

---

# Hydrocarbon Characterization for Use in the Hydrocarbon Risk Calculator and Example Characterizations of Selected Alaskan Fuels

## Technical Background Document and Recommendations

Prepared for  
**Alaska Statement of Cooperation Working Group**

September 2006

Prepared by  
**Geosphere, Inc.**  
**CH2MHILL**

## **Preface**

This document was created under the Alaska Statement of Cooperation (SOC), which is an agreement between the Alaska Department of Environmental Conservation (ADEC), the U.S. Environmental Protection Agency (EPA), the Departments of the Army, Air Force, Navy, Military and Veterans Affairs (Army National Guard), Interior, and the Federal Aviation Administration (FAA) and U.S. Coast Guard. The objective of the agreement is to work cooperatively to identify and resolve issues affecting human health and the environment through promoting compliance with environmental laws, preventing pollution, creating partnerships to identify and cleanup contaminants and pollution, promoting training and coordinating with affected Tribes. A subcommittee or “working group” was formed under the SOC to evaluate the characterization and fate and transport of petroleum hydrocarbons spilled in the environment, and the risks posed by petroleum contamination. FAA contracted with Geosphere and CH2M Hill to research the issues and develop eight technical issue papers. The paper titles are listed below. Staff from ADEC, FAA, the Army and Army Corps of Engineers, and the Army National Guard reviewed and provided feedback on the draft papers. These papers provide sound scientific and technical information along with recommendations for use and/or future consideration.

## **ADEC Disclaimer**

This paper does not constitute ADEC guidance, policy, or rule making, nor does it create any rights or benefits, substantive or procedural, enforceable at law or in equity, by any person. ADEC may take action at variance with this paper.

## **Statement of Cooperation Working Group Paper Titles**

1. Three- and Four-Phase Partitioning of Petroleum Hydrocarbons and Human Health Risk Calculations, Technical Background Report Document and Recommendations
2. Hydrocarbon Characterization for Use in the Hydrocarbon Risk Calculator and Example Characterizations of Selected Alaskan Fuels, Technical Background Document and Recommendations
3. Dilution-Attenuation Factors at Fuel Hydrocarbon Spill Sites, Technical Background Document and Recommendations
4. Maximum Allowable Concentration, Residual Saturation, and Free-Product Mobility, Technical Background Document and Recommendations
5. Groundwater Sampling Techniques for Site Characterization and Hydrocarbon Risk Calculations, Technical Background Document and Recommendations
6. Migration to Indoor Air Calculations for Use in the Hydrocarbon Risk Calculator, Technical Background Document and Recommendations
7. Site Conditions Summary Report for Hydrocarbon Risk Calculations and Site Status Determination, Technical Background Document and Recommendations
8. Proposed Environmental Site Closeout Concepts, Criteria, and Definitions, Technical Background Document and Recommendations

# Contents

---

Section	Page
<b>1 Introduction</b> .....	<b>1</b>
1.1 Purpose and Objectives .....	1
<b>2 Refineries, Fuel Types, and Volumes of Fuels Used in Alaska</b> .....	<b>2</b>
<b>3 Phase Partitioning Review</b> .....	<b>3</b>
<b>4 Petroleum Hydrocarbon Chemistry</b> .....	<b>5</b>
4.1 Petroleum Hydrocarbon Aromatics and Aliphatics .....	5
4.1.1 Aromatics.....	5
4.1.2 Aliphatics .....	5
4.2 Equivalent Carbon Number .....	6
4.3 Polar Fraction.....	7
<b>5 Fuel Hydrocarbon Characterization Assumptions &amp; Fractions</b> .....	<b>9</b>
5.1 Existing Oil Character Assumptions .....	9
5.2 Hydrocarbon Characterization Using Representative Fractions.....	9
5.3 Recommended Hydrocarbon Fractions .....	10
<b>6 Laboratory Test Methods to Assess Hydrocarbon Fractions</b> .....	<b>12</b>
6.1 Washington and Oregon “Northwest VPH” Test .....	12
6.2 Washington and Oregon “Northwest EPH” Test.....	12
6.3 Massachusetts and the TPHCWG Test Methods.....	13
6.4 Use of VPH and EPH Soils Data .....	14
6.5 Use of VPH and EPH Groundwater Data .....	16
<b>7 Example Alaskan Fuel Analyses</b> .....	<b>17</b>
7.1 Oil Analysis Methods .....	17
7.2 Reduction of the Oil Analysis Data .....	18
7.3 Oil Analyses Results .....	18
7.3.1 Example of the Oil Analyses Results .....	19
7.3.2 Equivalent Carbon Mass Fractions and Cumulative Mass Fraction .....	20
7.3.3 Boiling Point Curve .....	20
7.3.4 Percent Aromatics and Aliphatics .....	21
7.3.5 GRO, DRO, and RRO Content of Selected Alaskan Fuels .....	21
7.3.6 BTEX, GRO and DRO Effective Solubility of Selected Alaskan Fuels .....	21
7.3.7 $C_{sat}$ (Soil Saturation Concentration) .....	22
7.3.8 PAH .....	23
7.4 Comparison of Results with TPHCWG Characterization of Fuels.....	23
<b>8 SOCWG Recommendations</b> .....	<b>25</b>
<b>9 References</b> .....	<b>26</b>

**Tables**

- 1 Alaska Fuel Consumption History 1983 to 1998
- 2 Alaska Prime Supplier Fuel Sales 1998 to 2002
- 3 Alaska Refineries Approximate Capacities and Products
- 4 Representative Properties of the Hydrocarbon Fractions
- 5 Fuel Sample 1, Regular Gasoline Characterization
- 6 Fuel Sample 2, Premium Gasoline Characterization
- 7 Fuel Sample 3, JP4 Fuel Characterization
- 8 Fuel Sample 4, DF1 Characterization
- 9 Fuel Sample 5, DF2 Characterization
- 10 Fuel Sample 6, Regular Gasoline Characterization
- 11 Fuel Sample 7, Premium Gasoline Characterization
- 12 Fuel Sample 8, Aviation Gasoline Characterization
- 13 Fuel Sample 9, Jet A Characterization
- 14 Fuel Sample 10, Diesel Fuel Characterization
- 15 Fuel Sample 11, Jet A Characterization
- 16 Fuel Sample 12, DF2 Characterization
- 17 Mass Fractions in Equivalent Carbon and Boiling Temperature Groups
- 18 Summary of Mass Fractions in the Recommended Aromatic and Aliphatic Equivalent Carbon Groups
- 19 Summary of Effective Solubilities in the Recommended Aromatic and Aliphatic Equivalent Carbon Groups
- 20 Summary of Vadose Zone  $C_{sat}$  Values in the Recommended Aromatic and Aliphatic Equivalent Carbon Groups
- 21 Summary of Saturated Zone  $C_{sat}$  Values in the Recommended Aromatic and Aliphatic Equivalent Carbon Groups
- 22 Summary of PAH Mass Fractions in Selected Alaskan Fuels
- 23 PAH Concentrations in a Soil Containing 10,000 mg/kg NAPL of Selected Alaskan Fuels
- 24 Carbon Numbers and Equivalent carbon Numbers of the PAH Compounds

**Figures**

- 1 Alaska Fuel Consumption History
- 2 Average Fuel Sales Percentage by Fuel Type, 1998 to 2002
- 3 Solubilities of Hydrocarbon Fractions
- 4 Compilation of Laboratory Test Results into Recommended Hydrocarbon Fractions
- 5 Mass Fraction vs. Equivalent Carbon Number
- 6 Cumulative Mass Fraction vs. Equivalent Carbon Number
- 7 Cumulative Mass Fraction vs. Boiling Temp
- 8 Aromatic and Aliphatic Distribution in Selected Alaskan Fuels
- 9 Average Percent Aromatic & Aliphatics in Selected Alaskan Gasolines
- 10 Average Percent Aromatic & Aliphatics in Selected Alaskan Diesel & Jet Fuels
- 11 GRO, DRO & RRO Content of Selected Alaskan Fuels
- 12 Percent GRO, DRO and RRO in Selected Alaskan Gasolines

---

13	Percent GRO, DRO and RRO in Selected Alaskan Diesel & Jet Fuels
14	BTEX, GRO & DRO Solubility of Selected Alaskan Fuels
15	BTEX Solubilities of Selected Alaskan Fuels
16	Average GRO and DRO Solubility in Selected Alaskan Gasolines
17	Average GRO and DRO Solubility in Selected Alaskan Diesel & Jet Fuels
18	Soil Saturation Concentration ( $C_{sat}$ ) Values for Selected Alaskan Fuels
19	Average Vadose Zone $C_{sat}$ Values in Selected Alaskan Gasolines
20	Average Vadose Zone $C_{sat}$ Values in Selected Alaskan Diesel & Jet Fuels

# Acronyms and Abbreviations

---

AAC	Alaska Administrative Code
ADEC	Alaska Department of Environmental Conservation
AWQC	ambient water quality criteria
BTEX	benzene, toluene, ethylbenzene, and total xylenes
cm	centimeter
C <sub>sat</sub>	saturation concentration
DRO	Diesel-range organics
DF1	Arctic Grade Diesel Fuel or Diesel Fuel Number 1
DF2	Diesel Fuel Number 2, commonly used as heating oil
EC	equivalent carbon
EPA	U.S. Environmental Protection Agency
EPH	extractable petroleum hydrocarbon
FID	flame ionization detector
GC	gas chromatograph
GC/MS	gas chromatograph/mass spectrometer
GRO	gasoline-range organics
Jet A	Commercial Aviation Jet Fuel (similar to Military JP8)
JP4	Military Jet Fuel
MCL	maximum contaminant level
mg/kg	milligrams per kilogram
mg/L	milligrams per liter
NAPL	nonaqueous phase liquid
OH	oxygen and hydroxyl ions
PAH	polynuclear aromatic hydrocarbon
PID	photoionization detector
RRO	residual-range organics
S	Solubility
SOCWG	Alaska Statement of Cooperation Working Group
SVE	soil vapor extraction
TAH	total aromatic hydrocarbons
TAqH	total aqueous hydrocarbons
TPHCWG	The Petroleum Hydrocarbon Criteria Working Group
UCL	upper confidence level
VPH	volatile petroleum hydrocarbon

# Introduction

---

As described in the technical background document on phase partitioning, nonaqueous phase liquids (NAPL) exist in most soils at the lowest gasoline-range organics (GRO), diesel-range organics (DRO), and residual-range organics (RRO) cleanup level concentrations listed in Table B2 of 18 Alaska Administrative Code (AAC) 75. When fuel hydrocarbon NAPL is present in the soil, the individual hydrocarbon constituents are distributed between the dissolved, vapor, adsorbed and NAPL phases according to 4-phase partitioning equations and Raoult's Law. The accuracy of hydrocarbon phase partitioning calculations (which are used in the migration to groundwater; outdoor and indoor air inhalation exposure routes; soil vapor extraction [SVE] and air sparging remediation modeling; and hydrocarbon fate and transport modeling) depend in part on the accuracy of the NAPL characterization used as input to the 4-phase calculations. This technical background document describes the petroleum hydrocarbon characterization that is recommended for use in 4-phase calculations using Raoult's Law (e.g., the type of calculation done by the hydrocarbon risk calculator).

## 1.1 Purpose and Objectives

The purpose and objectives of this technical background document are as follows:

- Document the volumes of different fuel types refined and used in Alaska
- Provide some simple background information on the chemistry of petroleum hydrocarbons and the "equivalent carbon" number characterization of petroleum hydrocarbons
- Describe the aromatic and aliphatic equivalent carbon (EC) groups used to characterize fuel hydrocarbons in the hydrocarbon risk calculator
- Describe the commercial test methods available to characterize the fuel hydrocarbons present at contaminated sites
- Characterize selected Alaska fuels to help understand fuel hydrocarbon chemistry, as a general reference on Alaskan fuels, and potentially for use in hydrocarbon risk calculations when site-specific data are not available

This technical background document builds on the information presented in the technical background document on phase partitioning and provides details on the hydrocarbon characterization that is recommended in the technical background document on site characterization.

## SECTION 2

# Refineries, Fuel Types, and Volumes of Fuels Used in Alaska

---

Knowing the quantities, types, and sources of fuel used in Alaska may help environmental scientists understand the character of the fugitive hydrocarbons found at spill sites. The Alaska Department of Revenue, Alaska Division of Oil and Gas, and Alaska Oil and Gas Commission maintain limited records on the use and refining of fuels in Alaska. The Alaska Department of Revenue maintains the only public data on fuel consumption in Alaska and their records differentiate fuels based primarily on the taxes applicable to the fuels. Their fuel consumption records document the use of fuels such as gasoline, diesel, and jet; the mode of transportation that uses the fuels, such as the aviation industry, marine, and highway transportation (these are taxed fuels); and include many categories of tax-exempt fuels (such as heating oil, jet fuel used by foreign flights, and fuels used by government agencies). Records of fuel consumption (based on the Department of Revenue fuel consumption categories and records) for the period from 1983 to 1998 are listed in Table 1 and graphed in Figure 1. The Department of Revenue data do not include fuels purchased outside Alaska but consumed in Alaska. Table 2 and Figure 2 summarize transportation fuel use from 1998 to 2002 based on data in an Alaska Division of Oil and Gas report (Annual Report for 2003). Tables 1 and 2 and Figures 1 and 2 clearly show that jet fuel is the most common type of fuel consumed in Alaska, followed by diesel fuels and heating oils, and then gasolines.

Most of the fuel consumed in Alaska is refined in Alaska. The state is home to six refineries: the Flint Hills refinery in North Pole Alaska, the Tesoro refinery in Kenai, Petrostar refineries in North Pole and Valdez, and small refineries in the Prudhoe Bay and Kuparak oil fields on the North Slope. The Prudhoe Bay and Kuparak refineries are owned by the oil field operators, produce only arctic diesel fuel, and all of the fuel produced is consumed in North Slope oil field operations. Products from the other refineries are sold throughout Alaska. Table 3 summarizes the production capacities and the general types of fuel produced by the Alaskan refineries. Jet fuel and diesel are the dominant products of the refineries.



## SECTION 3

# Phase Partitioning Review

---

Fuel hydrocarbons may be present in the soil environment in four phases: dissolved phase, vapor phase, adsorbed phase and NAPL. Hydrocarbon phase partitioning describes the movement and redistribution of hydrocarbon molecules between the phases to establish equilibrium. The movement of molecules between the phases occurs continuously in the soil environment as a result of the thermal energy of the molecules. Phase equilibrium exists when the movement into each phase equals the rate of movement out of the phase. The hydrocarbon concentrations in each phase at equilibrium are defined by the phase partitioning relationships.

The solubility of a compound (S) describes the maximum concentration of the compound that can be dissolved in water. If a given hydrocarbon compound is mixed with water (only) at concentrations above its solubility limit, the compound will dissolve in the water to its solubility limit and the remainder of the compound will be present as NAPL or free product. Solubility values for common fuel hydrocarbons range over many orders of magnitude; for example, the solubility of benzene is about 1,750 milligrams per liter (mg/L) and the solubility of hexadecane (C16 aliphatic) is about 0.00005 mg/L. The Henry's Constant relates the dissolved concentration to the vapor concentration and the soil water partitioning coefficient ( $K_d$ ) relates the soil concentration to the adsorbed concentration. The ability of a soil to hold dissolved, vapor, and sorbed hydrocarbon is finite, and the maximum holding capacity of the soil for dissolved-, vapor-, and sorbed-phase hydrocarbons is described as the soil saturation concentration, which is abbreviated as  $C_{sat}$ . The  $C_{sat}$  of a compound may be calculated as follows:

$$C_{sat} = (S \cdot n_w / \rho_b) + (S \cdot H' \cdot n_a / \rho_b) + (foc \cdot K_{oc} \cdot S)$$

Which reduces to:

$$C_{sat} \text{ (mg/kg)} = S / \rho_b \cdot (K_d \cdot \rho_b + n_w + H' \cdot n_a)$$

Where:  $S$  = compound solubility in water (mg/L)

$\rho_b$  = soil dry bulk density (kilograms per liter [kg/L] or milligrams per cubic centimeter [mg/cm<sup>3</sup>])

$K_d$  = soil-water partitioning coefficient (L/kg)

$n_w$  = water-filled porosity (L water/L soil)

$H'$  = dimensionless Henry's Constant

$n_a$  = air-filled porosity (L air/L soil)

At hydrocarbon concentrations below the saturation concentration ( $C_{sat}$ ), all hydrocarbon present in the soil is distributed between the dissolved, vapor, and sorbed phases and the distribution of hydrocarbon may be referred to as a 3-phase problem. At hydrocarbon concentrations above the saturation concentration, nonaqueous phase hydrocarbon is present in addition to the dissolved, vapor, and sorbed phases, and the distribution of hydrocarbon may

be referred to as a 4-phase problem. Calculation of soil saturation concentrations ( $C_{sat}$ ) values for a variety of GRO and DRO compounds shows that GRO, DRO and RRO NAPL is likely present at even the lowest cleanup levels listed in Table B2 of 18 AAC 75.

Gasoline, jet fuel, diesel fuel and crude oil are complex mixtures of hundreds of individual hydrocarbon compounds. When NAPL in a soil is composed of more than one compound, the effective solubility and vapor concentrations of the compounds vary from their pure-phase solubility and vapor concentration according to Raoult's Law. Raoult's Law relates the effective solubility and vapor concentration of a hydrocarbon constituent to the mole fraction of the constituent in the NAPL:

$$S_{\text{effective}} = X_i * S$$

Where  $S$  = theoretical or maximum solubility (mg/L)

$X_i$  = mole fraction of compound X in the multiconstituent NAPL

= (moles of  $X_i$  / total moles of NAPL)

Because many of the most hazardous compounds in gasoline and diesel (such as the benzene, toluene, ethylbenzene and total xylenes [BTEX] compounds) are present as only a small fraction of the fuel mass (and moles), these compounds generally are present in the groundwater and soil vapor at only a small fraction of their theoretical solubility and volatility. Because the risk associated with the vapor inhalation and migration to groundwater exposure pathways is a function of the dissolved and vapor concentrations, the failure to use Raoult's Law to assess the vapor concentration and dissolved concentration may result in overestimating the risk associated with the vapor inhalation and migration to groundwater exposure pathways by one or more orders of magnitude (compared to the 3-phase equations used to calculate Tables B1 and B2 of 18 AAC 75). Hence, Raoult's Law must be applied to the gasoline, jet fuel, diesel fuel and crude oil spills in soils to represent the processes that occur when NAPL is present and to more accurately assess the fate and transport and the risk associated with multi-constituent petroleum hydrocarbons.

# Petroleum Hydrocarbon Chemistry

---

A brief discussion of petroleum hydrocarbon chemistry is provided to define selected terms and aid communication and understanding of the subsequent sections. The Alaska Statement of Cooperation Working Group (SOCWG) understands that the following discussion only touches on a very detailed and complex field, and that some terms may be used differently in general chemistry than they might be when addressing petroleum refining.

## 4.1 Petroleum Hydrocarbon Aromatics and Aliphatics

Petroleum hydrocarbons are molecules that by definition contain only carbon and hydrogen, although crude oil and refined products can contain a minor amount of impurities (primarily sulfur, nitrogen, oxygen, and some metals). The carbon atom has a valence of 4 and hence each carbon atom in a hydrocarbon molecule has four bonds to other atoms.

### 4.1.1 Aromatics

Aromatic and aliphatic hydrocarbons are two groups of hydrocarbons distinguished by their chemical structure. Aromatic compounds contain a six-carbon atom benzene ring structure. In benzene the carbon atom ring structure is hexagonal, lies in a single plane, and is distinguished by the double carbon bonds between every other pair of carbon atoms. Polynuclear aromatic hydrocarbons (PAHs) contain two or more linked benzene rings.

### 4.1.2 Aliphatics

In contrast, aliphatic compounds do not have the benzene ring structure and generally consist of straight chains, branched chains, or (nonbenzene) rings of carbon atoms (with single bonds). Alkanes, alkenes, and alkynes are aliphatic hydrocarbons that form homologous series. A homologous series is a series of compounds that vary by a constant number of atoms from the preceding compound in the series.

The n-alkane homologous series has a general formula of  $C_nH_{2n+2}$  and includes methane, ethane, propane, butane, pentane, hexane, heptane, octane, nonane, decane, etc. Alkanes are often referred to as paraffins and are characterized by single carbon-carbon bonds and carbon-hydrogen bonds that are identical in stability and reactivity. The ends of some alkanes may be joined to form rings called cycloalkanes (e.g., cyclopentane and cyclohexane). The cycloalkanes may also be referred to as naphthenes (not to be confused with naphthalene, the 2-ring aromatic).

Alkenes are aliphatic hydrocarbons with a general formula of  $C_nH_{2n}$ . The bonds in alkenes are not uniform in stability and reactivity; rather, alkenes are characterized by one double carbon-carbon bond with the remaining bonds in the homologous series being similar to the bonds in the alkanes. Alkenes are commonly referred to as olefins. Alkynes are aliphatic hydrocarbons with a general formula of  $C_nH_{2n-2}$ . The bonds in alkynes are also not uniform in stability and reactivity; rather, alkynes are characterized by at least one triple carbon-carbon bond.

Alkanes and cycloalkanes are described as “saturated hydrocarbons” because the carbon-carbon bonds are single bonds only and the molecule holds the maximum amount of hydrogen possible. In contrast, the alkenes, alkynes, and aromatics are described as unsaturated hydrocarbons because they contain some double or triple carbon-carbon bonds and hence they do not hold the maximum amount of hydrogen possible. Isomers are compounds with the same molecular formula but different structures. The phenomenon helps account for the tremendous variety of organic compounds and the complex naming conventions used in organic chemistry.

Aromatic and aliphatic hydrocarbons generally have very different fate and transport properties (e.g., solubilities, Henry’s values, and soil-water partitioning coefficients) and different toxicities, and hence have very different human health and ecological screening levels.

## 4.2 Equivalent Carbon Number

EC numbers are related to the boiling point of a hydrocarbon normalized to the boiling point of the n-alkanes or the retention time in a boiling point gas chromatograph (GC). For chemicals whose boiling points are known, an EC can be readily calculated. For example, hexane contains six carbon atoms and has a boiling point of 69° C, and its EC is six. Heptane contains seven carbon atoms and has a boiling point of 98° C, and its EC is seven. Benzene also contains six carbon atoms but has a boiling point of 80° C. Based on benzene’s boiling point and its retention time in a boiling point GC column (between hexane C6 and heptane C7), benzene’s EC number is 6.5 (TPHCWG, 1996).

The Petroleum Hydrocarbon Criteria Working Group (TPHCWG) developed regression equations to relate a variety of chemical properties of petroleum hydrocarbons to their equivalent carbon number. These regression equations are used to calculate solubilities, volatilities, organic carbon partitioning coefficients, molecular weights, and boiling temperatures for any hydrocarbon fraction. As described previously and as shown below, the aromatics and aliphatics have different solubilities and organic carbon partitioning coefficients and hence have different regression equations for the aromatic and aliphatic fractions. In addition, as shown below, although aromatics and aliphatics have similar vapor pressures, the vapor pressure regression equation is different for fractions with an EC above 12 than it is for fractions with an EC below 12.

Water Solubility (mg/L)

$$\text{for aromatics: } \log_{10}S = -0.21 * EC + 3.7 \text{ (R}^2 = 0.89\text{)}$$

$$\text{for aliphatics: } \log_{10}S = -0.55 * EC + 4.5 \text{ (R}^2 = 0.94\text{)}$$

Organic Carbon Partitioning Coefficient, K<sub>ow</sub> (ml/g)

$$\text{for aromatics: } \log_{10}K_{oc} = 0.10 * EC + 2.3 \text{ (R}^2 = 0.81\text{)}$$

$$\text{for aliphatics: } \log_{10} K_{oc} = 0.45 * EC + 0.43 \text{ (R}^2 = 0.94\text{)}$$

Vapor Pressure:      for EC ≤ 12:  $\log_{10}VP = -0.50 * EC + 2.3 \text{ (R}^2 = 0.99\text{)}$

$$\text{for EC > 12: } \log_{10}Vp = -0.36 * EC + 0.72 \text{ (R}^2 = 0.96\text{)}$$

Molecular Weight (g/mole)

$$\text{for aromatics: } \ln \text{MW} = 0.65 * \ln(\text{EC}) + 3.31$$

$$\text{for aliphatics: } \ln \text{MW} = 0.97 * \ln(\text{EC}) + 2.74$$

Henry's Law Constant ( $\text{cm}^3/\text{cm}^3$ ; the Henry's Law constant used in the hydrocarbon risk calculator is calculated from the vapor pressure and solubility values, as per its definition, rather than using a regression equation)

$$H = (\text{VP} * \text{MW}) / (\text{S} * \text{R} * \text{T})$$

where EC = equivalent carbon number

H = Henry's Constant ( $\text{cm}^3/\text{cm}^3$ )

VP = vapor pressure (atm)

MW = molecular weight (g/mole)

S = solubility (mg/L)

R = gas constant (0.08205 L\*atm / mole\* °K)

T = temperature (°K)

## 4.3 Polar Fraction

As described above, fresh hydrocarbon fuels are assumed to consist almost entirely of compounds containing only hydrogen and carbon and all of the hydrocarbon mass may be classified as aromatic or aliphatic hydrocarbons (recall that a small fraction of nitrogen- and sulfur-containing compounds may exist naturally in crude oil and refined products). However, fugitive hydrocarbons in the soil environment are subject to chemical and biological processes that change the composition and structure of the hydrocarbons. Biodegradation, chemical oxidation, and hydrolysis tend to attach oxygen atom and hydroxyl (OH) ions to the fugitive hydrocarbons, thereby forming phenols, alcohols, and organic acids. Collectively, these chemical oxidation, hydrolysis, and biodegradation products may be referred to as a "polar fraction" because the molecules are charged (although it is questionable whether these polar compounds should be described as hydrocarbons because, by definition, hydrocarbons contain only hydrogen and carbon). Regardless, this polar fraction is thought to partition into the dissolved, vapor, adsorbed and NAPL phases within hydrocarbon soil source areas and to be detected and quantified primarily as DRO and RRO by the existing AK102 and AK103 test methods. The polar fraction compounds likely form homologous series similar to the aliphatic n-alkane series. The polar nature of these modified hydrocarbon compounds tends to make the compounds relatively soluble compared to the non-polar aromatic and aliphatic compounds. Hence, even a small mass fraction of polar compounds in the hydrocarbon NAPL at a contaminated site will tend to result in relatively high dissolved phase concentrations of the polar compounds compared to the non-polar aromatic and aliphatic compounds. The polar fraction has not been extensively studied. Currently there are no widely accepted test methods available to directly measure the polar hydrocarbon concentration, there are no widely accepted

regression equations available to predict the behavior of the polar fraction, and there are no widely accepted toxicity values assigned to the polar hydrocarbons.

# Fuel Hydrocarbon Characterization Assumptions & Fractions

---

## 5.1 Existing Oil Character Assumptions

The assumptions regarding GRO, DRO, and RRO used in developing Table B2 are as follows:

- Fuel hydrocarbons are characterized using six fractions – GRO aromatics and GRO aliphatics; DRO aromatics and DRO aliphatics; and RRO aromatics and RRO aliphatics
- Cleanup level calculations were made for the six fuel fractions as if each fraction was a single pure chemical in the soil environment and there was no solubility or vapor pressure limit for the fractions (i.e., 3-phase partitioning equations were used and Raoult's Law was not considered)
- GRO is assumed to include the C6 to C10 range; DRO is assumed to include the C10 to C25 range; and RRO is assumed to include the C25 to C35 range
- GRO aromatics and aliphatics are assumed to have an equivalent carbon number of 8, DRO aromatics and aliphatics are assumed to have an equivalent carbon number of 14, and RRO aromatics and aliphatics are assumed to have an equivalent carbon number of 30.5
- When calculating cleanup levels for GRO, DRO, and RRO, the assumption is made that GRO is 50 percent aromatic and 50 percent aliphatic, DRO is 40 percent aromatic and 60 percent aliphatic, and RRO is 30 percent aromatic and 70 percent aliphatic.

Note that because 4-phase equations and Raoult's Law are not applied to the six hydrocarbon fractions, Table B2 tends to over-estimate risk for each fraction. Also note that the assumptions are not sensitive to the wide range of solubilities and vapor pressures within the GRO, DRO, and RRO fractions. For example, DRO aromatic solubilities range from 40 to 0.03 mg/L (3+ orders of magnitude) and DRO aliphatic solubilities range from 0.1 to 0.00000003 mg/L (6+ orders of magnitude). Better characterization of the NAPL at spill sites combined with use of 4-phase partitioning equations will result in a better understanding of the risk posed by fugitive hydrocarbons and a better understanding of the remediation and fate and transport of fugitive hydrocarbons.

## 5.2 Hydrocarbon Characterization Using Representative Fractions

The gasoline, diesel fuel, and crude oil present in Alaskan soils due to spills and leaks are mixtures of several hundred compounds with individual properties, such as solubility, volatility, organic carbon partitioning, and toxicity, ranging over many orders of magnitude. Because assessing the initial concentration, fate and transport, risk and remediation of several

hundred individual compounds is impractical, the petroleum hydrocarbon fuels must be characterized into a smaller number of hydrocarbon fractions or groups that represent the variability of the fuel constituents. Ideally these hydrocarbon groups or fractions should do the following:

- Represent or include the entire mass of the hydrocarbon present
- Emphasize the more soluble and volatile, and therefore higher human health risk compounds (i.e., the BTEX compounds)
- Correlate with regulatory criteria (give benzene, toluene, ethylbenzene, xylene, GRO, DRO, RRO, PAH, and total aromatic hydrocarbon [TAH] concentrations etc.)
- Limit the range of solubilities and vapor pressures within a hydrocarbon fraction (especially when the vapor pressure and or solubility for the fraction have the potential to exceed the risk-based criteria for that fraction; if the fraction does not have the potential to exceed risk criteria, then a wider range of solubilities or vapor pressures is acceptable)

### 5.3 Recommended Hydrocarbon Fractions

For fate and transport and risk calculations, the gasoline, diesel, and residual hydrocarbon ranges have been divided into 16 different aromatic and aliphatic equivalent carbon groups. The diesel range is divided into three aromatic and three aliphatic fractions; the gasoline range is divided into five aromatic and three aliphatic fractions; and the residual-range hydrocarbons are divided into one aromatic and one aliphatic fraction. The groups were selected to represent both the more mobile, higher- risk compounds and the bulk hydrocarbon. The hydrocarbon groups are listed in Table 4 and are identical to the Washington State Department of Ecology groups and similar to the groups recommended by the TPHCWG. Note that some hydrocarbon fractions or groups may contain only a single compound. For example, the only compound in the C<sub>6</sub> to C<sub>7</sub> aromatic hydrocarbon group is benzene, and the only compound in the C<sub>7</sub> to C<sub>8</sub> aromatic group is toluene. Other equivalent carbon groups may contain dozens of compounds. The differences between the TPHCWG-recommended EC fractions and the EC fractions used here is that the TPHCWG suggested one C<sub>8</sub> to C<sub>10</sub> aromatic fraction, while the system used in this document and in the hydrocarbon risk calculator subdivides the C<sub>8</sub> to C<sub>10</sub> aromatic fraction into three fractions: ethylbenzene (C<sub>8.5</sub>), xylene (C<sub>8.63</sub>), and C<sub>9</sub> to C<sub>10</sub> aromatics. This change allows the phase partitioning, fate and transport, and risk calculations to match the existing U.S. Environmental Protection Agency (EPA) and Alaska Department of Environmental Conservation (ADEC) regulations that identify groundwater maximum contaminant levels (MCLs), surface water ambient water quality criteria (AWQC), and soil screening/cleanup levels for both ethylbenzene and xylene. In addition, note that on Table 4 the DRO fraction is characterized as being C<sub>10</sub> to C<sub>21</sub>, while the current ADEC characterization of DRO is C<sub>10</sub> to C<sub>25</sub>. Dividing the DRO fractions from the RRO fraction at C<sub>21</sub> matches the TPHCWG recommendations, the Washington and Oregon regulations, the quantitation criteria used in existing laboratory “EPH” test methods (used in Washington and Oregon) and, as described in subsequent sections, has little impact in Alaska because typical Alaskan fuels have little hydrocarbon mass in the C<sub>21</sub> to C<sub>25</sub> range.



The molecular weights, solubilities, vapor pressures, Henry's Constant, and Koc of the fractions are summarized on Table 4. Note that the properties for benzene, toluene, ethylbenzene and xylene are based on values listed in the ADEC guidance on cleanup equations (which in turn are based on several chemical references), while the TPHCWG regression equations were used to calculate the properties for the other aromatic and aliphatic fractions. Figure 3 graphs the range in solubilities represented within each fraction and the representative solubility used to characterize the fraction. Note there is a relatively small (order of magnitude or less) range in solubilities in the lower EC groups and a larger relative change in the higher EC groups.

# Laboratory Test Methods to Assess Hydrocarbon Fractions

---

The distribution of hydrocarbon mass into the aromatic and aliphatic equivalent carbon groups ideally should be based on analysis of NAPL, soil, and groundwater samples collected during site investigation work (i.e., site specific data). Alternatively, BTEX, GRO, DRO, and RRO data from the site may be combined with existing analyses of fresh Alaskan fuels to assess the mass fraction in each hydrocarbon fraction. The Washington Department of Ecology, Oregon Department of Environmental Conservation, Massachusetts Department of Environmental Protection and TPHCWG have developed laboratory test methods to assess the concentration in the aromatic and aliphatic equivalent carbon fractions. These test methods are briefly described below.

## 6.1 Washington and Oregon “Northwest VPH” Test

The Northwest volatile petroleum hydrocarbon (VPH) test is a purge and trap gas chromatograph method available for NAPL, soil, and water samples (the analysis is similar to the AK101 A&A test method). The test uses a gas chromatograph with dual flame ionization and photoionization detectors. The flame ionization detector (FID) is considered to be a nonspecific carbon counter and hence gives a measure of the total hydrocarbon mass within an equivalent carbon range. The photoionization detector (PID) is assumed to detect or measure only the aromatic compounds. The aromatic concentrations are derived directly from the PID time and intensity data, while the aliphatic concentrations are derived by subtracting PID time and intensity data from the FID time and intensity data. The mass fraction or concentration in equivalent carbon ranges is based on the gas chromatograph retention times from GC analyses of synthetic matrix spike samples containing C5, C6, C8, C10, C12, and C13 n-alkane markers and several aromatic markers. The test is usually run in conjunction with a BTEX analyses and provides concentrations for the following EC fractions: benzene, toluene, ethylbenzene, xylene, C8 to C10 aromatics; C10 to C12 aromatics; C12 to C13 aromatics; C5 to C6 aliphatics; C6 to C8 aliphatics; C8 to C10 aliphatics; C10 to C12 aliphatics; and C12 to C13 aliphatics.

## 6.2 Washington and Oregon “Northwest EPH” Test

The Northwest extractable petroleum hydrocarbon (EPH) test is an extraction and gas chromatograph method available for NAPL, soil, and water samples (the analysis is similar to the AK102 A&A test method). The basic EPH method involves extraction of the hydrocarbon from the soil or water using methylene chloride, then a blow-down concentration step followed by analysis of a portion of the extract to yield the total EPH concentration. The separation and quantitation of the aromatic and aliphatic fractions is accomplished in several steps, including two solvent exchange and concentration steps (exchanging from methylene chloride to hexane); adsorption of the aromatics and aliphatics in a silica gel column; removal of the aromatics from the silica gel using hexane; removal of the aliphatics using methylene chloride; removal of the

polar fraction using methanol (optional); and injection of a consistent volume of extract into a gas chromatograph with a FID. The mass fraction or concentration of aromatics and aliphatics in equivalent carbon ranges is based on the gas chromatograph retention times from GC analyses of synthetic matrix spike samples containing n-alkane and aromatic markers and surrogates. The EPH test uses a synthetic calibration standard composed of all of the C8 to C35 n-alkanes for the aliphatic fraction and a synthetic calibration standard composed of all 18 PAH compounds for the aromatic fraction. In addition the EPH gas chromatographs are tested daily to ensure that the sum of the EPH aromatic and aliphatic in the EC groups correlates with a diesel fuel #2 standard. (In contrast the AK102 test uses a diesel fuel #2 calibration standard). The test provides concentrations for the following EC fractions: C8 to C10 aromatics; C10 to C12 aromatics; C12 to C16 aromatics; C16 to C21 aromatics; C21 to C35 aromatics; C8 to C10 aliphatics; C10 to C12 aliphatics; C12 to C16 aliphatics; C16 to C21 aliphatics; and C21 to C35 aliphatics.

### 6.3 Massachusetts and the TPHCWG Test Methods

Massachusetts and the TPHCWG also have test methods to quantify aromatics and aliphatics in different equivalent carbon groups. The Massachusetts approach uses two steps--- a VPH analysis and an EPH analysis. The VPH analysis uses a direct purge and trap method for water samples and a methanol extraction followed by a purge and trap for soil samples. The VPH test uses PID and FID detectors in series. The Massachusetts VPH test quantifies the benzene, toluene, ethylbenzene, xylene, naphthalene, MTBE, aromatics, and alkenes in the C9 to C10 range; alkanes and cyclo-alkanes in the C5 to C8 range and C9 to C12 ranges. The Massachusetts EPH test uses a methylene chloride extraction for both water and soil samples, followed by a Kudera-Danish concentration step, a solvent exchange to hexane and a silica gel cartridge to temporarily retain the aromatics and aliphatics. The aromatics and aliphatics are removed from the silica gel by hexane and methylene chloride rinses before passing through a GC with an FID detector. The Massachusetts EPH test results include PAHs, alkanes/cyclo-alkanes in the C9 to C18 and C19 to C36 ranges, and aromatics/alkenes in the C10 to C22 range.

The TPHCWG test method uses n-pentane to extract the hydrocarbon from both water and soil samples, a silica gel column to separate the aromatics and aliphatics, solvents to remove the aromatics and aliphatics from the silica gel, and a GC equipped with an FID for analysis. The test results include the C5 to C7, C7 to C8, C8 to C10, C10 to C12, C12 to C16, C16 to C21 and C21 to C35 aromatic fractions, and the C5 to C6, C6 to C8, C8 to C10, C10 to C12, C12 to C16, and C16 to C21 aliphatic fractions.

The Massachusetts test method was developed before the TPHCWG and Washington and Oregon methods, and emphasizes the human health risk posed by the hydrocarbon fractions, while the TPHCWG and the Washington and Oregon methods emphasize the fate and transport properties of the fractions (and then assign an appropriate toxicity to the fractions). The TPHCWG test method differs from the Washington and Oregon and AK102 and AK103 test methods in that it uses n-pentane for the initial extraction from the soil or water sample (not methylene chloride) and thereby eliminates a solvent exchange step. The aromatic and aliphatic equivalent carbon groups used in the hydrocarbon risk calculator are similar to the TPHCWG fractions with the primary differences being the division of the TPHCWG C8 to C10 aromatic group into ethylbenzene, xylene, C9 to C10 aromatics, and the inclusion of a C21 to C35

aromatic fraction. These modifications of the TPHCWG fractions were made to correlate with the ADEC Table B1 and B2 criteria. The Northwest VPH and EPH test methods were used in the testing conducted for this project because the methods provide concentration data in the desired aromatic and aliphatic equivalent carbon groups, the tests use extraction methods identical to the AK102 and AK103 methods and the tests are conducted by a commercial laboratory with offices in Alaska.

## 6.4 Use of VPH and EPH Soils Data

Within the existing regulatory framework, the VPH and EPH soils data are used differently than the GRO, DRO, and RRO data derived from the AK101, AK102, and AK103 test methods. The BTEX, GRO, DRO, and RRO results from the EPA 8021, AK101, AK102, and AK103 analysis methods would be used to identify the NAPL-contaminated soil source area and to calculate the 95 percent upper confidence level (UCL) on the mean soil concentrations for the NAPL-contaminated soil source area. The 95 percent UCL concentrations from the GRO, DRO, and RRO data would be used as the source area concentration input to the human health risk calculations. The objective of the VPH and EPH testing is to characterize the chemistry of the fugitive hydrocarbon by assessing the mass fraction of hydrocarbon in the 16 aromatic and aliphatic equivalent carbon fractions (the fraction of the GRO, DRO, and RRO that is aromatic versus aliphatic, and the fraction of the GRO and DRO aromatics and aliphatics within each equivalent carbon group). The mass fractions in the aromatic and aliphatic equivalent carbon groups are used as input in to the phase partitioning calculations. Note that the GRO, DRO, and RRO analyses are required by the existing regulations, while the VPH and EPH analyses are supplemental data. The SOCWG suggests that the VPH and EPH analyses be conducted on duplicate or co-located samples.

Not every sample needs to be tested by the Northwest VPH and EPH test methods; rather, it is expected that at both new and old spill investigation sites the majority of the soil sample analysis would be by the EPA 8021, AK101, and AK102 analysis methods and that VPH and EPH testing would be conducted on a limited number of samples from the core of the NAPL-contaminated soil source area. A specific number of samples needed to characterize the NAPL chemistry in a particular source area is not specified by the SOCWG, but the number of VPH and EPH analyses is likely a function of the variability of results within the particular source area. In general, several EPH analyses are recommended to represent each NAPL source area and larger source areas likely warrant more analyses than small source areas. In addition, the number of VPH analyses needed to characterize old diesel or jet fuel spill sites may be lower than the number of EPH analyses required to characterize the site, because the BTEX and GRO test results more fully define the GRO aromatic and aliphatic equivalent carbon groups and because the source areas tend to become depleted in GRO range hydrocarbons through time. If the investigators think that the NAPL source area is the result of overlapping NAPL plumes from different fuel types, then more VPH and EPH analysis may be needed to assess the character of the NAPL in each part of the NAPL source area and separate risk calculations should be performed on each part of the NAPL source area.

Figure 4 shows how the data from the BTEX, GRO, DRO, RRO, VPH, and EPH tests are used to derive mass fractions and concentrations in each of the 16 aromatic and aliphatic equivalent carbon groups. The distribution of hydrocarbon mass into the 16 aromatic and aliphatic

equivalent carbon groups is calculated using the site-specific BTEX, GRO, DRO, and RRO data and site-specific VPH and EPH data or VPH and EPH data from the analyses of fresh Alaskan fuel products as follows:

- The site-specific BTEX 95 percent UCL data defines the mass fraction and concentration in the BTEX groups
- The site-specific GRO, DRO, and RRO data are used to define the total concentration of GRO, DRO, and RRO in the site soils
- The NAPL characterization data from the site specific VPH and EPH test results or from a representative fresh fuel analysis are then used to assign a mass fraction to the GRO aromatic C9 to C10 group, the GRO aliphatic EC groups, DRO aromatic and aliphatic EC groups, and RRO aromatic and aliphatic EC groups.

For example, if the site specific EPH testing or a fresh fuel analysis show that the DRO portion (the C10 to C21 fraction) of a # 2 diesel is composed of 20 percent aromatics and 80 percent aliphatics, and that within the C10 to C21 aromatic portion there is 25 percent of the mass in the C10 to C12 fraction, 45 percent of the mass in the C12 to C16 fraction, and 30 percent of the mass in the C16 to C21 fraction, then the C10 to C12 aromatic fraction at the subject site will equal the AK102 DRO concentration multiplied by 0.20 (the DRO aromatic fraction) multiplied by 0.25 (the fraction of the DRO aromatics in the C10 to C12 range) . The use of fresh fuel, relative to a weathered diesel, to characterize the DRO and RRO aromatic and aliphatic EC distribution is thought to be conservative based on the following discussion.

The distribution of mass in aromatic and aliphatic equivalent carbon groups tends to change through time at gasoline and diesel fuels spills sites. The change in the distribution of mass in aromatic and aliphatic equivalent carbon groups may be described as “weathering” and involves mass loss from the NAPL phase primarily by the processes of volatilization, dissolution, and biodegradation. The weathering that occurs at a particular site is dependent on the site conditions but in general patterns of fuel hydrocarbon weathering may be discerned as follows:

- The lower EC aromatic and aliphatic groups have higher vapor pressures than the higher EC aromatic and aliphatic groups; therefore, lower EC aromatics and aliphatic tend to volatilize more readily than higher EC groups.
- Lower EC aromatics dissolve more readily than relatively higher EC aromatics; therefore, lower EC aromatics are lost to dissolution faster than relatively higher EC aromatics.
- Lower EC aliphatics dissolve more readily than relatively higher EC aliphatics; therefore, lower EC aliphatics are lost to dissolution faster than relatively higher EC aliphatics.
- Aromatics have higher solubilities than similar EC aliphatics; therefore, aromatics are lost to dissolution faster than similar EC aliphatics.
- Loss of mass at spills site due to biodegradation is more complex than loss of mass due to volatilization and dissolution, but several generalizations may be made as follows:
  - BTEX compounds biodegrade under both aerobic and anaerobic conditions at most sites (with aerobic reactions tending to be faster)

- Benzene commonly biodegrades more slowly than the other BTEX compounds (Suarez and Rafai, 1999).
- n-alkanes biodegrade relatively readily while other aliphatics such as cyclo-alkanes, tend to biodegrade more slowly or undergo the initial steps of biodegradation to water and carbon dioxide and then become recalcitrant (Salanitro, 2001)

The combination of dissolution, volatilization, and biodegradation appear to cause the NAPL at some recently studied diesel fuel spill sites to become relatively concentrated in the higher EC aromatic and aliphatic groups and to have relatively higher aliphatic concentrations compared to fresh fuels (Geosphere, 2006; CH2M HILL, 2000.) (Note that the above information suggests that diesel NAPL at old spill sites may be relatively more concentrated in the multi-ring PAH compounds and recall that the risk posed by the PAH compounds is addressed based on the measured PAH concentrations).

## 6.5 Use of VPH and EPH Groundwater Data

Risk-based concentrations for the intake of GRO, DRO, and RRO aromatics and aliphatics via the groundwater ingestion route are readily calculated by equations 1 and 2 of the ADEC Guidance on Cleanup Standards Equations and Input Parameters (ADEC, 2004). Calculations for the DRO range hydrocarbons yield groundwater ingestion risk-based levels of 1.46 mg/L DRO aromatics and 3.65 mg/L DRO aliphatics (recall that equations 1 and 2 calculate risk-based groundwater ingestion levels for DRO aromatics and aliphatics, not total DRO, and note that the Table C DRO aliphatic cleanup level of 0.1 mg/L is based on the solubility of a C14 aliphatic and is not a risk-based value). Unfortunately the AK101, AK102, and AK103 test methods quantitate aromatics, aliphatics, and polar compounds as undifferentiated “GRO, DRO, and RRO”. In contrast the VPH and EPH tests provide a direct measure of the GRO, DRO, and RRO aromatic and aliphatic concentrations in the different ranges; therefore, the VPH and EPH tests are better suited to assess if groundwater at a site is in compliance with the risk-based levels for DRO aromatics and aliphatics than the AK test methods. Given that current regulations require the analysis of groundwater by the AK methods, the SOCWG recommends collecting supplemental, duplicate water samples for VPH and EPH analysis and using the VPH and EPH results to characterize groundwater ingestion risks. Compliance with any non-risk-based Table C criteria and pollution prevention issues indicated by AK102 DRO test results would be addressed separately from the assessment of human health risk (e.g., the EPH test data may show that a site is in compliance with risk-based aromatic and aliphatic but the AK102 test result may yield a test result above the Table C total DRO criteria possibly indicating the presence of a polar fraction. The exceedance of the DRO criteria must be addressed with the ADEC regulator separate from the human health criteria).

# Example Alaskan Fuel Analyses

---

Samples of 12 different Alaskan fuels were analyzed in a laboratory to demonstrate the use of the aromatic and aliphatic equivalent carbon groups, to improve the general understanding of commonly used Alaskan fuels, and potentially for use in hydrocarbon risk calculations when site-specific data are not available. The 12 samples were donated by the Tesoro, Flint Hills, and Petrostar refineries, and include five gasoline samples and seven diesel / jet fuel samples. The following fuel analyses results should be considered “example analyses.” The results are subject to analytical variability and season variability in the fuel composition.

## 7.1 Oil Analysis Methods

The laboratory analyses were conducted at the North Creek Analytical laboratory in Portland, Oregon, under the direction of Steve Bonde. The analyses involved several steps, as follows:

- A laboratory control sample consisting only of n-alkanes (C5 to C35, minus heptane C7) was run through a “boiling point” GC to define the times that the n-alkanes eluted on the boiling point GC
- A sample of each oil was injected directly into a “boiling point” GC to yield a chromatogram of the whole oil or “neat product”
- The chromatograms of the oil product and the laboratory n-alkane control chromatograph were compared and the areas under the oil chromatogram curve within each n-alkane equivalent carbon number were quantified
- The area under the oil chromatogram curve within each equivalent carbon number divided by the total area under the chromatogram curve was assumed to be equal to the mass fraction within the equivalent carbon number
- The equivalent carbon mass fraction data were used to graph the mass fraction versus EC number; cumulative mass fraction versus EC number; and boiling temperature versus EC number
- The mass fraction of the oil, that is composed of benzene, toluene, ethylbenzene, xylene and individual PAH compounds, was assessed by analyzing a sample of the whole oil or neat product in a gas chromatograph/mass spectrometer (GC/MS) and by conducting a VPH-BTEX test on the neat product.

A separate series of analyses was conducted to assess the concentration of the BTEX compounds and the distribution of aromatic and aliphatics in the individual equivalent carbon groups.

- The gasoline samples were analyzed primarily by a modification of the BTEX and VPH test method. In an initial step the oil was dissolved in methanol and water and was injected into the GC for the purge and trap and dual FID/ PID analysis.

- The diesel and jet fuel samples were analyzed using a modified EPH method and by analyzing for BTEX as described above. In an initial step oil was dissolved in hexane and then passed through a silica gel column that adsorbed/retained the aromatics and aliphatics (the initial methylene chloride extraction and solvent exchange steps were eliminated). The aromatics were then extracted from the silica gel by hexane and the aliphatics were extracted from the silica gel by methylene chloride. The hexane and aromatics fractions were injected in the GC to yield a chromatograph of the aromatic fraction only. Then the methylene chloride and aliphatics fractions were injected in the GC to yield a chromatograph of the aliphatic fraction only. The mass fraction of aromatics and aliphatics in equivalent carbon ranges was based on the gas chromatograph retention times from GC analyses of synthetic matrix spike samples containing several n-alkane and aromatic markers.

## 7.2 Reduction of the Oil Analysis Data

The oil analyses data were reduced to provide a “best characterization” of the oil. The assumptions concerning the oil analyses data and the decisions made during the data reduction are as follows:

- The chromatograph of the whole oil product was assumed to provide the best characterization of the mass fraction of the oil in each equivalent carbon group and the best boiling point curve data. (This is because the extraction and “blow-down” concentration steps in the aromatic and aliphatic analyses allow a portion of the more volatile fractions to be lost.)
- The BTEX-VPH test data are assumed to provide best characterization of the BTEX concentrations because these results provided the better correlation with the dissolved concentrations measured in subsequent testing, (Geosphere and CH2M HILL, 2006) and the GC-MS data are interpreted to adequately characterize the PAH mass fractions.
- The aromatic and aliphatic data provide the best (and only) measure of the relative proportion of aromatics and aliphatics in the C5 to C35 range within each equivalent carbon number. Hence, the percentage of aromatics and aliphatics within each equivalent carbon number, multiplied by the mass fraction of the total oil within each equivalent number, provided the mass fraction of aromatics and aliphatics within each equivalent carbon group (e.g., the C11 to C12 aromatic mass fraction is calculated as the C11 to C12 mass from the direct oil injection GC run multiplied by the aromatic fraction in the C11 to C12 range during the aromatic and aliphatic silica gel separation GC runs).

## 7.3 Oil Analyses Results

Each oil analysis result is presented in a table that shows the mass fraction in each proposed aromatic and aliphatic equivalent carbon group and also shows calculated properties of the fuel such as solubility, vapor pressure, and  $C_{sat}$  (Tables 5 through 16). In addition, the equivalent carbon distribution and boiling point curves of the fuels and their calculated properties are compared in Figures 5 through 7.



### 7.3.1 Example of the Oil Analyses Results

The tables presenting the oil analyses results are discussed here for one of the fuels as an introduction to the data in the individual oil analyses results tables. The oil test results are then compared and contrasted in the following section. The sample discussed is Sample 4, a diesel fuel #1 sample (Table 8). The refiner of Sample 4 reports that their diesel fuel #1 is essentially the same product as their Jet A fuel. The data presented in the numbered columns of Table 8 are discussed below:

- The aromatic and aliphatic equivalent carbon groups or fractions are listed in column one. A total for the aromatics and a total for the aliphatics are provided below the aromatic and aliphatic groups. Near the bottom of the Table the fractions making up GRO, DRO, RRO, and TAH are summed to provide data on these groups of hydrocarbon fractions.
- The second column lists the equivalent carbon number that is considered representative of the fraction and that is substituted into the regression equations to calculate the properties of the hydrocarbon fraction (the values for the BTEX compounds are published pure compound values).
- The third column displays the percent mass of each aromatic and aliphatic equivalent carbon group in the fuel sample (i.e., in NAPL of the fresh fuel product). As shown in the third column the sample contains about 12.9 percent aromatics and about 87.1 percent aliphatics.
- The fourth column lists the approximate soil concentration of each fraction that would be measured in a soil sample containing 10,000 milligrams per kilogram (mg/kg) of the fuel type (this column of data is presented to demonstrate the relative proportion of each fraction in terms that may be commonly presented; that is, a benzene concentration of 2.6 mg/kg in a soil containing 10,000 mg/kg of the diesel fuel #1). Near the bottom of the Table in column 4 the results show that about 1,063 mg/kg of the diesel fuel is in the GRO range, 8,934 mg/kg is in the DRO range, and 2 mg/kg is in the RRO range.
- The representative molecular weights (calculated from the regression equations or based on the compound formula) are shown in column 5. The moles of each hydrocarbon fraction in a soil containing 10,000 mg/kg of the diesel fuel NAPL are listed in column 6 and the mole fraction of the each hydrocarbon group is listed in column 7.
- The single component solubilities of the BTEX compounds and representative solubilities of the aromatic and aliphatic equivalent carbon groups are listed in column 8.
- Column 9 shows the effective solubility of each fraction based on Raoult's Law (the effective solubility of each fraction is calculated as the single component solubility multiplied by the mole fraction). As shown in columns 8 and 9 of Table 8, although benzene has a pure phase or single component solubility of about 1750 mg/L, the effective solubility of benzene as a constituent of the Sample 4 diesel fuel is only about 0.98 mg/L, because the mole fraction of benzene in the diesel #1 NAPL is low. In addition, Table 8 shows that the dissolved phase concentration in equilibrium with the diesel #1 NAPL should be about 7.67 mg/L aromatics and 0.14 mg/L aliphatics; the dissolved GRO concentration should be about 6.04 mg/L and the dissolved DRO concentration would be about 1.77 mg/L.

- The single component vapor pressure, Raoult's Law or effective vapor pressure, Henry's Law Constants and diffusion coefficients in air and water are listed in columns 10 through 16.
- Column 16 displays the organic carbon partitioning coefficient for each compound or aromatic and aliphatic equivalent carbon group, and column 17 displays the soil-water partitioning coefficient assuming an organic carbon content of 0.001 by weight in the soil (0.001 is the ADEC default value).
- The soil saturation concentration, or  $C_{sat}$ , describes the capacity of a soil to hold dissolved-phase, vapor-phase and adsorbed-phase hydrocarbon. Below the  $C_{sat}$  concentration, all of the hydrocarbon mass is distributed between the dissolved, vapor, and adsorbed phases. Above the  $C_{sat}$  concentration, NAPL is present. Columns 18 and 19 show the concentration of each aromatic and aliphatic equivalent carbon fraction held in the dissolved, vapor, and adsorbed phases in a soil in equilibrium with a NAPL having the Sample 4 diesel #1 composition (the soil properties match the ADEC default soil assumptions). As shown, vadose zone soils (column 18) and saturated zone soils (column 19) have a limited capacity to hold dissolved-, vapor-, and adsorbed-phase diesel fuel. Table 8 indicates that vadose and/or saturated zone soils in equilibrium with Sample 4 diesel #1 would hold a total of about 6 or 8 mg/kg of GRO and about 9 mg/kg DRO in the dissolved, vapor, and adsorbed phases, indicating that most of the GRO and DRO mass in soils at contaminated sites is present as NAPL.

### 7.3.2 Equivalent Carbon Mass Fractions and Cumulative Mass Fraction

The distribution of hydrocarbon mass in single equivalent carbon groups is shown in Table 17 and Figures 5 and 6 for the 12 fuel samples analyzed. Figure 5 graphs the hydrocarbon mass fraction in increments of one equivalent carbon. Figure 6 graphs the cumulative mass fraction against equivalent carbon number. In general, the gasoline samples show significant hydrocarbon mass (10 to 30 percent) in the highly volatile C5 fraction, appear to peak in the C8 fraction, and show a tail beyond C10. The diesel #1 and Jet A samples appear to rise at about C8, peak in the C10 to C11 range, and tail off at about C17. The diesel fuel #2 samples appear to rise at about C10, peak in the C17 to C18 range, and tail off at about C21.

The JP 4 sample and the Sample 10 diesel fuel were distinct from the other fuel samples. The JP 4 sample has an equivalent carbon distribution similar to gasoline in the early portion of its curve (C6 to C8) but has a long tail in the C10 to C17 range. The sample 10 diesel fuel rises at about C8, reaches a low peak at about C12, and has a long tail in the C14 to C20 range.

### 7.3.3 Boiling Point Curve

Boiling point curves relate the cumulative mass fraction to the temperature at which the fractions boil, as shown in Figure 7. Because the initial steps in crude oil refining involve distillation by boiling, and because the boiling temperature is important to understanding how a hydrocarbon fuel volatilizes and combusts in an engine, the boiling point curve is a common tool used to classify fuels. The boiling point curve presented in Figure 7 looks like the cumulative mass fraction versus EC number in Figure 6 because there is a strong correlation between the boiling temperature and the EC number. The boiling point curves show a similar family of curves for the gasoline samples, a family of curves for the diesel #1 and Jet A samples,

and a family of curves for the diesel #2 samples. As described previously the JP4 and Sample 10 diesel fuels appear to have a broader range of boiling temperatures and equivalent carbon numbers and hence are between the gasoline and Jet A, and diesel #1 and diesel #2 curves, respectively.

### 7.3.4 Percent Aromatics and Aliphatics

Table 18 presents hydrocarbon mass fraction data in the recommended aromatic and aliphatic equivalent carbon groups. This information is essentially the same as that presented in Table 17 and Figures 5 and 6 except that the mass fractions are differentiated using the aromatic and aliphatic data, and summed within each equivalent carbon group. At the bottom of the aromatics section and at the bottom of the aliphatics section of Table 18, the mass fractions in the aromatic and aliphatic groups are listed for each fuel sample. The average aromatic mass fraction for the gasoline and diesel fuel samples is also presented at the bottom of Table 18. As shown in Table 18 and Figures 8 and 9, the gasoline samples range in aromatic fraction from about 13 to 48 percent and average about 37 percent aromatics. As shown in Table 18 and Figures 8 and 10, the diesel fuel and Jet A samples range in aromatic fraction from about 7 to 17 percent and average about 14 percent aromatics. This aromatic fraction is lower than that measured in several other Alaskan diesel and jet fuels reported by Geosphere (2002, 2003).

### 7.3.5 GRO, DRO, and RRO Content of Selected Alaskan Fuels

Table 18 also summarizes hydrocarbon data as GRO, DRO, and RRO (at the bottom of the table). As shown, gasoline samples contain some DRO range compounds, and diesel and jet samples contain some GRO and RRO compounds. The percent of each sample in the GRO, DRO, and RRO ranges is graphed in Figure 11, and the average GRO, DRO, and RRO content of the gasoline and diesel and Jet A samples are summarized in Figures 12 and 13. As shown in Table 18 and Figures 11 and 12, the gasoline samples range in GRO fraction from about 81 to 99 percent GRO and average about 88 percent GRO. As shown in Table 18 and Figures 11 and 13, the diesel fuel and Jet A samples range in DRO fraction from about 88 to 95 percent DRO and average about 92 percent DRO. The gasoline samples contained essentially no RRO, while the diesel and Jet A samples contained about 2 percent RRO (but much of this could be due to the GC baseline assumed for the analyses).

#### C21 versus C25 DRO versus RRO Break Point

Recall that the recommended aromatic and aliphatic equivalent carbon groups differentiate the DRO/RRO fractions at C21, while the existing criteria differentiate the DRO from the RRO fraction at C25. The mass fraction and equivalent carbon data (Tables 17 and 18) show that only diesel #2 fuels contain any appreciable mass in the C21 to C25 equivalent carbon range (about 4 to 5 percent). The impact of this relatively small mass on the effective solubility of the DRO fraction is negligible. Therefore, we conclude that differentiating DRO from RRO at C21 has little to no effect on site characterization or risk calculations.

### 7.3.6 BTEX, GRO and DRO Effective Solubility of Selected Alaskan Fuels

Table 19 summarizes the effective solubilities or the Raoult's Law solubilities of the aromatic and aliphatic equivalent carbon groups and the sum of the fractions composing, for example, the GRO, DRO, and BTEX fractions. Note that the solubility data in Table 19 and the related Figures are calculated based on the composition of the fuel and not directly measured in water

samples. Measured solubility data is presented in the SOCWG paper on groundwater sampling (Geosphere and CH2M HILL, 2006). The data in Table 19 are graphed in Figures 14 through 17. Figure 14 shows the total petroleum hydrocarbon (TPH) solubility, the GRO solubility, DRO solubility, and total BTEX solubility (note that the y-axis of the graph is log scale). The figure shows that the GRO samples have much higher solubilities than the diesel and jet samples, and that most of the solubility of the gasoline samples is due to their BTEX content. (Note that the BTEX concentrations are included in the GRO fraction and that the GRO fraction is included in the TPH value). Figure 15 shows the pure phase solubility and the effective solubility of the BTEX compounds in the fuel samples. As shown, the pure phase solubilities of the BTEX compounds are orders of magnitude higher than the effective solubilities in the fuels because the BTEX compounds represent only a minor fraction of the moles in the NAPL.

As shown in Table 19 and Figures 14 and 16, the gasoline samples range in GRO solubility from about 88 to 220 mg/L, and have an average GRO solubility of about 166.5 mg/L. The DRO solubility in the gasoline samples averaged about 1.0 mg/L. As shown in Table 19 and Figures 14 and 17, the diesel and Jet A samples range in DRO solubility from about 0.5 to 2.3 mg/L, and have an average DRO solubility of about 1.2 mg/L. The GRO solubility in the diesel and Jet A samples ranged from about 1.4 to 8.3 mg/L averaged about 4.7 mg/L.

Note that the DRO solubilities of the fresh diesel and Jet A fuel samples in this data set are close to the human health risk-based groundwater ingestion level of 1.5 mg/L aromatics and that the diesel #2 samples had DRO solubilities below the risk-based groundwater ingestion level. This indicates that the diesel #2 cannot cause groundwater to exceed risk-based standards even when there is NAPL on the water table, and that none of the diesel or jet samples would be expected to cause an exceedance of the groundwater criteria when the NAPL was in the vadose zone (given the current dilution-attenuation assumptions).

### 7.3.7 $C_{\text{sat}}$ (Soil Saturation Concentration)

Tables 20 and 21 list the vadose zone and saturated zone soil saturation concentrations or  $C_{\text{sat}}$  values for the analyzed fuel samples, respectively. The  $C_{\text{sat}}$  is defined as the mass of hydrocarbon held in the dissolved, vapor, and adsorbed phases in a soil in phase equilibrium with the NAPL of the analyzed fuel samples. The calculations are for a soil having the ADEC default soil characteristics (except that the saturated zone soil is assumed to be saturated). The soil saturation concentrations or  $C_{\text{sat}}$  values for the fuel samples are graphed in Figure 18. Figures 18 and 19 show that the gasoline samples had GRO  $C_{\text{sat}}$  values in the vadose zone ranging from about 75 to 134 mg/kg and averaging about 118 mg/kg, and that the gasoline samples had DRO  $C_{\text{sat}}$  values ranging from about 0.05 to 4.9 mg/kg and averaging about 2.7 mg/kg. Figures 18 and 20 show that the diesel and Jet A samples had GRO  $C_{\text{sat}}$  values in the vadose zone ranging from about 1.2 to 11.1 mg/kg and averaging about 5.5 mg/kg, and that the diesel and Jet A samples had DRO  $C_{\text{sat}}$  values ranging from about 4.8 to 10.3 mg/kg and averaging about 7.5 mg/kg. As shown on Table 21  $C_{\text{sat}}$  values in the saturated zone are slightly lower than those calculated for the vadose zone. The vadose zone and saturated zone  $C_{\text{sat}}$  values indicate that NAPL is present at the lowest cleanup levels listed in Tables B1 and B2 of 18 AAC 75.

### 7.3.8 PAH

Table 22 lists the mass fractions of PAHs measured in the fuel samples and Table 23 lists the PAH concentration in a soil sample given a total hydrocarbon concentration of 10,000 mg/kg. Of the thirteen PAH compounds listed by ADEC on Table B1, only five were detected in the fuels, and these compounds (naphthalene, acenaphthene, fluorene, anthracene, and fluoranthene) are lower equivalent carbon number PAHs. This result should be expected because the Alaskan fuels tend to have little mass in the RRO range where many of the PAH compounds would be expected to elute. Table 24 lists the number of carbon atoms in the 16 PAH compounds included in the total aqueous hydrocarbons (TAqH) criteria and the equivalent carbon number of each PAH compound. Table 24 shows that all but one of the PAH compounds which were detected in the fuel samples had equivalent carbon numbers below 20 and that all the PAHs which were not detected had equivalent carbon numbers above 20. Naphthalene was detected in every fuel sample and was typically present at the highest concentrations, yet the naphthalene represented such a small mass fraction of the fresh fuel that the fresh fuel would have to be present in the soil at a concentration of over 1,000,000 mg/kg for the soil to exceed the soil ingestion criteria for the compounds. Similarly, phase partitioning calculations indicate that none of the PAH compounds would not be expected to partition into groundwater from NAPL of the selected fuels at concentrations that would exceed the Table C standards. These results suggest that the PAH constituents in the Alaskan fuels present only a very limited human health risk.

## 7.4 Comparison of Results with TPHCWG Characterization of Fuels

The TPHCWG presents a brief characterization of selected gasoline, jet and diesel fuels (1998) as follows:

- Automotive gasolines are blended products having constituents in the C4 to C12 range, and are typically composed of about 40 to 70 percent straight, branched, and cyclic alkanes, generally less than 10 percent alkenes and about 20 to 50 percent aromatics.
- Aviation gasolines are typically composed of about 50 to 60 percent saturated hydrocarbons, 20 to 30 percent cyclo-alkanes, and only about 10 percent aromatics.
- JP4 jet fuel has constituents in the C5 to C14 range and is typically composed of about 2/3rds gasoline and 1/3 diesel range constituents. Aromatics generally compose less than about 20 percent of the fuel mass.
- Jet A and JP8 have constituents in the C8 to C17 range and are typically composed of about 80 to 90 percent saturated aliphatics and 10 to 20 percent aromatics.
- Diesel fuel #1 is similar to Jet A, has constituents in the C8 to C17 range and is typically composed of about 60 to 90 percent saturated aliphatics and 10 to 40 percent aromatics.
- Diesel fuel #2 has constituents in the C8 to C26 range with most of its mass in the C10 to C20 range and is typically composed of about 60 to 90 percent saturated aliphatics and 10 to 40 percent aromatics.

The fuel analysis conducted for this report correlates reasonably well with the general descriptions of the hydrocarbon products; however, additional or repeated testing of Alaska fuels is recommended to allow a more complete understanding of the average composition of Alaskan fuels and of the seasonal variation in composition.

## SECTION 8

# SOCWG Recommendations

---

Based on the information presented in this report, the SOCWG requests that ADEC consider the following recommendations:

- Use the sixteen hydrocarbon fractions listed herein for 4-phase fate and transport and risk calculations
- Accept the Northwest VPH and EPH test methods as valid tests for differentiating the concentration within the aromatic and aliphatic equivalent carbon groups (other test methods, such as that used by TPHCWG, should also be accepted for the same purpose)
- Where practical or when possible, use site specific data Northwest VPH and EPH test method to assess the mass fraction present in each of the aromatic and aliphatic equivalent carbon groups. When site specific data are not available use an appropriate fuel analysis from the fresh fuel analyses presented herein or another source to assess the mass fraction present in each of the aromatic and aliphatic equivalent carbon groups.
- Retest selected Alaskan fuels to assess seasonal variability in fuel composition and to assess analytical variability in the test results.

## SECTION 9

# References

---

- Alaska Department of Environmental Conservation. 1998. *Guidance on Cleanup Standards Equations and Input Parameters*. September 16, 1998.
- Alaska Department of Environmental Conservation. 1999. "Oil Spill and Hazardous Substances Pollution Control Regulations." *Alaska Administrative Code*. Title 18, Chapter 75. January 22, 1999.
- Alaska Department of Environmental Conservation. 2002. Cumulative Risk Guidance.
- Alaska Division of Oil and Gas. 2003. Division of Oil and Gas Annual Report for 2003.
- CH2M HILL. 2000. Fort Wainwright OU5 Site Conditions & Remediation Monitoring Report. A report prepared for the US Army.
- Cline, P. V., J. J. Delfino, and P. S. C. Rao. 1991. "Partitioning of aromatic constituents into water from gasoline and other complex solvent mixtures." *Environmental Science Technology*. Vol. 25, No. 5: pp. 914-920.
- Geosphere. 2002. Alaska Railroad Gold Creek Site 2001 Site Conditions, Groundwater Monitoring, and Hydrocarbon Fate and Transport Modeling Results. A report prepared for the ARRC.
- Geosphere. 2004. Assessing Hydrocarbon Cleanup Levels Appropriate for North Slope Gravel Pads. A report prepared for BPXA.
- Geosphere. 2006. FAA Strawberry Point Station Environmental Closure Investigation and Report. A report prepared for the Federal Aviation Administration.
- Keenan, Charles W., and Jesse Wood. 1971. *General College Chemistry*. Harper & Row, Publishers, Inc. New York, N. Y.
- Lee, L. S., M. Hagwell, J. J. Delfino, and P. S. C. Rao. 1992. "Partitioning of Polycyclic Aromatic Hydrocarbons from Diesel Fuel into Water." *Environmental Science Technology*. Vol. 26, No. 11: pp. 2104-2110.
- Mariner, P. E., M. Jin, and R. E. Jackson. 1997. "An Algorithm for the Estimation of NAPL Saturation and Composition from Typical Soil Chemical Analyses." *Ground Water Monitoring Review*. Vol. 17, No. 1: pp. 122-129.
- Mott, H. V. 1995. "A Model for the Determination of the Phase Distribution of Petroleum Hydrocarbons at Release Sites." *Ground Water Monitoring Review*. Vol. 15, No. 3: pp. 157-167.
- Park, Hun Seak, and C. San Juan. 2000. "A Method for Assessing Leaching Potential for Petroleum Hydrocarbons Release Sites: Multiphase and Multisubstance Equilibrium Partitioning." *Soil and Sediment Contamination*. Vol. 9, No. 6: pp. 611-632.



- Salanitro, Joseph. 2001. Biodegradation of Petroleum Hydrocarbons in Soil. *Advances in Agronomy*. Volume 72, page 53.
- Suarez, Monica, P. and Hanadi Rafai. 1999. Biodegradation Rates for Fuel Hydrocarbons and Chlorinated Solvents in Groundwater. *Bioremediation Journal*. Vol. 3, Issue 4, Pages 337-362.
- Trotten, George E. 2003. *Fuels and Lubricants Handbook*. ASTM International, West Conshohocken, PA.
- TPH Criteria Working Group. 1996. *Selection of Representative TPH Fractions Based on Fate and Transport Considerations*. Volume 3. Amherst Scientific Publishing.
- TPH Criteria Working Group. 1998. *Analysis of Petroleum Hydrocarbons in Environmental Media*. Volume 1. Amherst Scientific Publishing.
- U.S. Environmental Protection Agency. 1996. *Soil Screening Guidance: Technical Background Document*.

# Tables

---



**Table 3 Alaska Refineries Approximate Capacities and Products**  
**from: Division of Oil & Gas 2003 Annual Report**

<b>Refining Capacities</b>						
	<b>Flint Hills Resources</b>	<b>Petro Star Fairbanks</b>	<b>Petro Star Valdez</b>	<b>Tesoro</b>	<b>COTU Kuparik</b>	<b>COTU Prudhoe Bay</b>
Refinery North Slope Crude Flow-through Volume (barrels/day)	220,000	15,000	40,000	0	14,000	14,000
North Slope Oil Volume returned to Pipeline (barrels/day)	146,000	11,250	30,000	0	10,500	10,500
Throughput Capacity used in manufacture of refined products (barrels/day)	74,000	3,750	10,000	72,000	3,500	3,500
Refined Products Produced (barrels/day)	64,000	3,750	10,000	50,000	3,500	3,500
Oil volume used in manufacture of refined products (gallons/day)	2,688,000	157,500	420,000	2,100,000	147,000	147,000

<b>Products by Refinery</b>						
	<b>Flint Hills Resources</b>	<b>Petro Star Fairbanks</b>	<b>Petro Star Valdez</b>	<b>Tesoro</b>	<b>COTU Kuparik</b>	<b>COTU Prudhoe Bay</b>
Gasoline & Naphtha	19%			25%		
Jet Fuel	57%					
Diesel	19%				100%	100%
Jet, Diesel, Fuel Oil Combined		100%	100%	45%		
Gas Oil	4%					
Asphalt	1%					
Bottoms & Residual				30%		

**Table 4 Representative Properties of the Hydrocarbon Fractions**

	Equivalent Carbon Range	Median Equivalent Carbon	Molecular Weight	Maximum Solubility in Fraction (mg/L)	Minimum Solubility in Fraction (mg/L)	Representative Solubility for Fraction (mg/L)	Single Component Vapor Pressure (atm)	Henry's Constant (cm <sup>3</sup> /cm <sup>3</sup> )	Henry's Constant (atm m <sup>3</sup> /mole)	K <sub>oc</sub> (ml/g)	Example Compounds
<b>Aromatics</b>	C <sub>5</sub> -C <sub>7</sub> Benzene	6.50	78	1.75E+03	1.75E+03	1.75E+03	1.30E-01	2.59E-01	5.80E-03	5.89E+01	Benzene
	C <sub>7</sub> -C <sub>8</sub> Toluene	7.58	92	5.26E+02	5.26E+02	5.26E+02	3.80E-02	2.97E-01	6.66E-03	1.82E+02	Toluene
Gasoline Range	C <sub>8</sub> -C <sub>9</sub> Ethylbenzene	8.50	106	1.69E+02	1.69E+02	1.69E+02	8.10E-03	2.27E-01	5.09E-03	2.78E+02	Ethylbenzene
	C <sub>8</sub> -C <sub>9</sub> Xylene	8.63	106	1.61E+02	1.61E+02	1.61E+02	9.66E-03	2.84E-01	6.36E-03	1.46E+03	Xylene, & Styrene
	C <sub>9</sub> -C <sub>10</sub>	9.50	118	6.46E+01	3.98E+01	5.07E+01	3.55E-03	3.69E-01	8.28E-03	1.78E+03	Trimethylbenzenes, Methyl-Ethylbenzenes, Propylbenzenes
	C <sub>10</sub> -C <sub>12</sub>	11.00	130	3.98E+01	1.51E+01	2.45E+01	6.31E-04	1.49E-01	3.35E-03	2.51E+03	Naphthalene, Methyl-Naphthalene, Indan
Diesel Range	C <sub>12</sub> -C <sub>16</sub>	13.00	145	1.51E+01	2.19E+00	9.33E+00	1.10E-04	7.60E-02	1.70E-03	3.98E+03	Acenaphthylene, Acenaphthene
	C <sub>16</sub> -C <sub>21</sub>	17.00	173	2.19E+00	1.95E-01	1.35E+00	3.98E-06	2.27E-02	5.10E-04	1.00E+04	Fluorene, Methylfluorene
Residual Range	C <sub>21</sub> -C <sub>35</sub>	24.00	216	1.95E-01	2.24E-04	4.57E-02	1.20E-08	2.54E-03	5.68E-05	5.01E+04	Anthracene, Phenanthrene, Pyrene, Fluoranthene, Methylphenanthrene, Methyl-anthracene

<b>Aliphatics</b>	Equivalent Carbon Range										
	C <sub>5</sub> -C <sub>6</sub>	5.50	81	5.62E+01	1.58E+01	2.99E+01	3.55E-01	4.29E+01	9.62E-01	8.04E+02	Pentane, Hexane, Branched Chain Alkanes (Isopentane), Cycloalkanes, Straight Chain Alkenes
Gasoline Range	C <sub>6</sub> -C <sub>8</sub>	7.00	102	1.58E+01	1.26E+00	4.47E+00	6.31E-02	6.44E+01	1.44E+00	3.80E+03	Heptane, Branched Chain Alkanes (Isopentane), Cycloalkanes, Straight Chain Alkenes
	C <sub>8</sub> -C <sub>10</sub>	9.00	130	1.26E+00	1.00E-01	3.55E-01	6.31E-03	1.04E+02	2.32E+00	3.02E+04	Octane, Nonane, Branched Chain Alkanes, Cycloalkanes
	C <sub>10</sub> -C <sub>12</sub>	11.00	159	1.00E-01	7.94E-03	2.82E-02	6.31E-04	1.58E+02	3.55E+00	2.40E+05	Decane, Undecane, Branched Chain Alkanes
Diesel Range	C <sub>12</sub> -C <sub>16</sub>	13.00	186	7.94E-03	5.01E-05	2.24E-03	1.10E-04	4.07E+02	9.13E+00	1.91E+06	Dodecane, Tridecane, Tetradecane, Pentadecane, Branched Chain Alkanes
	C <sub>16</sub> -C <sub>21</sub>	17.00	242	5.01E-05	8.91E-08	1.41E-05	3.98E-06	3.04E+03	6.82E+01	1.20E+08	Hexadecane, Heptadecane, Octadecane, Nonadecane, Branched Chain Alkanes
Residual Range	C <sub>21</sub> -C <sub>35</sub>	24.00	338	8.91E-08	1.78E-15	2.00E-09	1.20E-08	9.08E+04	2.04E+03	1.70E+11	Eicosane, Heneicosane, Docosane, Tetracosane, Branched Chain Alkanes

























**Table 15 Fuel Sample 11, Jet A Characterization (Based on Product Analysis and Raoult's Law)**

1 Fraction	2 Median Equivalent Carbon	3 Percent Mass	4 Initial Concentrations at 10,000 mg/kg TPH (mg/kg)	5 Molecular Weight (g/mole)	6 Moles	7 Initial Mole Fraction	8 Single Component Solubility (mg/L)	9 Raoult's Law Solubility (mg/L)	10 Single Component Vapor Pressure (atm)	11 Raoult's Law Vapor Pressure (atm)	12 Henry's Constant (cm <sup>3</sup> /cm <sup>3</sup> )	13 Henry's Constant (atm m <sup>3</sup> /mole)	14 Diffusion Coefficient in Air (Dia) (cm <sup>2</sup> /sec)	15 Diffusion Coefficient in Water (Diw) (cm <sup>2</sup> /sec)	16 K <sub>oc</sub> (ml/g)	17 Coventional K <sub>D</sub> (=K <sub>oc</sub> *0.001)	18 Vadose C <sub>sat</sub> (mg/kg) (foc=0.001)	19 Saturated C <sub>sat</sub> (mg/kg) (foc=0.001)
<b>Aromatics</b>																		
Benzene	6.50	0.0077%	0.8	78	9.82E-06	1.65E-04	1.75E+03	0.29	1.30E-01	2.15E-05	2.59E-01	5.80E-03	8.80E-02	1.00E-05	5.89E+01	5.89E-02	0.05	0.07
Toluene	7.58	0.2220%	22.2	92	2.41E-04	4.05E-03	5.26E+02	2.13	3.80E-02	1.54E-04	2.97E-01	6.66E-03	8.70E-02	1.00E-05	1.82E+02	1.82E-01	0.62	0.79
Ethylbenzene	8.50	0.2670%	26.7	106	2.51E-04	4.23E-03	1.69E+02	0.72	8.10E-03	3.43E-05	2.27E-01	5.09E-03	8.00E-02	1.00E-05	2.78E+02	2.78E-01	0.27	0.33
Xylene	8.63	1.9300%	193.0	106	1.82E-03	3.07E-02	1.61E+02	4.93	9.66E-03	2.96E-04	2.84E-01	6.36E-03	1.00E-01	1.00E-05	1.46E+03	1.46E+00	7.71	8.11
C <sub>9</sub> -C <sub>10</sub>	9.25	0.1811%	18	116	1.56E-04	2.62E-03	5.72E+01	0.15	4.73E-03	1.24E-05	4.29E-01	9.62E-03	1.00E-01	1.00E-05	1.68E+03	1.68E+00	0.27	0.28
C <sub>10</sub> -C <sub>12</sub>	10.50	3.3750%	337	126	2.67E-03	4.50E-02	3.13E+01	1.41	8.71E-04	3.92E-05	1.57E-01	3.52E-03	1.00E-01	1.00E-05	2.24E+03	2.24E+00	3.28	3.41
C <sub>12</sub> -C <sub>16</sub>	13.00	7.6514%	765	145	5.27E-03	8.88E-02	9.33E+00	0.83	1.10E-04	9.74E-06	7.60E-02	1.70E-03	1.00E-01	1.00E-05	3.98E+03	3.98E+00	3.37	3.45
C <sub>16</sub> -C <sub>21</sub>	16.25	1.3844%	138	168	8.25E-04	1.39E-02	1.94E+00	0.03	7.41E-06	1.03E-07	2.86E-02	6.41E-04	1.00E-01	1.00E-05	8.41E+03	8.41E+00	0.23	0.23
C <sub>21</sub> -C <sub>35</sub>	28.00	0.0159%	2	239	6.68E-06	1.12E-04	6.61E-03	0.00	4.37E-10	4.91E-14	7.04E-04	1.58E-05	1.00E-01	1.00E-05	1.26E+05	1.26E+02	0.00	0.00
<b>Aromatics</b>		<b>15.0345%</b>	<b>1503</b>			<b>1.13E-02</b>		<b>10.48</b>		<b>5.67E-04</b>							<b>15.79</b>	<b>16.68</b>
<b>Aliphatics</b>																		
C <sub>5</sub> -C <sub>6</sub>	5.50	0.0151%	2	81	1.87E-05	3.14E-04	2.99E+01	0.01	3.55E-01	1.11E-04	4.29E+01	9.62E-01	1.00E-01	1.00E-05	8.04E+02	8.04E-01	0.05	0.01
C <sub>6</sub> -C <sub>8</sub>	7.00	0.5124%	51	102	5.01E-04	8.43E-03	4.47E+00	0.04	6.31E-02	5.32E-04	6.44E+01	1.44E+00	1.00E-01	1.00E-05	3.80E+03	3.80E+00	0.42	0.15
C <sub>8</sub> -C <sub>10</sub>	9.00	9.0957%	910	130	6.97E-03	1.17E-01	3.55E-01	0.04	6.31E-03	7.40E-04	1.04E+02	2.32E+00	1.00E-01	1.00E-05	3.02E+04	3.02E+01	1.75	1.27
C <sub>10</sub> -C <sub>12</sub>	11.00	29.4493%	2,945	159	1.86E-02	3.13E-01	2.82E-02	0.01	5.75E-04	1.80E-04	1.44E+02	3.24E+00	1.00E-01	1.00E-05	2.40E+05	2.40E+02	2.26	2.12
C <sub>12</sub> -C <sub>16</sub>	14.00	39.3882%	3,939	200	1.97E-02	3.31E-01	6.31E-04	0.00	4.79E-05	1.58E-05	6.78E+02	1.52E+01	1.00E-01	1.00E-05	5.37E+06	5.37E+03	1.14	1.12
C <sub>16</sub> -C <sub>21</sub>	19.00	6.5017%	650	269	2.41E-03	4.06E-02	1.12E-06	0.00	7.59E-07	3.08E-08	8.13E+03	1.82E+02	1.00E-01	1.00E-05	9.55E+08	9.55E+05	0.04	0.04
C <sub>21</sub> -C <sub>35</sub>	28.00	0.0032%	0	392	8.11E-07	1.37E-05	1.26E-11	0.00	4.37E-10	5.96E-15	6.07E+05	1.36E+04	1.00E-01	1.00E-05	1.07E+13	1.07E+10	0.00	0.00
<b>Aliphatics</b>		<b>84.9655%</b>	<b>8,497</b>			<b>4.81E-02</b>		<b>0.10</b>		<b>1.58E-03</b>							<b>5.67</b>	<b>4.71</b>
<b>Total Hydrocarbon</b>		<b>100.0000%</b>	<b>10,000</b>			<b>5.94E-02</b>	<b>Total Hydrocarbon</b>	<b>10.58</b>		<b>2.15E-03</b>					<b>Total Hydrocarbon</b>		<b>21.45</b>	<b>21.38</b>
<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>			<b>1223</b>				<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>	<b>8.31</b>		<b>1.90E-03</b>					<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>		<b>11.14</b>	<b>11.00</b>
<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>			<b>8775</b>				<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>	<b>2.27</b>		<b>2.45E-04</b>					<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>		<b>10.31</b>	<b>10.38</b>
<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>			<b>2</b>				<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>	<b>0.00</b>		<b>6.E-14</b>					<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>		<b>0.00</b>	<b>0.00</b>
<b>TAH (BTEX)</b>			<b>243</b>				<b>TAH (BTEX)</b>	<b>8.07</b>										
																	<b>8.80</b>	<b>9.47</b>





**Table 17 Mass Fractions in Equivalent Carbon and Boiling Temperature Groups**

EC Number	Boiling Temp (C°)	#10 DF	#11 Jet A	#12 DF2	# 3 JP4	#9 Jet A	#5 DF2	#8 Av Gas	#1 Regular Gas	#2 Premium Gas	#6 Regular Gas	#7 Premium Gas	#4 DF1/Jet A
5	36	4.3E-04	1.5E-04	4.1E-04	5.8E-02	4.2E-04	2.3E-04	1.4E-01	3.0E-01	2.6E-01	2.1E-01	1.6E-01	4.4E-04
6	69	9.4E-04	3.7E-04	5.9E-04	9.9E-02	1.0E-03	2.3E-04	6.4E-02	7.2E-02	5.7E-02	9.8E-02	6.6E-02	1.4E-03
7	98	5.8E-03	7.1E-03	1.6E-03	1.5E-01	6.3E-03	8.5E-04	3.0E-01	1.1E-01	1.1E-01	1.4E-01	1.3E-01	9.0E-03
8	126	1.4E-02	1.6E-02	3.8E-03	2.3E-01	1.5E-02	2.0E-03	4.5E-01	1.7E-01	1.7E-01	2.6E-01	2.9E-01	2.1E-02
9	151	4.9E-02	9.8E-02	5.8E-03	1.6E-01	5.1E-02	4.6E-03	2.8E-02	1.8E-01	2.2E-01	2.1E-01	2.3E-01	7.5E-02
10	174	9.2E-02	1.7E-01	8.2E-03	4.1E-02	1.4E-01	8.6E-03	2.9E-03	8.8E-02	9.9E-02	4.3E-02	7.1E-02	1.6E-01
11	196	1.1E-01	1.6E-01	1.1E-02	3.3E-02	2.2E-01	1.3E-02	8.0E-04	7.2E-02	8.0E-02	2.8E-02	4.3E-02	1.6E-01
12	216	1.1E-01	1.3E-01	1.7E-02	5.3E-02	2.1E-01	2.1E-02	9.7E-04	8.8E-03	7.2E-03	2.4E-03	4.4E-03	1.4E-01
13	235	1.0E-01	1.3E-01	2.9E-02	5.4E-02	1.7E-01	3.3E-02	2.2E-04	1.1E-03	6.1E-04	6.4E-04	1.1E-03	1.3E-01
14	254	9.1E-02	1.1E-01	5.0E-02	4.8E-02	9.5E-02	5.1E-02	1.1E-04	1.9E-05	6.7E-06	3.8E-04	5.3E-04	1.1E-01
15	271	8.8E-02	9.2E-02	9.2E-02	4.1E-02	5.3E-02	7.8E-02	7.8E-05	4.5E-06	4.5E-06	3.7E-04	4.0E-04	9.2E-02
16	287	8.3E-02	5.0E-02	1.4E-01	2.6E-02	2.8E-02	1.1E-01	4.8E-05	4.7E-06	3.8E-06	3.9E-04	4.1E-04	6.0E-02
17	302	8.3E-02	2.0E-02	1.7E-01	1.1E-02	1.2E-02	1.8E-01	2.8E-05	7.6E-06	2.5E-06	3.3E-04	3.6E-04	2.8E-02
18	316	7.7E-02	6.6E-03	1.8E-01	3.1E-03	4.0E-03	2.1E-01	2.6E-05	2.2E-05	5.7E-06	2.2E-04	2.6E-04	9.8E-03
19	330	4.9E-02	1.9E-03	1.5E-01	4.6E-04	8.4E-04	1.6E-01	1.7E-05	1.6E-05	9.8E-06	9.0E-05	1.2E-04	1.9E-03
20	344	2.5E-02	5.4E-04	9.3E-02	3.9E-05	1.3E-04	8.4E-02	8.1E-06	2.4E-05	1.5E-05	4.8E-05	7.4E-05	2.3E-04
21	356	1.2E-02	1.5E-04	4.1E-02	2.0E-07	1.1E-05	3.2E-02	5.9E-06	3.4E-05	2.5E-05	2.2E-05	4.2E-05	6.3E-06
22	369	4.6E-03	3.4E-05	1.1E-02	1.1E-05	1.4E-06	8.7E-03	1.2E-05	6.0E-05	5.0E-05	2.5E-05	3.4E-05	2.7E-06
23	380	1.6E-03	2.7E-06	2.4E-03	2.8E-05	6.9E-07	1.8E-03	5.6E-06	7.3E-05	5.6E-05	1.8E-05	2.6E-05	2.7E-05
24	391	2.3E-04	2.0E-07	2.5E-04	5.8E-05	4.0E-06	1.4E-04	1.1E-05	1.2E-04	6.7E-05	2.9E-05	3.1E-05	7.1E-05
25	402	9.5E-06	1.2E-06	1.6E-06	9.8E-05	1.8E-05	3.9E-07	2.3E-05	1.7E-04	9.0E-05	4.8E-05	4.4E-05	1.3E-04

**Table 18 Summary of Mass Fractions in the Recommended Aromatic and Aliphatic Equivalent Carbon Groups**

<b>Aromatic Fractions</b>	Median Equivalent Carbon	#1 Regular Gas	#2 Premium Gas	#3 JP4	#4 DF1 (Jet A)	#5 DF2	#6 Regular Gas	#7 Premium Gas	#8 Av Gas	#9 Jet A	#10 DF	#11 Jet A	#12 DF2
Benzene	6.5	2.74E-02	2.42E-02	4.72E-03	2.55E-04	5.77E-05	3.85E-02	3.97E-02	5.35E-04	1.06E-04	1.89E-04	7.67E-05	1.52E-04
Toluene	7.58	1.05E-01	1.27E-01	1.22E-02	2.16E-03	4.28E-04	1.19E-01	1.42E-01	1.28E-01	1.14E-03	1.94E-03	2.22E-03	8.35E-04
Ethylbenzene	8.5	2.37E-02	2.94E-02	3.19E-03	1.48E-03	2.20E-04	2.21E-02	2.75E-02	3.07E-04	1.16E-03	1.44E-03	2.67E-03	2.95E-04
Xylene	8.63	1.11E-01	1.40E-01	1.54E-02	8.96E-03	1.12E-03	1.15E-01	1.44E-01	1.43E-03	6.75E-03	8.21E-03	1.93E-02	1.60E-03
C <sub>9</sub> -C <sub>10</sub>	9.25	7.23E-02	8.63E-02	3.26E-03	1.01E-03	2.39E-05	7.51E-02	6.79E-02	3.26E-04	2.23E-04	5.89E-04	1.81E-03	6.55E-06
C <sub>10</sub> -C <sub>12</sub>	10.5	6.39E-02	7.16E-02	1.40E-02	2.33E-02	5.31E-04	2.49E-02	3.37E-02	5.93E-04	1.25E-02	1.43E-02	3.37E-02	3.18E-04
C <sub>12</sub> -C <sub>16</sub>	13	3.99E-03	3.13E-03	4.10E-02	6.50E-02	8.65E-03	1.32E-03	1.88E-03	0.00E+00	4.08E-02	4.57E-02	7.65E-02	1.06E-02
C <sub>16</sub> -C <sub>21</sub>	16.5	2.99E-05	1.49E-05	1.63E-02	2.67E-02	1.32E-01	3.79E-04	3.59E-04	0.00E+00	1.14E-02	6.50E-02	1.38E-02	1.20E-01
C <sub>21</sub> -C <sub>35</sub>	25	1.86E-04	1.15E-04	1.88E-04	9.29E-05	2.67E-08	4.93E-05	5.18E-05	2.05E-07	1.01E-06	9.93E-03	1.59E-04	3.74E-02
<b>Sum of Aromatics</b>		4.07E-01	4.81E-01	1.10E-01	1.29E-01	1.43E-01	3.96E-01	4.57E-01	1.31E-01	7.41E-02	1.47E-01	1.50E-01	1.72E-01
<b>Aliphatic Fractions</b>													
C <sub>5</sub> -C <sub>6</sub>	5.5	2.98E-01	2.59E-01	5.75E-02	4.39E-04	2.31E-04	2.11E-01	1.60E-01	1.44E-01	4.24E-04	4.27E-04	1.51E-04	4.12E-04
C <sub>6</sub> -C <sub>8</sub>	7	5.11E-02	1.80E-02	2.33E-01	7.93E-03	5.93E-04	8.03E-02	2.45E-02	2.39E-01	6.12E-03	4.63E-03	5.12E-03	1.23E-03
C <sub>8</sub> -C <sub>10</sub>	9	1.41E-01	1.29E-01	3.60E-01	8.41E-02	5.17E-03	2.63E-01	2.74E-01	4.81E-01	5.80E-02	5.22E-02	9.10E-02	7.67E-03
C <sub>10</sub> -C <sub>12</sub>	11	9.58E-02	1.07E-01	6.04E-02	2.96E-01	2.08E-02	4.63E-02	7.85E-02	3.10E-03	3.42E-01	1.86E-01	2.94E-01	1.88E-02
C <sub>12</sub> -C <sub>16</sub>	14	5.98E-03	4.70E-03	1.54E-01	4.09E-01	1.74E-01	2.45E-03	4.40E-03	1.38E-03	4.86E-01	3.49E-01	3.94E-01	1.78E-01
C <sub>16</sub> -C <sub>21</sub>	16.5	4.48E-05	2.23E-05	2.51E-02	7.37E-02	6.13E-01	7.03E-04	8.37E-04	1.28E-04	3.39E-02	2.53E-01	6.50E-02	6.04E-01
C <sub>21</sub> -C <sub>35</sub>	25	2.79E-04	1.73E-04	6.49E-06	1.43E-04	4.27E-02	9.15E-05	1.21E-04	5.73E-05	3.40E-05	8.13E-03	3.18E-05	1.81E-02
<b>Sum of Aliphatics</b>		5.93E-01	5.19E-01	8.90E-01	8.71E-01	8.57E-01	6.04E-01	5.43E-01	8.69E-01	9.26E-01	8.53E-01	8.50E-01	8.28E-01
<b>Total Hydrocarbon</b>		1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>		8.30E-01	8.13E-01	6.89E-01	1.06E-01	7.85E-03	9.24E-01	8.80E-01	9.95E-01	7.39E-02	6.96E-02	1.22E-01	1.22E-02
<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>		1.70E-01	1.87E-01	3.11E-01	8.93E-01	9.49E-01	7.61E-02	1.20E-01	5.19E-03	9.26E-01	9.12E-01	8.77E-01	9.32E-01
<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>		4.66E-04	2.88E-04	1.95E-04	2.36E-04	4.27E-02	1.41E-04	1.73E-04	5.75E-05	3.50E-05	1.81E-02	1.91E-04	5.55E-02
<b>TAH (BTEX)</b>		2.67E-01	3.20E-01	3.55E-02	1.29E-02	1.83E-03	2.94E-01	3.54E-01	1.30E-01	9.16E-03	1.18E-02	2.43E-02	2.88E-03

<b>Summary of GRO, DRO &amp; RRO Distribution</b>	<b>Gasoline Samples</b>		<b>Diesel &amp; Jet A Samples</b>	
	<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>	88%	<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>	7%
	<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>	12%	<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>	92%
	<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>	0%	<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>	2%

<b>Summary of Aromatic &amp; Aliphatic Distribution Distribution</b>	<b>Gasoline Samples</b>		<b>Diesel &amp; Jet A Samples</b>	
	<b>Aromatics</b>	37%	<b>Aromatics</b>	14%
	<b>Aliphatics</b>	63%	<b>Aliphatics</b>	86%

**Table 19 Summary of Effective Solubilities in the Recommended Aromatic and Aliphatic Equivalent Carbon Groups**

<b>Aromatic Fractions</b>	Median Equivalent Carbon	Single Component Solubility (mg/L)	#1 Regular Gas	#2 Premium Gas	#3 JP4	#4 DF1 (Jet A)	#5 DF2	#6 Regular Gas	#7 Premium Gas	#8 Av Gas	#9 Jet A	#10 DF	#11 Jet A	#12 DF2
Benzene	6.5	1750.00	62.55	55.95	13.43	0.98	0.30	89.44	94.96	1.30	0.41	0.80	0.29	0.78
Toluene	7.58	526.00	61.02	74.76	8.84	2.11	0.57	70.39	86.56	78.95	1.13	2.09	2.13	1.09
Ethylbenzene	8.5	169.00	3.84	4.83	0.64	0.40	0.08	3.65	4.66	0.05	0.32	0.43	0.72	0.11
Xylene	8.63	161.00	17.18	21.94	2.97	2.33	0.40	18.06	23.36	0.23	1.78	2.35	4.93	0.56
C <sub>9</sub> -C <sub>10</sub>	9.25	5.7E+01	3.62	4.39	0.20	0.09	0.00	3.83	3.56	0.02	0.02	0.05	0.15	0.00
C <sub>10</sub> -C <sub>12</sub>	10.5	3.1E+01	1.61	1.83	0.44	0.99	0.03	0.64	0.89	0.02	0.54	0.67	1.41	0.02
C <sub>12</sub> -C <sub>16</sub>	13	9.3E+00	0.03	0.02	0.33	0.72	0.13	0.01	0.01	0.00	0.46	0.56	0.83	0.16
C <sub>16</sub> -C <sub>21</sub>	16.5	1.9E+00	0.00	0.00	0.02	0.05	0.35	0.00	0.00	0.00	0.02	0.14	0.03	0.32
C <sub>21</sub> -C <sub>35</sub>	25	6.6E-03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<b>Sum of Aromatics</b>			149.85	163.72	26.89	7.67	1.86	186.01	214.02	80.56	4.68	7.09	10.48	3.04
<b>Aliphatic Fractions</b>														
C <sub>5</sub> -C <sub>6</sub>	5.5	3.0E+01	11.20	9.86	2.69	0.03	0.02	8.08	6.29	5.75	0.03	0.03	0.01	0.03
C <sub>6</sub> -C <sub>8</sub>	7	4.5E+00	0.23	0.08	1.29	0.06	0.01	0.36	0.11	1.13	0.05	0.04	0.04	0.01
C <sub>8</sub> -C <sub>10</sub>	9	3.5E-01	0.04	0.04	0.12	0.04	0.00	0.07	0.08	0.14	0.03	0.03	0.04	0.00
C <sub>10</sub> -C <sub>12</sub>	11	2.8E-02	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00
C <sub>12</sub> -C <sub>16</sub>	14	6.3E-04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C <sub>16</sub> -C <sub>21</sub>	16.5	1.1E-06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C <sub>21</sub> -C <sub>35</sub>	25	1.3E-11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<b>Sum of Aliphatics</b>			11.47	9.98	4.11	0.14	0.03	8.52	6.49	7.02	0.11	0.10	0.10	0.05
<b>Total Hydrocarbon</b>			161.32	173.70	31.00	7.81	1.89	194.53	220.51	87.58	4.79	7.19	10.58	3.09
<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>			159.68	171.85	30.20	6.04	1.38	193.88	219.61	87.56	3.77	5.82	8.31	2.60
<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>			1.64	1.85	0.80	1.77	0.51	0.65	0.90	0.02	1.03	1.37	2.27	0.50
<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<b>TAH (BTEX)</b>			144.59	157.48	25.88	5.83	1.34	181.53	209.56	80.53	3.65	5.67	8.07	2.54

<b>Gasoline Samples</b>		<b>Diesel &amp; Jet A Samples</b>	
Average GRO Solubility (mg/L)	166.5	Average GRO Solubility (mg/L)	4.7
Average DRO Solubility (mg/L)	1.0	Average DRO Solubility (mg/L)	1.2

**Table 20 Summary of Vadose Zone Csat Values in the Recommended Aromatic and Aliphatic Equivalent Carbon Groups**

<b>Aromatic Fractions</b>	Median Equivalent Carbon	#1 Regular Gas	#2 Premium Gas	#3 JP4	#4 DF1 (Jet A)	#5 DF2	#6 Regular Gas	#7 Premium Gas	#8 Av Gas	#9 Jet A	#10 DF	#11 Jet A	#12 DF2
Benzene	6.5	10.14	9.07	2.18	0.16	0.05	14.51	15.40	0.21	0.07	0.13	0.05	0.13
Toluene	7.58	17.67	21.65	2.56	0.61	0.16	20.39	25.07	22.87	0.33	0.60	0.62	0.32
Ethylbenzene	8.5	1.45	1.82	0.24	0.15	0.03	1.38	1.76	0.02	0.12	0.16	0.27	0.04
Xylene	8.63	26.82	34.26	4.64	3.64	0.62	28.20	36.49	0.37	2.78	3.67	7.71	0.87
C <sub>9</sub> -C <sub>10</sub>	9.25	6.52	7.90	0.37	0.15	0.00	6.90	6.42	0.03	0.03	0.10	0.27	0.00
C <sub>10</sub> -C <sub>12</sub>	10.5	3.75	4.27	1.03	2.30	0.07	1.49	2.07	0.04	1.26	1.56	3.28	0.04
C <sub>12</sub> -C <sub>16</sub>	13	0.11	0.08	1.36	2.91	0.53	0.04	0.05	0.00	1.85	2.26	3.37	0.64
C <sub>16</sub> -C <sub>21</sub>	16.5	0.00	0.00	0.20	0.45	3.01	0.00	0.00	0.00	0.19	1.20	0.23	2.71
C <sub>21</sub> -C <sub>35</sub>	25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.03
<b>Sum of Aromatics</b>		66.47	79.07	12.58	10.38	4.47	72.90	87.27	23.53	6.64	9.70	15.79	4.78
				0.00									
<b>Aliphatic Fractions</b>				0.00									
C <sub>5</sub> -C <sub>6</sub>	5.5	64.45	56.75	15.50	0.16	0.11	46.48	36.21	33.07	0.16	0.17	0.05	0.20
C <sub>6</sub> -C <sub>8</sub>	7	2.54	0.91	14.46	0.66	0.07	4.07	1.28	12.63	0.52	0.43	0.42	0.14
C <sub>8</sub> -C <sub>10</sub>	9	1.65	1.53	5.22	1.65	0.14	3.12	3.34	5.95	1.15	1.13	1.75	0.20
C <sub>10</sub> -C <sub>12</sub>	11	0.44	0.51	0.35	2.31	0.22	0.22	0.38	0.02	2.71	1.60	2.26	0.20
C <sub>12</sub> -C <sub>16</sub>	14	0.01	0.01	0.34	1.20	0.70	0.00	0.01	0.00	1.45	1.13	1.14	0.70
C <sub>16</sub> -C <sub>21</sub>	16.5	0.00	0.00	0.01	0.05	0.57	0.00	0.00	0.00	0.02	0.19	0.04	0.55
C <sub>21</sub> -C <sub>35</sub>	25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<b>Sum of Aliphatics</b>		69.10	59.70	35.88	6.03	1.81	53.89	41.23	51.66	6.01	4.64	5.67	1.99
<b>Total Hydrocarbon</b>		135.57	138.77	48.45	16.42	6.27	126.79	128.49	75.20	12.64	14.34	21.45	6.78
<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>		131.26	133.90	45.17	7.19	1.18	125.03	125.97	75.14	5.16	6.39	11.14	1.90
<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>		4.31	4.87	3.29	9.23	5.09	1.75	2.52	0.05	7.48	7.94	10.31	4.85
<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.03
<b>TAH (BTEX)</b>		56.09	66.81	9.62	4.57	0.86	64.47	78.72	23.46	3.30	4.57	8.64	1.36

<b>Gasoline Samples</b>		<b>Diesel &amp; Jet A Samples</b>	
<b>Average GRO Csat (mg/L)</b>	118.3	<b>Average GRO Csat (mg/L)</b>	5.5
<b>Average DRO Csat (mg/L)</b>	2.7	<b>Average DRO Csat (mg/L)</b>	7.5

**Table 21 Summary of Saturated Zone Csat Values in the Recommended Aromatic and Aliphatic Equivalent Carbon Groups**

<b>Aromatic Fractions</b>	Median Equivalent Carbon	#1 Regular Gas	#2 Premium Gas	#3 JP4	#4 DF1 (Jet A)	#5 DF2	#6 Regular Gas	#7 Premium Gas	#8 Av Gas	#9 Jet A	#10 DF	#11 Jet A	#12 DF2
Benzene	6.5	1.54E+01	1.38E+01	3.31E+00	2.41E-01	7.40E-02	2.60E+01	2.34E+01	3.19E-01	1.02E-01	1.97E-01	7.13E-02	1.93E-01
Toluene	7.58	2.25E+01	2.76E+01	3.27E+00	2.41E-01	2.10E-01	1.70E+00	3.20E+01	2.92E+01	4.18E-01	7.72E-01	7.88E-01	4.05E-01
Ethylbenzene	8.5	1.79E+00	2.25E+00	3.00E-01	2.41E-01	3.79E-02	2.97E+01	2.17E+00	2.46E-02	1.49E-01	2.01E-01	3.33E-01	5.02E-02
Xylene	8.63	2.82E+01	3.60E+01	4.88E+00	2.41E-01	6.49E-01	7.15E+00	3.84E+01	3.86E-01	2.93E+00	3.87E+00	8.11E+00	9.18E-01
C <sub>9</sub> -C <sub>10</sub>	9.25	6.76E+00	8.19E+00	3.80E-01	2.41E-01	5.09E-03	1.55E+00	6.65E+00	3.24E-02	3.56E-02	1.02E-01	2.80E-01	1.38E-03
C <sub>10</sub> -C <sub>12</sub>	10.5	3.91E+00	4.44E+00	1.07E+00	2.41E-01	7.41E-02	3.66E-02	2.16E+00	3.85E-02	1.31E+00	1.62E+00	3.41E+00	4.39E-02
C <sub>12</sub> -C <sub>16</sub>	13	1.09E-01	8.68E-02	1.39E+00	2.41E-01	5.39E-01	3.90E-03	5.39E-02	0.00E+00	1.90E+00	2.32E+00	3.45E+00	6.54E-01
C <sub>16</sub> -C <sub>21</sub>	16.5	3.02E-04	1.53E-04	2.06E-01	2.41E-01	3.04E+00	1.78E-05	3.81E-03	0.00E+00	1.97E-01	1.22E+00	2.32E-01	2.75E+00
C <sub>21</sub> -C <sub>35</sub>	25	6.62E-05	4.16E-05	8.34E-05	2.41E-01	2.16E-08	8.82E+01	1.93E-05	7.74E-08	6.13E-07	6.54E-03	9.36E-05	3.00E-02
<b>Sum of Aromatics</b>		7.87E+01	9.24E+01	1.48E+01	2.41E-01	4.63E+00	0.00E+00	104.81	3.00E+01	7.04E+00	1.03E+01	1.67E+01	5.04E+00
<b>Aliphatic Fractions</b>													
C <sub>5</sub> -C <sub>6</sub>	5.5	1.11E+01	9.77E+00	2.67E+00	2.41E-01	1.96E-02	1.45E+00	6.24E+00	5.70E+00	2.69E-02	2.95E-02	9.30E-03	3.46E-02
C <sub>6</sub> -C <sub>8</sub>	7	9.06E-01	3.24E-01	5.15E+00	2.41E-01	2.40E-02	2.25E+00	4.56E-01	4.50E+00	1.85E-01	1.52E-01	1.50E-01	4.93E-02
C <sub>8</sub> -C <sub>10</sub>	9	1.19E+00	1.10E+00	3.77E+00	2.41E-01	9.93E-02	2.05E-01	2.42E+00	4.30E+00	8.33E-01	8.13E-01	1.27E+00	1.46E-01
C <sub>10</sub> -C <sub>12</sub>	11	4.16E-01	4.74E-01	3.27E-01	2.41E-01	2.07E-01	4.29E-03	3.57E-01	1.43E-02	2.54E+00	1.50E+00	2.12E+00	1.85E-01
C <sub>12</sub> -C <sub>16</sub>	14	1.03E-02	8.22E-03	3.31E-01	2.41E-01	6.85E-01	2.90E-04	7.93E-03	2.51E-03	1.43E+00	1.11E+00	1.12E+00	6.93E-01
C <sub>16</sub> -C <sub>21</sub>	16.5	1.81E-05	9.17E-06	1.27E-02	2.41E-01	5.67E-01	3.26E-06	3.55E-04	5.50E-05	2.34E-02	1.90E-01	4.35E-02	5.52E-01
C <sub>21</sub> -C <sub>35</sub>	25	9.79E-06	6.15E-06	2.83E-07	2.41E-01	3.41E-03	1.19E+01	4.44E-06	2.13E-06	2.03E-06	5.27E-04	1.84E-06	1.43E-03
<b>Sum of Aliphatics</b>		1.36E+01	1.17E+01	1.23E+01	2.41E-01	1.61E+00	1.00E+02	9.48	1.45E+01	5.03E+00	3.79E+00	4.71E+00	1.66E+00
<b>Total Hydrocarbon</b>		9.2E+01	1.0E+02	2.7E+01	4.8E-01	6.2E+00	1.0E+02	1.1E+02	4.4E+01	1.2E+01	1.4E+01	2.1E+01	6.7E+00
<b>GRO (C<sub>5</sub> to C<sub>10</sub>)</b>		8.8E+01	9.9E+01	2.4E+01	1.9E+00	1.1E+00	7.0E+01	1.1E+02	4.4E+01	4.7E+00	6.1E+00	1.1E+01	1.8E+00
<b>DRO (C<sub>10</sub> to C<sub>21</sub>)</b>		4.4E+00	5.0E+00	3.3E+00	1.4E+00	5.1E+00	4.5E-02	2.6E+00	5.5E-02	7.4E+00	8.0E+00	1.0E+01	4.9E+00
<b>RRO (C<sub>21</sub> to C<sub>35</sub>)</b>		7.6E-05	4.8E-05	8.4E-05	4.8E-01	3.4E-03	1.0E+02	2.4E-05	2.2E-06	2.6E-06	7.1E-03	9.5E-05	3.1E-02
<b>TAH (BTEX)</b>		6.8E+01	8.0E+01	1.2E+01	9.7E-01	9.7E-01	6.5E+01	9.6E+01	3.0E+01	3.6E+00	5.0E+00	9.3E+00	1.6E+00

<b>Gasoline Samples</b>		<b>Diesel &amp; Jet A Samples</b>	
Average GRO Csat (mg/L)	82.6	Average GRO Csat (mg/L)	4.4
Average DRO Csat (mg/L)	2.4	Average DRO Csat (mg/L)	6.2

**Table 22 Summary of PAH Mass Fractions in Selected Alaskan Fuels**

Compound	Equivalent Carbon	#1 Regular Gas	#2 Premium Gas	#3 JP4	#4 DF1 (Jet A)	#5 DF2	#6 Regular Gas	#7 Premium Gas	#8 Av Gas	#9 Jet A	#10 DF	#11 Jet A	#12 DF2
Naphthalene	11.69	4.7E-05	1.4E-03	5.1E-03	3.3E-03	1.2E-04	2.9E-03	3.9E-03	1.4E-04	2.4E-03	1.6E-03	2.7E-03	5.0E-04
2-Methyl naphthalene	12.84	2.6E-03	3.5E-05	7.1E-03	8.0E-03	3.4E-03	1.2E-03	1.3E-03	4.0E-05	6.7E-03	5.8E-03	8.2E-03	3.3E-03
Acenaphthene	15.5	ND	ND	ND	ND	ND	ND	ND	ND	8.9E-05	2.5E-04	4.5E-04	2.3E-04
Fluorene	16.55	ND	ND	2.8E-04	7.5E-04	1.3E-03	0.0E+00	0.0E+00	ND	4.6E-05	2.2E-04	8.1E-05	2.6E-04
Phenanthrene	19.36	ND	ND	4.7E-05	2.4E-04	3.8E-03	1.7E-04	1.4E-04	ND	1.4E-05	7.8E-05	ND	1.5E-04
Anthracene	19.43	ND	ND	ND	ND	2.7E-04	ND	ND	ND	ND	4.0E-04	2.8E-05	8.3E-04
Fluoranthene	21.85	ND	ND	ND	ND	2.6E-05	ND	ND	ND	ND	ND	ND	ND

The PAH concentration expressed as mg of PAH per kg of fuel maybe calculated by multiplying the mass fraction by 1,000,000 mg per kg; mg of PAH per liter of fuel may be calculated by multiplying the mg/kg concentration by the specific gravity of the fuel. Gasolines typically have specific gravities in the 0.75 to 0.8 range and diesel and jet fuels typically have specific gravities in the 0.8 to 0.85 range.

**Table 23 PAH Concentrations in a Soil Containing 10,000 mg/kg NAPL of Selected Alaskan Fuels**

Compound	Table B1 Soil Ingestion Conc. (mg/kg)	Table B1 Migration to Groundwater Conc. (mg/kg)	#1 Regular Gas	#2 Premium Gas	#3 JP4	#4 DF1 (Jet A)	#5 DF2	#6 Regular Gas	#7 Premium Gas	#8 Av Gas	#9 Jet A	#10 DF	#11 Jet A	#12 DF2
Naphthalene	4,100	43	0.466	14.039	51.069	33.000	1.209	28.967	39.257	1.369	23.559	15.560	27.240	5.006
2-Methylnaphthalene	2030	60.9	26.058	0.348	70.526	80.368	33.796	12.468	13.326	0.402	67.021	57.541	82.293	33.081
Acenaphthene	6100	210									0.888	2.484	4.509	2.342
Fluorene	4,100	270			2.787	7.540	12.795	0.000	0.000		0.459	2.156	0.814	2.626
Phenanthrene	30000	4300			0.472	2.408	37.886	1.722	1.434		0.136	0.777		1.499
Anthracene	30,000	4,300					2.695					4.007	0.283	8.325
Fluoranthene	30,000	2,100					0.256							

**Table 24 Carbon Numbers and Equivalent Carbon Numbers of the PAH compounds**

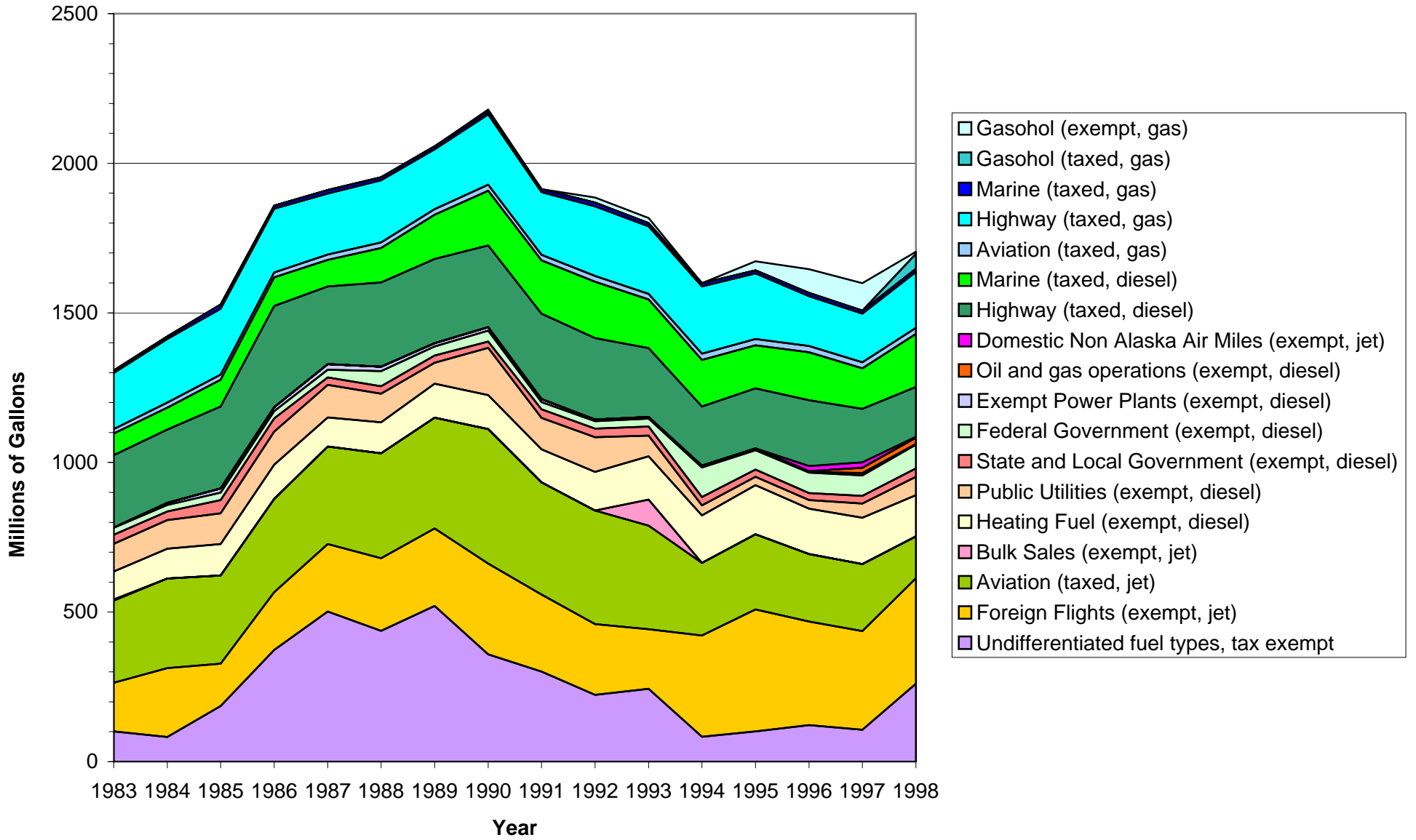
Compound	# of carbon atoms	EC #
Naphthalene	10	11.69
2-methylnaphthalene	11	12.84
1-methylnaphthalene	11	12.99
Acenaphthylene	12	15.06
Acenaphthene	12	15.5
Fluorene	13	16.55
Phenanthrene	14	19.36
Anthracene	14	19.43
Fluoranthene	16	21.85
Pyrene	16	20.8
Benzo (a) Anthracene	18	26.37
Chrysene	18	27.41
Benzo (b) fluoranthene	20	30.14
Benzo (k) fluoranthene	20	30.14
Benzo (a) pyrene	20	31.34
Indeno (1,2,3-cd) pyrene	22	35.01
Dibenz (a,h) anthracene	22	34.01
Benzo(g,h,i)perylene	22	34.01

# Figures

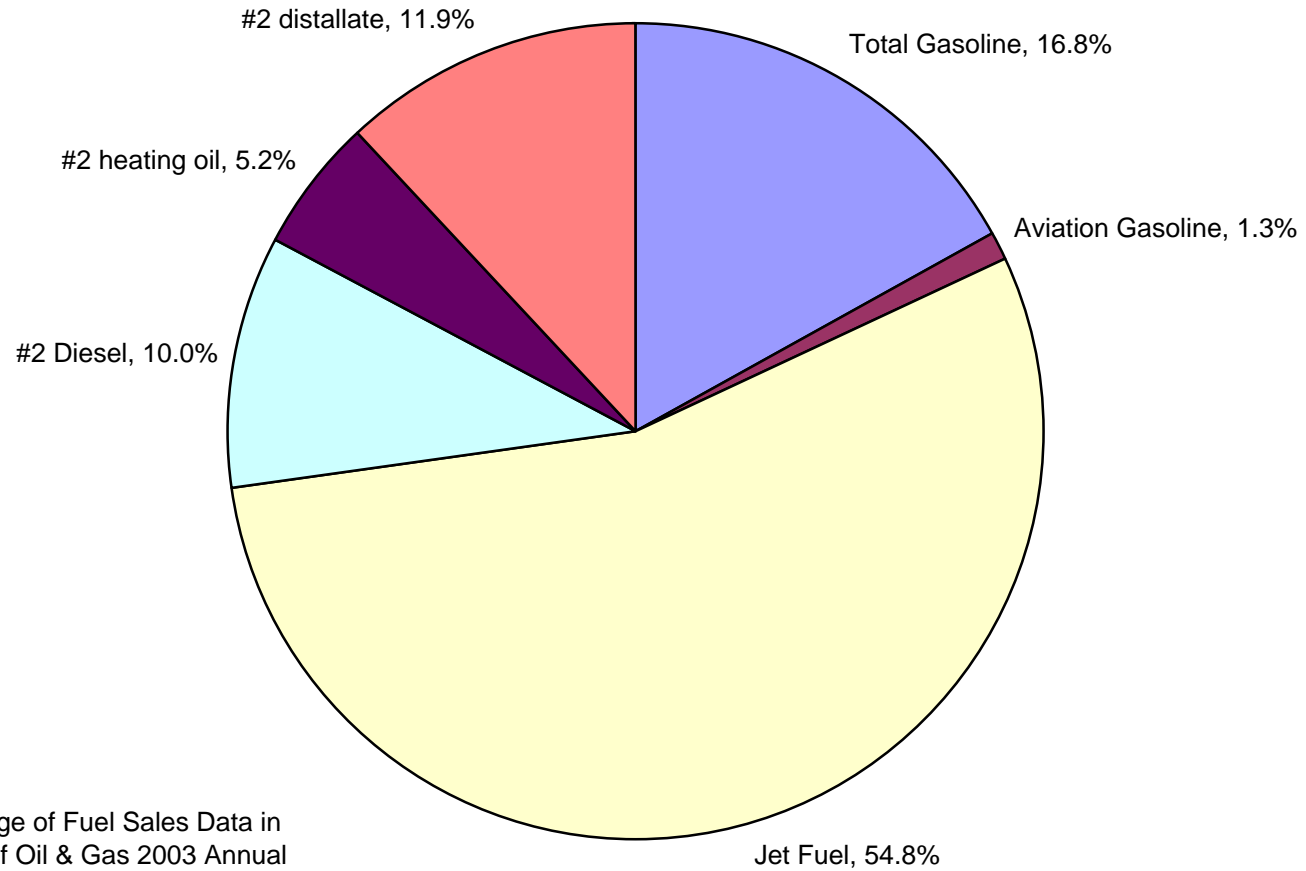
---



Figure 1 Alaska Fuel Consumption History

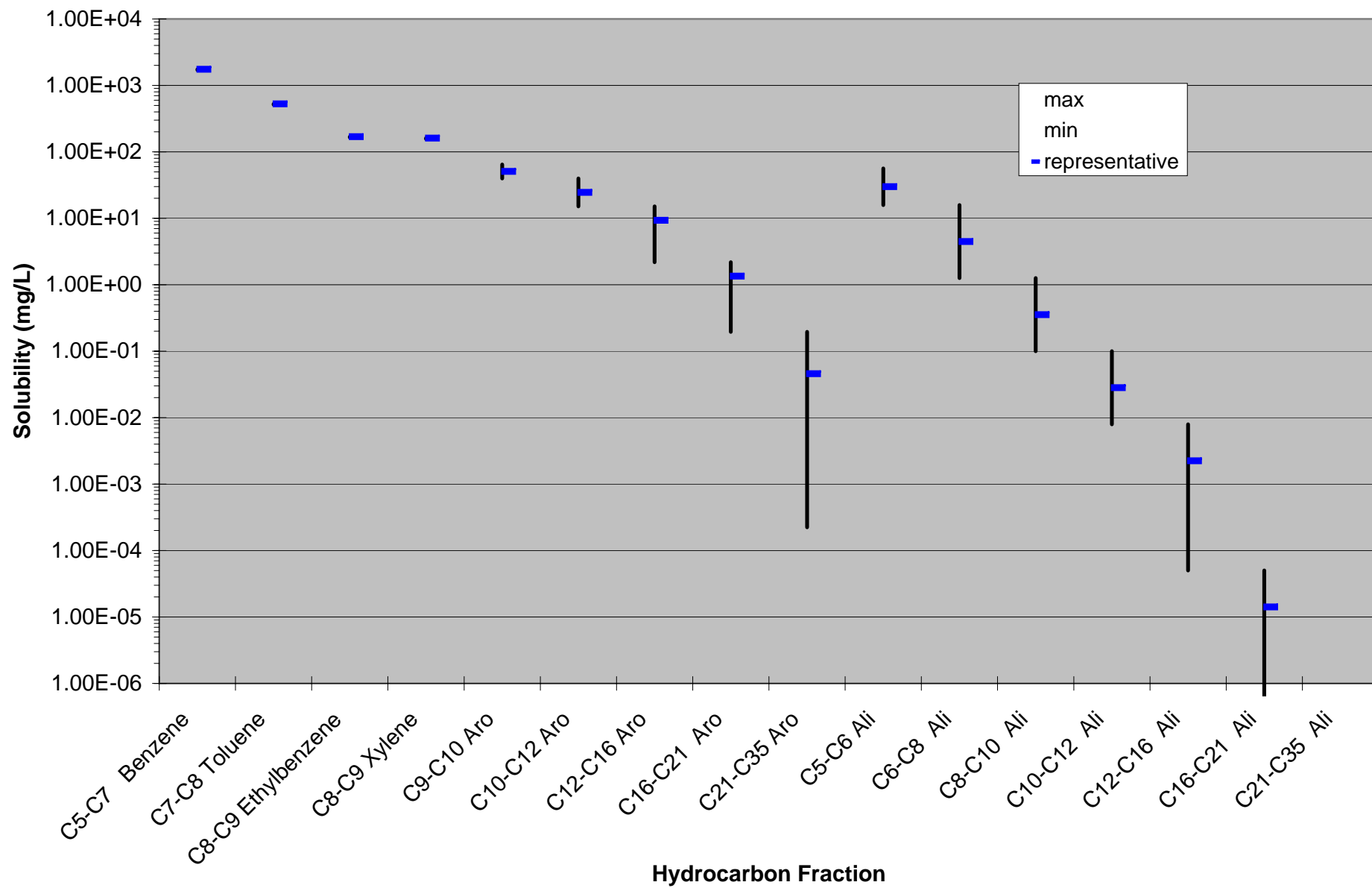


**Figure 2 Average Fuel Sales by Fuel Type, 1998 to 2002**



5 Year Average of Fuel Sales Data in  
the Division of Oil & Gas 2003 Annual  
Report

Figure 3 Solubilities of Hydrocarbon Fractions



**Figure 4 Compilation of Laboratory Test Results into Recommended Hydrocarbon Fractions**

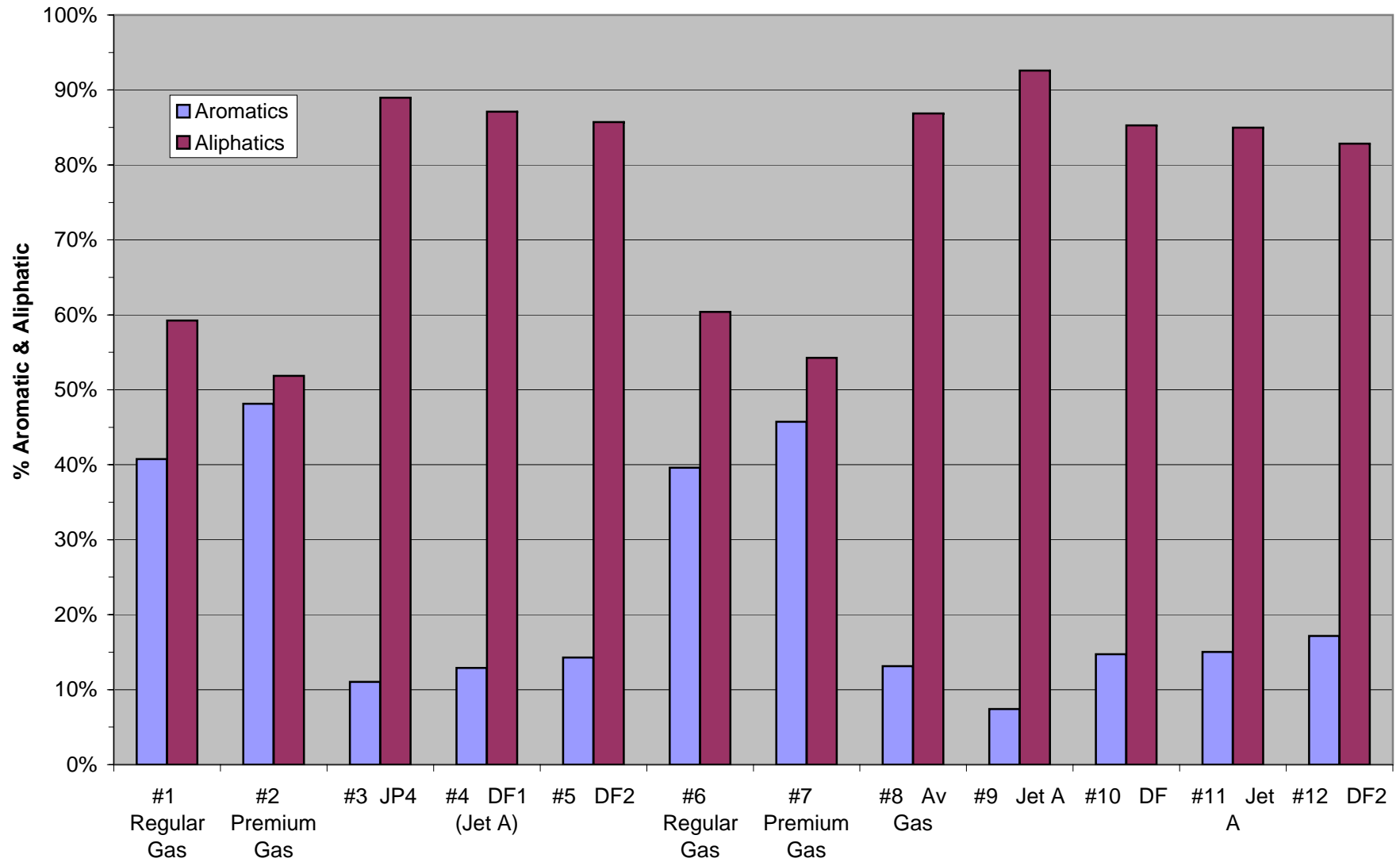
Equivalent Carbon Number	GRO AK101	DRO AK102	RRO AK103	GRO AK101 A&A	DRO AK102 A&A	RRO AK103 A&A	Washington VPH Test	Washington EPH Test	BTEX Test	Recommended Characterization (combines VPH, EPH, BTEX, GRO, DRO and RRO data)			
5										= C5 to C6 fraction of GRO aliphatics * AK 101 GRO concentration			
6	C6 to C10 aromatics & aliphatics			C6 to C10 aromatics	C6 to C10 aliphatics		C5 to C6 aliphatics		benzene	= benzene concentration			
7							C6 to C8 aliphatics		toluene	= toluene concentration			
8									C8 to C10 aromatics	C8 to C10 aromatics	ethylbenzene	= ethylbenzene concentration	
9										C8 to C10 aliphatics	xylene	= xylene concentration	
10		C10 to C25 aromatics & aliphatics			C10 to C25 aromatics	C10 to C25 aliphatics	C8 to C10 aromatics	C8 to C10 aromatics			= C8 to C10 fraction of GRO aromatics * GRO concentration - (ethylbenzene + xylene)		
12									C10 to C12 aromatics	C10 to C12 aromatics			= C10 to C12 fraction of DRO aromatics (more conservative value from VPH or EPH test) * AK 102 DRO concentration
13									C12 to C13 aromatics				= C12 to C16 fraction of DRO aromatics * AK 102 DRO concentration
16										C12 to C16 aromatics	C12 to C16 aromatics		= C16 to C21 fraction of DRO aromatics * AK 102 DRO concentration
21								C16 to C21 aromatics	C16 to C21 aromatics	= C16 to C21 fraction of DRO aliphatics * AK 102 DRO concentration			
25										= C21 to C35 fraction of RRO aromatics * AK 103 RRO concentration			
35			C25 to C35 aromatics & aliphatics							= C21 to C35 fraction of RRO aromatics * AK 103 RRO concentration			







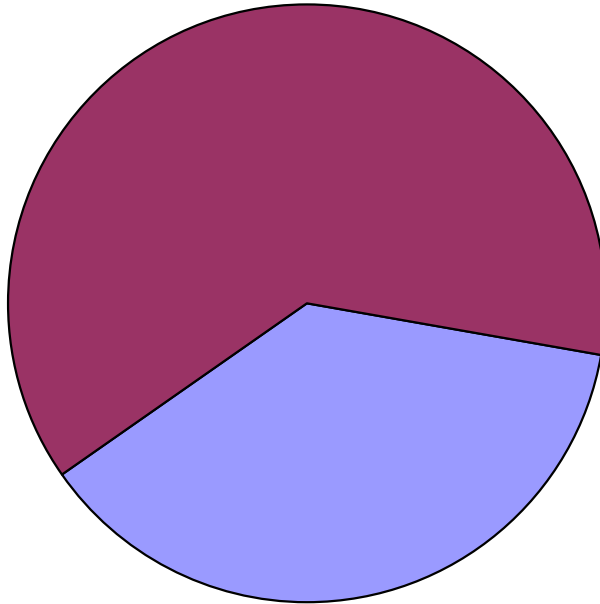
Figure 8 Aromatic and Aliphatic Distribution in Selected Alaskan Fuels





**Figure 9 Average Percent Aromatic & Aliphatics in Selected Alaskan Gasolines**

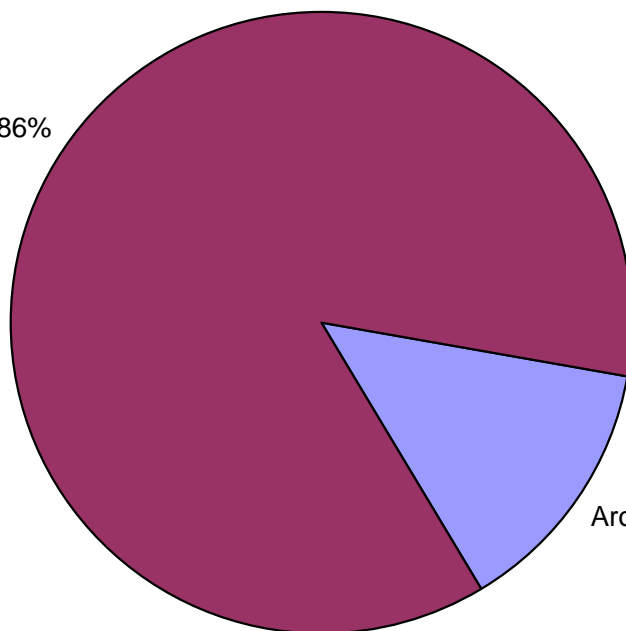
Aliphatics, 63%



Aromatics, 37%

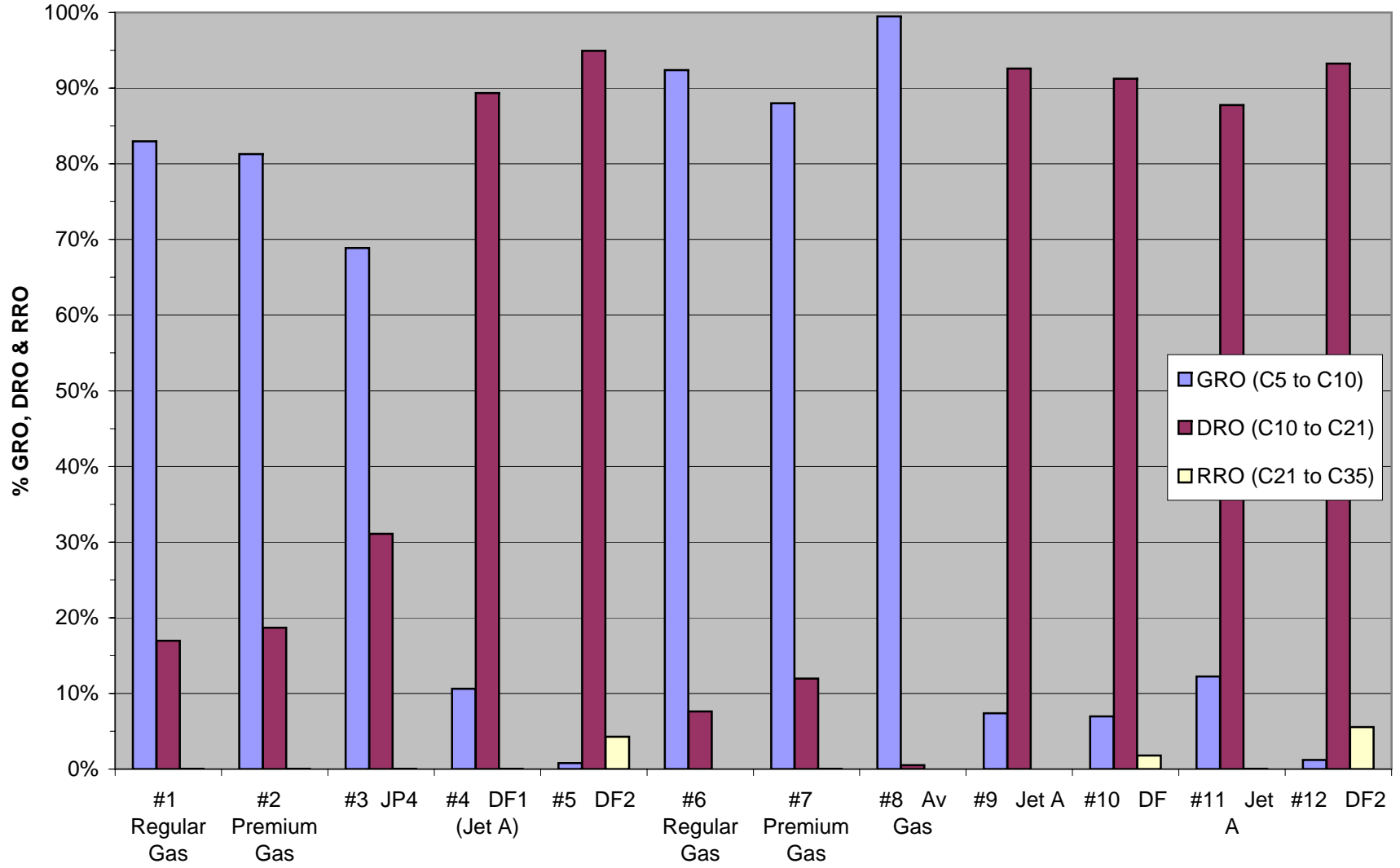
**Figure 10 Average Percent Aromatic & Aliphatics in Selected Alaskan Diesel & Jet Fuels**

Aliphatics, 86%

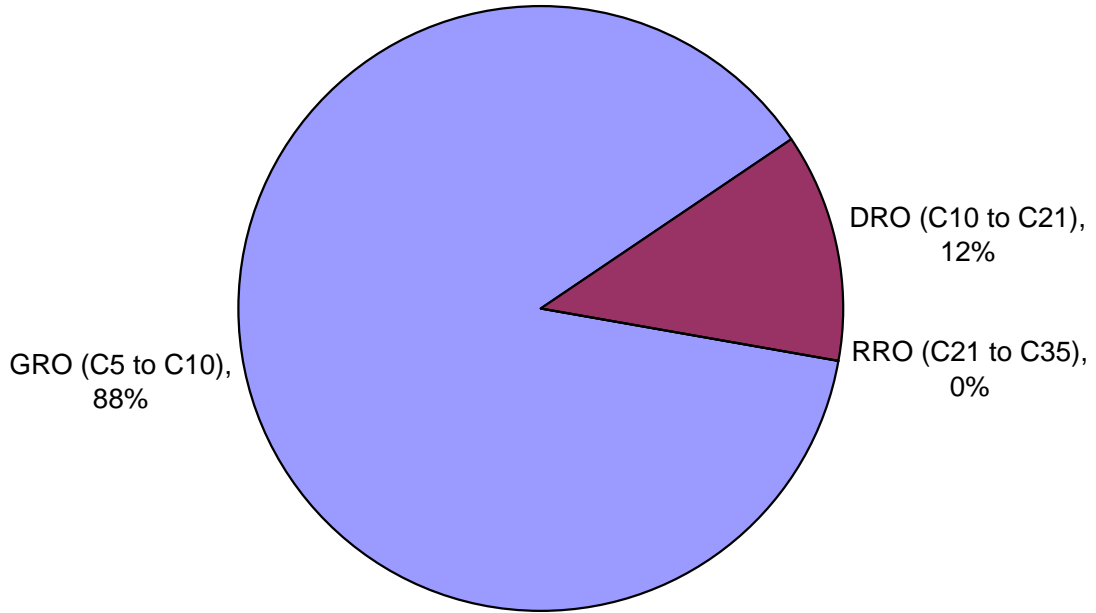


Aromatics, 14%

Figure 11 GRO, DRO & RRO Content of Selected Alaskan Fuels



**Figure 12 Percent GRO, DRO and RRO in Selected Alaskan Gasolines**



**Figure 13 Percent GRO, DRO and RRO in Selected Alaskan Diesel & Jet Fuels**

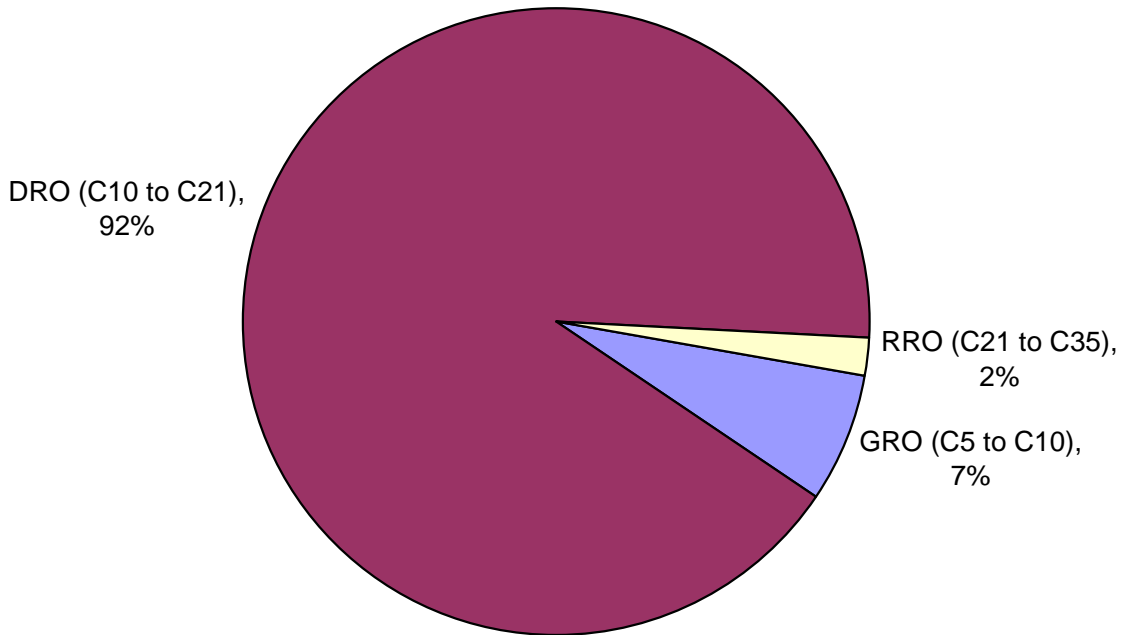


Figure 14 BTEX, GRO & DRO Solubility of Selected Alaskan Fuels

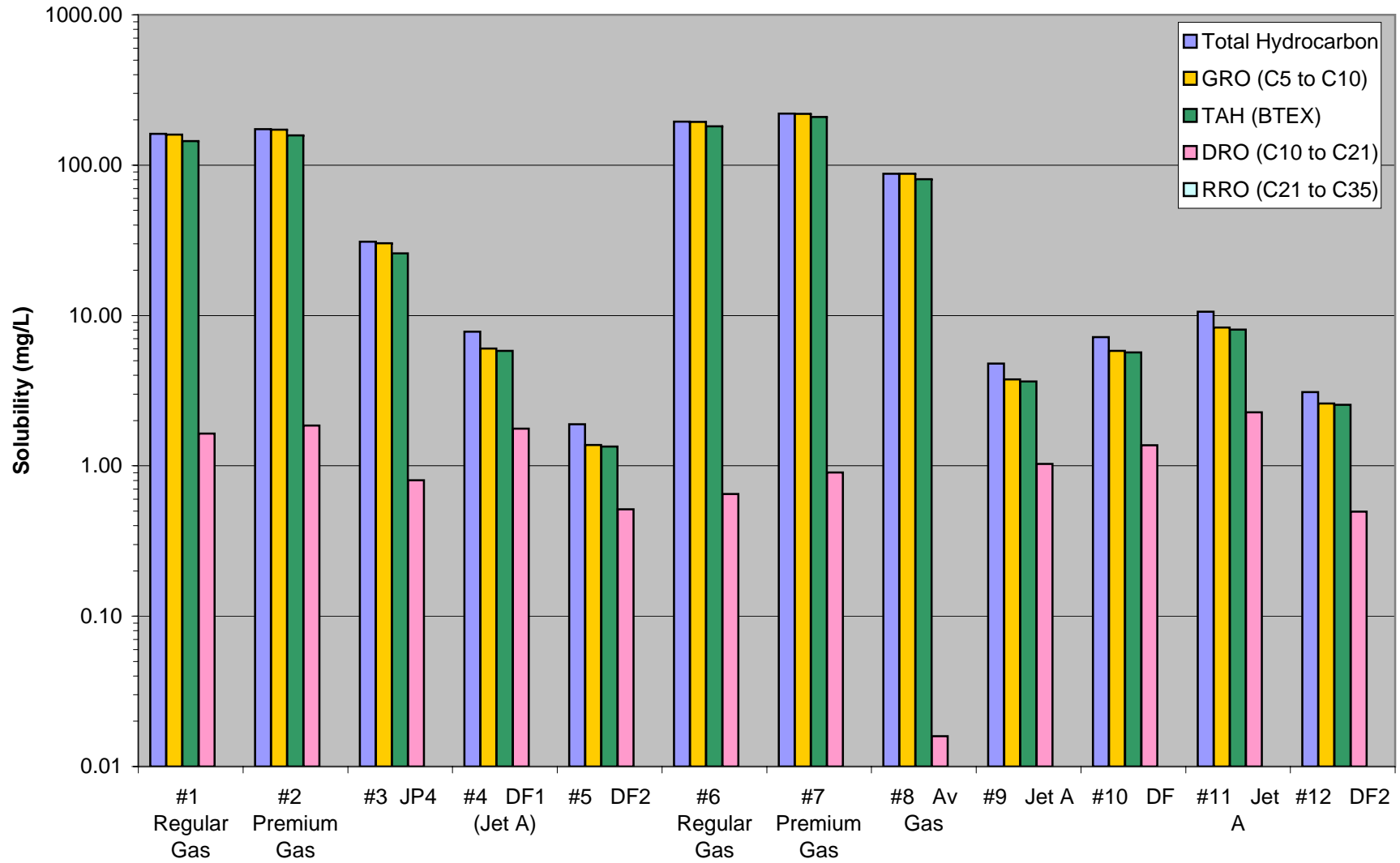
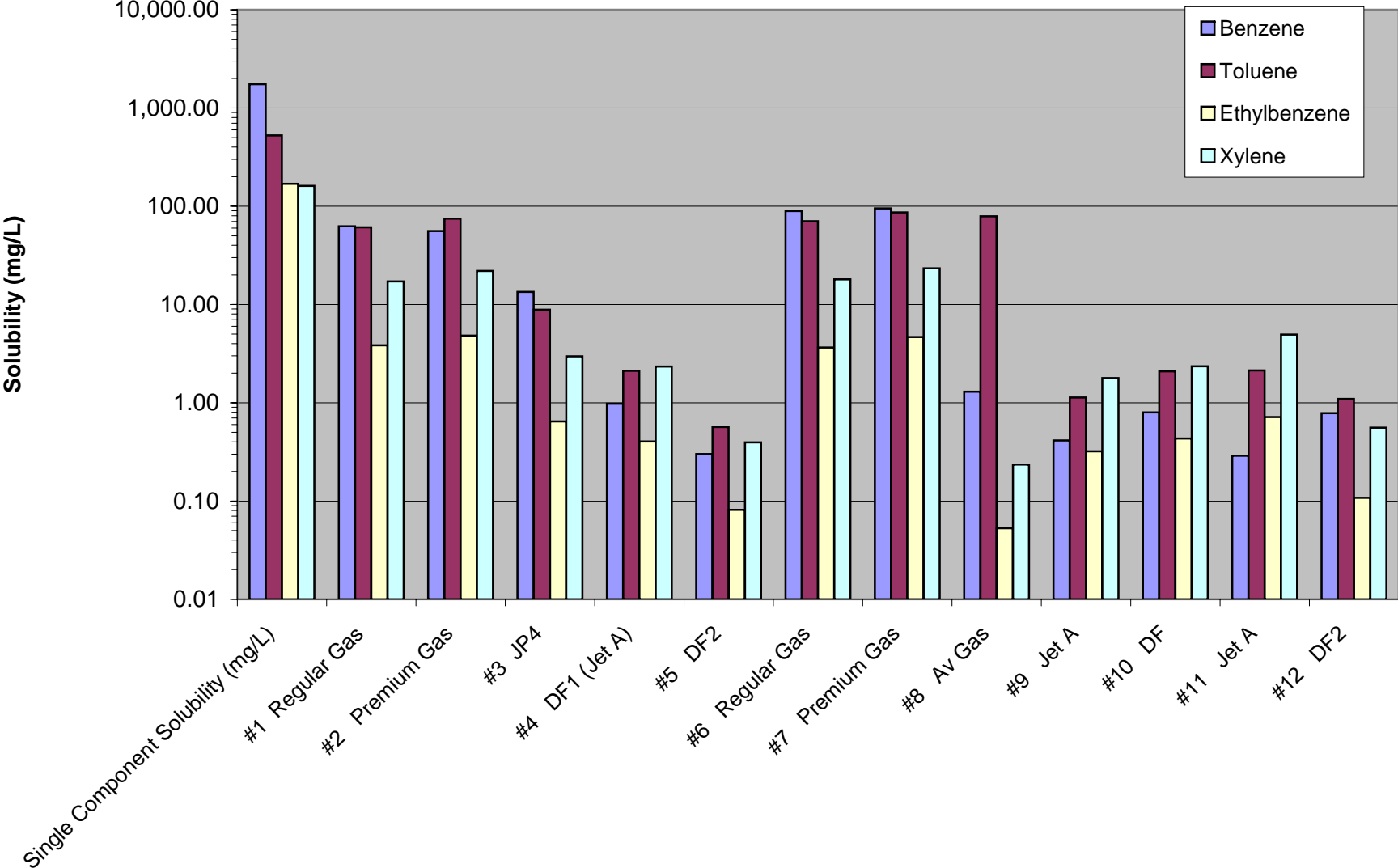
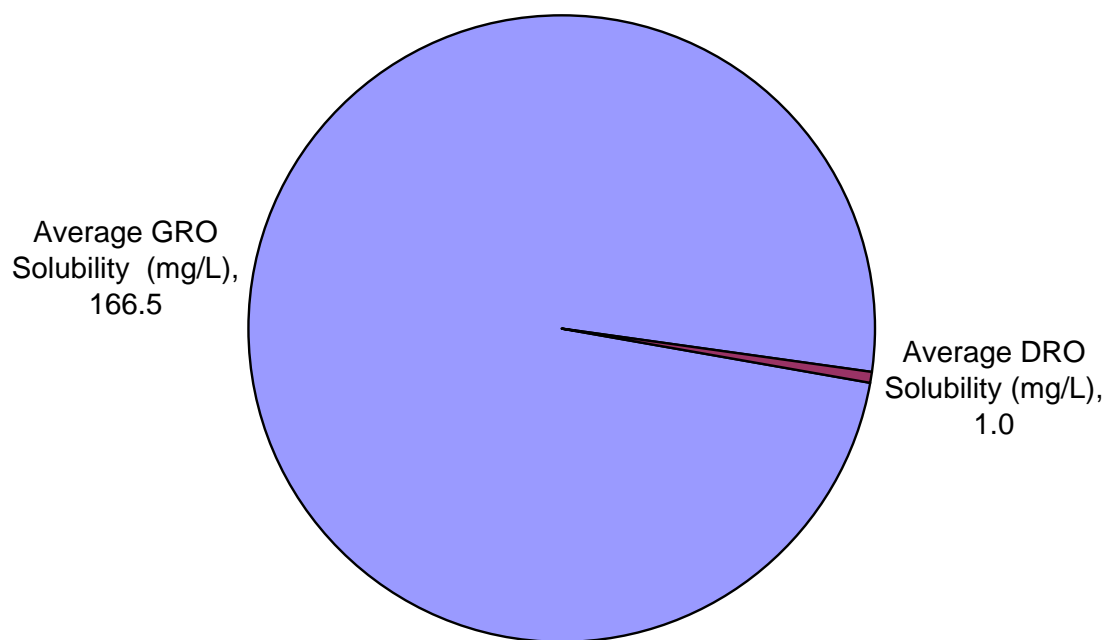


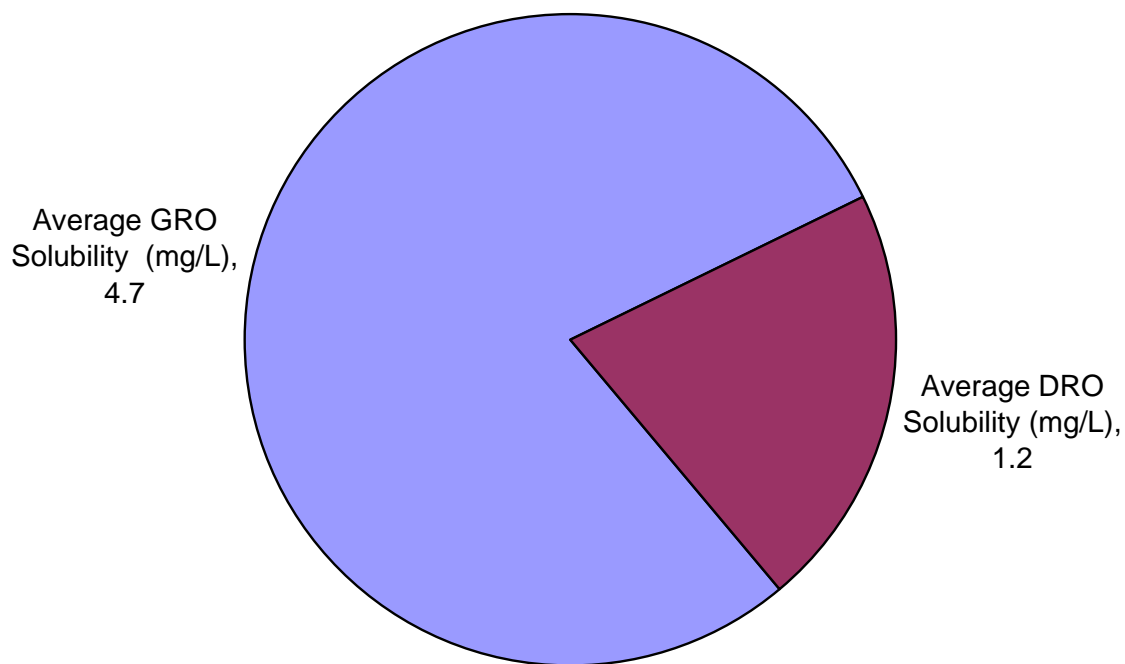
Figure 15 BTEX Solubilities of Selected Alaskan Fuels



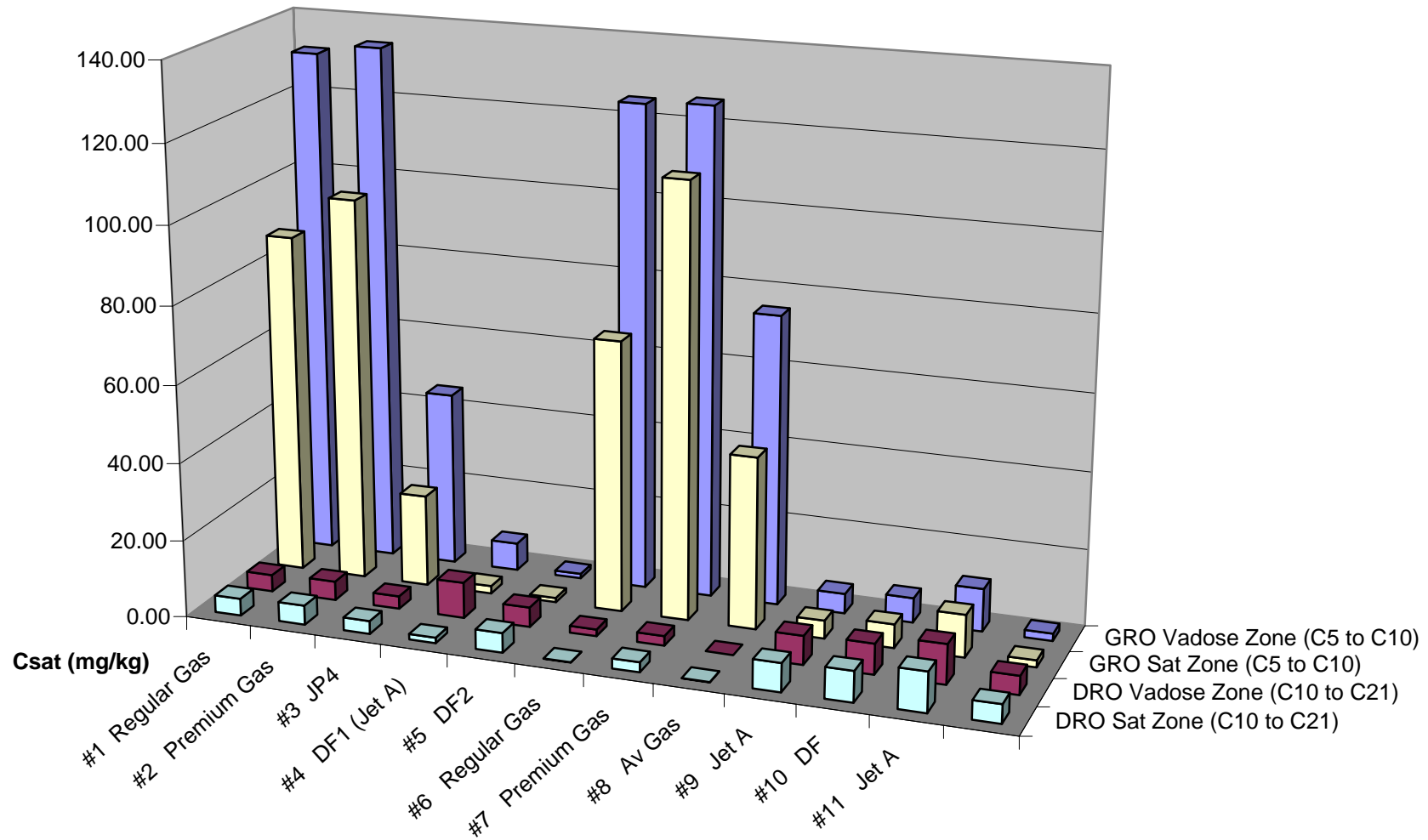
**Figure 16 Average GRO and DRO Solubility in Selected Alaskan Gasolines**



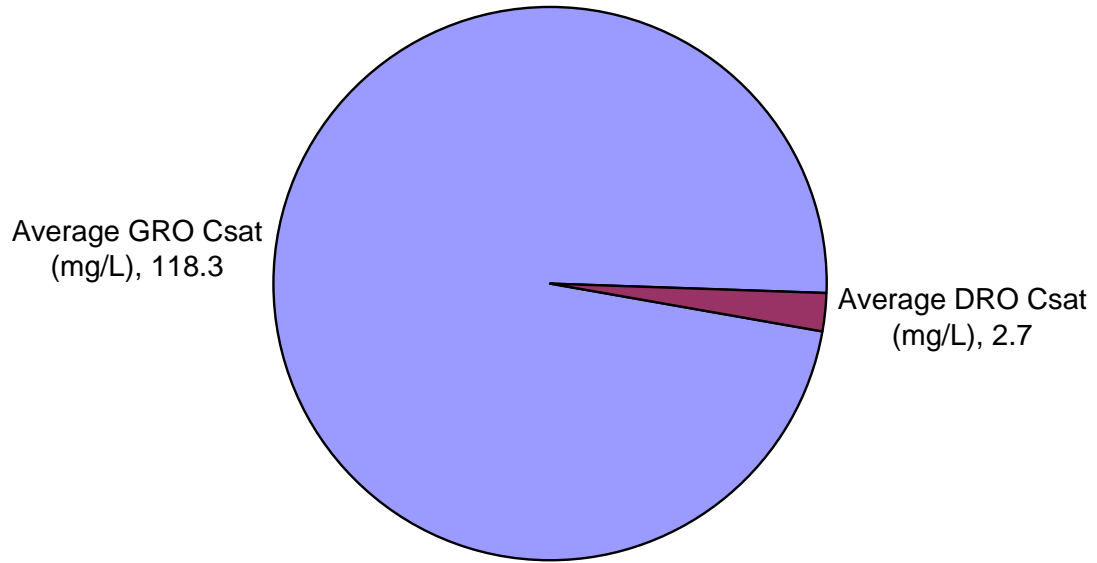
**Figure 17 Average GRO and DRO Solubility in Selected Alaskan Diesel & Jet Fuels**



**Figure 18 Soil Saturation Concentration (C<sub>sat</sub>) Values for Selected Alaskan Fuels**



**Figure 19 Average Vadose Zone Csat Values in Selected Alaskan Gasolines**



**Figure 20 Average Vadose Zone Csat Values in Selected Alaskan Diesel & Jet Fuels**

