

# KEROSENE/JET FUEL CATEGORY ASSESSMENT DOCUMENT

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## SUMMARY

The Kerosene/Jet Fuel category covers refinery streams and finished products commonly referred to by the generic term “kerosene”. The substances in this category are complex petroleum derived substances, have a boiling range of approximately 302 to 554 °F (150 to 290 °C) and a carbon range of approximately C9 – C16. At ambient temperatures, all the substances in this category are liquids with low vapor pressures. The substances in this test plan share many physical properties that make them suitable as blending components for finished fuels such as aviation turbine fuels (jet fuels), No. 1-K kerosene (for heating and illumination), and No. 1 grades of fuel oil, diesel fuel, and gas turbine oil.

The kerosene-range substances have broadly overlapping chemical composition and closely related physical properties. The Petroleum HPV Testing Group (Testing Group) believes the physical and chemical similarities among the streams in this category allow toxicology data on one material to be extrapolated to the others.

### Physical-Chemical Properties:

Substances in the Kerosene/Jet Fuel Category are liquids composed of individual hydrocarbons that boil within the general range of 150°C to 290°C at atmospheric pressure. Measured vapor pressures ranged from 3 hPa to 35 hPa, indicating limited tendency to volatilize. Partition coefficients of constituent hydrocarbons making up these streams ranged from 3.3 to >6. Water solubility measurements taken from water soluble fractions ranged from approximately 5 to 12 mg/L.

### Environmental Fate:

If Kerosene/Jet Fuel category members enter the environment, individual components will disperse and partition according to their individual physical-chemical properties. Their final dispositions are determined by both abiotic and biotic processes. Based on modeling individual structures encompassing the different types and molecular weights of hydrocarbon constituents of kerosenes, volatilization to the atmosphere is an important fate process. Residence times in the atmosphere are relatively short due to indirect photodegradation reactions. In water, hydrolysis is not likely to occur, as the chemical linkages of hydrocarbons do not allow for hydrolytic processes. However, biodegradation data show that these substances can exhibit a moderate to rapid rate of biodegradation and are considered at least inherently biodegradable.

### Ecotoxicity:

The substances in the Kerosene/Jet Fuel Category are expected to produce a similar range of toxicity for the aquatic species when studies using similar solution preparation and exposure techniques are compared. The endpoint values reflect the loading rates of the test substance added to exposure solutions. Termed water accommodated fractions, the WAF preparation is the most appropriate procedure for testing complex substances having low water solubility. The results of studies of representative substances confirmed that the range of acute toxicities was similar for the three trophic levels (fish, invertebrates, and algae) when similar testing methods were used. The “read-across” ranges of acute toxicity endpoints (expressed as lethal loading rates, LL/EL50 values) that are proposed as representative of the potential aquatic toxicity are:

Fish	18 – 25 mg/L
Invertebrates	1.4 – 21 mg/L
Algae	5.0 – 11 mg/L

### Human Health Effects:

The low vapor pressures of substances in this category make dermal the most likely route of exposure

both in the workplace and the general population. LOAEL and NOAEL designations for repeated dose and developmental/ reproduction studies for read-across to untested category members are derived from dermal results.

Acute Dermal Toxicity: LD50 >2000 mg/kg

Repeated Dose Dermal Toxicity: Substances in the Kerosene/Jet Fuel Category are skin irritants upon repeated exposure. Studies up to 13-weeks duration in rats with kerosene substances have not reported significant systemic effects including neurotoxicity or effects on the reproductive organs of either sex. The read-across NOAEL value for untested category members is 495 mg/kg/d dermal exposure.

In Vitro Genetic Toxicity – Gene mutation: The potential in vitro genotoxicity of kerosene and jet fuel has been evaluated in a variety of studies. Standard Ames assays, optimized Ames assays, mouse lymphoma assays, and sister chromatid exchange assays have been conducted with predominately negative results. The read-across conclusion for untested substances in this category is that kerosenes are not genetic toxicants under in vitro conditions.

In Vivo Genetic Toxicity – Cytogenetics: Many in vivo genotoxicity studies have been done on a variety of kerosene-based materials. Bone marrow cytogenetic tests, sister chromatid exchange assays, dominant lethal assays, and red blood cell micronucleus studies have been conducted with predominately negative results. The read-across conclusion for untested substances in this category is that kerosenes are not genetic toxicants under in vivo conditions.

Developmental Toxicity: There were no significant effects on fetal development or growth in an OECD 421 reproductive-developmental screening study on hydrodesulfurized kerosene. Both oral and inhalation studies with kerosenes have also been conducted without evidence of significant effects on the fetus. The read-across NOAEL value for developmental toxicity for untested substances in this category is 495 mg/kg/d dermal exposure.

Reproductive Toxicity: There were no significant effects on the reproductive organs of male and female rats exposed for 13-weeks to hydrodesulfurized kerosene (NOAEL 495 mg/kg/d). An OECD 421 reproductive-developmental screening test on hydrodesulfurized kerosene had a NOAEL 495 mg/kg/d. The read-across NOAEL value for reproductive toxicity for untested substances in this category is 495 mg/kg/d dermal exposure.

## 1.0 DESCRIPTION OF THE KEROSENE/JET FUEL CATEGORY

The Kerosene/Jet Fuel category covers substances and finished products commonly referred to by the generic term “kerosene”. The specific CAS numbers and descriptions of category members are detailed in Appendix A. The generic term “kerosene” is used to describe the fraction of crude oil that boils approximately in the range of 302 to 554 °F (150 to 290°C) and consists of hydrocarbons approximately in the range of C9-C16. Kerosenes are the lighter end of a group of petroleum substances known as middle distillates, the heavier end being gas oils (See Figure 2).

The predominant use of kerosene in the U.S.A is aviation turbine fuel for civilian (using Jet A or Jet A-1) and military (using JP-8 or JP-5) aircraft. Kerosenes are also used as diesel fuel (No. 1), domestic heating fuel (Fuel oil No. 1), and illuminating kerosene (No.1-K). Kerosene-based fuels differ from each other in performance specifications (primarily freezing point or sulfur concentration) and minor amounts of performance additives that may be added (generally less than 0.1% v/v) (CONCAWE 1995, 1999, ASTM, 2001a,b; 2002).

The Testing Group has utilized information on the kerosene-type jet fuels in assessing effects on category members although these fuels do not appear by name among the Chemical Abstract Services (CAS) numbers covered in this category (see Table 1.) Kerosene-type jet fuels (such as Jet A & JP-8) do not have CAS numbers and are not specifically identified on the Toxic Substances Control Act’s (TSCA) Chemical Inventory of Substances. However, the Testing Group believes testing done on a kerosene-type jet fuel can be extrapolated to all the substances in this Category. Products from the refining of crude oil are rarely, if ever, sold by TSCA Inventory identifiers. The refining and sale of petroleum products pre-dates development of CAS and TSCA nomenclature. The fungible products that leave a refinery are sold based on the product meeting certain performance, physical, or chemical specifications which make them fit for purpose (i.e., “on-road” diesel fuel, illumination grade kerosene, and USP white mineral oil). The standard specifications for the primary kerosene products used in the USA are found in Table 2.

**Table 1. Kerosene/Jet Fuel Category Members and Supporting Substances**

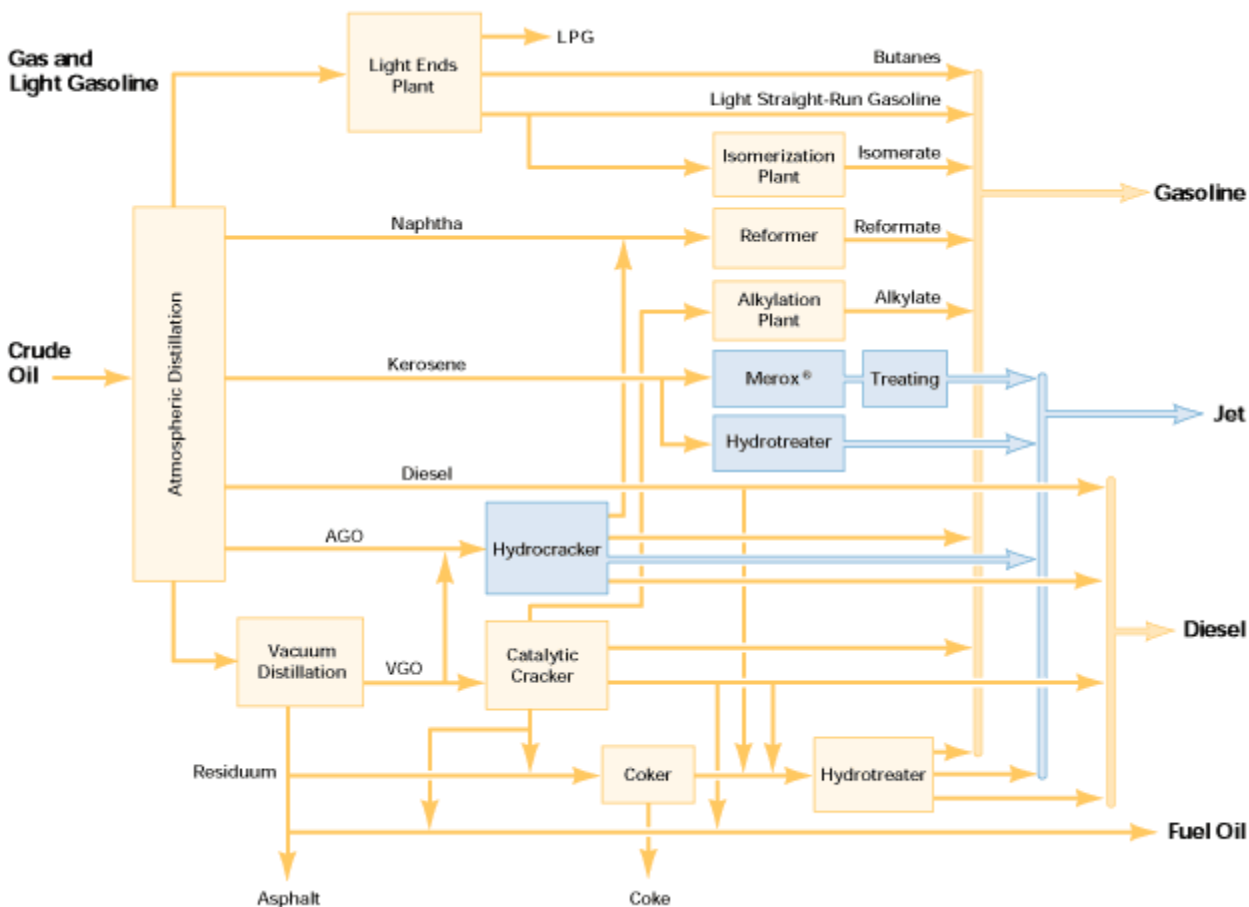
CAS #	NAME	
8008-20-6	Kerosene (petroleum)	Category member
64742-14-9	Acid Treated Light Distillate, Light	Category member
64742-31-0	Distillates (petroleum), chemically neutralized light	Category member
64742-81-0	Kerosene (petroleum), hydrodesulfurized	Category member
64742-47-8	Distillates (petroleum), hydrotreated light	Category member
64742-96-7	Solvent naphtha (petroleum), heavy aliph.	Category member
91770-15-9	Kerosene (petroleum), sweetened	Supporting substance
101316-80-7	Solvent naphtha (petroleum), hydrocracked heavy arom.	Supporting substance
NONE	Aviation Turbine Fuels (ASTM or USA Military specification)	Supporting materials

**Table 2. Kerosene Product Specifications**

<b>Product</b>	<b>Standard</b>	<b>Designation</b>
Kerosene No. 1-K or No. 2-K	ASTM	D 3699
Jet A or Jet A-1	ASTM	D 1655
JP-8 and JP-8+100	DOD	MIL-DTL-83133F
JP-5	DOD	MIL-DTL-5624 U
Diesel Fuel No. 1-D	ASTM	D 975
Gas Turbine Fuel Oil No. 1-GT	ASTM	D 2880
Fuel Oil No. 1	ASTM	D 396

As can be seen in Figure 1, there are several refinery processes that make hydrocarbon streams suitable for blending kerosene-range products (White, 1999). Kerosene may be obtained either from the atmospheric distillation of crude oil (straight-run kerosene) or from cracking of heavier petroleum streams (cracked kerosene). The kerosenes can be further treated by a variety of processes to remove or reduce the levels of undesirable components, e.g. sulfur, nitrogen or olefinic materials. This additional processing also reduces compositional variation and enriches components that improve performance (cycloalkanes and isoalkanes). In practice, the major refining processes used are hydrodesulfurization (treatment with hydrogen to remove sulfur components), washing with caustic soda solution (to remove mercaptans and other sulfur-containing components), and hydrotreating (to remove olefins, sulfur- and nitrogen-containing components). For instance, hydrodesulfurized kerosene (CAS no. 64742-81-0) is obtained by treating a kerosene-range petroleum stock with hydrogen to convert organic sulfur to hydrogen sulfide, which is then removed. These subsequent treatments may blur the distinction between “straight-run” and “cracked” kerosenes (CONCAWE 1995, 1999).

**Figure 1. Kerosene/Jet Fuel Processing**



ChevronTexaco, 2003  
 Note: Mercox® = mercaptan oxidation – reduces mercaptan levels

Although straight run kerosene can be marketed directly, more commonly, several kerosene-range streams may be blended to produce desired products. However, whether straight run or blended, all kerosene-based fuels are produced to meet the appropriate specifications for heating and illumination fuels, diesel fuels, or aviation turbine fuels (ASTM 2001a,b, 2002). Since specifications for both the heating and transportation fuels are similar; it is often possible for refiners to satisfy the performance requirements of both applications with the same substance or blend of process streams. The final products are essentially the base kerosene with additives (if necessary and allowed) for the intended use. Otherwise these petroleum substances and kerosene fuel products are virtually indistinguishable on the basis of physical or chemical properties (CONCAWE 1995, 1999).

While kerosenes are similar in composition, the precise composition of a specific kerosene-range refinery stream depends on the crude oil from which the kerosene was derived and on the refinery processes used for its production. Because they are complex petroleum derived hydrocarbons, substances in this category are typically not defined by detailed compositional data but instead by process history, physical properties, and product-use specifications (ASTM 2001a,b, 2002). General compositional information (Table 3) on representative kerosene-range refinery streams and fuels illustrates the fact that the members of this category are all similar in their physical properties and composition (API, 1987b); Dickson, 2002,



CONCAWE, 1995);. Regardless of the crude oil source or processing history, the major components of all kerosenes are branched and straight chain paraffins and naphthenes (cycloparaffins), which normally account for at least 70% by volume. Aromatic hydrocarbons in this boiling range, such as alkylbenzenes (single ring) and alkylnaphthalenes (double ring) do not normally exceed 25% by volume of kerosene streams. Olefins are usually not present at more than 5% by volume. This is illustrated by an analysis of fourteen samples of Jet A conducted by a Petroleum HPV Testing Group member company (Table 4). The samples were from seven different refineries across the USA using different crude oils and refining processes. A published analysis of a sample of hydrodesulfurized kerosene also illustrates these same properties (Table 5).

**Table 3. Compositional Data on Representative Kerosene-Range Materials**

	<b>8008-20-6</b>	<b>64742-81-0</b>	<b>Jet A</b>	<b>JP-8</b>	<b>91770-15-9</b>	<b>101316-80-7</b>
API gravity	41.8 – 44.9	39 – 45.5	37.2- 46.1	37.0 – 46.7	45.3	43.8
Aromatic content, vol. %	15.5 – 19.6	18 – 21.4	11.6 – 24.0	13.6 – 22.1	18	19.3
Olefin content, vol %	1.3 - 2.5	1.0 – 1.66	0.0 – 4.1	0.6 – 3.0	1.0	1,7
Saturates content, vol %	79 - 82	77.2 – 82	71.9 - 88.4	74.9 - 85.8	81	79
Distillation, °F						
10%	320 - 377	329 -406	294 – 394	333 – 390	332	368
Final	468 - 538	451 - 568	404 – 510 (90%)	419 – 474 (90%)	495	550

**Table 4. Fuel Survey Results for Jet A**

Measurement	Average n=14	Min	Max
Specific Gravity, D 1298 or D 4052	0.81	0.80	0.82
Viscosity, 40C,D 445, CST	1.39	1.27	1.51
Distillation, D 86, F			
Initial BP	312.1	281.0	331.0
10%	353.7	332.0	376.5
50%	409.5	391.0	424.0
90%	481.1	458.0	498.0
End Pt	524.1	489.0	551.0
Recovery, Vol %	98.2	97.5	99.3
Residue, Vol %	1.0	0.5	1.3
Loss, Vol %	0.8	0.0	1.5
Extended FIAM by HPLC, Vol %			
Aromatics	21.18	17.90	27.20
Olefins	0.00	0.00	0.00
Par/NP	78.82	72.80	82.10
Mass Spec, D 2425, Wt %			
Paraffins	46.66	32.60	59.10
Monocycloparaffins	26.19	13.80	34.20
Dicycloparaffins	5.89	4.10	8.50
Tricycloparaffins	0.77	0.40	1.40
Benzenes	12.99	9.50	16.50
Indans/Tetralins	4.05	2.50	6.60
CnH2n-10	0.96	0.60	1.80
Naphthalene	0.44	0.00	1.10
Naphthalenes	1.46	0.90	2.00
CnH2n-14	0.34	0.20	0.50
CnH2n-16	0.23	0.00	0.50
CnH2n-18	0.00	0.00	0.00
Total Saturates	78.82	72.80	82.10
Total Aromatics	21.18	17.90	27.20
Aromatics, D 5769, WT%			
Total	10.46	7.55	16.49
BENZENE	0.01	0.00	0.02
TOLUENE	0.14	0.06	0.50
ETHYLBENZENE	0.15	0.08	0.26
M,P-XYLENE	0.54	0.24	1.25
1,2-DIMETHYLBENZENE	0.24	0.11	0.51
ISOPROPYL-BENZENE	0.07	0.05	0.11
PROPYL-BENZENE	0.14	0.06	0.25
1-METHYL-3-ETHYLBENZENE	0.50	0.21	1.02
1-METHYL-4-ETHYLBENZENE	0.13	0.04	0.24
1,3,5-TRIMETHYLBENZENE	0.25	0.11	0.65

	1-METHYL-2-ETHYLBENZENE	0.18	0.02	0.30
	1,2,4-TRIMETHYLBENZENE	0.94	0.50	1.78
	1,2,3-TRIMETHYLBENZENE	0.33	0.20	0.43
	INDAN	0.06	0.00	0.12
	ALKYL INDANS	0.61	0.06	1.13
	1,4-DIETHYL+BUTYLBENZENE	0.32	0.11	0.50
	1,2-DIETHYLBENZENE	0.18	0.02	0.41
	1,2,4,5-TETRAMETHYLBENZENE	0.11	0.09	0.20
	1,2,3,5-TETRAMETHYLBENZENE	0.46	0.08	0.72
	C10 BENZENES	1.34	0.10	2.76
	C11 BENZENES	2.88	0.69	4.53
	C12 BENZENES	0.18	0.07	0.34
	NAPHTHALENE	0.18	0.07	0.30
	2-METHYL-NAPHTHALENE	0.38	0.18	0.57
	1-METHYL-NAPHTHALENE	0.28	0.13	0.37

Data provided by a member company of Petroleum HPV Testing Group

**Table 5. Chemical Composition of a Hydrodesulfurized Kerosene Sample**

<b>Component<sup>a</sup></b>	<b>Weight percent</b>
Nonaromatics	80.27
Saturates	78.61
Olefins	1.66
Aromatics	19.72
Less than three-ring PAC <sup>b</sup>	≈19.72
Three- to seven-ring PAC <sup>b</sup>	<0.01

<sup>a</sup>Analyzed by ASTM Method D1319-1, Fluorescent indicator Adsorption.

<sup>b</sup>Polycyclic aromatic compounds.

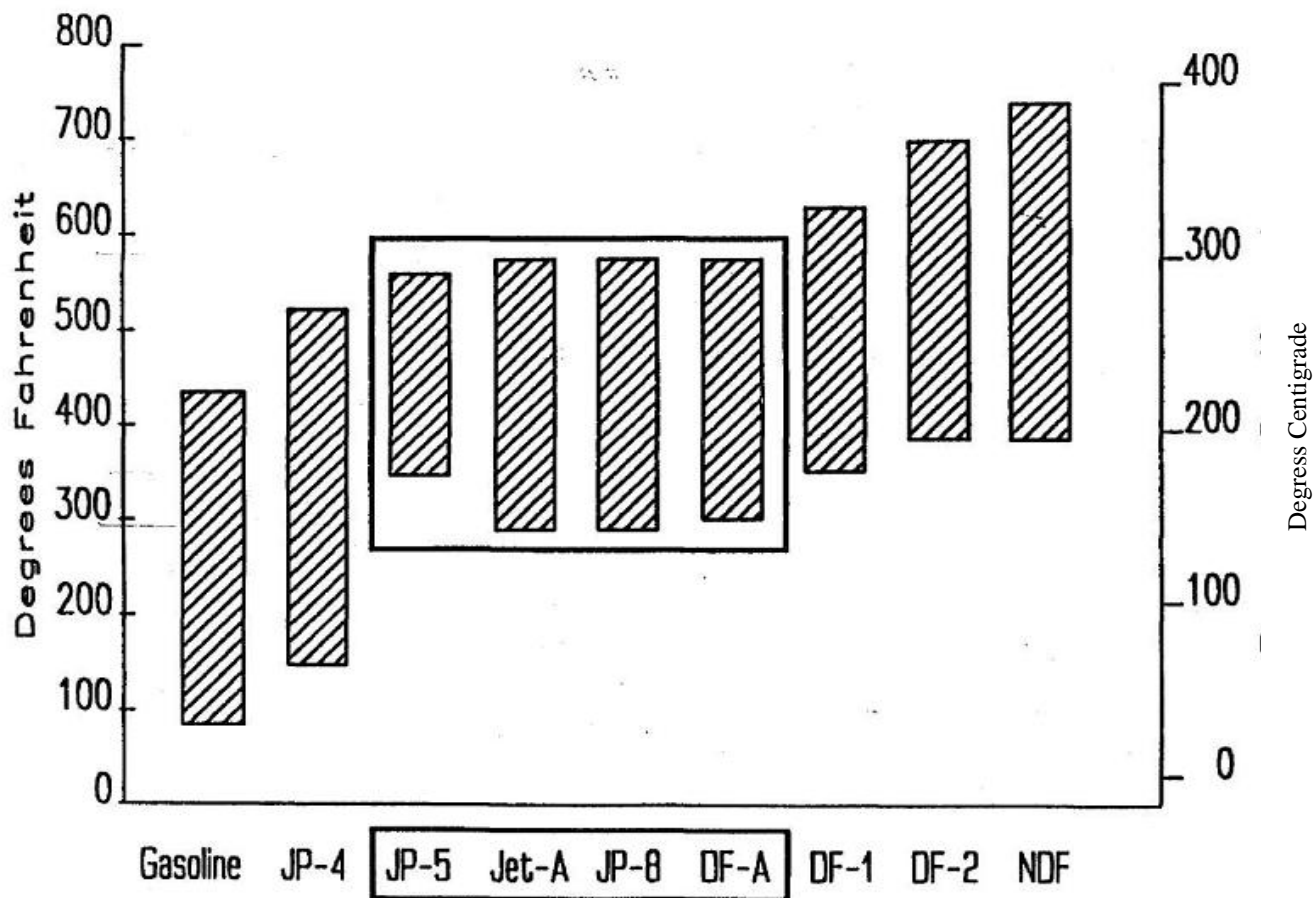
(Schreiner et al., 1997)

The distillation range of kerosenes is such that benzene (80 °C boiling point) and n-hexane (69 °C boiling point) concentrations are typically below 0.01 % by mass. The boiling points of the 3 - 7 fused-ring polycyclic aromatic compounds (PACs) are well above the boiling range of straight-run kerosene streams. Consequently, the concentrations of 3 - 7 PACs found in kerosenes are very low, if not below the limits of detection of the available analytical methods (CONCAWE 1995, 1999). This is also demonstrated in Table 6 where the Testing Group analyzed a series of kerosenes using the ASTM E1687 method which separated aromatic-ring classes (ARC) by boiling point after extraction with DMSO. Only 1-ring and 2-ring compounds were found.

**Table 6. Analysis of Kerosene/Jet Fuels for Polycyclic Aromatic Compounds by ASTM E 1687**

<b>Substance/Product</b>	<b>DMSO Extractable wt.%</b>	<b>% ARC 1</b>	<b>% ARC 2</b>	<b>% ARC 3</b>	<b>% ARC 4</b>	<b>% ARC 5</b>	<b>% ARC 6</b>	<b>% ARC 7</b>
Jet A	2.6	0.5	2.1	0.0	0.0	0.0	0.0	0.0
JP-8 (unadditized)	2.9	0.6	2.3	0.0	0.0	0.0	0.0	0.0
No. 1-K Kerosene	1.9	0.6	1.4	0.0	0.0	0.0	0.0	0.0
Kerosene (petroleum), hydrodesulfurized	1.9	0.4	1.5	0.0	0.0	0.0	0.0	0.0
Kerosene (petroleum), hydrodesulfurized	3.4	1.0	2.4	0.0	0.0	0.0	0.0	0.0
Kerosene (petroleum), hydrodesulfurized	2.0	0.6	1.4	0.0	0.0	0.0	0.0	0.0
Kerosene (petroleum), hydrodesulfurized	2.2	0.7	1.6	0.0	0.0	0.0	0.0	0.0
Kerosene (petroleum), hydrodesulfurized	4.3	0.4	3.9	0.0	0.0	0.0	0.0	0.0

Figure 2. Boiling Ranges of Fuels



U.S. Army, 2001

## 2.0 CATEGORY DEFINITION AND JUSTIFICATION

The Kerosene/Jet Fuel category covers substances and finished products commonly referred to by the generic term “kerosene”. The finished products meet performance, physical, and chemical specifications appropriate for their use. The materials in this category are complex petroleum substances, with boiling ranges of approximately 302 to 554 °F (150 to 290 °C) and carbon numbers in the range of approximately C9 – C16. Because the HPV substances included in the Category are related by physical-chemical properties and product blending utility, toxicology data on one substance can be considered as representative of other category members. The Testing Group believes the existing physicochemical, environmental data, and toxicology information is sufficient to characterize the SIDS endpoint hazards under the HPV Challenge program.

### 3.0 PHYSICAL-CHEMICAL PROPERTIES

The physicochemical endpoints for the EPA HPV chemical program include melting point, boiling point, vapor pressure, octanol/water partition coefficient (log Kow), and water solubility.

Although some data exist for some substances in this category, not all of these endpoints are defined and a consensus database for physical-chemical values for all substances in this category does not exist. Further, because of the complex nature of the substances in the category, some physical-chemical properties are best represented by a range of values depending on the specific constituents and their concentrations in the various substances. For example, a complex substance containing a number of individual chemical constituents does not have a single boiling point, but a range of boiling points reflecting the constituent properties. Therefore, measured data were provided when available, calculations based on representative constituents were made when necessary, and technical discussions were given in those situations which do not apply to the substances in the category.

For the physical-chemical properties that cannot be defined for complex substances, ranges of endpoint values were reported for representative paraffinic, naphthenic, olefinic, and aromatic hydrocarbons compounds (PONA) covering the molecular weight ranges (C9 to C16 carbon atoms) in these streams. Individual compounds were chosen from detailed hydrocarbon analyses of selected streams using gas chromatography. The EPI-Suite™ computer model (EPA, 2000), as discussed in the US EPA document entitled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program" (EPA, 1999) was used to calculate physical-chemical properties of representative hydrocarbon constituents in these substances. When the physical-chemical attributes are compared across the various substances that are characterized and described in the robust summaries, it is evident that their physical-chemical properties are similar.

#### 3.1 Melting Point

For complex substances like petroleum products, there is no single melting point; rather, melting occurs over a range of temperatures reflecting the melting points of the individual components. To better describe the physical phase or flow characteristics of petroleum products, the pour point is routinely used. The pour point is the lowest temperature at which movement of the test specimen is observed under prescribed conditions of the test (ASTM, 1999). The product's viscosity decreases as the pour point temperature falls. Pour point values for a variety of kerosenes or jet fuels have been reported in the literature. The pour point of a sample of straight-run kerosene (CAS no. 8008-20-6) with 15 - 20% aromatics was measured by API (1987b) to be -55 °C. The pour point values for three jet fuels reported by Jokuty et al. (2002) ranged from -50 to -47 °C. This narrow range of pour points is indicative of the relative homogeneity of the composition of jet fuel products.

An alternative measure of this endpoint commonly used for aviation fuels is the freezing point, which is defined as the temperature below which solid hydrocarbon crystals may form in aviation fuels (ASTM method D2386; ASTM, 2006). The ASTM and military specifications for freezing point are either -40°C max (Jet A) or -47°C max (JP-8).

### **3.2 Boiling Point**

Like most refinery streams, kerosenes do not have a single numerical value for boiling point, but rather a boiling or distillation range that reflects the individual components in each substance. Distillation ranges for a variety of jet fuels and kerosene blending streams have been reported (CONCAWE, 1995; Jokuty et al., 2002, API, 1987b). These values are generally consistent with the distillation range of 150 to 290 °C described by the Chemical Abstract Services definitions for the general category of kerosenes having hydrocarbon components predominantly in the range of C9 to C16 (Appendix 1).

### **3.3 Vapor Pressure**

Raoult's Law states that the vapor pressure of solutions is the sum of the products of the vapor pressures of each individual constituent times its mole fraction in the mixture. Because kerosene is composed of hydrocarbons with appreciable individual vapor pressures, the streams in this category also would be expected to have measurable vapor pressures. Kerosenes generally are expected to have measurable vapor pressures due to their boiling range (150 to 290 °C) and molecular weights of the constituent hydrocarbons (C9 – C16 carbon atoms). The vapor pressures of kerosene (CAS # 8008-20-8) (API, 1987b) and Jet A/A-1 (Jokuty et al., 2002) measured at 37.8 °C using ASTM D323 were 14 hPa and >10 hPa, respectively. Vapor pressure values from the U.S. Air Force for jet fuels JP5 and JP8 at 21 °C were 3 - 35 hPa (U.S. Air Force, 1989). These directly-measured values are considered to be representative of the general category of kerosenes and jet fuels and the petroleum refining streams that produce them.

### **3.4 Octanol:Water Partition Coefficient**

The percent distribution of the hydrocarbon groups (i.e., paraffins, olefins, naphthenes, and aromatics) and the carbon chain lengths of hydrocarbon constituents in kerosenes and jet fuels largely determine the partitioning characteristics of the mixture. Generally, hydrocarbon chains with fewer carbon atoms tend to have lower partition coefficients than those with higher carbon numbers (CONCAWE, 2001). Because kerosenes are complex substances, it is not possible to determine their log Kow values. Rather, partition coefficients have been calculated for individual component hydrocarbons from known hydrocarbon composition (CONCAWE, 1995) to establish a range of calculated Kow values from 3.3 to >6 for straight-run and hydrodesulfurized kerosene (both 82% saturated hydrocarbons). Those estimates are in agreement with a range of log Kow values of 3.3 to >6 determined by the Testing Group using EPI-Suite™ (EPA, 2000) for various C9 to C16 hydrocarbon components in kerosenes. Given that the ranges of log Kow values for the different hydrocarbon molecules are similar (see robust summary, Appendix C), kerosenes with varying proportions of saturated, aromatic, and olefinic hydrocarbons would be expected to have log Kow ranges of 3.3 to > 6.

### **3.5 Water Solubility**

Water solubility values for the individual hydrocarbon constituents making up kerosenes vary by orders of magnitude. For individual compounds, both molecular weight and chemical structure influence the degree of solubility (Shiu, et al., 1990; Yaws, et al., 1994). The total solubility of all components in these substances will be affected by component composition and the loading rates of water to oil. For many types of petroleum substances, Shiu et al. (1990) concluded that maximum dissolution of hydrocarbons can be obtained at water/oil ratios of  $\leq 40:1$ . An indication of kerosene's water solubility was shown in aquatic toxicity studies that used water soluble fractions created from mixing and then separating the dissolved aqueous fraction from the kerosene product. Environment Canada (1994) measured approximately 10.4 mg/L of total petroleum hydrocarbons in the water soluble fraction (40:1 water/oil ratio) of Jet A-1 fuel. Measurements were verified by purge and trap GC-FID analyses. Lockhart et al.

(1987) measured approximately 5.2 mg/L of total hydrocarbons in an 80:1 water soluble fraction of fuel oil no. 1. Aside from having a higher dilution ratio than what Shiu et al. (1990) showed as being optimum, Lockhart et al. (1987) employed an analytical method that limited detection to a maximum of C12 hydrocarbons. Therefore, this value may be lower than what might be considered a solubility limit for their particular sample. Rozkov, et al. (1998) measured 4.78 mg/L of total hydrocarbons in culture medium used in biodegradation testing. They used a 200:1 medium/oil ratio and GC-FID analysis of the soluble fraction of a kerosene-type aviation fuel (distillation range 200 - 300°C). Due to the high medium/oil ratio, this value may be lower than what might be achieved using a lower ratio. Klein and Jenkin (1983) used a solubilizing apparatus that employed five columns in series to produce saturated solutions of JP-8. The generator contained very low water/oil ratios used continuously to create water soluble fractions of the fuel. The concentration of the total dissolved hydrocarbon fraction decreased some over time, but initial measurements (18 hours after initiation of the generator) averaged 12.44 mg/L ( $\pm 0.71$  mg/L) while measurements taken after seven days averaged 10.67 mg/L ( $\pm 0.71$  mg/L). The water soluble fractions were measured by GC-FID analysis. Other sources reporting somewhat similar values may be found in the public domain. For example, the Agency for Toxic Substances and Disease Registry (ATSDR, 1998) reported a water solubility value of 5 mg/L for kerosene. However, the original data reported by the U.S. Air Force (1989) could not be reviewed or verified.

### **3.6 Assessment Summary for Physical Chemical Endpoints**

Substances in the Kerosene/Jet Fuel Category are liquids composed of numerous individual hydrocarbons that boil within the approximate range of 150°C to 290°C at atmospheric pressure. Measured vapor pressures on samples of whole product ranged from 3 hPa to 35 hPa, indicating limited tendency to volatilize. Partition coefficients of constituent hydrocarbons making up these streams ranged from 3.3 to >6. Water solubility measurements taken from water soluble fractions ranged from approximately 5 to 12 mg/L.

## **4.0 ENVIRONMENTAL FATE**

To assess the environmental fate properties for the HPV program, the U.S. EPA has selected important fate endpoints by which these substances may be characterized. Thus, environmental fate endpoints include photodegradation, stability in water (hydrolysis), environmental distribution (fugacity), and biodegradation.

In determining these fate characteristics for members of the Kerosene/Jet Fuel Category, a high reliance was placed on predicted properties of the individual hydrocarbon constituents of these complex substances. Because it would be impractical to conduct an environmental fate assessment on a component by component basis, specific hydrocarbons were selected from detailed hydrocarbon analyses of the whole product to serve as representative structures. These constituents were selected to span the typical ranges of molecular weights and hydrocarbon types that constitute these category members. Therefore, the package of computer programs contained in EPI Suite<sup>TM</sup> (US EPA, 2000) was used to estimate the properties of photodegradation, stability in water, and environmental distribution. Measured data, when available, were also included in the assessment. For the assessments of biodegradation, the approach taken was to characterize the biodegradability potential of the whole product.

### **4.1 Photodegradation**

Direct photodegradation



The direct aqueous photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation. Only light energy at wavelengths between 290 and 800 nm can result in photochemical transformations in the environment, although absorption is not always sufficient for a chemical to undergo photochemical degradation. Saturated and one-ring aromatic hydrocarbons do not show absorbance in the 290 to 800 nm range and would not be expected to be directly photodegraded. Polyaromatic hydrocarbons, on the other hand, have shown absorbance of the 290 to 800 nm range of light energy and could potentially undergo photolysis reactions. The degree and rate at which these compounds photodegrade depend upon whether environmental conditions allow penetration of light with sufficient energy to effect a change. The fraction of aromatic hydrocarbons in kerosenes is typically <25%, and is made up of mostly single-ring aromatics (alkylbenzenes). Concentrations of polyaromatic hydrocarbons in these substances are quite low (e.g., Table 2); hence direct photodegradation would not be expected to be a significant fate mechanism for this category.

#### Indirect Photodegradation

Components in kerosenes that do not directly photodegrade (e.g., paraffins, naphthenes, and one-ring aromatic compounds) may still be subject to indirect photodegradation. Indirect photodegradation is the reaction with light-potentiated oxygen in the atmosphere in the form of hydroxyl radicals ( $\text{OH}^-$ ). The potential to undergo indirect photodegradation can be estimated using the atmospheric oxidation potential (AOP) model subroutine (AOPWIN V1.90) in EPI-Suite<sup>TM</sup> (EPA, 2000), which calculates a chemical half-life and an overall  $\text{OH}^-$  reaction rate constant based on a 12-hour day and a given  $\text{OH}^-$  concentration. Atmospheric oxidation rates and half-lives were calculated for the low and high end of the range of molecular weight constituents of kerosenes (e.g., C9 and C16 hydrocarbon structures). AOP half-life estimates for these compounds ranged from 0.2 (for C16 2-ring aromatic compounds) to 1.5 days (for a C9 alkylbenzene).

Conclusion: Direct photodegradation is not expected to play an important role in the environmental fate of kerosene/jet fuel category substances. Indirect photodegradation via reaction with hydroxyl radicals and ozone (for olefinic constituents) may be important in the gas-phase degradation of hydrocarbons that volatilize to the troposphere. Atmospheric half-lives of 0.2 to 1.5 days have been calculated for representative C9 and C16 hydrocarbon components of kerosenes.

#### 4.2 Stability in Water

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Harris, 1982). Because kerosenes do not contain significant levels of constituents with these functional groups, substances in the kerosenes category are not subject to hydrolysis.

Conclusion: The substances in the kerosene category do not contain chemical moieties that undergo hydrolysis and, therefore, this process would not be expected to be an important fate pathway.

#### 4.3 Transport Between Environmental Compartments (Fugacity Modeling)

Equilibrium models can provide information on where a chemical is likely to partition in the environment. These data are useful in identifying environmental compartments to which substances are likely to distribute. A widely used fugacity model is the EQC (Equilibrium Criterion) model (Mackay et al., 1997). In its guidance document for HPV data development, the U.S. EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The EQC model is a Level I model that describes the equilibrium distribution of a fixed quantity of conserved (i.e., non-reacting) chemical at steady state within a closed environment with assumed volumes of air, water, soil and sediment. The

model assumes the chemical becomes instantaneously distributed to an equilibrium condition using physical-chemical properties to quantify the chemical's behavior. The model does not include degrading reactions, advective processes or inter-media transport between compartments.

The EQC model was used by the Testing Group to estimate the percent distribution in environmental media (i.e., air, water, soil, sediment, and fish) of various C9 to C16 compounds representing the different classes of hydrocarbons found in kerosenes (e.g., paraffins, naphthenes, and aromatics). Hydrocarbons having nine carbon atoms showed a tendency to partition to air (up to 99%). Constituents with molecular weights > C9 have an increasing tendency to partition to soil, although, even the highest molecular weight constituents, the C16 isoparaffins, 2- and 3-ring naphthenes, and monoaromatics, also partition to the air compartment to a significant extent (13 - 60%). Partitioning to water is <10% at equilibrium, while partitioning to sediment is  $\leq 2\%$  and to biota (fish) is  $\leq 0.1\%$

Conclusion: Fugacity modeling for those constituents in the kerosene/jet fuel category indicates that, at steady state, hydrocarbons having nine carbon atoms showed a tendency to partition to air (up to 99%). Increasing molecular weight of the hydrocarbon classes increases partitioning to soil, though the C16 isoparaffins, 2- and 3-ring naphthenes, and monoaromatics. For these C16 molecules, estimated distributions to air range from (13 - 60%). Partitioning to water is <10% at equilibrium, while partitioning to sediment is  $\leq 2\%$  and to biota (fish) is  $\leq 0.1\%$ .

#### **4.4 Biodegradation**

Limited specific biodegradation data from studies utilizing standard test methodology are available for identified CAS numbers in the kerosene/jet fuels category. Data are available on the behavior of one category member (straight-run kerosene, CAS no. 8008-20-6) following OECD 301F ready biodegradability test guidelines, indicating the refining stream is inherently, though not readily, biodegradable with an average 58.6% of theoretical oxygen consumption in 28 days (Mobil, 1999). Aviation turbine fuel was tested in a 10-day BOD respirometry test using enriched and un-enriched seawater and enriched fresh water at 30 °C according to ASTM D2329-68 closed-bottle respirometry guidelines. The fuel was degraded by 46 - 53% in the enriched waters in the 10-day interval; however, degradation in un-enriched seawater was only 2%, indicating nutrient limitation may play a role in hindering biodegradation of petroleum hydrocarbons (Bridie and Bos 1971).

There are numerous literature reports on biodegradation or bioremediation of kerosene or jet fuels in environmental media (e.g., Song, et al., 1990); many of the environmental factors affecting the biodegradability of petroleum hydrocarbons are described in the context of applied bioremediation in Hinchee et al. (1995). In general, kerosene/jet fuel components biodegrade significantly under aerobic conditions provided sufficient nutrients are present for conversion of the hydrocarbons to microbial biomass. There is a complex interplay between partitioning, and thus bioavailability, and biodegradation in the various media in the environment. Lower molecular-weight, linear paraffinic hydrocarbons are most readily biodegraded but tend to partition to air rather than water (e.g., see Spain and Somerville, 1985), while more complex, higher molecular weight polynuclear aromatics and substituted aromatics tend to sorb to soil or sediment (Spain et al., 1983); sorption limits bioavailability and can slow biodegradation. The constituents of kerosenes are generally not inhibitory to microbial activity (Aelion and Bradley 1991; Song and Bartha 1990) though changes in microbial community composition may occur in spill or impacted areas due to the selection for species that can biodegrade the compounds (Song and Bartha 1990).

Petroleum hydrocarbon biodegradability is governed by the molecular structure of individual hydrocarbons and the metabolic capability of the exposed microbial community. In general, the smaller

and simpler molecules (e.g., short-chain normal paraffins) are most readily degraded, while increased molecular weight, branching, presence of aromatic structures, and substitution tend to decrease the rate and sometimes the extent of biodegradation of hydrocarbons of the same carbon number (Atlas, 1981). The biodegradability of a substance such as kerosene would be the sum of the partial biodegradability of each individual component. Most of the kerosenes contain relatively narrow ranges of olefins (<1 -7%) and aromatics (18 - 25%, Table 1). The biodegradability of C9 to C16 olefins is documented in the HPV submission from the American Chemistry Council Higher Olefins Panel (AR201-13116a, July 2001) where they are noted to be at least inherently and, in some cases, readily biodegradable. The low aromatic content of CAS no. 64742-96-7 is not expected to significantly alter the biodegradability of that kerosene relative to those with higher aromatic content because the balance is made up by saturates.

Conclusion: Adequate data regarding the biodegradability of kerosene components and jet fuel products are available to demonstrate kerosenes are inherently biodegradable, with a generally high degree of complete biodegradation.

#### **4.5 Assessment Summary for Environmental Fate**

If Kerosene/Jet Fuel category members enter the environment, individual components will disperse and partition according to their individual physical-chemical properties. Their final dispositions are governed by both abiotic and biotic processes. Based on modeling individual structures encompassing the different types and molecular weights of hydrocarbons making up kerosenes, volatilization to the atmosphere is an important fate process. Residence times in the atmosphere are relatively short due to indirect photodegradation reactions. In water, hydrolysis is not likely to occur, as the chemical linkages of hydrocarbons are stable. However, biodegradation data show that these substances can exhibit a moderate to rapid rate of biodegradation and are considered at least inherently biodegradable.

### **5.0 ENVIRONMENTAL EFFECTS**

#### **5.1 Acute Aquatic Toxicity**

The HPV Chemical Test Program includes acute toxicity endpoints for a freshwater fish, a freshwater invertebrate, and a freshwater alga. Substances in the kerosene/jet fuels category would be expected to produce a similar range of toxicity for these three endpoints based on results of studies using comparable standardized test methods and exposure solution preparation procedures. This is predicted because the majority of constituents in kerosenes are neutral organic hydrocarbons that act in a common mode of action termed "non-polar narcosis", which is brought about by disruption of biological membrane function (van Wezel and Opperhuizen 1995). Similarities in the range of toxic response elicited by exposure to complex petroleum substances may also be predicted based on physical-chemical properties and acute toxicities of the individual hydrocarbons (Peterson, 1994, CONCAWE, 1996a).

For the assessment of ecotoxicity of poorly water-soluble mixtures such as petroleum products, "loading rate" is now generally accepted for how study results should be expressed (OECD, 2000). The "loading rate" is defined as the amount of the substance equilibrated with the aqueous test medium, and the aqueous phase at equilibrium is termed the water-accommodated fraction (WAF) for the loading rate (OECD, 2000). Toxicological endpoints such as the lethal loading rate (LL<sub>50</sub>) or effective loading rate (EL<sub>50</sub>) are used to express the loading rate of the substance that is lethal or produces a specific effect to 50% of the test organisms. Studies in which the results are expressed in terms of dilutions of a water-soluble fraction (WSF) do not allow the ecotoxicity of a substance to be expressed in terms of the amount

of the product required to produce a particular effect. Such test data are not comparable to results obtained by other exposure methods Girling and Whale (1994). An additional recommendation for testing substances that contain volatile components is to use sealed test vessels with minimal headspace (OECD 2000). This procedure should be used in preparation of the exposure solutions as well as during testing, as studies have clearly documented the loss of volatile hydrocarbons with open-air vessels or use of aeration during testing (Anderson et al., 1974; Lockhart et al., 1987; Tsvetnenko and Evans, 2002).

The aquatic toxicity database used to characterize the ecotoxicological hazards of the kerosene/jet fuel category include multiple tests of one category member, hydrodesulfurized kerosene (CAS no. 64742-81-0). The studies on this substance employed the recommended testing methods for complex substances having limited water solubility (i.e., WAF preparations and sealed test vessels with no headspace) and are identified as key studies in the robust summary file. Additional studies of other kerosene-type substances not included in the HPV category were used as supporting substances when the same test methodologies were employed. These included the following:

- Kerosene, sweetened (CAS no. 91770-15-9) and
- Solvent naphtha, hydrocracked heavy aromatic (CAS no. 101316-80-7).

The inclusion of these two substances to support the aquatic toxicity hazard characterization for all members of the kerosene/jet fuel category is warranted because these substances are classified as kerosene by CONCAWE (2001), and therefore are legitimate representatives of these materials. Additionally, the carbon number range and proportions of major hydrocarbon classes (e.g., alkanes and aromatic hydrocarbons) of these two substances are similar to other members of this HPV category (CONCAWE, 1996). Table 7 presents the ecotoxicological endpoints for the category member and supporting substances used to characterize the aquatic hazard of all category members.

**Table 7. Ecotoxicology Hazard Data for the Kerosene/Jet Fuel Category**

CAS No.	Substance Description	Ecotoxicological Endpoints (95% Confidence Interval)			Reference
		Fish	Invertebrate	Algae	
<b>CATEGORY MEMBER</b>					
64742-81-0	Kerosene (petroleum), hydrodesulfurized	96-h LL50 = 20 mg/L (6.8 – 34 mg/L)	48-h EL50 = 1.4 mg/L (1.0 – 2.0 mg/L)	96-h EL <sub>R</sub> 50 = 6.2 mg/L (ND) 96-h EL <sub>B</sub> 50 = 11 mg/L (0 – 42 mg/L)	Exxon, 1995a,b,c  Shell Research Ltd., 1995
		96-h LL50 = >10mg/L, <100 mg/L	48-h LL50 = >40, <89 mg/L	72-h EL <sub>R</sub> 50 = >10, <30 mg/L 72-h EL <sub>B</sub> 50 = >10, <30 mg/L	
<b>SUPPORTING SUBSTANCES</b>					
91770-15-9	Kerosene (petroleum), sweetened	96-h LL50 = 18 mg/L (13-24 mg/L)	48-h EL50 = 21 mg/L (17 – 27 mg/L)		Exxon, 1995d,e

101316-80-7	Solvent naphtha (petroleum), hydrocracked	96-h LL50 = 25 mg/L (20 – 32 mg/L)	48-h EL50 = 1.9 mg/L (1.3 – 4.3 mg/L)	96-h EL <sub>R</sub> 50 = 5.0 mg/L (0.5 – 131 mg/L)  96-h EL <sub>B</sub> 50 = 5.9 mg/L (ND)	Exxon, 1995f,g,h
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ND = not determined or calculated.

Two sets of aquatic toxicity studies (fish, invertebrate, and algae) were reported for hydrodesulfurized kerosene (CAS no. 64742-81-0). Fish tests were run on rainbow trout, with Exxon (1995a) reporting a 96-h LL50 of 20 mg/L. Using a similar WAF methodology, Shell Research (1995) reported that the 96-h LL50 fell between the limits of 10 and 100 mg/L based on the dose-response pattern of the test. Fish tests run on the two kerosenes used as supporting substances (CAS no. 91770-15-9, sweetened kerosene; CAS no. 101316-80-7, hydrocracked naphtha) resulted in toxicity endpoints similar to the category member. The LL50 values were 18 mg/L and 25 mg/L, respectively for the two materials (Exxon, 1995d,f).

Tests with aquatic invertebrates resulted in some of the lowest toxicity endpoints for the three species but also some of the most variable. Exxon (1995b) reported an EL50 of 1.4 mg/L for hydrodesulfurized kerosene, while Shell Research (1995) reported the EL50 to lie between 40 and 89 mg/L. Some of the difference in the data may be due to the type of tests that were run. Exxon (1995b) conducted a semi-static test that renewed the exposure solutions after 24 hours, while Shell Research (1995) did not renew the exposure solutions. Data on the two supporting substances showed 48-h EC50 values of 1.9 mg/L (hydrocracked solvent naphtha) and 21 mg/L (sweetened kerosene) (Exxon, 1995e,g).

The toxicity to algae of these substances did not differ a great deal from fish or invertebrates. Exxon (1995c) cited toxicity endpoints of 6.2 mg/L based on algal growth rate (EL<sub>R</sub>50) and 11 mg/L (EL<sub>B</sub>50) based on area under the growth curve. Shell Research (1995) data approximated those values and reported that both EL<sub>R</sub>50 and EL<sub>B</sub>50 values lay between 10 mg/L and 30 mg/L. The test with the supporting substance, hydrocracked naphtha, reinforced the data on the category member. Exxon (1995h) obtained EL<sub>R</sub>50 and EL<sub>B</sub>50 values of 5.0 mg/L and 5.9 mg/L, respectively.

There is considerable data regarding toxicity of jet fuels to aquatic organisms, which has been summarized by CONCAWE (1995). Many of the studies used dilutions of a single water-soluble fraction, in which the aqueous fraction of a single loading rate of test substance is diluted to varying percentages (concentrations are expressed as either percent WSF or mg/L corresponding to the dilution). This approach can provide an indication of the relative toxicity of different insoluble products or the relative sensitivity of different organisms to a single test material, but is not useful for quantifying the amount of the material that must be added to a given volume of aqueous medium to produce the effect. In general these studies indicate similar results when compared on equivalent exposure units (e.g., %WSF or measured hydrocarbons).

## 5.2 Chronic Aquatic Toxicity

In order to characterize the chronic aquatic toxicity of members of the kerosene/jet fuel category, the Testing Group conducted a 21-day reproduction test (OECD 211) with *Daphnia magna* with hydrodesulfurized kerosene (CAS no. 64742-81-0) (Exxon, 2010). The study employed independent WAF preparations for the exposure solutions, and the total dissolved hydrocarbons in each WAF

treatment was measured by gas chromatography. The toxicity endpoints of survival and reproduction were calculated based on the WAF loading rates and the mean measured concentrations of total petroleum hydrocarbons. When expressed as the WAF loading rate, kerosene produced EL50 values of 0.89 mg/L for reproduction and 0.81 mg/L for immobilization. The LOELR and NOELR were 1.2 mg/L and 0.48 mg/L, respectively. These values were the same when based on immobilization, reproduction, or growth of adult daphnids. When expressed as mean measured concentrations of dissolved hydrocarbons, kerosene produced EC50 values of 0.16 mg/L for reproduction and 0.15 mg/L for immobilization. The LOELR and NOELR were 0.23 mg/L and 0.092 mg/L, respectively. These values were the same when based on immobilization, reproduction, or growth of adult daphnids.

Conclusion: Adequate data regarding the ecotoxicity of kerosenes and jet fuels are available to demonstrate moderate acute toxicity to aquatic organisms.

### 5.3 Assessment Summary for Environmental Effects

The substances in the Kerosene/Jet Fuel Category are expected to produce a similar range of toxicity for the aquatic species when studies using similar solution preparation and exposure techniques are compared. The endpoint values reflect the loading rates of the test substance added to exposure solutions. Termed water accommodated fractions, the WAF preparation is recommended as the appropriate procedure for testing complex substances having low water solubility. The range of acute toxicities was similar for the three trophic levels (fish, invertebrates, and algae) based on similar testing methodology using water-accommodated fractions (WAF). The proposed ranges of acute toxicity endpoints (expressed as lethal loading rates) that are expected to represent the potential toxicity are:

- Fish 18 – 25 mg/L
- Invertebrates 1.4 – 21 mg/L
- Algae 5.0 – 11 mg/L

## 6.0 HUMAN HEALTH ENDPOINTS

A substantial body of data ranging from acute to long-term carcinogenicity studies has been compiled on selected kerosene-range substance and products. Additional reviews by various expert panels have also been published (ACGIH, 2003; ATSDR, 1995; CONCAWE, 1995,1999; EPA, 2002; IARC, 1989; NRC, 1996; NRC, 2003; Zeiger, et al., 1998). Because No. 1 fuel oil, kerosene and jet fuels (kerosene type) are virtually indistinguishable on the basis of their gross physical or chemical properties (IARC, 1988), data generated on any of these materials can be used to characterize the toxicity of all other kerosenes and similar substances.

### 6.1 Acute Toxicity

Oral LD50s for three kerosenes (Jet A, CAS no. 8008-20-6 and CAS no. 64742-81-0) ranged from > 2 to >20 g/kg bw (API, 1980a, 1982, 1985a). Note that the apparent differences in LD50 values were the consequence of the protocols utilized and do not imply differences in inherent toxicity among the various substances tested. The dermal LD50s of the same three kerosenes were all >2.0 g/kg bw (API, 1980a; 1982, 1985a). Inhalation LC50 values in Sprague-Dawley rats for straight run kerosene (CAS no. 8008-20-6) and hydrodesulfurized kerosene (CAS no. 64742-81-0) were reported to be > 5 and > 5.2 mg/l, respectively (API, 1983, 1987a). Carpenter et al, (1976) reported no mortalities in rats when they were exposed for eight hours to saturated vapor of deodorized kerosene (probably a sweetened kerosene, CAS

no. 91770-15-9). Six hour exposures of cats to the same material produced an LC50 of >6.4 mg/l (Carpenter et al, 1976).

When tested in rabbits for skin irritation, straight run kerosene (CAS no. 8008-20-6) produced “moderate” to “severe” irritation (API, 1985a). Six additional skin irritation studies on a range of kerosenes produced “mild” to “severe” irritation (API, 1980a, 1982; Shell, 1991a,b,c,d).

An eye irritation study in rabbits of straight run kerosene (CAS no. 8008-20-6) produced Draize scores of 0.7 and 2.0 (unwashed and washed eyes) at 1 hour (API, 1985a). By 24 hours, the Draize scores had returned to zero. Eye irritation studies on hydrodesulfurized kerosene and jet fuel reported them to be mildly irritating (Draize scale) (API, 1980a, 1982).

Straight run kerosene (CAS no. 8008-20-6), Jet A, and hydrodesulfurized kerosene (CAS no. 64742-81-0) have not produced sensitization when tested in guinea pigs (API, 1980a, 1984a, 1985a).

Conclusion: Multiple acute toxicity studies have been reported on a variety of kerosene streams and fuels demonstrating low acute toxicity but with the potential to cause skin irritation. Skin sensitization studies were negative.

## 6.2 Repeated Dose Toxicity

Dermal irritation from repeated exposure to middle distillate hydrocarbons (kerosenes and gas oils) is recognized as a significant experimental toxicology issue (Nessel, 1999). Repeated application will cause severe skin injury in many common animal models. Some methods of mitigating Jet A dermal irritation in rats were explored by Mann et al., 2008, including rotating the site of application, diluting 50% with 4:1 acetone:olive oil, and diluting 50% with mineral oil. Only the use of mineral oil resulted in an acceptable degree of skin irritation over 28-days of repeated application. Similar experience is reported by Schreiner et al, 1997 and Nessel et al, 1999.

This potential to cause severe dermal irritation with repeated treatment is illustrated by two kerosene samples that were tested in rabbits; a straight run kerosene (CAS 8008-20-6) and a hydrodesulfurized kerosene (CAS 64742-81-0) (API 1985b; API unpublished data). The test materials were applied undiluted to the skin of male and female New Zealand white rabbits 3x/week for 28 days at 200, 1000, and 2000 mg/kg. Several treatment-related deaths occurred in both studies and humane euthanasia of ten animals was done because of severe dermal irritation caused by the hydrodesulfurized kerosene sample. Findings with the straight run kerosene included weight loss, cracked, flaky and/or leathery skin, crusts and/or hair loss. Clinical signs that were considered to be treatment-related included: nasal discharge, lethargy, soiled anal area, anal discharge, and wheezing. Reductions in red blood cell number, hemoglobin and hematocrit were seen in the male dose groups. There were no treatment related effects on a variety of clinical chemistry values. Absolute and relative weights for a number of organs were normal, with the following exceptions that were judged to be treatment-related:

- increased relative heart weights for the mid- and high- dose males and females,
- increased absolute and relative spleen weights in treated females, and
- differences in absolute and relative adrenal weights in both male and female treated animals (considered to be stress-related and therefore, indirectly related to treatment).

The severity of the dermal irritation in both these studies makes problematic the use of the systemic effects observed in these studies for hazard and risk assessment purposes.

A13-week subchronic toxicity/neurotoxicity study was conducted with a sample of hydrodesulfurized kerosene (HDS), CAS number 64742-81-0 (Battelle, 1997). The sample met the specifications for

aviation turbine fuel (Jet A). HDS kerosene was diluted in USP grade mineral oil and applied to the shaved backs of Sprague-Dawley CD rats, 12/sex/group, 6 hr/d, 5 d/wk. Doses of 0 (vehicle control), 165 mg/kg (20% HDS kerosene), 330 mg/kg (40% HDS kerosene), or 495 mg/kg (60% HDS kerosene) were used. The high dose was determined in previous studies demonstrating an acceptable level of dermal irritation when HDS kerosene was diluted below 60% with moderate viscosity (340 SUS) USP mineral oil. Additional rats (12/sex) in the control and high dose groups were held after final treatment for a 4-week recovery period. Standard parameters of toxicity were measured throughout the study. At necropsy, organs were weighed and tissues processed for microscopic evaluation. Neurotoxicity evaluations consisted of motor activity and a functional operational battery measured pretest, throughout exposure and after the recovery period. There were no apparent test substance-related effects on mortality, clinical observations (excepting slight dermal irritation), body weight, or coagulation and clinical chemistry values. HDS kerosene produced a dose-related increase in skin irritation at the site of administration with an apparent greater effect in males. Histopathology confirmed minimal, reversible, skin lesions. Hematology results were unremarkable except for an elevation in the mean neutrophil values for the high dose females and possibly males. All hematology values were normal after 4-weeks recovery. There were no apparent test-related effects on neurotoxicological endpoints and no gross or microscopic findings in peripheral or central nervous system tissues. Statistically significant increases in relative spleen weight at treatment termination and in absolute spleen weight after the recovery period were observed in high dose females without gross or microscopic correlate. The NOAEL for neurotoxicity was 495 mg/kg/day and for subchronic toxicity (excluding skin irritation) the NOAEL was 330 mg/kg/day.

A sample of hydrodesulfurized kerosene (CAS no. 64742-81-0) has also been tested in a four week inhalation study (API, 1986). In the study, Sprague-Dawley rats were exposed to a nominal concentration of 24 mg/m<sup>3</sup> kerosene. Exposures were for 6 hr/day, five days each week for four consecutive weeks. There were no treatment-related effects on clinical condition, growth rates, absolute or relative organ weights, or any of the hematological or clinical chemistry determinations. Microscopic examination found no treatment-related changes observed in any tissues. The NOAELs for both local and systemic effects were >24 mg/m<sup>3</sup>.

Conclusion: Standard hazard screening studies in rats by dermal and inhalation routes have shown minimal systemic effects from hydrodesulfurized kerosene. The dermal NOAEL was 495 mg/kg.

### 6.3 Genetic Toxicity In Vitro

Standard Ames assays on two kerosene samples and a sample of Jet A produced negative results with/without activation (API, 1977, 1978, 1979a). Optimized Ames assays on four kerosenes also produced negative results (with/without activation) except for one positive assay that occurred with activation (Blackburn, et al., 1986; CONCAWE, 1991). The testing of five kerosene and jet fuel samples in mouse lymphoma assays produced a mixture of negative and positive results (API, 1977, 1979a, 1984b, 1985c; NTP, 1986). Hydrodesulfurized kerosene tested in a sister chromatid exchange assay produced negative results (with/without activation) (API, 1988a).

The genotoxicity of several military fuels has been tested in bacterial and mammalian cells (Brusick and Matheson, 1978 as cited in NRC, 1996). In the tests on JP-8, in vitro assays used microbial and mammalian cells in culture, and in vivo assays measured potential germ-cell effects in mice and rats. JP-8 fuel did not induce mutagenicity in *Salmonella typhimurium* in the Ames assay; however, it did have toxic effects in most of the bacterial strains at concentrations above 1 µg per plate. In the mouse lymphoma assay, JP-8 did not induce gene mutations in L5178Y mouse lymphoma cells at the TK locus but did induce moderately toxic effects at 0.16 µL/mL. JP-8 induced significant increases of <sup>3</sup>H-



thymidine in WI-38 cells. The genotoxicity was moderate and not dose-related. There was clear evidence of cytotoxicity at 5.0  $\mu\text{L}/\text{mL}$ .

Tests on JP-5 also did not result in evidence of mutagenicity. JP-5 was tested in the Ames assay with *Salmonella typhimurium* TA-1535, TA-1537, TA-97, TA-98, and TA-100 at concentrations of 100-10,000  $\mu\text{g}$  per plate in the presence or absence of metabolic activation systems from rat or hamster liver (NTP, 1986).

McKee et al. (1994) evaluated five middle distillate materials, including Jet A, in *Salmonella* strain TA98 and found that they were nonmutagenic; that is, they induced less than a doubling of revertant colonies.

The ability of JP-8 to induce DNA damage in cultured mammalian cells has been investigated with the Comet (single-cell gel electrophoresis) assay. Grant et al. (2001) tested JP-8 in H4IIE rat hepatoma cells, which are capable of expressing many of the metabolic enzymes, including cytochrome P450-dependent oxidases, normally expressed in liver in vivo. JP-8, solubilized in ethanol at 0.1% (v/v), was applied to the H4IIE cells at 0-20  $\mu\text{g}/\text{mL}$  for 4 hr, after which DNA damage was assessed with the Comet assay. JP-8 induced a dose-dependent increase in mean Comet tail moments in H4IIE cells; this indicates DNA damage. The authors reported that comet tail lengths increased and DNA strand breaks accumulated in the presence of DNA-repair inhibitors and JP-8 and concluded that JP-8 induces DNA damage, which can be mitigated by DNA repair. Neither cytotoxicity nor significant apoptosis was induced by JP-8.

#### 6.4 Genetic Toxicity In Vivo

Deodorized kerosene (probably a sweetened kerosene, CAS no. 91770-15-9) and Jet A produced negative results in dominant lethal assays (API, 1973, 1980b). The deodorized kerosene was administered either ip or subcutaneously in rats and mice respectively at 1 g/kg. The Jet A was administered to mice by inhalation of 100 or 400 ppm for six hours a day for eight weeks.

JP-8 was found to be negative in the dominant lethal assays in both mice and rats (Brusick and Matheson, 1978 as cited by NRC, 1996). The mice were administered 0.13, 0.4, or 1.3 mL/kg of body weight per day orally for 5 days. The concentrations administered to rats were 0.1, 0.3, or 1.0 mL/kg per day orally for 5 days.

McKee et al. (1994) evaluated five middle distillate materials, including Jet Fuel A, administered by gavage, in the CD-1 mouse bone marrow micronucleus test. No increases in the frequency of MNs were observed for any of the test materials in assessments 24, 48, or 72 hr after treatment. The authors did not see any evidence of bone marrow depression. Vijayalaxmi et al., (2006) investigated the genotoxic potential of jet fuels, JP-8 and Jet-A. Mice were treated dermally with either a single or multiple applications of these jet fuels. Peripheral blood and bone marrow smears were prepared to examine the incidence of micronuclei (MN) in polychromatic erythrocytes (PCEs). In all experiments, using several different exposure regimens, no statistically significant increase in the incidence of MN was observed in the bone marrow and/or peripheral blood of mice treated with JP-8 or Jet-A when compared with those of untreated control animals. The data in mice treated with a single dose of JP-8 or Jet-A did not confirm the small but statistically significant increase in micronuclei reported in a previous study by the same authors (Vijayalaxmi et al., 2004).

Hydrodesulfurized kerosene produced a positive response in male mice and negative results in females when tested in a sister chromatid exchange assay (API, 1988b). The mice were administered a single dose of 0.4, 2.0 or 4.0 g/kg of body weight ip.

Deodorized kerosene (probably a sweetened kerosene, CAS no. 91770-15-9) and hydrodesulfurized kerosene were negative in in vivo bone marrow cytogenetic tests in Sprague-Dawley rats (API, 1977, 1985d). The test materials had been administered by single ip injection up to 3 g/kg. Jet A was reported as positive for bone marrow cytogenetic abnormalities after inhalation exposure to either 100 ppm for 19 day or 400 ppm for 5 days (Conway et al., 1982). The same “positive” study results have been cited in IARC, 1989, and Koschier, 1999. In the Conway et al., paper, the control values for many of the studies reviewed were less than 1% aberrant cells (typical control values). But there were a number of samples with higher control values. The highest was for Jet A with a control value of 9.2 % aberrant cells. A subsequent review of the original photomicrographs and discussions with the testing laboratory determined that turnover in laboratory personnel had compromised the evaluation and the results were simply unreliable. The Testing Group believes this bone marrow cytogenetic study on Jet A should not be used in the hazard assessment of the Kerosene/Jet Fuel Category.

Conclusion: Existing in vitro and in vivo studies are adequate to characterize the genotoxicity of kerosene and jet fuels. The overall conclusion from these studies is that kerosene(s) are not genotoxic under both in vitro and in vivo conditions.

### **6.5 Reproductive and Developmental Toxicity**

A reproductive/developmental screening study in Sprague-Dawley rats of hydrodesulfurized kerosene (Schreiner et al., 1997) was performed in accordance with OECD Guideline 421, except males were treated for 8 weeks to improve the quality of the assessment of the potential for kerosene to affect on the male reproductive system. Either 0, 20, 40 or 60% (v/v) kerosene in mineral oil was applied to the skin of the rats. The doses per body weight equivalents were 0, 165, 330 and 495 mg/kg. Test material was applied daily, 7 days/week from 14 days pre mating through 20 days of gestation. There were no treatment-related effects on mortality and no clinical signs of toxicity were observed. Compound-related skin irritation (usually graded as slight) was seen in both males and females. At the terminal sacrifice, no findings were reported except for those on the skin. Over the course of the 8 weeks, high dose males gained less weight than the controls; however, body weights and food consumption were unaffected by treatment. High dose males had a higher mean relative kidney weight than controls, this being attributed to the lower mean final body weights of the high dose group. Microscopic changes were found in the skin of males in the vehicle control and all kerosene-treated groups. In females, the skin changes were observed only in the high dose group, but there were no other effects. No test-material-related microscopic changes were observed in the testes or epididymides of adult male rats or in the ovaries of adult female rats. There were no compound-related effects on any of the reproductive/developmental parameters. The authors concluded that the no observable effect level (NOEL) for reproductive/developmental toxicity of HDS kerosene under the treatment conditions of the study was 495 mg/kg/day.

The National Toxicology Program reported no histological changes in the reproductive systems of B6C3FI mice dermally exposed to 2 to 8 g/kg of JP-5 for 13-weeks (NTP, 1986).

Developmental toxicity screening studies by inhalation have been reported in which kerosene and Jet A were tested (API, 1979b,c). In both studies, presumed-pregnant female rats were exposed via inhalation to nominal concentrations of either 100 or 400 ppm of kerosene/jet fuel vapor for 6 hours/day on days 6 through 15 of gestation. On day 20 of gestation, the animals were killed and the visceral and thoracic organs were examined. The contents of the uteri were also examined. Live and dead fetuses, and resorption sites were noted. The fetuses were examined externally for abnormalities and then weighed. Selected fetuses were examined for either soft tissue changes or skeletal abnormalities. There were no compound-related deaths in either study. While kerosene produced no clinical signs, the jet fuel produced

a dose-related eye irritation (or infection). The signs of irritation lasted from 2 to 8 days with most animals showing signs for 3 days. Neither of the test materials had an effect on body weights or food consumption. Examination of offspring at delivery did not reveal any treatment-related abnormalities, soft tissue changes or skeletal abnormalities. The sex ratio of the fetuses was also unaffected by treatment with either of the compounds. The NOAEL was 400 ppm, the highest concentration tested.

NRC, 2003 reviews several studies on JP-8 using oral administration to evaluate reproductive and developmental effects (specifically Mattie et al., 1995; Mattie et al., 2000; Cooper and Mattie, 1996). Since this route of exposure is not expected, limited data is summarized here and no robust summaries are included. None of the studies report specific adverse effects on male or female reproductive parameters at doses of up to 1,500 mg/k for 90 days. Maternal and fetal body weights were decreased at doses above 500 mg/kg but the number and type of fetal malformation and variations were not affected.

Conclusion: A dermal screening study in rats for reproduction and developmental toxicity reported a NOAEL of 495 mg/kg for hydrodesulfurized kerosene.

## 6.6 Health Effects Other

### Dermal Carcinogenesis:

A number of dermal carcinogenicity studies have been performed on kerosenes or jet fuels. Although carcinogenicity is not a required endpoint of the HPV program, the Testing Group believes the results may be useful in evaluating the repeated dose endpoint. These studies have been fully summarized and reviewed elsewhere (ATSDR, 1995; CONCAWE, 1996; IARC, 1988). When it was discovered that hydrodesulfurized (HDS) kerosene caused skin tumors in lifetime mouse skin painting studies, the role of dermal irritation in tumor formation was extensively studied (API, 1989a; CONCAWE, 1996; Freeman et al., 1993). HDS kerosene proved to be a mouse skin tumor promoter rather than initiator, and this promotion required prolonged dermal irritation (Nessel et al., 1999). If the equivalent dose of kerosene was applied to the skin in manner that did not cause significant skin irritation (eg, dilution with a mineral oil) no skin tumors occurred (CONCAWE, 1996). Dermal bioavailability studies in rats confirmed that mineral oil did not significantly decrease skin penetration of kerosene components (Schreiner et al., 1997). The effect of chronic acanthosis on the dermal tumorigenicity of a hydrodesulfurized kerosene was studied and the author concluded that hyperplasia was essential for tumor promotion. However, the author also concluded that subacute inflammation did not appear to be a significant factor (Skisak, 1991).

A sample of a hydrodesulfurized kerosene has been tested in an initiation-promotion assay in male CD-1 mice (API, 1989b). Survival was not affected by exposure to the kerosene. The study's authors concluded that the kerosene was not an initiator but it did show tumor promoting activity.

## 6.7 Assessment Summary for Health Effects

The vapor pressures of substances in the category make dermal exposure the most likely route of exposure for humans both in the workplace and the general population. Studies employing the oral or inhalation routes are included for completeness and to address unusual exposure scenarios (cold engine start where unburned fuel can be aerosolized by jet engines). LOAEL and NOAEL designations for repeated dose and developmental/ reproduction studies for read-across to untested category members are derived from results of dermal studies.

Acute Dermal Toxicity: LD50 >2000 mg/kg

**Repeated Dose Dermal Toxicity:** The read-across NOAEL value for untested category members is 495 mg/kg/d dermal exposure.

**In Vitro Genetic Toxicity – Gene mutation:** The read-across conclusion for untested substances in this category is negative for in vitro genetic toxicity.

**In Vivo Genetic Toxicity – Cytogenetics:** The read-across conclusion for untested substances in this category is negative for in vivo genetic toxicity.

**Developmental Toxicity:** The read-across NOAEL value for developmental toxicity for untested substances in this category is 495 mg/kg/d dermal exposure.

**Reproductive Toxicity:** The read-across NOAEL value for reproductive toxicity for untested substances in this category is 495 mg/kg/d dermal exposure.

## **7.0 HUMAN EXPOSURE SUMMARY**

### **7.1 Occupational Exposure**

An occupational exposure standard for Kerosene/jet fuels of 200 mg/m<sup>3</sup> (8-hour time weighted average for hydrocarbon vapor) has been recommended by ACGIH (2003). The Department of Defense has an interim Permissible Exposure Limit of 350 mg/m<sup>3</sup> (8-hour time weighted average for hydrocarbon vapor) for JP-8.

Hazard evaluation and labeling of kerosene and kerosene containing materials in the workplace is regulated by the Occupational Health and Safety Administration in the Department of Labor.

A summary of occupational exposure to kerosene was recently released which includes both published studies and unpublished data developed by individual companies and CONCAWE (CONCAWE, 2007). Table 7 contains data reproduced from that CONCAWE report which summarizes inhalation and dermal exposure to kerosene in common industrial situations. The inhalation exposure estimates are modeled full-shift exposures based on frequency and duration per task. The dermal exposure estimates are modeled full-shift exposures based on highest task-based exposure estimate assuming individuals do not wear gloves.

**Table 8. Occupational Exposure To Kerosene**

Job title	EASE model inhalation exposure estimate (mg/m <sup>3</sup> )
1.1 Production / On-site operator	1 – 9
1.2 Tank farm / Off-site operator	4 – 20
1.3 Mechanical maintenance	1 – 15
1.4 Laboratory technician	1 – 8
1.7 Jetty staff	0.5 – 3
2.1 Road tanker driver (top loading)	5 – 26
2.1 Road tanker driver (bottom loading)	0.5 – 1.3
2.2 Subsidiary road tanker driver (bottom loading, vapour recovery)	10 – 63
2.2 Subsidiary road tanker driver (bottom loading, remote venting)	11 – 67
2.2 Subsidiary road tanker driver (top loading)	14 – 81
2.3 Terminal operator (with drum filling)	0.5 – 19
2.3 Terminal operator (no drum filling)	0.2 – 6.5
2.4 Terminal rack operator (top loading)	25 – 94
2.4 Terminal rack operator (bottom loading)	0 – 0.5
2.5 Rail car operator (with vapour recovery)	0 – 13
2.5 Rail car operator (no vapour recovery)	50 – 100
2.6 Ship deck crew	0 – 9
2.7 Jetty staff	0 – 7
2.8 Terminal vehicle mechanic	5 – 11
2.9 Terminal equipment maintenance	50 – 100
3.1 Aircraft refueller	13 – 25
3.2 Yard operator	3 – 44
3.3 Airport rail car operator	0 – 0.5
3.4 Airport vehicle mechanic	5 – 23
3.5 Airport tank/interceptor cleaning/inspection	50 – 100
3.6 Airport terminal operator	5 – 43
3.7 Aircraft maintenance worker	50 – 100
4.1 Domestic heating oil supplier	0 – 50
4.2 Domestic heating engineer	0 – 0.5

Job title	Typical estimates		RWC dermal exposure (mg.d <sup>-1</sup> )
	Type of contact	Surface (cm <sup>2</sup> )	
Manufacturing			
Production/On-site operator	Incidental	840	84
Tank farm/Off-site operator	Intermittent	420	420
Mechanical maintenance	Intermittent	420	420
Laboratory technician	Incidental	420	42
Rail car operator	Intermittent	420	420
Jetty staff	Intermittent	420	420
Distribution operations			
Road tanker driver	Incidental	840	84
Subsidiary / Commercial road tanker driver	Incidental	420	42
Terminal operator	Intermittent	840	840
Rack operator	Intermittent	420	420
Rail car operator	Intermittent	420	420
Deck crew: ships / barges	Intermittent	420	420
Jetty staff	Incidental	420	42
Vehicle mechanic	Intermittent	420	420
Equipment maintenance	Incidental	840	84
Aviation refuelling operations			
Aircraft refueller	Incidental	420	42
Yard operator	Incidental	840	84
Rail car operator	Incidental	420	42
Vehicle mechanic	Intermittent	420	420
Terminal operator	Intermittent	840	840

RWC = Realistic Worst-Case

Exposure to jet fuel by military personnel has been reported by Chao et al., (2005) and others (NRC, 2003). Military requirements and procedures result in exposures that are not typical for industrial and consumer applications.

The long history of petroleum refining has resulted in the development of recommended practices (RP) and standards (STD) to improve safety within the facilities. API has been a leader in developing these standards for both Upstream and Downstream operations. Listed below are groups of STDs and RPs that help ensure safe operation of the plant and reduce exposures to workers and the surrounding community.

API PERSONNEL SAFETY SET

PERSONNEL SAFETY INCLUDES THE FOLLOWING API STANDARDS: STD 2217A, RP 2016, STD 2220RP 2221, RP 54, RP 74, STD 2015

#### API PROCESS SAFETY SET

PROCESS SAFETY INCLUDES THE FOLLOWING API STANDARDS: PUBL 770, PUBL 9100, RP 751 RP 752

#### API SAFETY & FIRE SET

SAFETY AND FIRE - INCLUDES THE FOLLOWING API STANDARDS: 54, 74, 751, 752, 770, 2001, 2003, 2009, 2015, 2016, 2021, 2021A, 2023, 2026, 2027, 2028, 2030, 2201, 2207, 2210, 2214, 2216, 2217A 2218, 2219, 2220, 2221, 2350, 2510A, 9100

### **7.2 Consumer Exposure**

Kerosene is available for purchase at the retail level for various domestic uses. Kerosene is used in portable heaters, stoves, and lanterns, as charcoal lighter fluid, and as an ingredient in consumer products like furniture polish. Labeling and packaging of kerosene containing consumer products in the USA is regulated by the Consumer Product Safety Commission (CPSC). Any use of kerosene in pesticide products as a carrier is regulated by EPA under FIFRA. Transportation of kerosene containing products would also be regulated by the Department of Transportation.

### **7.3 Exposure to Children**

There are no known uses of kerosene in products intended for use by children. Because kerosene or kerosene-containing products can be stored in the home, accidental ingestion and aspiration by children is a recognized hazard. In the USA, product labeling and child-proof container requirements are required by CPSC for most kerosene containing products.

## **8.0 CATEGORY ANALYSIS CONCLUSIONS**

Sufficient data is available on SIDS endpoints for the Kerosene/Jet Fuel Category to satisfy the requirements of EPA's HPV Challenge program. Appendix B is a data matrix which summaries key study results that can be used to read-across to untested substances in the Category. Current regulations by EPA, CPCS, DOT, and OSHA limit the environmental and human health risk to communities, workers, consumers, and children.

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## 10.0 LIST OF APPREVIATIONS AND ACRONYMS

API – American Petroleum Institute

BOD – biological oxygen demand

Btu/lb – British thermal unit per pound

Btu/scf – British thermal unit per standard cubic feet

AUGC – area under the growth curve

CAS RN/CAS #/CAS No. - Chemical Abstract Service Registry Number

oC – degrees Celsius

CONCAWE – Conservation of Clean Air and Water in Europe

d - day

DMSO – Dimethyl sulfoxide

EINECS – European Inventory of Existing Commercial Chemical Substances

EL50 – effective loading rate lethal to 50% of the test population

EbL50 – effective loading rate that causes 50% reduction in algal cell biomass

ErL50 – effective loading rate that causes 50% reduction in algal growth rate

EPA/US EPA – United States Environmental Protection Agency

g/cm<sup>3</sup> – grams per cubic centimeter

h - hour

HLS – Huntingdon Life Sciences

HPV – High Production Volume

IRDC – International Research and Development Corporation  
oK – degrees Kelvin  
kPa - kilopascal  
LC50 – lethal concentration for 50% of the test population  
LD50– lethal dose level for 50% of the test population  
LL50 – lethal loading rate for 50% of the test population  
Loading Rate – total amount of test substance added to dilution water to prepare water accommodated fractions (WAFs) for ecotoxicity testing  
LOAEL – lowest observable adverse effect level  
mg/kg – milligrams per kilogram  
mg/L – milligrams per liter  
mg/m<sup>3</sup> – milligrams per cubic meter  
mL - milliliter  
mm - millimeter  
nm - nanometer  
NOAEL – no observable adverse effect level  
NOEC – no observable effect concentration  
NOELR – no observable effect loading rate  
OECD – Organization for Economic Cooperation and Development  
OPPTS – US EPA Office of Prevention, Pesticides and Toxic Substances  
PAC - Polycyclic aromatic compound  
PAH – polycyclic aromatic hydrocarbon  
PNA – polynuclear aromatic  
ppm – part per million  
SIDS – Screening Information Data Set  
US EPA – United States Environmental Protection Agency  
UV - ultraviolet  
WAF – water accommodated fraction  
wt% - weight percent  
µg - microgram  
µg/L – microgram/liter  
> greater than  
< less than  
= equal to

## 11.0 GLOSSARY

**NOTE:** *The following terms are used in this document. To the extent possible definitions were taken from relevant authoritative sources such as US EPA, OECD, ASTM and IUPAC.*

**Alpha 2-microglobulin mediated nephropathy:** also identified as light hydrocarbon-induced nephropathy (LHN) is a species and sex-specific syndrome induced in male rats resulting from repeated exposure to volatile petroleum naphthas in the gasoline blending stream range. The syndrome is characterized by excessive formation of hyaline droplets comprised of the unique sex-hormone dependent alpha 2-microglobulin, in the epithelium of the proximal convoluted tubules leading to degenerative changes in these tubules in the renal cortex and tubular dilatation and necrosis at the corticomedullary junction. Evaluation of nephrotoxicity of volatile hydrocarbons in male rats and comparison of effects in female rats and both sexes of other species (Alden et al., 1984) has confirmed the specificity of this

syndrome for male rats and has resulted in the US EPA determination that alpha 2-microglobulin mediated nephrotoxicity is not relevant to health effects in humans. (US EPA, 1991).

**Bioavailability:** The state of being capable of being absorbed and available to interact with the metabolic processes of an organism. Typically a function of chemical properties, physical state of the material to which an organism is exposed, and the ability of the individual organism to physiologically take up the chemical. Also, the term used for the fraction of the total chemical in the environmental that is available for uptake by organisms. (AIHA 2000)

**Category Member:** The individual chemical or substance entities that constitute a chemical category.

**Category:** A chemical category, for the purposes of the HPV Challenge Program, is a group of chemicals whose physicochemical and toxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity. These structural similarities may create a predictable pattern in any or all of the following parameters: physicochemical properties, environmental fate and environmental effects, and/or human health effects. (US EPA 2007)

**Dose:** The amount of a substance available for interactions with metabolic processes or biologically significant receptors after crossing the outer boundary of an organism. The **potential dose** is the amount ingested, inhaled, or applied to the skin. The **applied dose** is the amount presented to an absorption barrier and available for absorption (although not necessarily having yet crossed the outer boundary of the organism). The **absorbed dose** is the amount crossing a specific absorption barrier (e.g., the exchange boundaries of the skin, lung, and digestive tract) through uptake processes. **Internal dose** is a more general term denoting the amount absorbed without respect to specific absorption barriers or exchange boundaries. The amount of the chemical available for interaction by a particular organ or cell is termed the delivered or **biologically effective dose** for that organ or cell (US EPA 2002).

**Dose-Response Relationship:** The relationship between a quantified exposure (dose) and the proportion of subjects demonstrating specific biological changes in incidence or in degree of change (response) (US EPA 2002).

#### **Ecological Effects – all endpoints (OECD definitions)**

**Fish, Acute Toxicity Test:** In a four-day exposure, acute toxicity is defined by the LC<sub>50</sub>, the concentration of test substance in water which kills 50% of the test population of fish. Test methodology is described in OECD Guideline 203, in OECD Guidelines for the Testing of Chemicals.

**Daphnia sp., Acute Immobilization Test:** In a one or two-day exposure, acute toxicity is defined by the EC<sub>50</sub>, the concentration of test substance in water which causes immobilization to 50% of the test population of invertebrates. Test methodology is described in OECD Guideline 202, Part 1, in OECD Guidelines for the Testing of Chemicals.

**Alga, Growth Inhibition Test:** In a three-day exposure, growth inhibition is defined by the EC<sub>50</sub>, the concentration of test substance in growth medium which results in a 50% reduction in either alga cell growth or growth rate relative to a control group. Test methodology is described in OECD Guideline 201, in OECD Guidelines for the Testing of Chemicals.

**Endpoint:** In the context of the EPA High Production Volume Challenge Program, an endpoint is a physical-chemical, environmental fate, ecotoxicity, and human health attribute measurable by following an approved test methodology (e.g., OECD Guidelines for Testing of Chemicals). Melting point, biodegradation, fish acute toxicity, and genetic toxicity are examples of endpoints that are measured by an approved test method. (US EPA 1999)

#### **Environmental Fate Effects – all endpoints (OECD definitions)**



**Photodegradation:** The photochemical transformation of a molecule into lower molecular weight fragments, usually in an oxidation process. This process may be measured by Draft OECD Guideline, “*Phototransformation of Chemicals in Water – Direct and Indirect Photolysis*”. This process also may be estimated using a variety of computer models.

**Stability in Water:** This environmental fate endpoint is achieved by measuring the hydrolysis of the test substance. Hydrolysis is defined as a reaction of a chemical RX with water, with the net exchange of the group X with OH at the reaction center. Test methodology for hydrolysis is described in OECD Guideline 111, in OECD Guidelines for the Testing of Chemicals.

**Transport Between Environmental Compartments:** This endpoint describes the distribution of a chemical between environmental compartments using fugacity-based computer models. The results of the model algorithms provide an estimate of the amount of the chemical within a specific compartment. The environmental compartments included in many models are air, water, soil, sediment, suspended sediment, and aquatic biota.

**Biodegradation:** Breakdown of a substance catalyzed by enzymes *in vitro* or *in vivo*. As an endpoint in EPA’s HPV program, biodegradation is measured by one of six methodologies described in OECD Guidelines 301A-F, in OECD Guidelines for the Testing of Chemicals.

**Exposure:** Contact made between a chemical, physical, or biological agent and the outer boundary of an organism. Exposure is quantified as the amount of an agent available at the exchange boundaries of the organism (e.g., skin, lungs, gut). (US EPA 2002).

**Feedstock:** A refinery product that is used as the raw material for another process; the term is also generally applied to raw materials used in other industrial processes. (Speight, 2007).

**Female Mating Index:** Number of females with confirmed mating (sperm and/or vaginal plug)/number of females placed with males. (US EPA 1996).

**Formulated Gasoline:** Unleaded automotive fuel formulated by blending paraffinic, olefinic, naphthenic and aromatic petroleum naphtha that does not contain oxygenates (e.g. methyl tertiary butyl ether, ethanol, etc.).

**Hazard Assessment:** The process of determining whether exposure to an agent can cause an increase in the incidence of a particular adverse health effect (e.g., cancer, birth defect) and whether the adverse health effect is likely to occur in humans (US EPA 2002).

**Hazard Characterization:** A description of the potential adverse health effects attributable to a specific environmental agent, the mechanisms by which agents exert their toxic effects, and the associated dose, route, duration, and timing of exposure (US EPA 2002).

**Hazard:** A potential source of harm (US EPA 2002).

#### **Health Effects – all endpoints (OECD definitions, unless otherwise specified)**

**Acute Toxicity:** The adverse effects occurring within a short time-frame of administration of a single dose of a substance, multiple doses given within 24 hours, or uninterrupted exposure over a period of 24 hours or less. Exposure may be via oral, dermal or inhalation routes as described in OECD Guidelines 401, 402, 403, and 420 in OECD Guidelines for the Testing of Chemicals.

**Developmental Toxicity:** Adverse effects on the developing organism that may result from exposure prior to conception (either parent), during prenatal development, or postnatally until the time of sexual maturation. The major manifestations of developmental toxicity include death of the developing organism, structural abnormality, altered growth, and functional deficiency. (US NLM 2007)

**Genetic Toxicity *in vivo* (Chromosomal Aberrations):** The assessment of the potential of a chemical to exert adverse effects through interaction with the genetic material of cells in the whole animal. Genotoxicity may be studied in the whole animal using methods described in OECD Guideline 475, in OECD Guidelines for the Testing of Chemicals.

**Genetic Toxicity *in vitro* (Gene Mutations):** The assessment of the potential of a chemical to exert adverse effects through interaction with the genetic material of cells in cultured mammalian cells. Genotoxicity may be studied in cultured cells using methods described in OECD Guideline 476, in OECD Guidelines for the Testing of Chemicals.

**Repeated Dose Toxicity:** The adverse effects occurring due to repeated doses that may not produce immediate toxic effects, but due to accumulation of the chemical in tissues or other mechanisms, produces delayed effects. Repeated dose toxicity may be studied following methods described in OECD Guidelines 407, 410, or 412 in OECD Guidelines for the Testing of Chemicals.

**Reproductive Toxicity:** The occurrence of biologically adverse effects on the reproductive systems of females or males that may result from exposure to environmental agents. The toxicity may be expressed as alterations to the female or male reproductive organs, the related endocrine system, or pregnancy outcomes. The manifestation of such toxicity may include, but not be limited to, adverse effects on onset of puberty, gamete production and transport, reproductive cycle normality, sexual behavior, fertility, gestation, parturition, lactation, developmental toxicity, premature reproductive senescence, or modifications in other functions that are dependent on the integrity of the reproductive systems. **(US EPA 1996)**

**Light hydrocarbon induced nephrotoxicity (LHN): also identified as** alpha 2-microglobulin mediated nephropathy. See definition above.

**Lowest-Observed-Adverse-Effect Level (LOAEL):** The lowest exposure level at which there are statistically or biologically significant increases in frequency or severity of adverse effects between the exposed population and its appropriate control group **(US EPA 2002)**.

**No-Observed-Adverse-Effect Level (NOAEL):** The highest exposure level at which there are no biologically significant increases in frequency or severity of adverse effects between the exposed population and its appropriate control group; some effects may be produced at this level, but they are not considered adverse or precursors to adverse effects **(US EPA 2002)**.

**Petroleum** (crude oil): A naturally occurring mixture of gaseous, liquid, and solid hydrocarbon compounds usually found trapped deep underground beneath impermeable cap rock and above a lower dome of sedimentary rock such as shale; most petroleum reservoirs occur in sedimentary rocks of marine, deltaic, or estuarine origin **(Speight 2007)**.

**Portal of Entry Effect:** A local effect produced at the tissue or organ of first contact between the biological system and the toxicant **(US EPA 1994a)**.

**Read Across:** Read-across can be regarded as using data available for some members of a category to estimate values (qualitatively or quantitatively) for category members for which no such data exist. **(OECD 2007)**

**Systemic Effects or Systemic Toxicity:** Toxic effects as a result of absorption and distribution of a toxicant to a site distant from its entry point **(US EPA 2002)**.

**Target Organ:** The biological organ(s) most adversely affected by exposure to a chemical or physical agent **(US EPA 2002)**.

## Appendix 1 – Kerosene/Jet Fuel Category Members

The CAS numbers and definitions of refinery streams were developed in response to Section 8(b) of the Toxic Substances Control Act. This section of TSCA required identification and registration with the Environmental Protection Agency before July 1979 of each “chemical substance” being manufactured, processed, imported or distributed in commerce. Due to analytical limitations and known variability in refinery stream composition, identification of every specific individual molecular compound in every refinery process stream under all processing conditions was impossible. Recognizing these problems, the American Petroleum Institute (API) recommended to the EPA a list of generic names for refinery streams consistent with industry operations and covering all known processes used by refiners. The list, including generic names, CAS numbers and definition of each stream, was published by the EPA as “Addendum I, Generic Terms Covering Petroleum Refinery Process Streams.”

Because of the variability inherent in the processing of petroleum materials, the definitions API developed for the CAS numbers are qualitative in nature, written in broad, general terms. The definitions often contain only ranges of values for carbon numbers, with little if any quantitative analytical information or concern for possible compositional overlaps. As a result, the CAS descriptions are not useful in determining the exact composition of any specific refinery stream.

8008-20-6

Kerosene (petroleum)

A complex combination of hydrocarbons produced by the distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150°C to 290°C (320°F to 554°F).

064742-14-9

Acid Treated Light Distillate, Light

A complex combination of hydrocarbons obtained as a raffinate from a sulfuric acid treating process. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150°C to 290°C (302°F to 554°F).

064742-31-0

Distillates (petroleum), chemically neutralized light

A complex combination of hydrocarbons produced by a treating process to remove acidic materials. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150°C to 290°C (302°F to 564°F).

064742-47-8

Distillates (petroleum), hydrotreated light

A complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150°C to 290°C (302°F to 554°F).

064742-81-0

Kerosene (petroleum), hydrodesulfurized

A complex combination of hydrocarbons obtained from a petroleum stock by treating with hydrogen to convert organic sulfur to hydrogen sulfide which is removed. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150°C to 290°C (302°F to 554°F).

064742-96-7

Solvent naphtha (petroleum), heavy aliph.

A complex combination of hydrocarbons obtained from the distillation of crude oil or natural gasoline. It consists predominantly of saturated hydrocarbons having carbon numbers predominantly in the range of C11 through C16 and boiling in the range of approximately 190°C to 290°C (374°F to 554°F).

**Appendix 2 - Data Matrix**

	Category Member	Category Member	Category Member	Category Member	Category Member	Category Member	Supporting Material	Supporting Material	Supporting Material	Supporting Material	Supporting Material	Read Across Range to Untested Category Members
<b>CASRN</b>	8008-20-6	64742-81-0	64742-14-9	64742-31-0	64742-47-8	64762-96-7	No CASRN	No CASRN	No CASRN	91770-15-9	101316-80-7	
<b>CAS Name</b>	Kerosine (petroleum)	Kerosine (petroleum), hydrodesulfurized	Distillates (petroleum), acid-treated light	Distillates (petroleum), chemically neutralized light	Distillates (petroleum), hydrotreated light	Solvent naphtha (petroleum), heavy aliph.	Jet Fuel A <sup>2</sup>	JP-8 <sup>3</sup>	JP-5 <sup>4</sup>	Kerosine (petroleum), sweetened	Solvent naphtha (petroleum), hydrocracked heavy arom.	
<b>Endpoint PHYSICAL CHEMICAL PROPERTIES</b>												
Melting Point (°C)												not relevant
Pour Point (°C)	-55 (min)						-47	-47 to -50				-55 to -47
Freezing Point (°C)							-40 (max)	-47 (max)	-46 (max)			-47 to -40
Boiling Point (°C)	164 - 271 (10% and final BP)	183 - 279 (initial and final BP)					205 - 300 (maximum 10% and final BPs)	175 - 300 (typical initial and final BP)	206 - 300 (maximum 10% and final BPs)	152 - 257	187 - 288	150 - 290
Vapor Pressure (hPa)	14 (38°C)							3 - 35 (21°C)	3 - 35 (21°C)			3 to 35
Partition Coefficient <sup>1</sup>	3.3 to >6	3.3 to >6										3.3 to >6
Water Solubility <sup>1</sup> (mg/L)	5.5						4.8 - 10.4	12.4				4.8 - 12.4
<b>ENVIRONMENTAL FATE</b>												
Photodegradation, OH <sup>-</sup> reaction T <sub>1/2</sub> <sup>1</sup> (h or d)	0.2 - 1.5 days (modeled data)											0.2 to 1.5



Rat Acute (mg/m <sup>3</sup> )	LC50 >5280 (4hr)	LC50 >5200 (4hr)									LC50 >5,000
Rat Acute Oral (mg/kg)	LD50 >5000	LD50 >5000					LD50 >20000				LD50 >5,000
Rat Acute Dermal (mg/kg)	LD50 >2000	LD50 >2000					LD50 >4000				LD50 >2,000
Inhalation Rat Repeated-Dose (mg/m <sup>3</sup> )		NOAEL >24									NOAEL >24
Dermal Rat Repeated-Dose (mg/kg/d)		NOAEL 495									NOAEL 495
Genotoxicity, <i>in vitro</i>	equivocal	negative			negative		equivocal		negative	negative	negative
Genotoxicity, <i>in vivo</i>	negative	negative					equivocal	negative			negative
Dermal Reproductive toxicity (mg/kg/d)		NOAEL 495									NOAEL 495
Inhalation Developmental toxicity (PPM)	NOAEL >364						NOAEL >395				NOAEL >364 PPM
Dermal Developmental toxicity (mg/kg/d)		NOAEL 495									NOAEL 495

blank cells = no data; value will be read across range

<sup>1</sup> Level 1 fugacity model output. Range of values based upon characteristics of individual hydrocarbon constituents.

<sup>2</sup> ASTM D1655

<sup>3</sup> MIL-PRF-83133

<sup>4</sup> MIL-PRF-5624

<sup>5</sup> NOTE - when multiple studies for one CASRN, used key study