated or discussed.

Chemical components of products in this category will partition primarily to the air. Therefore, their fate in air is of environmental interest. In addition, preliminary distribution data suggest that they will not partition to suspended organic matter in air and precipitate to aquatic and terrestrial compartments.

In all cases, based on physicochemical characteristics, these substances will partition to the air at a rapid rate if released to the environment. As a result, the aquatic and terrestrial environments will not be the compartments of concern when evaluating the potential environmental impact of these substances.

Physicochemical data for the Propylene Streams category will be developed using the EPIWIN[12] model, as discussed in the EPA document titled "*The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemical Challenge Program.*"[13] In addition, measured data will also be provided for selected products in this category where readily available.

<u>Mammalian/Human Health Effects and Test Strategy</u>

Existing mammalian toxicity data suggests that propylene is not acutely toxic. [1,2] At very high exposure levels, propylene produces an anesthetic effect and in fact, propylene has been used as an anesthetic agent. Long-term animal studies in which rats and mice were exposed to high dose levels of propylene show no statistically significant increase in tumor incidence nor was there evidence of adverse systemic health effects. [3,4,5] Two chronic animal inhalation studies have found low-grade irritation of the nasal mucosa in rats and mice at exposures of 5,000 and 10,000

ppm. The mice also reportedly had an inflammatory change of the kidney; however, the toxicological significance and treatment-relatedness of this effect is questioned. Propylene has also been shown not to cause genetic effects;[6, 7, 8] however, available data is very limited - comprised only of gene mutation assays *in vitro*.

There is very little metabolism of propylene in animals.[9, 10, 11] Most of the propylene is exhaled unchanged. A small fraction, however, is metabolized to propylene oxide (PO). PO can react with DNA and is demonstrated to be mutagenic *in vitro*, weakly mutagenic *in vivo*, and produces local site of contact tumors. Evidence for conversion to PO in propylene-exposed animals includes direct measurement of propylene oxide in the blood and low level binding of propylene oxide to blood cells and DNA in various organs. Conversion that occurs has not been found to result in any health effects in the two-year cancer studies or studies of potential adverse genetic effects. Studies of petroleum workers, who are exposed to many different chemicals, show no increase in cancer rates that can be associated with propylene exposure.

The strategy for characterizing the hazards of this category consists of evaluating the data on propylene as a major component of the streams in this category and to a lesser extent the data on propane for some of the mixed streams in the category. The existing data and data under development under the ICCA program for propylene and evaluation of propane by the API Petroleum HPV Testing Group will be sufficient to adequately characterize the toxicity of the substances included in the category and the associated potential human health effects; thus, further testing of the Propylene Streams category is not recommended.

Ecotoxicity

Aquatic toxicity endpoints for the HPV Chemical Program include acute toxicity to a freshwater fish and invertebrate, and toxicity to a freshwater alga. 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. However, the OECD aquatic toxicity test methods were not designed to assess the acute toxicity of gaseous substances like those in the Propylene Streams 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.[12]

Environmental Fate

Environmental fate endpoints for the HPV Chemical Program include biodegradation, photodegradation, hydrolysis, and fugacity. The products in the Propylene Streams category are gaseous at environmentally relevant temperatures Therefore, their degradation in the environment will result primarily from physical processes, which will be addressed under the photodegradation endpoint discussed below. Data and/or information in the form of a technical discussion will be provided for photodegradation.

Chemicals in this category are not subject to hydrolysis at measurable rates, therefore information for this endpoint will be summarized in a technical review document.

Equilibrium models are used to calculate chemical fugacity, which can provide information on where a chemical is likely to partition in the environment. Fugacity data can only be calculated. For the HPV Program, environmental partitioning data will be calculated for selected chemical components using a widely accepted fugacity computer model. Preliminary data from this model show that several chemicals in the Propylene Streams category are calculated to partition to the air to a significant extent. Because the air phase may be the primary partitioning compartment for many chemical components in this category, data characterizing their potential for physical degradation in the atmosphere will be developed (this is discussed below under photodegradation).

1. Biodegradation

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 inorganic forms 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. However, substances in this category are gaseous at room temperature and development of biodegradation data would not provide relevant information for use in a hazard or risk assessment. In addition, standard biodegradation test methods were not designed to assess the relative biodegradability of gaseous materials. To provide relevant information for this endpoint, a technical 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 can degrade through hydroxyl radical attack, which is briefly described under *Photodegradation* below.

2. Photodegradation – Photolysis

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 lead to its 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.[14]

The UV light absorption of selected chemicals in products from the Propylene Streams category will be evaluated to identify those chemicals with a potential to degrade in solution. When possible, first order reaction rates will be calculated for chemicals identified to have a potential for direct photolysis in water. If instead, a low potential for direct photolysis is suggested by the evaluation, a technical discussion will be prepared to summarize the findings.

3. Photodegradation – Atmospheric Oxidation

Photodegradation can be measured (EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the EPA.[15] 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. AOP valuess can be calculated using a computer model. Hydrocarbons, such as those in the Propylene Streams category, have the potential to volatilize to air. In air, chemicals may undergo reaction with photosensitized oxygen in the form of ozone and hydroxyl radicals. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows)[12] is used by OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant at a given OH- concentration. This calculation will be performed for the representative chemical components of products in the Propylene Streams category.

4. 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.[16]

Chemical stability in water can be measured (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA.[15] 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)[12] is used for this purpose by OPPTS.

All of the chemical structures included in the Propylene Streams category are 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 that discusses 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.

5. 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.[17] The U.S. EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data*,[15] which was prepared as guidance for the HPV Program.

In its document, U.S. 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 of chemical partitioned to 6 compartments described above within a defined 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, melting point, vapor pressure, and water solubility to calculate distribution within a unit world. This model will be used to calculate distribution values for representative chemical components identified in products from this category. A computer model, EPIWIN version 3.04,[12] will be used to calculate the physicochemical properties needed to run the Level I EQC model.

Physicochemical Properties

The physicochemical (PC) endpoints for the HPV chemical program include melting point, boiling point, vapor pressure, water solubility, and octanol/water partition coefficient (K_{ow}). Although some data exist for products in the Propylene Streams category, not all of these endpoints are defined and a consensus data set does not exist. Therefore, calculated data will be developed for a group of selected chemicals contained by products in this category to provide a consistent, representative data set. Also, existing measured data will be identified where readily available.

Calculated PC data for selected chemical components in the Propylene Streams category will be developed using the EPIWIN computer model,[12] as discussed in the U.S. EPA document entitled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program."[13] The use of computer modeling for the development of these data is justified since components of the streams in this category are chemically related and expected to exhibit relatively similar environmental properties. The calculated and measured PC data will be included in robust summaries, which will be prepared for each endpoint prior to the completion of the HPV program for this category.

IV. TEST PLAN SUMMARY

The plan proposes addressing the category using toxicological data for propylene and propane. Propylene is sponsored in the ICCA Program by the CEFIC Lower Olefins Sector Group and propane is sponsored in the HPV Challenge Program by the API Petroleum HPV Testing Group.

The following testing, modeling, and technical discussions will be developed for the Propylene Streams category:

- Robust summaries for new (developmental toxicity test and mouse micronucleus test in bone marrow) and existing studies on propylene will become available through the ICCA program.
- Robust summaries for new and existing studies on propane will become available through the EPA HPV Challenge Program.
- Prepare a technical discussion evaluating the propylene streams based on data on propylene and propane.

- Prepare a technical discussion on the potential aquatic toxicity of selected chemical components comprising streams in this category using modeled data.
- 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 biodegradation of chemical components of streams in this category.
- Calculate fugacity data for selected chemical components of streams in this category.
- Calculate physicochemical data as described in the EPA document titled *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program*. Identify valid measured data for chemical components and products where readily available and prepare robust summaries of the calculated and measured data.

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

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Table 3. Typical Composition Ranges (%) for Propylene Streams

Component Name	Polymer Grade Propylene	Chemical Grade Propylene	Propylene Stream	Light ends from BD unit
Compositions, wt %				
Methane		0.5		
Ethylene		0.1 - 1		
Ethane		0.1 - 1		0 - 2
Propylene	95 - 100	90 - 99.8	85	25 - 40
Propane	0.1 - 0.5	0.2 - 10	12	60 - 70
Methylacetylene & Propadiene			3	

Note 1: The composition data shown above are composites of reported values.
Note 2: The streams may contain 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 the highs and lows of the reported values.

Table 4. Assessment Plan for Propylene Stream under the Program. Robust summaries for propylene will become available as part of the ICCA Program and robust summaries for propane will become available as part of the EPA HPV Challenge Program.

Product Description	Human Health Effects						Ecotoxicity			Environmental Fate				
	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Repro-duction	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photo-deg.	Hydrol-ysis	Fugacity	Biodeg.
Propylene *	A[1]	A[1]	A[1]	A[1]	A[1]	A[1]	CM	CM	CM	CM[2]	TD	TD	CM	TD
Propylene Streams **	RA	RA	RA	RA	RA	RA	RA	RA	RA	RA	TD	TD	RA	TD
Propane	A[3]	A[3]	A[3]	A[3]	A[3]	A[3]	CM	CM	CM	CM[2]	TD	TD	CM	TD

A Adequate data available
CM Computer modeling proposed
RA Read across
TD Technical discussion proposed

[1]Robust summaries for new and existing data will become available as part of the ICCA program
[2]Identify and provide measured data with calculated data
[3]Robust summaries for new and existing data will become available as part of the EPA HPV Challenge Program

* Propylene is sponsored in the ICCA Program by the CEFIC Lower Olefins Sector Group
** Propane is sponsored in the EPA HPV Challenge Program by the API Petroleum HPV Testing Group

Table 5. Olefins Panel Sponsored Test Categories

Category Number	Category Description
1.	Crude Butadiene C4
2.	Low Butadiene C4
3.	C5 Non-Cyclics
4.	Propylene Streams (C3)
5.	High Benzene Naphthas (C6-C12, predominantly C6)
6.	Low Benzene Naphthas (C7-C12)
7, 8, 9	Resin Oils and Cyclodiene Dimer Concentrates
10.	Fuel Oils (C8+)
11.	Fuel Gases

Appendix I

ETHYLENE PROCESS DESCRIPTION

A. The 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 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. Refinery Gas Separation

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 offgas. 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 and then further processed. Product propylene and propylene streams from the ethylene unit and from down stream processing make up the Propylene Streams category.

The chemical process operations that are associa ted with the process streams in the Propylene Streams category are shown in Figure 1.
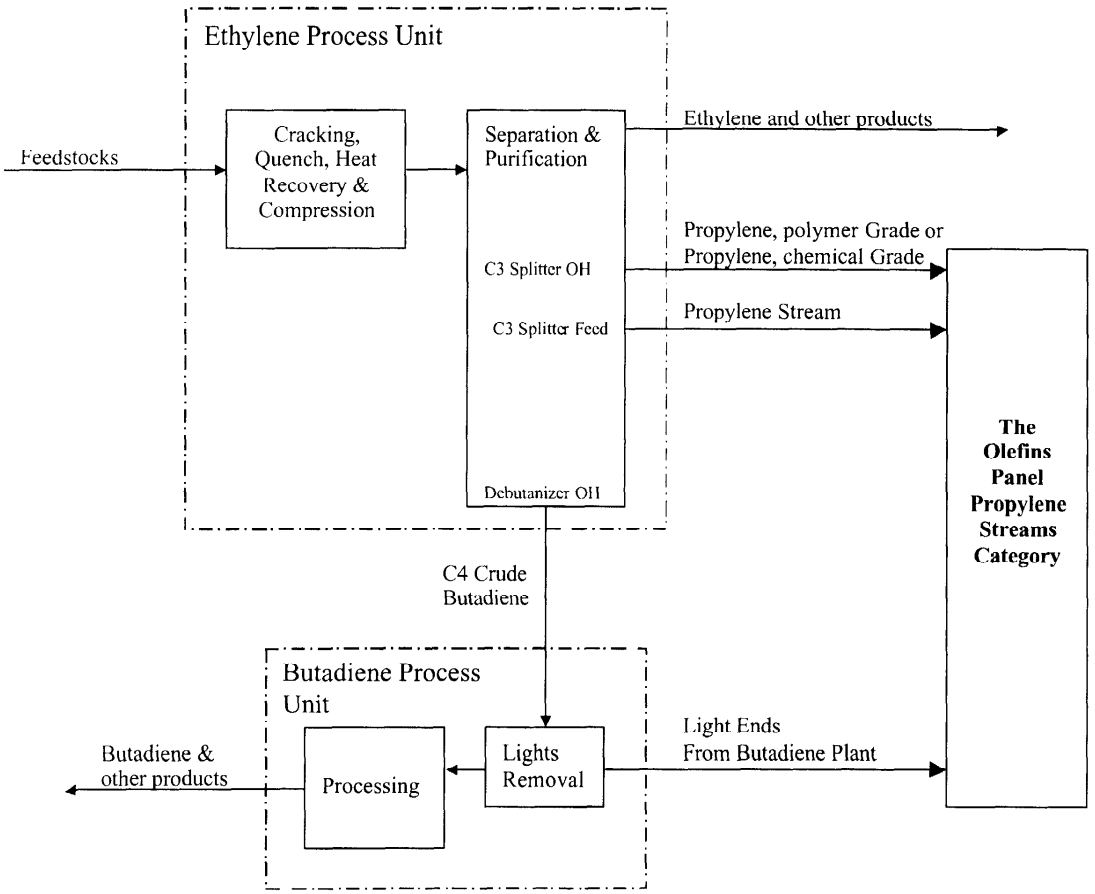
Figure 1: Chemical Process Operations Associated with Process Streams in the Propylene Streams Category