

201-16098A

HIGH PRODUCTION VOLUME (HPV) CHEMICAL CHALLENGE PROGRAM

TEST PLAN

Kerosene/Jet Fuel Category

Submitted to the US EPA

by

The Petroleum HPV Testing Group

www.petroleumhpv.org

Consortium Registration #

December 31, 2003

Updated December 16, 2005

RECEIVED
MPT CDIC
05 DEC 19 AM 8:04

Table of Contents

Plain Language Summary	3
Description of The Kerosene/Jet Fuel Category	4
Category Rationale	7
Evaluation of Existing Health Effects Data and Proposed Testing	8
Evaluation of Existing Physicochemical and Environmental Fate Data and Proposed Testing	11
Evaluation of Existing Ecotoxicity Data and Proposed Testing	14
Matrix of Available Data and Proposed Testing	16
References	17
Appendices	
Appendix A. CAS Numbers and Descriptions of Category Members	22
Appendix B. Links to Additional Resources	25
Appendix C. Chronology of the Development of Jet Fuels	26
Appendix D. Robust Summary (separate document)	27
Figures	
Figure 1. Kerosene/Jet Fuel Process Diagram	5
Figure 2. Boiling Ranges of Fuels	7
Tables	
Table 1. Compositional Data on Representative Kerosene- Range Materials	6
Table 2. Chemical Composition of Hydrodesulfurized Kerosene	6
Table 3. Matrix of Available Data and Proposed Testing	16

Plain Language Summary

The Kerosene/Jet Fuel category covers the kerosene-range refinery streams, commonly referred to by the generic term "kerosene". The refinery streams in this category are complex petroleum mixtures, have a boiling range of approximately 293 to 572 °F (145 to 300 °C) and a carbon range of C₅ - C₂₅. At ambient temperatures, all the substances in this category are liquids. The substances in this test plan share many physical properties that make them suitable for blending into kerosene fuels, but only a few are sold as finished light distillate (kerosene based) home heating oils and transportation fuels. When sold as fuels, the kerosene-range refinery streams are known as aviation turbine fuels (jet fuels), kerosene, and No. 1 grades of fuel oil, diesel fuel, and gas turbine oil.

The kerosene-range refinery streams are mixtures of petroleum hydrocarbons with broadly overlapping chemical composition, closely related physical properties, and generally similar toxicological effects. The Testing Group thinks the physical and chemical similarities among the streams in this category allow toxicology data on one material to be extrapolated to the others (White, 1999). Mammalian toxicity studies on jet fuel (composed almost entirely of kerosene or hydrodesulfurized kerosene) and two samples of kerosene produced by different refining processes support this position.

This test plan demonstrates that there are adequate data on kerosene and jet fuel (the two materials in this category with the greatest potential for public exposure) to characterize the potential hazards of kerosene-range refinery streams. The Testing Group thinks the existing physicochemical, mammalian toxicology and environmental data provide sufficient information to characterize the potential health and environmental effects of kerosene-range refinery streams. Therefore, the Testing Group is not proposing any additional mammalian, environmental fate, or ecotoxicity testing.

Description of the Kerosene/Jet Fuel Category

Based on their intended use, the streams in this category can be divided into two groups, those used primarily as fuels and those used primarily as solvents. The eight kerosene-range streams that are used as solvents are not primary products of the petroleum industry and therefore are not considered in detail in this Test Plan. Those eight streams are also being sponsored by either the International Hydrocarbon Solvents Consortium (IHSC) or the ACC Olefins Panel's (ACCOP) Low Benzene Naphtha group and are considered in test plans being developed by those two groups. The Petroleum HPV Testing Group is sharing information with the two other groups to avoid duplication of effort and unnecessary use of animals.

The Kerosene/Jet Fuel category includes both finished products (fuels) and the refinery streams from which they are blended. 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 293 to 572 °F (145 to 300°C) and consists of hydrocarbons primarily 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 heavier-weight gas oils, Diesel and Fuel Oil No. 2, Fuel Oil No. 4 and Fuel Oil No. 6 (heavy fuel oil) are covered in separate API HPV Test Plans.

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

In developing this Test Plan, the Testing Group has utilized information on the kerosene-based jet fuels although these fuels do not appear by name among the CAS numbers covered in this category. Kerosene-type jet fuels (such as Jet A & JP-8) are not specifically identified on the Toxic Substances Control Act's Chemical Inventory of Substances, and consequently do not have unique CAS numbers. However, because jet fuels are composed of kerosene (CAS no. 8008-20-6) or hydrodesulfurized kerosene (CAS no. 64742-81-0), the Testing Group thinks testing done on a kerosene-type jet fuel can be extrapolated to not only those two CAS numbers, but to other kerosene-range refinery streams as well.

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 are further treated by a variety of processes to remove or reduce the level of undesirable components, e.g. aromatic hydrocarbons, 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 processes used are hydrodesulfurization (treatment with hydrogen to remove sulfur components), washing with caustic soda solution (to remove sulfur components), and hydrogenation (to remove olefins, sulfur and nitrogen components). Aromatics that may have formed during the cracking process are removed via solvent extraction. 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).

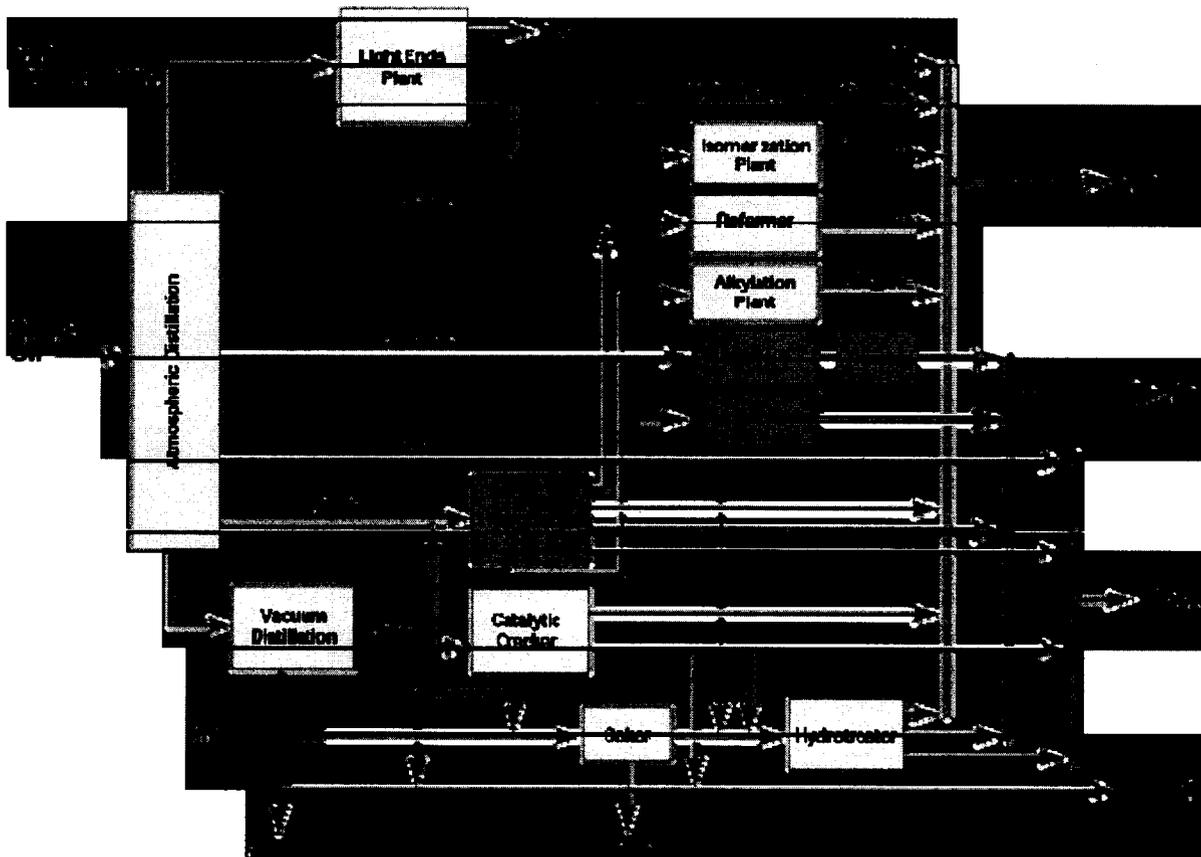
Links to additional resources on refining processes and petroleum-related glossaries are presented in Appendix B.

Although straight run kerosene can be marketed directly, more commonly, several kerosene-range streams may be blended to produce the final product. However, whether straight run or blended, kerosene-based fuels are produced to meet the ASTM specifications for fuel oils, 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 process stream or blend of process streams (ASTM 2000, 2001a,b). The final products are essentially the same kerosene with additives for the intended use. Otherwise these petroleum streams and kerosene fuel

products are virtually indistinguishable on the basis of physical or chemical properties (CONCAWE 1995, 1999).

While kerosenes are essentially 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 hydrocarbon mixtures, materials 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). Consequently, detailed compositional information for the streams in this category is limited. General compositional information (Table 1) on representative kerosene-range refinery streams and fuels illustrates the fact that the materials in this category are all similar in their physical properties and composition. 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 of a process stream. 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. The distillation range of kerosenes is such that benzene (80 °C boiling point) and n-hexane (69 °C boiling point) concentrations are always 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 PACs found in kerosenes are very low, if not below the limits of detection of the available analytical methods (CONCAWE 1995, 1999). A detailed analysis of a hydrodesulfurized kerosene illustrates this (Table 2).

Figure 1. Kerosene/Jet Fuel Processing



Note: Merox® = mercaptan oxidation – reduces mercaptan levels

Table 1. Compositional Data on Representative Kerosene- Range Materials

	8008-20-6	64742-96-7	64742-14-9	64742-31-0	64742-81-0	Jet A	JP-8
API gravity	41.8 – 44.9	38.4	42.8	43.91	39 – 45.5	37.2- 46.1	37.0 – 46.7
Aromatic content, vol. %	15.5 – 19.6	<1.0 - 13	21.52	13.9	18 – 21.4	11.6 – 24.0	13.6 – 22.1
Olefin content, vol %	1.3 - 2.5	-	2.29	7.15	1.0 – 1.66	0.0 – 4.1	0.6 – 3.0
Saturates content, vol %	79 - 82	99.16	76.19	78.95 %	77.2 – 82	71.9 - 88.4	74.9 - 85.8
Distillation, °F							
10%	320 - 377	385	376	377	329 -406	294 - 394	333 - 390
FBP	468 - 538	630	491 (90%)	487	451 - 568	404 – 510 (90%)	419 – 474 (90%)

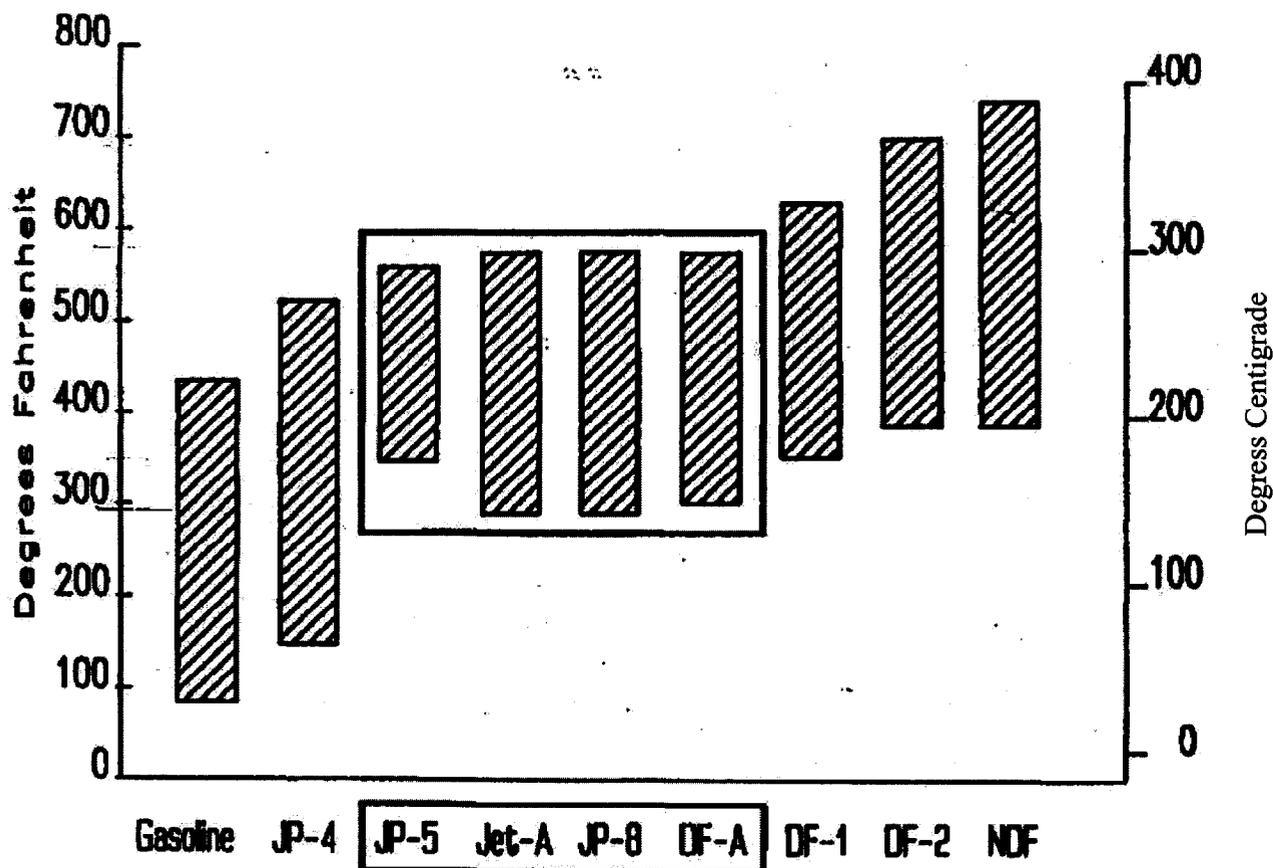
Table 2. Chemical Composition of Hydrodesulfurized Kerosene (CAS No 64742-81-0)

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

^aAnalyzed by ASTM Method D1319-1, Fluorescent indicator Adsorption.

^bPolycyclic aromatic compounds.

Figure 2. Boiling Ranges of Fuels



U.S. Army, 2001

Category Rationale

The Testing Group made the following assumptions when analyzing the existing data:

- The materials included in the Kerosene/Jet Fuel category are related from both process and physical-chemical perspectives;
- the physical and chemical similarities among the materials in this category allow toxicology data on one material to be extrapolated to the others;
- data developed on jet fuels can be used to characterize members of this category since jet fuels are essentially kerosene or hydrodesulfurized kerosene.

The Testing Group thinks the existing physicochemical, mammalian toxicology and environmental data on jet fuel and kerosene will provide sufficient information to characterize the potential health and environmental effects of kerosene-range refinery streams.

Evaluation of Existing Health Effects Data and Proposed Testing

General Evaluation

A substantial body of data ranging from acute to long-term carcinogenicity studies has been compiled on selected kerosene-range refinery streams and fuels. Additional reviews by various expert panels have also been published (ACGIH, 2003; ATSDR, 1998; Bogo, et al., 1983; Bruckner, et al., 2001; Carpenter, et al., 1976; CONCAWE, 1995,1999; EPA, 2002; Gaworski, et al., 1984; IARC, 1989; MacNaughton, et al., 1984; Nessel, 1999; NRC, 1996; Ritchie, et al., 2001; Zeiger, et al., 1998). Because No. 1 fuel oil, kerosene and jet fuels (kerosene based) are virtually indistinguishable on the basis of their gross physical or chemical properties (IARC, 1988), data generated on any of the materials can be used to characterize the toxicity of all the materials.

The Test Plan addresses the health effects endpoints of the category by:

- Evaluating the extensive toxicology database for the jet fuels and selected kerosene-range refinery streams, and
- Using read-across information whenever possible among category members.

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). 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, 1987). Carpenter et al, (1976) reported no mortalities in rats when exposed for eight hours to saturated vapor of deodorized kerosene (probably a desulfurized kerosene). 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, 1980, 1982; Shell, 1991a,b,c,d).

An eye irritation 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 have also been reported for hydrodesulfurized kerosene and jet fuel (API, 1980a, 1982). These materials produced more irritation in the unwashed eyes at 1 hour than had the straight run kerosene. The eye irritation persisted longer than that seen with straight run kerosene, but by day 7 had resolved.

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).

Summary: No additional testing is planned. Multiple acute toxicity studies have been reported on a variety of kerosene based streams. The Testing Group thinks the existing data is sufficient to characterize the acute toxicities of this category of materials.

Repeat-Dose Toxicity

Seven dermal toxicity studies have been reported for various kerosene based refinery streams and fuels. These dermal studies have utilized a number of species and have ranged in duration from one to thirteen weeks. A 28-day inhalation study has also been conducted. In preparing this Test Plan, the Testing Group has reviewed the available toxicology studies and included in the robust summary a detailed description(s) of the one study or a small number of studies that best address each SIDS Level 1 endpoint. Other studies are cited in the appropriate "Remarks" section of the Robust Summary and are intended to supplement the readers' knowledge. Therefore, the attached Kerosene/Jet Fuel Robust Summary (Appendix D) contains complete summaries for one 28-day and one 13 week study done via the dermal route. Results from the remaining five dermal studies are summarized on pages 52 and 53 of the Jet Fuel/kerosene Robust Summary. A complete summary of the 28-day inhalation study has also been included in the Robust Summary.

Dose levels of 200, 1000 and 2000 mg/kg_{bw} of a straight run kerosene (CAS no. 8008-20-6) were applied undiluted to the skin of male and female New Zealand white rabbits (API, 1985b). The test material was applied 3x/week for 28 days. One male and one female in the 2000 mg/kg_{bw} dose group found dead on days 10 and 24 respectively were thought to be treatment-related. Clinical signs that were considered to be treatment-related included: thinness, nasal discharge, lethargy, soiled anal area, anal discharge, wheezing. The high dose group appeared to have a treatment related mean body weight loss when compared to controls. Dose-related skin irritation was observed, ranging from "slight" to "moderate" in the low and high dose groups, respectively. Other treatment-related dermal findings included cracked, flaky and/or leathery skin, crusts and/or hair loss. Reductions in RBC, 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).

Gross necropsy findings were confined largely to the skin. Enlarged spleens were seen in the female groups. Microscopic examination of tissues taken at necropsy found proliferative inflammatory changes in the treated skin of all male and female animals in the high dose group. These changes were, in the majority of animals, accompanied by an increase in granulopoiesis of the bone marrow. Four of six high dose males had testicular changes (multifocal or diffuse tubular hypoplasia) that were considered by the study authors to be secondary to the skin and/or weight changes.

In a different study, hydrodesulfurized kerosene (CAS no. 64742-81-0) was tested in a thirteen-week dermal study using Sprague-Dawley rats (Battelle, 1997). Test material was applied 5x/week to the skin of male and female rats at dose levels of 165, 330 & 495 mg/kg_{bw}. Aside from skin irritation at the site of application, there were no treatment-related clinical signs during the study. Screening of all animals using a functional observation battery (FOB) did not find any substance-related effects. Ophthalmological examination of all animals also found no treatment-related effects. There were no treatment-related effects on growth rates, hematological or clinical chemical values, or absolute or relative organ weights. Microscopic examination of tissues from animals surviving to termination found no treatment-related changes, with the exception of a minimal degree of a proliferative and inflammatory changes in the skin.

A hydrodesulfurized middle distillate (CAS no. 64742-80-9) 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 25mg/m³ kerosene. Exposures were for approximately 6 hr/day, five days each week for four consecutive weeks. There were no treatment-related effects on clinical condition, growth rate, 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.

Carcinogenicity

In addition to the repeat-dose studies discussed above, 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 mice confirmed that the reduced irritation seen with samples in mineral oil was not due to decreased skin penetration (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). Animal survivals were not effected by exposure to the kerosene. The study's authors concluded that the kerosene was not an initiator but it did show tumor promoting activity.

Summary: No additional repeat-dose testing is planned for kerosene or jet fuel. Multiple repeat-dose toxicity studies have been reported on a variety of kerosenes or jet fuels. When applied dermally, kerosenes and jet fuels have been shown to produce dermal and systemic effects. The Testing Group thinks the existing data are sufficient to characterize the repeat-dose toxicity of this category of materials.

In-Vitro (Genotoxicity)

The potential *in vitro* genotoxicities of kerosene and jet fuel have been evaluated in a variety of studies. Standard Ames assays on two kerosene samples and a sample of Jet A produced negative results with/without activation (API, 1977, 1978, 1979a). Modified 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).

In-Vivo Genotoxicity

Multiple *in vivo* genotoxicity studies have been done on a variety of kerosene-based materials. Four samples of kerosene were negative and a sample of Jet A was positive in *in vivo* bone marrow cytogenetic tests in Sprague-Dawley rats (API, 1977, 1979a, 1984b, 1985d). One of the kerosene samples produced a positive response in male mice and negative results in females when tested in a sister chromatid exchange assay (API, 1988b). Both deodorized kerosene and Jet A samples produced negative results in dominant lethal assays (API, 1973, 1980b). The kerosene was administered to both mice and rats intraperitoneally, while the jet fuel was administered only to mice via inhalation.

Summary: No additional testing is planned. Existing *in vitro*, *in vivo* and carcinogenicity studies are adequate to characterize the genotoxicity of kerosene and jet fuels.

Reproductive/Developmental Toxicity

A reproductive/developmental screening study in Sprague-Dawley rats of hydrodesulfurized kerosene has been reported by Schreiner et al. (1997). The study was performed in accordance with OECD Guideline 421, except males were treated for 8 weeks to improve observation of effects on the reproductive system. Either 0, 20, 40 or 60% (v/v) kerosene in mineral oil was applied to the skin of the rats. The dose per body weight equivalents were 0, 165, 330 and 494 mg/kg_{bw}. 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 (up to moderate) 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. 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 494 mg/kg_{bw}/day.

Developmental toxicity screening studies on a kerosene and a sample of Jet A have been reported (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.

Summary: No additional reproductive/developmental toxicity testing is planned. Three reproductive/developmental tests have been reported on kerosenes or jet fuels. None of these studies have shown compound-related effects on any of the recorded reproductive or developmental parameters. The Testing Group thinks the existing data are sufficient to characterize the repeat-dose toxicity of this category of materials.

Evaluation of Existing Physicochemical and Environmental Fate Data and Proposed Testing

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. Environmental fate endpoints include photodegradation, hydrolysis, environmental transport and distribution (fugacity), and biodegradation.

Although some data exist for some products in this category, not all of these endpoints are defined and a consensus database for chemicals that represent products in this category does not exist. Therefore, calculated and measured representative data have been identified and a technical discussion provided, where appropriate. The EPIWIN[®] computer model, as discussed in the US EPA document entitled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program" has been used to calculate physical-chemical properties of representative constituents of kerosene and jet fuels (EPA, 2000).

The substances covered under this HPV testing plan are mixtures of paraffinic, naphthenic, olefinic, and aromatic (PONA) hydrocarbon compounds having predominantly nine to sixteen carbon atoms. Because of the diversity of compounds encompassing kerosenes and the fuel products derived from them, it is not feasible to model the physicochemical and environmental fate endpoints for each potential compound. Rather, modeling efforts done for those endpoints covered representative low and high molecular weight PONA components. This provided a range of values that were considered to encompass those characteristics for the majority of the hydrocarbon constituents in kerosenes.

Physicochemical Data

Melting Point

For complex mixtures 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 pour point temperature falls as an oil's viscosity increases. 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.

Summary: No additional testing is proposed. The pour points of various kerosenes and jet fuels have been adequately demonstrated and shall be considered representative of the melting point characteristic for these petroleum refining streams.

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 the hydrocarbon mixture. Distillation ranges for a variety of jet fuels and kerosene blending streams have been reported (CONCAWE, 1995; Jokuty et al., 2002, API, 1987b). Typical distillation ranges for blended fuels are within 125 - 300 °C for kerosenes and Jet A/A-1. These values are generally consistent with the distillation range of 145 to 300 °C described by CONCAWE (1995) for the general category of kerosenes and jet fuels having hydrocarbon components predominantly in the range of C₉ to C₁₆.

Summary: No additional testing is proposed. The distillation ranges of kerosenes and jet fuels have been adequately determined.

Vapor Pressure

For mixtures such as petroleum products, the vapor pressure of the mixture is the sum of the partial pressures of the individual components (Dalton's Law of Partial Pressures). Kerosenes generally are expected to have measurable vapor pressure due to their boiling range (145 to 300 °C) and molecular weights of the constituent hydrocarbons (C₉ - C₁₆ carbon atoms). Kerosene (API, 1987b) and narrow-cut jet fuel (Jet A/A-1, Jokuty et al., 2002) measured at 37.8 °C using ASTM D323 had vapor pressures of >1 to 1.4 kPa (Jokuty et al. 2002). Vapor pressure values from the US Air Force for jet fuels at 20 - 21 °C were 0.3 - 3.5 kPa for JP5 and JP8. 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.

Summary: No additional testing is proposed. The vapor pressures of representative distillate fuels have been adequately measured. These measurements are expected to approximate the vapor pressures of individual category members with similar carbon-number and boiling point ranges.

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 mixtures, 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 EPIWIN[®] (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 D), kerosenes with varying proportions of saturated, aromatic, and olefinic hydrocarbons would not be expected to have significantly different log Kow ranges.

Summary: No additional modeling is proposed. Partition coefficients (Kow) of 3.3 to >6.0 have been estimated for representative C₉ to C₁₆ PONA components of kerosenes.

Water Solubility

When released to water, kerosene will float and spread at a rate that is viscosity - and temperature-dependent. Component hydrocarbons in the products will partition to water according to their individual solubility values. For individual hydrocarbon constituents in middle distillates, water solubility values vary by orders of magnitude. Molecular weight and chemical structure have a great influence on the ultimate degree of solubility. Water solubility of component hydrocarbon molecules was estimated using EPIWIN[®], WSKOW V1.40 computer model (EPA, 2000). Water solubility ranged from <10⁻³ mg/L for the higher molecular weight n-alkanes (e.g., n-C₁₆) to approximately 52 mg/L for a C₉ alkylbenzene. Water solubility values from government/military sources or anecdotal evidence (e.g., spill events) were included in the robust summaries as supporting data for the modeled estimates. Those sources cited water solubility values ranging from 4.8 to 57 mg/L.

Summary: No additional modeling is proposed. Water solubility values have been calculated for various C₉ to C₁₆ PONA constituents of kerosenes.

Environmental Fate Data

The typical battery of tests used to measure the environmental fate of a material is not easily performed on the materials of this category because of their physical and chemical properties. Therefore, when measured data are not available to describe a fate process, characteristics of kerosene components will be modeled where appropriate using EPIWIN[®] (U.S. EPA, 2000).

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 depends 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.

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 (OH⁻). The potential to undergo indirect photodegradation can be estimated using the atmospheric oxidation potential (AOP) model subroutine (AOPWIN V1.90) in EPIWIN[®] (EPA, 2000), which calculates a chemical half-life and an overall OH⁻ reaction rate constant based on a 12-hour day and a given 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).

Summary: No additional modeling is proposed. Atmospheric half-lives of 0.2 to 1.5 days have been calculated for representative C₉ and C₁₆ hydrocarbon components of kerosenes.

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 these functional groups, materials in the kerosenes category are not subject to hydrolysis.

Summary: No additional modeling is proposed. The materials in the kerosene category do not contain chemical moieties that undergo hydrolysis.

Transport and Distribution in the Environment (Fugacity)

Fugacity-based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended solids, water and biota). The U.S. EPA has agreed that computer modeling techniques are an appropriate approach to estimating chemical partitioning. A widely used fugacity model is the EQC (Equilibrium Criterion) model. The EQC model is a Level 1 (i.e., steady state, equilibrium, closed system and no degradation) model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized unit environment. EPA cites the use of the EQC model in its document, "Determining the Adequacy of Existing Data", which was prepared as guidance for the HPV chemicals program. 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%). Increasing molecular weight of the hydrocarbon classes increases partitioning to soil, though the C₁₆ isoparaffins, 2- and

3-ring naphthenes, and monoaromatics exhibit significant distribution to air (13 - 60%). Partitioning to water is <10% at equilibrium, while partitioning to sediment is \leq 2% and to biota (fish) is \leq 0.1%

Summary: No further modeling is proposed. Fugacity modeling has been done to provide an estimate of the percent distribution in environmental media of various C₉ to C₁₆ PONA hydrocarbons found in kerosenes.

Biodegradation

Limited specific biodegradation data are available for identified CAS numbers in the kerosene/jet fuels category following standard test methodology. 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 (jet fuel, CAS number not reported) was tested in a 10-day BOD respirometry test using enriched and unenriched seawater and enriched fresh water at 30 °C according to ASTM D2329-68 closed-bottle respirometry guidelines, and found to degrade by 46 - 53% in the enriched waters in the 10-day interval; however, degradation in unenriched 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 contaminated 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, normal 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); both processes limit bioavailability and can slow biodegradation. The hydrocarbons in 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 proliferation of 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 mixture 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) and their biodegradability would primarily be governed by the biodegradability of the saturates in the mixtures. 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. The biodegradability of refined low-aromatic solvents containing mostly saturates [three different carbon-number cuts of CAS no. 64742-47-8, Mixed Alkanes (n-, iso-, and cycloparaffins)] in the same carbon number range will ultimately be addressed by the International Hydrocarbon Solvents Consortium HPV submissions to ICCA.

Summary: No further testing is proposed. 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.

Evaluation of Existing Ecotoxicology Data and Proposed Testing

Data for one category member (kerosene, hydrodesulfurized, CAS no. 64742-81-0) and two surrogate (non-HPV) kerosene streams are available. Both surrogate streams -- Sweetened Kerosene, CAS no. 91770-15-9 and Hydrocracked Heavy Naphtha, CAS no. 101316-80-7 -- are included in the CONCAWE (1995) dossier on kerosenes and jet fuels, and were assessed for ecotoxicity by Exxon (1995a-e), while the category

member was tested by both Exxon (1995f-h) and Shell (1995a-c). Robust summaries for the surrogate and category member studies are included in the Robust Summary, Appendix D. All studies used exposures to water accommodated fractions (WAFs) of the process streams. Each of the different streams exhibited similar toxicity to rainbow trout (*Oncorhynchus mykiss*, 96-hour EL50 values of 18 - 25 mg/L); likewise, toxicity to the alga *Selenastrum capricornutum*, with 96-hour growth rate EL50 values of 5.0 - 6.2 mg/L and biomass inhibition EL50 values of 5.9 - 11 mg/L, did not vary greatly among the streams. There was considerable variation in the measured toxicity of the category member (CAS no. 64742-81-0) to daphnids (*Daphnia magna*) when evaluated in different tests; in the test using daily renewal of freshly-prepared WAF (Exxon 1995g), the 48-hr EL50 was estimated at 1.4 mg/L, while in the test where solution was not renewed (Shell, 1995b) it was estimated at between 40 and 89 mg/L. In spite of daily renewal, a sample of sweetened kerosene (CAS no. 91770-15-9) exhibited considerably less toxicity than the hydrodesulfurized and hydrocracked materials tested in the same laboratory (Exxon 1995b), indicating the difference in that measurement is due to the nature of the sample rather than variations in the testing approach.

Two additional studies using the WAF methodology, summarized by CONCAWE (1995), indicate greater sensitivity of a marine amphipod (*Chaetogammarus marinus*) with an EL50 of 1.4 mg/L, than of the zebrafish (*Brachydanio rerio*), EL50 13.5 mg/L, to cracked kerosene (CAS no. 68477-39-4). These results are consistent with those summarized above and indicate measurable, moderate aquatic toxicity of kerosenes over a range of CAS numbers.

There is considerable data regarding toxicity of jet fuels to aquatic organisms, as summarized by CONCAWE (1995). Many of the studies used a water-soluble fraction, in which the aqueous fraction of a single loading rate of hydrocarbon, after equilibration, is diluted to varying percentages (expressed as either percent WSF or mg/L corresponding to the dilution) and used for exposure. 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 to those obtained using the WAF methodology, with generally similar toxicity among different jet fuel products for a given species or taxonomic group.

The similarity of PONA composition of the kerosene refining/processing streams and generally similar estimates of aquatic toxicity among those streams indicate the existing data can be used to estimate the toxicity of the remaining category members.

Summary: No further testing is proposed. Adequate data regarding the ecotoxicity of kerosenes and jet fuels are available to demonstrate moderate acute toxicity to aquatic organisms.

Matrix of Available Data and Proposed Testing

Table 3. Matrix of Available Data and Proposed Testing

	KEROSENE	JET FUEL
TEST		
Physical/Chemical Properties		
Melting Point	Adequate	Adequate
Boiling Point	Adequate	Adequate
Vapor Pressure	Adequate	Adequate
Water Solubility	Adequate	Adequate
Partition coefficient (log Kow)	Adequate	Adequate
Ecotoxicity		
Algae Growth Inhibition	Adequate	Read-Across ^a
Acute Freshwater Invertebrate	Adequate	Read-Across ^a
Acute Freshwater Fish	Adequate	Read-Across ^a
Environmental Fate		
Biodegradation	Adequate	Adequate
Stability in Water	N/A	N/A
Photodegradation (estimate)	Adequate	Adequate
Transport and Distribution	Adequate	Adequate
Mammalian Toxicity		
Acute	Adequate	Adequate
Repeat-dose	Adequate	Adequate
Reprod/Develop	Adequate	Adequate
Genotoxicity, <i>in vitro</i>	Adequate	Adequate
Genotoxicity, <i>in-vivo</i>	Adequate	Adequate

^aRead-across for jet fuels will be from kerosene stream data using WAF methodology

References

- ACGIH (American Conference Governmental Industrial Hygienists). 2003. Kerosene/Jet Fuels; Documentation of the TLV. Documentation of the TLVs® and BEIs® with Other Worldwide Occupational Exposure Values CD-ROM – 2003. Cincinnati, OH.
- Aelion C M; Bradley P M. 1991. Aerobic biodegradation potential of subsurface microorganisms from a jet fuel-contaminated aquifer. *Appl. & Envir. Micro.* 57(1) 57-63.
- API (American Petroleum Institute). 1973. Mutagenicity studies of thirteen petroleum fractions. *API Med. Res. Publ.* 26-60098, Washington D.C.
- API (American Petroleum Institute). 1977. Mutagenicity evaluation of kerosene. *API Med. Res. Publ.* 26-60017, Washington D.C.
- API (American Petroleum Institute). 1978. Estimation of the mutagenicity of hydrocarbon fractions utilizing the bacterial assay procedure with mammalian tissue metabolic activation. *API Med. Res. Publ.* 26-60103, Washington D.C.
- API (American Petroleum Institute). 1979a. In vitro and in vivo mutagenicity studies Jet Fuel A. *API Med. Res. Publ.* 27-30051, Washington D.C.
- API (American Petroleum Institute). 1979b. Teratology study in rats: Kerosene. *API. Med. Res. Publ.* 27-32175, Washington D.C.
- API (American Petroleum Institute). 1979c. Inhalation/teratology study in rats: Jet Fuel A. *API. Med. Res. Publ.* 27-32173, Washington D.C.
- API (American Petroleum Institute). 1980a. Acute toxicity tests of API Jet fuel A. *API Med. Res. Publ.* 27-32815, Washington D.C.
- API (American Petroleum Institute). 1980b. Mutagenicity evaluation of Jet fuel A in the mouse dominant lethal assay. *API Med. Res. Publ.* 28-31345, Washington D.C.
- API (American Petroleum Institute). 1982. Acute oral toxicity study in rats acute dermal toxicity study in rabbits primary dermal irritation study in rabbits primary eye irritation study in rabbits API 81-07 hydrodesulphurized kerosene (CAS 8008-20-6). *API Med. Res. Publ.* 30-31986, Washington D.C.
- API (American Petroleum Institute). 1983. LC50 Acute inhalation toxicity evaluation of a petroleum derived hydrocarbon in rats. Hydrodesulphurized kerosene API Sample 81-07. *API Med. Res. Publ.* 30-32855, Washington D.C.
- API (American Petroleum Institute). 1984a. Dermal sensitization study in guinea pigs, closed patch technique, API sample 81-07. *API Med. Res. Publ.* 31-31413, Washington D.C.
- API (American Petroleum Institute). 1984b. Mutagenicity evaluation studies in the rat bone marrow cytogenetic assay in the mouse lymphoma forward mutation assay Hydrodesulfurized kerosene API sample 81-07. *API Med. Res. Publ.* 32-30240, Washington D.C.
- API (American Petroleum Institute). 1985a. Acute oral toxicity study in rats acute dermal toxicity study in rabbits primary dermal irritation study in rabbits primary eye irritation study in rabbits dermal sensitization study in guinea pigs API 83-09 straight run kerosene (CAS 8008-20-6). *API Med. Res. Publ.* 32-32858, Washington D.C.
- API (American Petroleum Institute). 1985b. 28-day dermal toxicity study of API 83-09 in the rabbit. *API Med. Res. Publ.* 33-30443, Washington D.C.
- API (American Petroleum Institute). 1985c. L5178Y TK+/- Mouse lymphoma assay API 83-09, Straight run

kerosene (CAS 8008-20-6). API Med. Res. Publ. 32-32745, Washington D.C.

API (American Petroleum Institute). 1985d. The acute in vivo cytogenetics assay in male and female rats of API 83-09. API Med. Res. Publ. 32-31769, Washington D.C.

API (American Petroleum Institute). 1986. Four week subchronic inhalation toxicity study in rats: Final report. API 81-07 hydrodesulfurized kerosene (petroleum) (CAS 64742-81-0), API 81-09 hydrodesulfurized middle distillate (petroleum) (CAS 64742-80-9), API 81-10 hydrodesulfurized middle distillate (petroleum) (CAS 64742-80-9). API Med. Res. Publ. 33-32724, Washington D.C.

API (American Petroleum Institute). 1987a. Acute inhalation toxicity of a petroleum derived hydrocarbon in rats. API 83-09 Straight run kerosene (CAS 8008-20-6). API Med. Res. Publ. 34-30634, Washington D.C.

API (American Petroleum Institute). 1987b. Comprehensive analytical analysis of API generic petroleum streams. Washington, D.C.

API (American Petroleum Institute). 1988a. Sister chromatid exchange assay in Chinese hamster ovary cells with API 81-07: hydrodesulfurized kerosene. API Med. Res. Publ. 35-32482, Washington D.C.

API (American Petroleum Institute). 1988b. In vivo chromatid exchange assay with API 81-07 Hydrodesulfurized kerosene. API Med. Res. Publ. 36-30043, Washington D.C.

API (American Petroleum Institute). 1989a. Lifetime dermal carcinogenesis/chronic toxicity screening bioassay of refinery streams in C3H/HEJ mice. API Med. Res. Publ. 36-31364, Washington D.C.

API (American Petroleum Institute). 1989b. Short-term dermal tumorigenesis study of selected petroleum hydrocarbons in male CD-1 mice. Initiation and promotion phases. API Med. Res. Publ. 36-32643. Washington D.C.

ASTM (American Society for Testing and Materials). 1999. Standard Test Method for Pour Point of Petroleum Oils. ASTM D97, Volume 05.01. West Conshohocken, PA.

ASTM (American Society for Testing and Materials). 2001a. Standard Specification for Aviation Turbine Fuels. ASTM D1655-01. West Conshohocken, PA.

ASTM (American Society for Testing and Materials). 2001b. Standard Specification for Fuel Oils. ASTM D396-01. West Conshohocken, PA.

ASTM (American Society for Testing and Materials). 2002. Standard Specification for Diesel Fuel Oils. ASTM D975-02. West Conshohocken, PA.

Atlas, R.M. Microbial Degradation of Petroleum Hydrocarbons: an Environmental Perspective. Microbiological Reviews. 45: 180-209; 1981.

ATSDR (Agency for Toxic Substances and Disease Registry). 1998. Jet fuels (JP-5 and JP-8). U.S. Department of Health & Human Services.

Battelle. (1997). 13-Week subchronic dermal study with neurotoxicology evaluations of hydrodesulfurized kerosene in Sprague-Dawley rats: Final report. Battelle study No. N001450A. Battelle, Columbus, Ohio.

Blackburn, G. R., Deitch, R. A., Schreiner, C. A. and Mackerer, C. R. 1986. Predicting tumorigenicity of petroleum distillation fractions using a modified Salmonella mutagenicity assay. Cell Biol. Toxicol. Vol. 2. pp 63-84.

Bogo, V., R.W. Young, T.A. Hill, CX. Feser, J. Nold, G.A. Parker, R.M. Cartledge. 1983. The toxicity of petroleum and shale JP5. AFRRRI SR83-26; AD-A142 670. Armed Forces Radiobiology Research Institute, Bethesda, MD. See also: MacFarland, H.N. et al. (Eds.), Advances in Modern Environmental Toxicology, Vol. 6: Applied Toxicology of Petroleum hydrocarbons. Princeton Scientific Publishers, Princeton, NJ, pp. 17-32, 1982.

Bridie, A.L. and Bos, J. 1971. Biological degradation of mineral oil in sea water. *J Inst Petrol* 57(557):270-277.

Bruckner, J.V., and D. A. Warren. 2001. Chapter 24: Toxic effects of solvents and vapors. Pp. 869-916 in Casarett and Doull's *Toxicology: The Basic Science of Poisons*, 6th ed., CD. Klaassen, ed. New York: McGraw-Hill.

Carpenter, C.P., D.L. Geary, Jr., R.C. Myers, D.J. Nachreiner, L.J. Sullivan, and J.M. King. 1976. Petroleum hydrocarbon toxicity studies. XI. Animal and human response to vapors of deodorized kerosene. *Toxicol. Appl. Pharmacol.* 36:443-456.

CONCAWE. 1991. Middle distillates - a review of the results of a CONCAWE programme of short-term biological studies, CONCAWE report No. 91/51

CONCAWE. 1995. Kerosenes/jet fuels. Product Dossier No. 94/106. CONCAWE, Brussels.

CONCAWE. 1996. Overview of the CONCAWE Middle Distillate Program. Report No. 9662. CONCAWE, Brussels.

CONCAWE. 1999. Exposure Profile: kerosenes/jet fuels. Product Dossier No. 99/52. CONCAWE, Brussels.

CONCAWE. 2001. Environmental classification of petroleum substances - Summary data and rationale. Report No. 01/54. CONCAWE, Brussels.

Dickson, C.L. 2002. Aviation Turbine Fuels, 2001. TRW-224 PPS 2002/2. TRW Petroleum Technologies. Bartlesville, OK.

Exxon (Exxon Biomedical Sciences, Inc). 1995a. Fish, Acute Toxicity Test, Rainbow Trout – Renewal. Project No. 188358.

Exxon (Exxon Biomedical Sciences, Inc). 1995b. Daphnia acute toxicity test. Project No. 188342. Jersey.

Exxon (Exxon Biomedical Sciences, Inc). 1995c. Fish, Acute Toxicity Test, Rainbow Trout – Renewal. Project No. 188458A.

Exxon (Exxon Biomedical Sciences, Inc). 1995d. Daphnia acute toxicity test. Project No. 188442A.

Exxon (Exxon Biomedical Sciences, Inc). 1995e. Alga, Growth Inhibition Test. Project No. 188467A.

Exxon (Exxon Biomedical Sciences, Inc). 1995f. Fish, Acute Toxicity Test, Rainbow Trout – Renewal. Project No. 188558.

Exxon (Exxon Biomedical Sciences, Inc). 1995g. Daphnia acute toxicity test. Project No. 188542.

Exxon (Exxon Biomedical Sciences, Inc). 1995h. Alga, Growth Inhibition Test. Project No. 188567.

EPA (U.S. Environmental Protection Agency) 2000. Estimation Programs Interface (EPI) Suite, Version 3.10. U.S. Environmental Protection Agency, Washington, DC.

EPA (U.S. Environmental Protection Agency) 2002. Jet Propellant Fuel 8 (JP-8) (CAS Reg. No. 8008-20-6 [kerosene]): Proposed acute exposure guideline levels (AEGs). Public Draft. Office of Pollution Prevention and Toxics. Federal Register – January.

Gaworski, C.L., J.D. MacEwen, E.H. Vernot, R.H. Bruner, and M.J. Cowan, Jr. 1984. Comparison of the subchronic inhalation toxicity of petroleum and oil shale JP-5 jet fuels; In: MacFarland, H.N. et al., eds., *Advances in Modern Environmental Toxicology*, vol. VI, Applied Toxicology of Petroleum Hydrocarbons.

Princeton Scientific Publishers, Princeton, New Jersey, pp. 33-47.

Harris, J.C. 1982. Rate of Hydrolysis: In Handbook of Chemical Property Estimation Methods. Lyman, Reehl and Rosenblatt, eds. McGraw-Hill Book Co., New York.

Hinchee, R.E., J.A. Kittel and H.J. Reisinger. 1995. Applied Bioremediation of Petroleum Hydrocarbons. Columbus, OH: Battelle Press. 534 pp.

IARC. 1989. IARC Monographs on the Evaluation of Carcinogenic Risks to Humans: Occupational Exposures in Petroleum Refining; Crude Oil and Major Petroleum Fuels, Volume 45. International Agency for Research on Cancer, Lyon.

Jokuty, P., Whiticar S., Wang Z., Fingas M., Fieldhouse B., Lambert P., and Mullin J.. 2002. Properties of Crude Oils and Oil Products. Environmental Protection Service, Environment Canada, Ottawa, Ontario. Internet Version 2002 via <http://www.etcentre.org/spills>.

MacNaughton, M.G. and D.E. Uddin. 1984. Chapter IX: Toxicology of mixed distillate and high-energy synthetic fuels. Pp. 121-132 in Volume VI1 of Advances in Modern Environmental Toxicology: Renal Effects of Petroleum Hydrocarbons, Princeton Scientific Publishers, Inc., Princeton, NJ.

Mobil Corporation, 1999. 'Determination of the Aerobic Ready Biodegradability of MSDW Kerosene Mid Blend Using the OECD 301F Manometric Respirometry Test Method.' Mobil Business Resources Corp., Ecotoxicology Laboratory, Paulsboro, NJ, 1999.

Nessel, C.S. 1999. A comprehensive evaluation of the carcinogenic potential of middle distillate fuels. Drug Chem. Toxicol. 22:165-180.

NRC (National Research Council). 1996. Permissible Exposure Levels for Selected Military Fuel Vapors. Committee on Toxicology, Subcommittee on Permissible Exposure Levels for Military Fuels. Washington DC: National Academy Press.

NTP (National Toxicology Program). 1986. Toxicology and carcinogenesis studies of marine diesel fuel and JP-5 navy fuel (CAS No. 8008-20-6) in B6C3F1 mice (dermal studies). Technical report series No. 310. Research Triangle Park, NC, US Dept of Health and Human Resources

Ritchie, G.D., M.Y. Bekkedal, A.J. Bobb, and K.R. Still. 2001a. Biological and Health Effects of JP-8 Exposure. Report No. TOXDET-01-01, Naval Health Research Center Detachment (Toxicology) Wright-Patterson AFB, OH.

Schreiner, C., Bui, Q., Breglia, R., Burnett, D., Koschier, F., Podhasky, P., Lapadula, L., White, R., Feuston, M., Krueger, A. and Rodriguez, S. 1997. Toxicity evaluation of petroleum blending streams: reproductive and developmental effects of hydrodesulfurized kerosene. J. Tox. and Env. Health Vol 52, pp 211-229.

Shell (Shell Research Limited.). 1991a. The toxicology of petroleum products: the skin irritancy of odourless kerosene (white spirit). External report No. SBER 91-001. Shell Research, Sittingbourne.

Shell (Shell Research Limited.). 1991b. Toxicology of petrochemicals: the skin irritancy of hydrocracked kerosene. External report No. SBER 91-004. Shell Research, Sittingbourne.

Shell (Shell Research Limited.). 1991c. Toxicology of petroleum products: the skin irritancy of kerosene SG. External report No. SBER 91-003. Shell Research, Sittingbourne.

Shell (Shell Research Limited.). 1991d. Toxicology of petroleum products: the skin irritancy of AVTUR Jet A1. External report No. 91-005. Shell Research, Sittingbourne.

Shell (Shell Research Limited). 1995a. Acute toxicity of water accommodated fractions to *Oncorhynchus mykiss*. Study No. 6165, Report No. SBGR.94.001

Shell (Shell Research Limited). 1995b. Acute toxicity of water accommodated fractions to *Daphnia magna*. Study No. 6165, Report No. SBGR.94.001.

Shell (Shell Research Limited). 1995c. Acute toxicity of water accommodated fractions to *Raphidocelis subcapitata*. Study No. 6165, Report No. SBGR.94.001.

Skisak, C. 1991. The role of chronic acanthosis and subacute inflammation in tumor promotion in CD-1 mice by petroleum middle distillates. *Tox. and Appl. Pharmacol.* Vol 109, pp 399-411.

Song H-G; Wang X; Bartha R. 1990. Bioremediation potential of terrestrial fuel spills. *Appl. Environ. Microbiol.* Vol. 56, No. 3, pp. 652-656.

Song H-G; Bartha R. 1990b. Effects Of Jet Fuel Spills On The Microbial Community Of Soil. *Appl Environ Microbiol.* Vol. 56, No. 3, pp. 646-651.

Spain J C; Sommerville C C. 1985. Biodegradation of Jet Fuel by Aquatic Microbial Communities. *Govt Reports Announcements & Index (GRA&I)*. No. 16.

Spain J C; Somerville C C; Butler L C; Lee T J; Bourquin A W. 1983. Degradation of Jet Fuel Hydrocarbons by Aquatic Microbial Communities. *Govt Reports Announcements & Index (GRA&I)*, (1983). No. 14

U.S. Army. 2001. JP-8: The Single Fuel Forward U.S. Army Tank-automotive and Armaments Command Research, Development, and Engineering Center Warren, MI 48397-5000.

White, R.D. 1999. Refining and blending of aviation turbine fuels. *Drug and Chemical Toxicology*, 22(1), 143-153.

Zeiger, E., and L. Smith. 1998. The first international conference on the environmental health and safety of jet fuel. *Environ. Health Persp.* 106:763-764.

APPENDIX A.

CAS Numbers and Definitions of 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.

With regard to the Kerosene/Jet Fuel Category, it should be noted that jet fuels as such (Jet A, JP-8, etc.) are not on the Toxic Substances Control Act's Chemical Inventory of Substances, and consequently do not have CAS numbers. Thus, they are not listed as members of the Kerosene/Jet Fuel Category. However, because jet fuels are composed almost entirely of kerosene (CAS no. 8008-20-6) or hydrodesulfurized kerosene (64742-81-0), testing done on a jet fuel can be extrapolated to not only those two CAS numbers, but other kerosene-range refinery streams which are members of the kerosene/jet fuel HPV category.

CAS number

Addressed in Kerosene/Jet Fuel Test Plan

008008-20-6

Kerosine (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).

064742-81-0

Kerosine (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).

068477-58-7

Distillates (petroleum), steam-cracked petroleum distillates, C5-18 fraction

A complex combination of organic compounds obtained by the multiple distillation of steam-cracked distillates to which hydrocarbons having carbon numbers predominantly in the range of C5 through C12 from distillation of polymerized steam-cracked distillates may have been added. It consists of hydrocarbons having carbon numbers predominantly in the range of C5 through C18.

068333-23-3

Thermocracked Naphtha, Heavy Coker – C6-15, 315F- 550F
Naphtha (petroleum), heavy coker

A complex combination of hydrocarbons from the distillation of products from a fluid coker. It consists predominantly of unsaturated hydrocarbons having carbon numbers predominantly in the range of C6 through C15 and boiling in the range of approximately 157°C to 288°C (315°F to 550°F).

Addressed by International Hydrocarbon Solvents Consortium (IHSC) or the ACC Olefins Panel's (ACCOP) Low Benzene Naphtha Group Test Plans¹

064741-73-7

Distillates (petroleum), alkylate

A complex combination of hydrocarbons produced by distillation of the reaction products of isobutane with monoolefinic hydrocarbons usually ranging in carbon numbers from C3 through C5. It consists of predominantly branched chain saturated hydrocarbons having carbon numbers predominantly in the range of C11 through C17 and boiling in the range of approximately 205°C to 320 °C (401°F to 608°F).

Int'l Hydrocarbons Solvents HPV consortium -C14+ aliphatics (2% aromatics or less).

064741-85-1

Raffinates (petroleum), sorption process

A complex combination of hydrocarbons remaining after removal of normal paraffins in a selective adsorption process. It consists predominantly of branched chain and cyclic hydrocarbons having carbon numbers predominantly in the range of C5 through C25 and boiling in the range of approximately 35°C to 400°C (95°F to 752°F).

Int'l Hydrocarbons Solvents HPV consortium -C9-C13 aliphatics.

064741-98-6

Extracts (petroleum), heavy naphtha solvent

A complex combination of hydrocarbons obtained as the extract from a solvent extraction process. It consists predominantly of aromatic hydrocarbons having carbon numbers predominantly in the range of C7 through C12 and boiling in the range of approximately 90°C to 220°C (194°F to 428°F).

ACC Olefins Panel's Low Benzene Naphtha test plan.

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).

Int'l Hydrocarbons Solvents HPV consortium -C9-C13 aliphatics (2% aromatics or less).

064742-88-7

Solvent naphtha (petroleum), medium 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 C9 through C12 and boiling in the range of approximately 140°C to 220°C (284°F to 428°F).

Int'l Hydrocarbons Solvents HPV consortium -C9-C13 aliphatics (2% aromatics or less).

064742-94-5

Solvent naphtha (petroleum), heavy arom.

A complex combination of hydrocarbons obtained from distillation of aromatic streams. It consists predominantly of aromatic hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 165°C to 290°C (330°F to 554°F).

Int'l Hydrocarbons Solvents HPV consortium -C10-C12 aromatic hydrocarbon solvents.

068551-19-9

Alkanes, C12-14-iso-

NONE

Int'l Hydrocarbons Solvents HPV consortium -C14+ aliphatics (2% aromatics or less).

068551-20-2

Alkanes, C13-16-iso-

NONE

Int'l Hydrocarbons Solvents HPV consortium -C14+ aliphatics (2% aromatics or less).

Note 1

There are a total of fourteen CAS numbers included in the Kerosene/Jet Fuel Category. Of those, the eight materials listed below are being considered under complementary test programs not administered by the API HPV Test Group. The appropriate Test Consortium is listed under each of the CAS numbers. The API HPV Testing Group anticipates that the data generated under these complementary programs will provide the basis for establishing the SIDS endpoint values for these materials.

Appendix B.

Links to Additional Resources

Refining Processes: General Descriptions

http://www.chevron.com/about/learning_center/refinery
<http://www.lubrizol.com/lubetheory/default.htm>
<http://www.orionrefining.com/flow.htm>
http://www.osha-slc.gov/dts/osta/otm/otm_toc.html
http://www.shellglobalsolutions.com/base_oils/library/library.htm
<http://www.shell-lubricants.com/learningcenter/aboutoil.html>
http://www.shellus.com/welcome/history/hist_oil_main.html
<http://www.epa.gov/compliance/resources/publications/assistance/sectors/notebooks/petrefsnpt1.pdf>
http://www.mts.net/~dbrad1/base_oil.htm

Petroleum Related Glossaries

http://www.caltex.com.au/products_glo.asp
<http://www.citgo.com/CommunityInvolvement/Classroom/Glossary.jsp>
<http://www.epplp.com/gloss.html>
http://www.prod.exxon.com/exxon_productdata/lube_encyclopedia/
http://www.hellenic-petroleum.gr/english/glossary/gl_main.htm
http://www.prod.exxon.com/exxon_productdata/lube_encyclopedia/
<http://www.oilanalysis.com/dictionary>
<http://www.orionrefining.com/glossary.htm>
<http://www.gedolbear.com/glossary.htm>
http://www.shellglobalsolutions.com/base_oils/glossary/a_g.htm
http://www.ursa-texaco.com/English/glossary_a.html
http://www.eia.doe.gov/pub/oil_gas/petroleum/data_publications/petroleum_marketing_annual/current/pdf/glossary.pdf

Appendix C

Chronology of the Development of Jet Fuels

JP-1 (1944) was kerosene with a -77 °F freeze point and 109 °F (Min) flash point. Fuel availability was seriously limited.

JP-2 (1945) was an experimental fuel with unsuitable viscosity and flammability characteristics.

JP-3 (1947 to 1951) had a high vapor pressure, similar to avgas. Fuel boil-off loss and vapor lock were problems at high altitudes.

JP-4 (1951 to 1995), also designated as **Jet B**, is a blend of gasoline and kerosene. It has a Reid vapor pressure of 2-3 psi to reduce boil-off and vapor lock problems, and a -77 °F freeze point. Flash point (~ 0 °F) was not specified. An anti-static additive was introduced in the mid-1980s.

JP-5 (1952 to present) is the primary fuel for US Navy for ship-board aviation. It has a 140 °F (Min) flash point, -51 °F freeze point and contains no anti-static additive.

Jet A / Jet A-1 (1950s to present) are commercial airline kerosene fuels. Both have 100 °F (Min) flash point; Jet A has a -40 °F freeze point, whereas Jet A-1 is -53 °F. In the US, these fuels are not required to contain an anti-static additive.

JP-8 (1978/1995 to present) is the primary US Air Force and shore-based US Navy aviation fuel. JP-8 is very similar to Jet A/A-1; however, JP-8 contains anti-icing, corrosion/lubricity and anti-static additives.

JP-6 (1956), developed for the XB-70, is similar to JP-5 but with a lower -66 °F freeze point and improved thermal stability. Flash point was not specified.

JP-7 (1960s), developed for the SR-71, has low vapor pressure, high thermal stability, -47 °F freeze point and 140 °F flash point (Min).

JPTS (1956), developed for the U-2, is a "non-distillate" kerosene with a -64 °F freeze point, 109 °F flash point of (Min) and thermal stability add-pack (CJFA-5).

JP-8+100 (1994 to present) is JP-8 with a "+100" additive package designed to increase thermal stability (e.g., reduce fouling and coking) by 100 °F. The add-pack contains a detergent/dispersant, metal deactivator and antioxidant. The +100 additive is primarily used in Air Force fighter and trainer aircraft (256 ppm treat rate (per AFRL, <http://www.pr.wpafb.af.mil/JP8plus100.html>), and is commercially used in KLM Boeing 747s and Tampa FL police helicopters.

Appendix D.
Robust Summary
(Separate document)