HIGH PRODUCTION VOLUME (HPV) CHEMICAL CHALLENGE PROGRAM

GAS OILS CATEGORY ANALYSIS DOCUMENT AND HAZARD CHARACTERIZATION

Submitted to the US EPA

by

The American Petroleum Institute (API) Petroleum HPV Testing Group

www.petroleumhpv.org

Consortium Registration # 1100997

October 24, 2012

TABLE OF CONTENT

EXECUTIVE SUMMARY

EXECUTIVE SUMMARY

The Gas Oil Category includes 29 members comprised of 4 finished products (distillate fuels) and 25 refinery streams with similar carbon ranges. The category members are complex UVCB substances, containing variable amounts of alkanes, cycloalkanes, olefins, and aromatics. Gas oil streams are produced either by atmospheric distillation or by secondary processing of the materials derived from the vacuum distillation of the residuum from the atmospheric distillation of crude oil. Materials from this secondary processing may have higher aromatic and olefin contents than straight run gas oils. The distillate fuels may be straight run or a blend of various gas oil streams (both straight run and streams from secondary processing). In comparison to gas oil refinery streams that do not have product specifications, no. 2 diesel fuel and fuel oil must meet stringent ASTM and EPA specifications for commercialization. The boiling point specifications for these fuels essentially limit the aromatics to 1, 2 and 3-ring compounds with minimal 4-ring or higher polycyclic aromatic compounds (PAC). Physical properties, process history and product use specifications rather than composition define gas oils streams (ASTM, 2003) and provide the rationale for the composition of this category. Key parameters when analyzing this category for environmental hazards are the distribution of aromatic and saturated hydrocarbons, and for some mammalian endpoints (repeated-dose, developmental, reproduction, and mutagenicity) the content and distribution of PACs are important.

Physical-Chemical Properties: Gas oils are variable and complex substances of hydrocarbons, predominantly having carbon chains from C_9 to C_{30}, and boiling over the temperature range of approximately 150°C to 450°C. Vapor pressures are within a measurable range, with values of 0.4 kPa and 2 kPa being reported. Partition coefficients of constituent hydrocarbons range from 3.3 to >6. Water solubility values for components of these substances have been reported to range from 2.0 mg/L to 8.7 mg/L for different constituents.

Environmental Fate: If gas oils are released to the environment, individual components will disperse and partition according to their individual physical-chemical properties. Based on modeling individual structures encompassing the different types and molecular weights of hydrocarbons, volatilization to the atmosphere is an important process for the low molecular weight fractions. 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 these reactions. Components in gas oils will biodegrade, but it is unlikely that these substances would pass ready biodegradability criteria; however, available test data provide evidence for inherent biodegradability.

Environmental Effects: Multiple ecotoxicological studies on heating and transportation fuels (e.g., No. 2 fuel oil and diesel fuel) were reviewed and new tests of two gas oil streams having a high proportion of aromatic or saturated hydrocarbon content were conducted. Estimated lethal loading toxicity endpoints (LL/EL_{50}s) using the PETROTOX model and detailed 2D-GC-MS hydrocarbon analyses of the two gas oil streams were also calculated. When all LL/EL_{50} experimental data were combined with the modeled endpoints, the acute LL/EL_{50} toxicity values for the three trophic levels ranged from 0.18 mg/L to 125 mg/L for fish, 0.35 mg/L to 210 mg/L for invertebrates, and 0.20 mg/L to 78 mg/L for algae. The light catalytic cracked gas oil (high aromatic stream) was the most acutely toxic to all three trophic levels among the category members.

The chronic effects assessment included a fish growth test with no. 2 fuel oil and *D. magna* reproduction studies of light catalytic cracked gas oil and light hydrocracked gas oil. The LOELR based on reduction in fish growth was 3.0 mg/L while the NOELR was 1.2 mg/L. For invertebrates,

reduced reproduction in *D. magna* was observed at the LOELR of 0.10 mg/L. The NOELR was 0.05 mg/L. The NOELR based on the PETROTOX model was 0.06 mg/L for the catalytic cracked gas oil. The NOELR value of 0.05 mg/L for the light catalytic cracked gas oil sample was the lowest among the chronic effect endpoints and may be used as the chronic NOELR for the category.

Human Health Effects:

Gas Oil streams and fuels induce minimal acute toxicity by the oral, dermal and inhalation routes. Moderate to severe skin irritation has been reported from studies involving 24 hour exposure periods, but skin irritation would more likely be mild to moderate if these substances were tested under the 4 hour exposure conditions recommended for classification purposes. No dermal sensitization has been reported. Eye irritation was minimal to slight.

Some gas oil streams and distillate fuels induce gene mutation in bacterial and mammalian cells as demonstrated in both standard *in vitro* assays and the Optimized Ames Test. However fuels and streams in which the content of DMSO extractable aromatics is very low are not gene mutagens. Overall, the weight of evidence from studies for chromosome aberrations or micronucleus formation indicate that gas oils generally do not cause cytogenetic damage in animals

Repeated dose 13-week rat dermal studies on gas oil streams indicate LOAEL values of 125mg/kg with the exception of a light coker gas oil (CAS RN 64741-82-8 sample 87213) for which the LOAEL was 30mg/kg, the lowest dose tested, effects likely exacerbated by severe skin irritation at all dose levels. Skin irritation produced by other gas oils generally ranged from slight to moderate. NOAEL values of 25-30mg/kg were seen. The exception was an ultralow sulfur diesel fuel (CAS RN68334-30-5) which contained very low levels of DMSO-extractable aromatic hydrocarbons and did not produce any systemic effects (NOEL = 600mg/kg, the highest dose tested). The main systemic effects of exposure to gas oils occur in organ weights, primarily the liver, thymus and on hematologic parameters. Effects appear to be related to aromatic content and effects are more pronounced in gas oil streams with higher levels of aromatics. The 4 week duration rat dermal studies showed slight to moderate skin irritation and minimal systemic toxicity. No adverse effects were seen in reproductive organs in any rat dermal study. Supplemental studies of the effects of repeated dermal exposure in rabbits focused on irritation and mortality and are provided as supplementary information.

Some of the substances tested in the Gas Oil Category had developmental LOAELs ranging from 125 – 500mg/kg attributed primarily to fewer live offspring at delivery and lower fetal or pup body weight at delivery or Lactation days 0-4 and NOAELs ranging from 30 – 600mg/kg. Fetal malformations were reported only for CAS RN 64741-43-1 [an intermediate gas oil] and CAS RN 64741-49-7 [Vacuum Tower Overheads]. Developmental toxicity was seen primarily at doses that also produced maternal effects. Some gas oils showed no developmental toxicity at the highest doses tested even in the presence of maternal toxicity.

Reproductive parameters in developmental toxicity studies addressing fertility, successful insemination and implantation demonstrate that in general these endpoints are not adversely affected by treatment with gas oil streams. Three studies in which females were treated dermally for a week prior to mating through mating and gestation demonstrated that exposure to high concentrations of several gas oils did not adversely affect mating or establishment of pregnancy but did affect successful completion of pregnancy and pup viability at maternally toxic doses of 250mg/kg and above. Evaluation of reproductive organs and sperm morphology and motility from 13-week repeated dose studies consistently demonstrated no adverse effects on ovary or testes

weights, no abnormal histopathology and no effects on sperm at doses ranging up to 500-820mg/kg/day. The NOAELs for reproductive toxicity are not expected to be lower than the NOAELs for developmental toxicity because the most sensitive endpoints identified in the developmental and reproductive toxicity studies have been developmental effects, specifically reductions in fetal survival and growth resulting from *in utero* exposure.

Overall, for dermal repeated dose and developmental toxicity, effects appear to be related to aromatic content. The systemic effects seen in repeated dose studies may be considered generalized responses to total aromatics either adaptive or minimally toxic and reversible while effects in developmental studies are more associated with aromatics containing a higher distribution of 3 or more rings. Effects in developmental toxicity studies seem to require higher doses than in systemic toxicity studies and may not be induced even at doses that are systemically toxic to pregnant females.

The reported repeat dose dermal toxicity and developmental toxicity studies provide a spectrum of effects from virtually non-toxic for streams with minimal levels of DMSO extractable aromatics (e.g. Ultralow sulfur diesel fuel CAS RN 68334-30-5) to streams with higher DMSO extractable 1-3+ aromatic ring content which can be characterized as the potentially more hazardous of this category (e.g. light coker gas oil (light cycle oils CAS RN 64741-59-9)

Inhalation Studies: Two 4 week repeat dose inhalation studies with samples of hydrodesulfurized distillates administered at single concentrations of 25mg/m^3 and one developmental toxicity study of a marketplace sample of diesel fuel [CAS RN 68476-34-6] administered at 100 or 400ppm daily on gestation days 6-15 did not result in any toxicologically important substance induced effects.

Dermal carcinogenesis studies indicate that Gas Oils and distillate fuels can induce dermal tumors after repeated skin application but do not cause systemic tumors. The gas oils which contain 3 and higher ring PACs are mutagenic in Salmonella assays and show evidence of carcinogenic initiating potential when evaluated in initiation/promotion tests. Other gas oils may also produce tumors if repeatedly applied to mouse skin; however, the tumors produced gas oils that contain low or no PAC are likely due to a non-genotoxic, promotional effect and only observed in the in the presence of sustained skin irritation

Human Exposure

Because the No. 2 distillate fuels have widespread use in transportation and industrial and residential heating applications, both occupational and consumer exposures are possible. Exposure to children is not anticipated. The other substances in the Gas Oil Category are only used in industrial applications.

In conclusion, the information provided in this Gas Oils Category Assessment Document is sufficient to characterize physiochemical properties and to evaluate the environmental and human health hazards of gas oil refinery streams and distillate fuels. The more potentially hazardous of these substances are refinery blending streams which do not have compositional limitations (e.g. 64741-82-8; CAS RN 64741-59-9) but fuels that are introduced into commerce (e.g.68334-30-5, Ultra low sulfur diesel) have technical requirements that limit the content of higher boiling aromatics and do not induce significant mammalian toxicity.

1. DESCRIPTION OF THE GAS OILS CATEGORY

1.1. Nomenclature, Use, and Manufacture

The Gas Oils category includes both finished products (distillate fuels) and refinery streams (gas oils) . The specific CAS numbers and descriptions of category members are detailed in Appendix A.

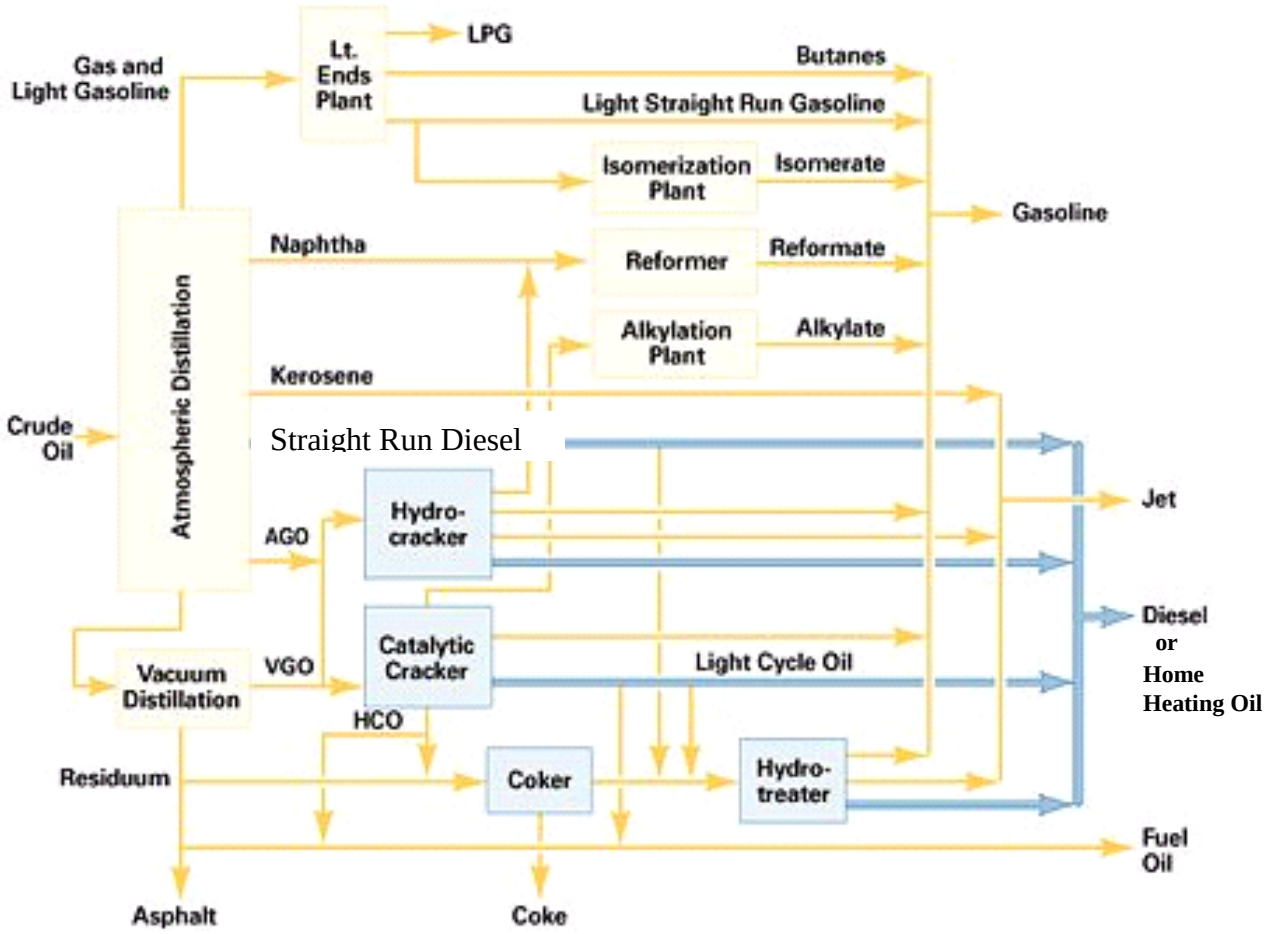
The distillate fuels covered in this category are used primarily as heating oils and as fuels in compression-ignition engines. Because they are manufactured to meet performance specification limits (and not specific chemical compositions), the chemical compositions of distillate fuels can vary since products with the desired fuel properties can be formulated in a number of ways. Distillate fuels are distinguished from each other based primarily on their boiling point ranges, aromatic content, and uses. However, whether straight run or blended, distillate fuels are produced to meet the ASTM specifications for either Fuel Oils (ASTM D396) or Diesel Fuel Oils (ASTM D975). The ASTM specification for diesel fuels limits the aromatic content low sulfur diesel fuels to a maximum 35% by volume (ASTM, 2002).

The boiling range of No. 2 Diesel Fuel [CAS RN 68476-34-6 or 68334-30-5] and No. 2 Fuel Oil [CAS RN 68476-30-2] are limited to a maximum T90 of 338 °C (640 °F). That specification essentially limits the aromatics to 1, 2, or 3-ring compounds. Four-ring aromatic compounds are theoretically possible, but are rarely found in commercial on-road diesel fuel [see Tables 1-3 On road Diesel Fuel #2 CAS RN 68334-30-5] This is not the case with Fuel oil No. 4 [CAS RN 68476-31-3] which does not have a specification for boiling range and could contain higher levels of aromatics with 4+ rings. While Fuel oil No. 4 is sponsored in the Gas Oil Category, no member of the Petroleum HPV Testing Group actually makes the substance and therefore no samples were available to analyze.

Diesel fuel No. 2 is used for automotive diesel engines while No. 4 diesel fuel is used for low and medium speed diesel engines in non-automotive applications. Fuel Oil No. 4 has been used in commercial and industrial burners to generate steam, for space and water heating, pipeline pumping, and gas compression (ASTM, 2001; 2002). Two other classes of fuel oils, Fuel Oil No. 1(also known as kerosene) and Fuel Oil No. 6 (heavy fuel oil) are covered in separate API HPV Category Closure Documents.

As shown in Figure 1, gas oil streams are produced either by atmospheric distillation or by secondary processing of the materials derived from the vacuum distillation of the residuum from the atmospheric distillation of crude oil. Materials from this secondary processing may have higher aromatic and olefin contents than straight run gas oils. Distillate fractions that require only minor or no additional processing are known as “straight run” gas oils. The distillate fuels may be straight run or a blend of various gas oil streams (both straight run and cracked). Historically, straight-run gas oils are the major components of the distillate fuels, but rising demand has made it necessary to use increasing volumes of streams derived from the secondary processing of heavier fractions. Cracking is a process that breaks (“cracks”) the heavier, higher boiling petroleum streams produced by atmospheric or vacuum distillation into lighter molecular weight materials such as gasoline, diesel fuel, jet fuel and kerosene. Thermal cracking uses heat to break molecular bonds and catalytic cracking uses a catalyst and heat to facilitate the cracking process. Figure 1b illustrates the distribution of CAS RNs in this category by manufacturing process

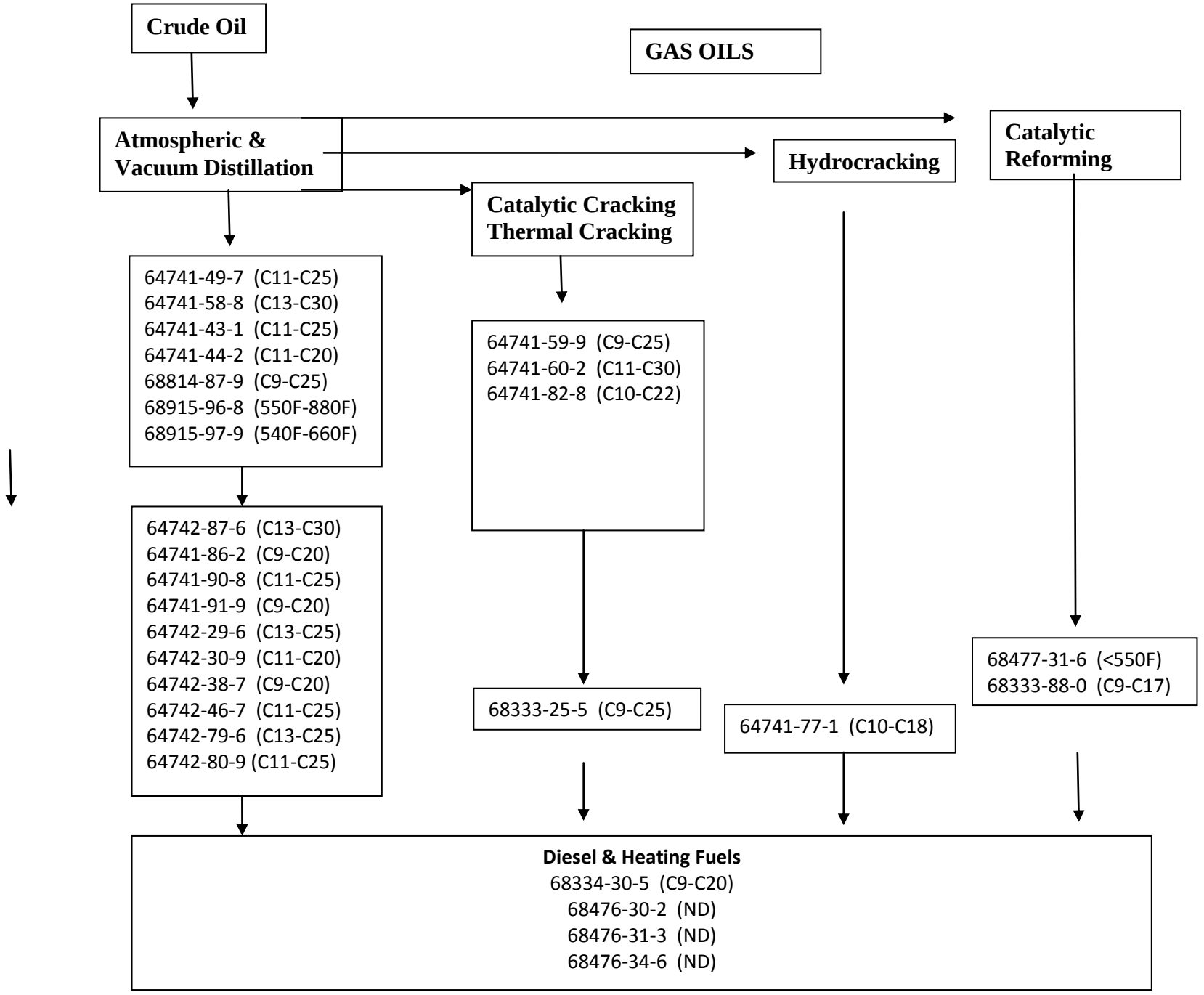
Figure 1. Gas Oils Process Diagram



ChevronTexaco, 2003

Note: AGO = atmospheric gas oil
VGO = vacuum gas oil
HCO = heavy cycle oil

Figure 1b. Gas Oil Process Diagram by CAS RN distribution

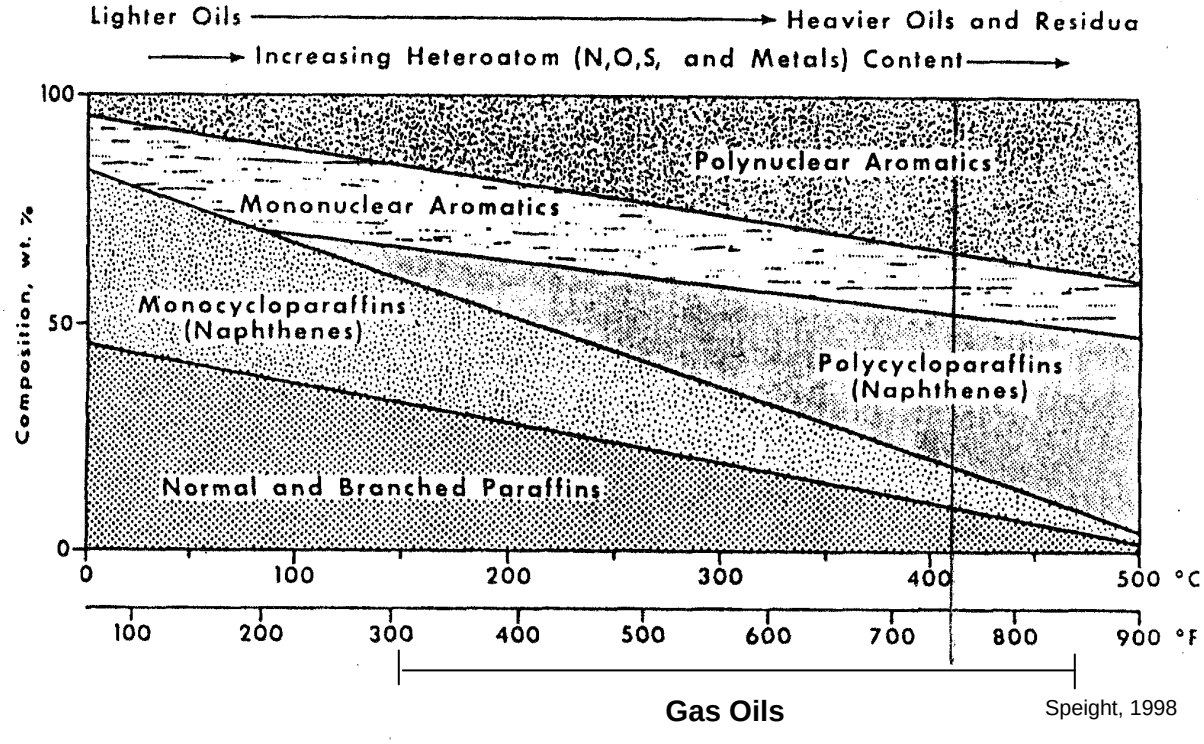


1.2 Analytical Characterization

The UVCB substances in this category boil over a range of approximately 300 to 880ºF (150 to 471ºC) and are composed primarily of saturated and/or aromatic hydrocarbons with carbon numbers ranging from C9 to C30. Gas oils contain straight and branched chain alkanes (paraffins, and cycloparaffins), cycloalkanes (naphthenes), aromatic hydrocarbons and mixed aromatic cycloalkanes. As the boiling ranges of the fractions increase, the levels of polycyclic aromatic compounds (PACs), polycycloparaffins and heteroatoms (Nitrogen, Oxygen, and Sulfur) increase, while the levels of paraffins decrease (Figure 2, Speight, 1998). Most commercial gas oils contain PACs. In light straight-run gas oils these are mainly 2 and 3-ring aromatic compounds, with much lower levels of PACs with 4 or more rings. The heavier atmospheric, vacuum or cracked gas oil components may contain increased levels of PACs with 4 or more rings, some of which are carcinogenic (CONCAWE, 1996). In general terms, petroleum streams from thermal or catalytic cracking processes have higher PAC content than straight-run distillation fractions or streams derived from other non-cracking processes (i.e., hydrotreating). However, because of the ASTM and EPA specifications for No. 2 Diesel Fuel and No. 2 Fuel Oil the aromatic constituents in these finished products are effectively limited to PACs with 1, 2 or 3 rings. Blended distillate fuels, in addition to containing the hydrocarbons from their blending stocks, may also contain low concentrations of performance additives such as flow improvers, corrosion inhibitors, defoamers, dyes/markers, anti-oxidants, stability improvers, cetane improvers, detergents and anti-static additives. These additives are not part of the CAS definitions and are outside the Petroleum industry HPV program. None of the samples tested for toxicity including the ultralow sulfur diesel (ULSD) product were additized.

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

Figure 2. Refinery Stream Composition – Boiling Range vs. General Composition



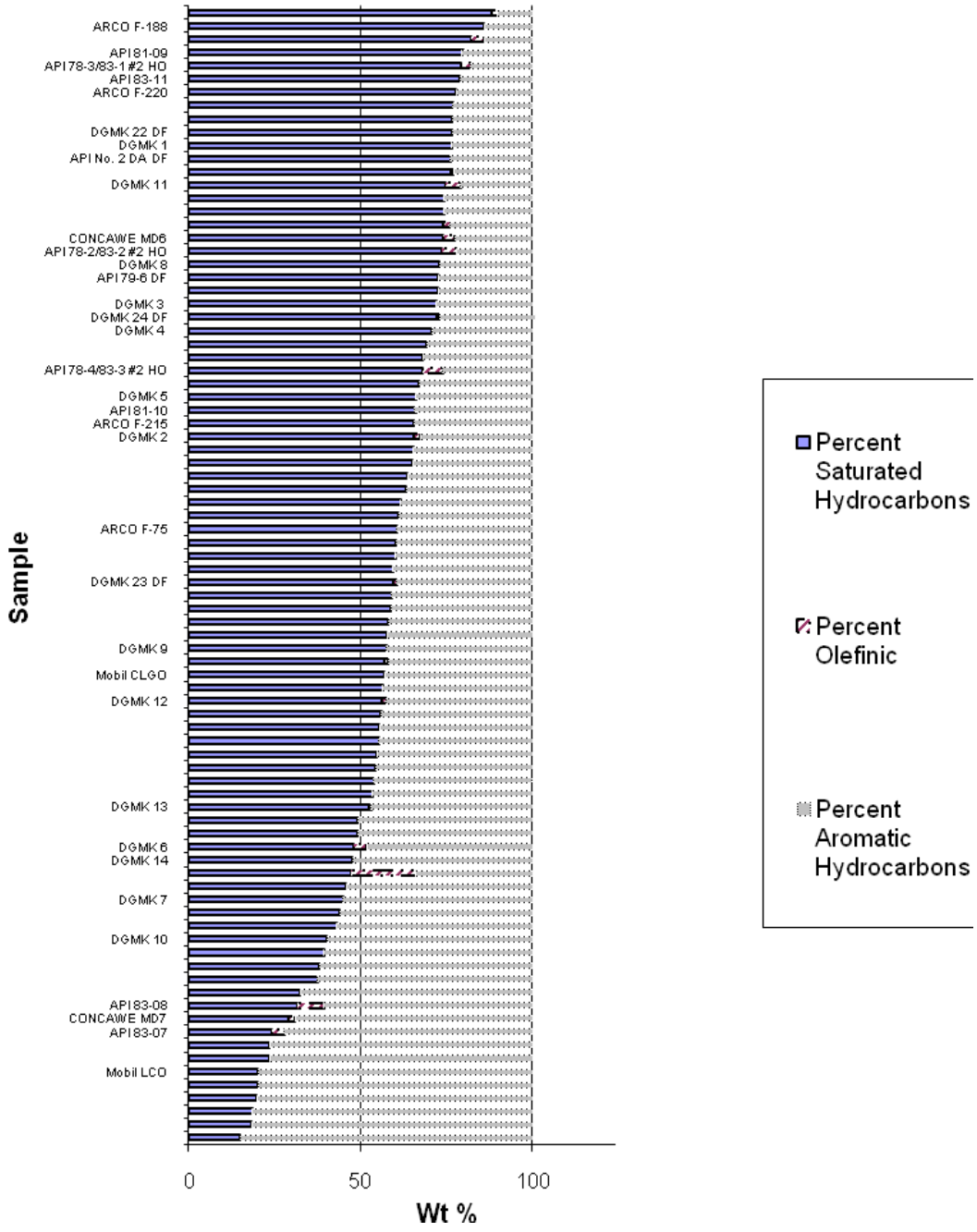
Because they are complex substances, the materials in this category are typically not defined by detailed compositional information but instead by process history, physical properties, and product use specifications (ASTM 2001, 2002). Whereas detailed compositional information may be limited, general compositional information can be inferred from the gas oil's physical properties and the type of processing it has undergone, e.g. the higher the boiling temperature range of a fraction, the higher the molecular weight of the oil's components. Similarly, streams that have been "cracked" have higher olefinic and aromatic hydrocarbon content while straight run gas oil streams that have undergone a limited amount of additional processing are composed predominantly of saturated hydrocarbons.

Compositional information on 86 gas oil samples (representing 15 of the CAS numbers in this category) showed that the range of hydrocarbon types was:

Saturates: 18 - 86%
Aromatics: 14 - 82 %

As shown in Figure 3, the saturate and aromatic hydrocarbon content of the Gas Oil category members forms a continuum from high saturate content to high aromatic content.

Figure 3. Composition of Representative Samples of Gas Oils and Distillate Fuels



Note: Samples shown with a descriptive title (I.e. ARCO F-188) are from studies described in the Robust summaries (Separate appendix). Compositional information for these 86 samples of gas oils and distillate fuels was obtained from publications and company reports.

An important compositional characteristic of gas oils is the presence of varying amounts of polycyclic aromatic compounds (PACs). PACs are a subset of the aromatic compounds presented in Figure 3 above. Although similar to polycyclic aromatic hydrocarbons (PAHs) that contain two or more fused-aromatic rings consisting only of carbon and hydrogen, PACs are a broader group of compounds that also includes heteroatomic compounds in which one or more of the carbon atoms in the PAH ring system are replaced by nitrogen, oxygen, or sulfur atoms. The distribution of PACs is dependent on the crude oil source and the nature and severity of refining processes and includes a complex variety of parent (i.e., unsubstituted) and alkylated structures. The alkyl-substitutions are usually one to four carbons long and can include non-carbon compounds such as sulfur. Multiple alkyl and cycloparaffin substitutions of the parent structure are also common, especially in higher boiling fractions of petroleum. The relative abundance of the alkylated polycyclic aromatics (C1-C4) in petroleum far exceeds the abundance of the parent compound (C0) (Speight, 2007). The fact that the levels of alkylated polycyclic aromatics are much greater than the parent polycyclic aromatics is the main feature of the PACs found in petroleum substances (Altgelt and Boduszynski, 1994). Studies in laboratory animals have demonstrated that samples with high aromatic content, particularly in the 3-7 ring range are likely to be more toxic than those high in saturates or containing primarily 1 and 2 ring PAC (Feuston et al.,1994).

Tables 1 to 3 summarize the composition of On Road Diesel Fuel No. 2 illustrating the limited aromatics content and profile of generally 1, 2, and 3-ring compounds and low sulfur content. In order to meet ASTM standards, commercial diesel fuels are much less variable in composition than refinery streams from which they are derived. The boiling point specifications for diesel fuel no. 2 (including Ultra Low Sulfur Diesel) limit the PAC content, minimizing the amount of PAC with 4-rings or higher. Comparison of the PAC analytical profiles of ULSD (CAS RN 68334-30-5) samples in Table 5 with refinery stream samples without product specifications further illustrates these differences.

Table 1. Typical Properties of On-Road Diesel Fuel No. 2 (ULSD, <15 PPM Sulfur)[a]

TEST DESCRIPTION	#2 REGULAR DIESEL S15		
	MINIMUM	MAXIMUM	AVERAGE
Number of Fuel Samples = 111			
Relative Density, 60/60 F	0.8239	0.8652	0.8458
Distillation, Deg F			
IBP	334	423	361
5 % rec.	367	447	396
10 % rec.	376	467	414
20 % rec.	402	488	440
30 % rec.	425	506	462
40 % rec.	446	527	484
50 % rec.	464	545	504
60 % rec.	483	564	525
70 % rec.	506	583	548
80 % rec.	534	604	574
90 % rec.	563	638	608
95 % rec.	586	669	637
EP	615	687	656
Kinematic Viscosity, @ 40 Deg C, cSt.	1.98	3.29	2.59

Cloud Point, Deg. F	-24	20	4
Nitrogen, Wt. %	<0.001	0.014	<0.002
Sulfur (D-5453), ppm wt.	<1	10	<6
Mono Aromatics Content (SFC)	14.9	28.5	21.7
Poly Aromatics (SFC)	0.8	8.5	3.9
Total Aromatics (SFC)	15.7	35.3	25.7

[a] Alliance of Automobile Manufacturers 2008 summer survey

Table 2. Hydrocarbon Composition of On-Road Diesel Fuel No. 2 (Low Sulfur, <500 PPM)[a]

Number of Fuel Samples = 12		Average	Min	Max
Extended FIAM by HPLC, Vol %				
	Aromatics, Vol %	29.3	11.9	46.6
	Olefins, Vol %	0.0	0.0	0.0
	Paraffins, Vol %	70.7	53.4	88.1
Total Aromatics, SFC		27.6	11.6	43.4
Monoaromatics, SFC		21.6	9.3	35.8
Polycyclic Aromatics, SFC		5.9	1.5	17.5
D2425 Mass Spec Group Type, Wt %				
	Paraffins	42.1	31.0	61.8
	Monocycloparaffins	20.6	14.8	31.0
	Dicycloparaffins	6.7	3.7	12.3
	Tricycloparaffins	1.2	0.6	2.9
	Benzenes	10.8	4.1	18.7
	Indans/Tetralins	8.4	2.1	13.0
	CnH2n-10	3.5	1.8	5.2
	Naphthalene	0.7	0.3	1.5
	Naphthalenes	2.8	0.5	9.0
	CnH2n-14	1.8	0.7	2.9
	CnH2n-16	1.3	0.2	2.8
	CnH2n-18	0.0	0.0	0.1
	Total Saturates	70.7	53.4	88.1
	Total Aromatics	29.3	11.9	46.6
D5769 Aromatics, Wt%				
	Benzene	0.008	0.000	0.025
	Toluene	0.062	0.000	0.178
	Ethylbenzene	0.047	0.016	0.070
	M,P-XYLENE	0.193	0.075	0.711
	1,2-DIMETHYLBENZENE	0.077	0.026	0.224
	ISOPROPYL-BENZENE	0.024	0.005	0.059
	PROPYL-BENZENE	0.075	0.011	0.285
	1-METHYL-3-ETHYLBENZENE	0.172	0.038	0.430
	1-METHYL-4-ETHYLBENZENE	0.042	0.006	0.099
	1,3,5-TRIMETHYLBENZENE	0.077	0.008	0.292
	1-METHYL-2-ETHYLBENZENE	0.070	0.000	0.173
	1,2,4-TRIMETHYLBENZENE	0.224	0.008	0.658
	1,2,3-TRIMETHYLBENZENE	0.074	0.008	0.209

	INDAN	0.040	0.007	0.102
	ALKYL INDANS	0.366	0.068	0.765
	1,4-DIETHYL+BUTYLBENZENE	0.109	0.029	0.245
	1,2-DIETHYLBENZENE	0.061	0.025	0.161
	1,2,4,5-TETRAMETHYLBENZENE	0.049	0.025	0.101
	1,2,3,5-TETRAMETHYLBENZENE	0.179	0.036	0.302
	C10 BENZENES	0.564	0.154	0.993
	C11 BENZENES	1.792	0.289	3.074
	C12 BENZENES	0.154	0.043	0.277
	NAPHTHALENE	0.060	0.021	0.179
	2-METHYL-NAPHTHALENE	0.275	0.040	1.426
	1-METHYL-NAPHTHALENE	0.171	0.028	0.824

[a] Unpublished data from Petroleum HPV Testing Group member company, 1997.

Table 3. Analysis of Metals in On-Road Diesel Fuel No. 2 (Low Sulfur, <500 PPM)[a]

	Average	Min	Max
Number of Fuel Samples = 12			
Al, PPM	0	< 1	0
As, PPM	0	< 0.5	0
Be, PPM	0	< 0.02	0
Ca, PPM	0	< 2	0
Trace Ca, PPM	0	< 0.020	0
Cd, PPM	0	< 0.03	0
Co, PPM	0	< 0.1	0
Cr, PPM	0	< 0.05	0
Cu, PPM	0	< 0.3	0
Cu, by GFAAS (PPM)	0	< 0.010	0
Hg, (NAA), PPM	0	< 0.009	0
K, PPM	0	< 3	0
Trace K, PPM	0.039	0.021	0.049
Li, PPM	0	< 1	0
Trace Li, PPM	0	< 0.020	0
Mn, PPM	0	< 0.02	0
Na, PPM	0	< 3	0
Trace Na, PPM	0	< 0.020	0
Ni, PPM	0	< 0.06	0
Pb, PPM	0	< 0.2	0
Pb, by GFAAS (PPM)	0	< 0.010	0
Sb, PPM	0	< 0.5	0
Se, PPM	0	< 1	0
Si, PPM	0	< 0.1	0
Sulfur, D 2622 PPM	302	63	671
V, PPM	0	< 0.2	0
V, by GFAAS (PPM)	0	< 0.030	0

[a] Unpublished data from Petroleum HPV Testing Group member company, 1997

Two Gas Oil samples were tested to expand the database for biodegradation and aquatic toxicity endpoints. CAS RN 64741-59-9 Light catalytic cracked gas oil and CAS RN 64741-77-1 light hydrocracked gas oil were analyzed using ASTM methods D1319 and D5186 (see Appendix C). The light hydrocracked gas oil contained a lower distribution of total aromatics approximately 21% by D5186, most of which were mono-aromatics than did the light catalytic cracked gas oil which was approximately 83% total aromatics.

Another direct approach to characterizing the aromatic composition of a wide range of high boiling petroleum streams and the fuels derived from them [PAC analytical Method II] involves a DMSO extraction procedure of samples supplied by US refineries based on the CAS RN assigned by the refineries. This method concentrates non-polar aromatics which are then analyzed by gas chromatography with flame ionization detection (GC/FID) or mass spectrometry (GC/MS) and the percentage of each ring distribution in the extract is calculated. Table 4 provides results for gas oil fuels and refinery stream PAC content by PAC analytical method II matched with aromatic content defined by ASTM method 5186. Comparison of the methods indicates that within the total wt % aromatic content there is a fairly high concentration of monoaromatics and although the D5186 characterization shows the highest PAC concentrations are of one and two rings, DMSO extraction tends underestimates the one-ring aromatic content.

Table 4. Aromatics Profile of Gas Oil Fuels and Refinery Streams

CAS RN/ Sample No.	DMSO Extract wt %[1]	DMSO ARC 1[2] wt.%	DMSO ARC 2 wt.%	DMSO ARC 3 wt.%	DMSO ARC 4 wt.%	DMSO ARC 5 wt.%	DMSO ARC 6 wt.%	DMSO ≥ARC 7 wt.%	D5186[3] Wt.% Total Aromatics	D5186 Wt.% Mono Aromatics	D5186 Wt.% Poly Aromatics
Distillate Fuels											
68334-30-5 Diesel Oils C9 – C20											
7 blend	2.8	0.1	2.2	0.6	0.0	0.0	0.0	0.0	26.4	21.8	4.6
1:5	3.4	0.2	2.7	0.3	0.0	0.0	0.0	0.0	26.4	23.3	3.1
10:4	2.5	0.2	1.8	0.5	0.0	0.0	0.0	0.0	16.7	12.5	4.2
32:4	2.8	0.1	2.0	0.6	0.1	0.0	0.0	0.0	21.2	16.6	4.6
68476-30-2 No 2 Fuel Oil											
17:4	3.4	0.3	2.4	0.6	0.0	0.0	0.0	0.0	33.9	27.7	6.3
20:1	3.8	0.2	3.0	0.6	0.0	0.0	0.0	0.0	32.1	26.4	5.6
26:15	2.3	0.1	1.4	0.7	0.0	0.0	0.0	0.0	25.1	20.7	4.4
26:22	4.7	0.7	3.6	0.4	0.0	0.0	0.0	0.0	34.2	29.2	5
68476-34-6 Fuels, diesel, no. 2											
19:1	6.7	0.1	3.2	3.4	0.0	0.0	0.0	0.0	33	20.9	12
24:2	2.7	0.2	2.2	0.3	0.0	0.0	0.0	0.0	29.1	25.4	3.7
33:5	3.3	0.2	3.0	0.1	0.0	0.0	0.0	0.0	21.9	18.2	3.7
37:9	0.5	0.0	0.4	0.1	0.0	0.0	0.0	0.0	8.3	8.3	<0.5
9:9	1.6	0.1	1.1	0.4	0.0	0.0	0.0	0.0	23.6	20.7	2.9
Refinery Streams											
64741-43-1 Gas Oil Intermediate C11 - C25											
12:12	5.1	0.1	2.1	2.6	0.2	0.0	0.0	0.0	27.9	16.4	11.5
16:3	4.5	0.1	2.0	2.4	0.0	0.0	0.0	0.0	25	14.8	10.2
23:14	3.3	0.0	0.6	2.5	0.2	0.0	0.0	0.0	22.8	13.6	9.2
26:6	4.8	0.1	2.4	1.9	0.1	0.0	0.0	0.0	25.2	16.5	8.8
30:1	7.1	0.0	0.6	6.4	0.2	0.0	0.0	0.0	36.9	18.2	18.7
8:4	6.1	0.1	3.6	2.3	0.1	0.0	0.0	0.0	39.1	19.7	19.4
64741-58-8 Vacuum Distillate, Light Vacuum C13 - C30											
1:9	5.2	0.0	0.8	2.6	1.1	0.5	0.1	0.0	71.8	62.7	9.1
16:6	7.2	0.1	2.9	3.6	0.4	0.1	0.0	0.0	40.3	21.2	19.1
23:12	4.4	0.0	0.1	4.4	0.1	0.0	0.0	0.0	28	15.5	12.5
25:17	6.4	0.0	1.3	3.6	1.1	0.4	0.1	0.0	79.7	59.6	20.1
26:8	8.9	0.1	4.5	4.5	0.0	0.0	0.0	0.0	41.3	22.4	18.9
28:6	8.1	0.0	2.7	4.8	0.6	0.0	0.0	0.0	44.3	21	23.2
4:3	6.2	0.0	0.2	3.7	1.9	0.6	0.1	0.0	40.8	19.2	21.6
41:1	9.2	0.1	3.7	4.6	0.6	0.1	0.0	0.0	48.9	22.9	26
8:2	9.1	0.1	3.8	4.1	0.9	0.2	0.0	0.0	49	22.8	26.2
64741-60-2 Catalytic Cracked Distillate, Intermediate C11- C30											
41:5	48.0	0.0	0.5	33.6	14.4	1.0	0.0	0.0	>75	7.1	>50

CAS RN/ Sample No.	DMSO Extract wt %[1]	DMSO ARC 1[2] wt.%	DMSO ARC 2 wt.%	DMSO ARC 3 wt.%	DMSO ARC 4 wt.%	DMSO ARC 5 wt.%	DMSO ARC 6 wt.%	DMSO ≥ARC 7 wt.%	D5186[3] Wt.% Total Aromatics	D5186 Wt.% Mono Aromatics	D5186 Wt.% Poly Aromatics
46:6	41.0	0.4	28.7	12.3	0.0	0.0	0.0	0.0	>75	11.2	>50
64741-77-1 Hydrocracked Distillate, light C10 – C18											
16:8	6.3	4.4	1.9	0.0	0.0	0.0	0.0	0.0	44.6	44.5	<0.5
25:3	8.6	1.7	6.9	0.0	0.0	0.0	0.0	0.0	64.3	61.5	2.8
32:5	4.8	1.4	3.4	0.0	0.0	0.0	0.0	0.0	39.9	39.4	0.5
7:3	2.1	0.6	1.5	0.0	0.0	0.0	0.0	0.0	21	20.8	<0.5
64741-82-8 Thermocracked Distillate, light C10 - C18											
12:5	9.8	0.5	7.9	1.0	0.0	0.0	0.0	0.0	37.2	23.2	14.0
2:7	12.0	3.6	4.8	3.6	0.0	0.0	0.0	0.0	40.9	26.1	14.8
30:4	12.0	0.1	6.0	6.0	0.0	0.0	0.0	0.0	40.6	19.9	20.6
34:3	8.6	0.2	5.2	3.4	0.3	0.0	0.0	0.0	31.3	20.4	10.9
43:3	9.8	0.9	6.9	2.0	0.0	0.0	0.0	0.0	34.3	22	12.3
9:4	7.9	0.3	4.0	3.2	0.2	0.0	0.0	0.0	38.6	21.4	17.2
64742-80-9 Hydrodesulfurized Distillate Middle, C11- C25											
12:18	7.4	0.2	3.7	3.7	0.0	0.0	0.0	0.0	39.9	24.8	15.2
28:8	2.5	0.2	2.0	0.5	0.0	0.0	0.0	0.0	27.6	23.5	4.1
3:2	3.4	0.0	2.4	1.0	0.0	0.0	0.0	0.0	30.1	23.2	6.9
32:6	7.0	0.2	4.2	2.7	0.0	0.0	0.0	0.0	48.5	34	14.5
64742-38-7 Clay treated distillate C9-C20											
48:1	3.6	0.7	2.9	0.0	0.0	0.0	0.0	0.0	22.5	19	3.5
68333-25-5 Hydrodesulfurized distillate , light catalytic cracked C9- C25											
25:6	9.4	0.5	6.6	2.8	0.0	0.0	0.0	0.0	43.1	29.5	13.7
31:7	2.1	0.0	1.5	0.4	0.0	0.0	0.0	0.0	25.7	21.8	4
68333-88-0 Aromatic hydrocarbons											
49:1	31.0	9.3	18.6	0.6	0.0	0.0	0.0	0.0	98.4	69.7	28.7
49:2	8.8	4.4	3.5	0.3	0.0	0.0	0.0	0.0	84.8	>75	7.8
49:3	4.9	3.4	1.5	0.1	0.0	0.0	0.0	0.0	87.4	>75	1.7
68477-31-6 Reformed Bottoms											
49:5	1.4	1.3	0.1	0.0	0.0	0.0	0.0	0.0	59.9	59.6	<0.5
49:4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	66	65.7	<0.5
68915-96-8 Gas Oil, Heavy [straight run distillate]											
12:9	5.7	0.0	0.5	2.3	2.9	0.2	0.0	0.0	35.5	16.5	19
14:2	7.8	0.0	0.8	2.3	3.9	0.8	0.0	0.0	38.1	17.8	20.4
26:24	5.4	0.2	1.6	2.2	1.1	0.5	0.1	0.0	40.3	19.8	20.5
30:7	4.7	0.0	0.9	1.9	0.9	0.5	0.2	0.0	39.2	17.3	22
43:1	5.0	0.1	1.0	2.0	1.0	0.5	0.1	0.0	30	18	12
64741-44-2 Gas Oil, light C11- C20											
2:5	5.8	0.1	3.6	2.2	0.0	0.0	0.0	0.0	34.6	20.3	14.3
23:16	3.4	0.0	1.9	1.4	0.0	0.0	0.0	0.0	20.3	12.6	7.7
25:14	5.8	0.0	1.9	3.9	0.0	0.0	0.0	0.0	31.7	16.2	15.5
26:3	5.7	0.1	2.9	2.8	0.0	0.0	0.0	0.0	30.7	16.6	14.1
28:9	6.1	0.1	3.2	2.9	0.0	0.0	0.0	0.0	35.6	20.1	15.4

CAS RN/ Sample No.	DMSO Extract wt %[1]	DMSO ARC 1[2] wt.%	DMSO ARC 2 wt.%	DMSO ARC 3 wt.%	DMSO ARC 4 wt.%	DMSO ARC 5 wt.%	DMSO ARC 6 wt.%	DMSO ≥ARC 7 wt.%	D5186[3] Wt.% Total Aromatics	D5186 Wt.% Mono Aromatics	D5186 Wt.% Poly Aromatics
32:7	6.8	0.3	6.3	0.2	0.0	0.0	0.0	0.0	27.7	19	8.7
41:3	9.7	0.4	6.2	3.1	0.0	0.0	0.0	0.0	49.4	33.2	16.1
9:6	5.3	0.0	0.4	2.1	1.6	0.5	0.2	0.0	32	17.8	14.3
64741-49-7 Vacuum Tower Condensate C11- C25											
12:14	7.7	0.0	4.6	3.1	0.0	0.0	0.0	0.0	33.3	16.6	16.7
64741-59-9 Catalytic Cracked Distillate, light C9-C25											
1:7	31.5	0.0	22.1	9.5	0.0	0.0	0.0	0.0	75.0	24.0	>50
16:4	30.0	1.2	24.9	4.2	0.0	0.0	0.0	0.0	80.6	30.8	49.8
17:5	23.9	2.4	16.7	4.8	0.0	0.0	0.0	0.0	65.0	28.9	36.1
25:11	36.0	0.4	22.3	13.3	0.0	0.0	0.0	0.0	78.5	17.7	60.7
26:18	32.5	3.3	19.5	9.8	0.0	0.0	0.0	0.0	80.9	35.3	45.7
28:2	39.8	0.4	27.9	8.0	0.0	0.0	0.0	0.0	91.0	23.1	>50
31:6	36.0	0.7	25.2	10.4	0.0	0.0	0.0	0.0	86.1	23.1	63
35:1	30.0	0.6	19.5	9.6	0.0	0.0	0.0	0.0	77.1	22.2	54.8
4:4	32.0	1.6	24.0	6.4	0.0	0.0	0.0	0.0	86.2	33.2	53
41:7	36.0	0.7	23.0	12.2	0.0	0.0	0.0	0.0	82.5	21.5	61
5:1	38.2	0.0	34.4	3.8	0.0	0.0	0.0	0.0	83.5	24.0	>50
64741-86-2 Sweetened Distillate C9-C20											
25:12	2.1	0.6	1.5	0.0	0.0	0.0	0.0	0.0	26.9	25.3	1.6
64742-46-7 Hydrotreated Distillate, Middle C11-C25											
11:2	4.9	0.2	3.4	1.2	0.0	0.0	0.0	0.0	34.3	24.9	9.4
12:1	0.3	0.0	0.2	0.1	0.0	0.0	0.0	0.0	<1.0	<1.0	<0.5
17:3	3.7	0.4	2.7	0.6	0.0	0.0	0.0	0.0	31.3	25.9	5.4
31:4	2.2	0.3	1.7	0.2	0.0	0.0	0.0	0.0	34.9	31.3	3.6
4:1	1.0	0.1	0.7	0.1	0.0	0.0	0.0	0.0	18.1	16.1	2
41:2	1.8	0.1	1.3	0.5	0.0	0.0	0.0	0.0	22.9	19.7	3.3
64742-87-6 Hydrodesulfurized Gas Oil, light vacuum C13- C30											
26:23	9.5	0.0	3.8	4.8	0.3	0.0	0.0	0.0	47.2	22.9	24.3
68814-87-9 Gas Oil, Intermediate C9- C25											
10:3	4.3	0.1	2.6	1.7	0.1	0.0	0.0	0.0	20.9	11.5	9.4
17:2	9.6	0.5	5.8	2.9	0.1	0.0	0.0	0.0	35.8	19	16.7
26:1	14.0	0.7	9.8	4.2	0.0	0.0	0.0	0.0	46.8	22.2	24.6
64742-79-6 Hydrodesulfurized Gas Oil C13 – C25											
55:1	5.0	0.4	3.0	1.7	0.0	0.0	0.0	0.0	49.5	38.6	10.9

1 – Percent of DMSO-extractable PACs as determined by PAC-2 Method.

2 – ARC is “aromatic ring class”. ARC 1 (%) is the weight percent of PACs that have 1 aromatic ring within the total sample; “ARC 2 (%) is the percent of PACs with 2 aromatic rings, and so forth to 7 aromatic rings determined by the PAC-2 method.

3 – ASTM D5186 Standard Test Method for Determination of Aromatic Content and Polynuclear Aromatic Content of Diesel Fuels and Aviation Turbine Fuels by Supercritical Fluid Chromatography

Table 5 provides similar analytical profiles for retail samples of Ultralow Sulfur Diesel fuel marketed in the US in 2008.

Table 5. Aromatics Profile of Marketed ULSD Fuels in the United States

State Purchased	AF ID	DMSO extract Wt %								ASTM D5186 Wt % Aromatics		
		Total Extract	ARC 1	ARC 2	ARC 3	ARC 4	ARC 5	ARC 6	ARC ≥7	Total Arom	Mono Arom	Poly Arom
New Mexico	5537	4.30	0.4	3.0	0.9	0.0	0.0	0.0	0.0	24.9	20.1	4.8
New Mexico	5538	3.66	0.3	2.2	1.1	0.0	0.0	0.0	0.0	24.6	20.5	4.1
Georgia	5540	4.26	0.4	3.0	0.9	0.0	0.0	0.0	0.0	31.1	26.3	4.8
Montana	5541	2.42	0.1	1.7	0.5	0.0	0.0	0.0	0.0	23.4	20.7	2.7
Montana	5542	2.49	0.2	2.0	0.2	0.0	0.0	0.0	0.0	24.0	22.0	2.0
Massachusetts	5543	3.16	0.3	2.2	0.6	0.0	0.0	0.0	0.0	24.9	21.9	3.0
Massachusetts	5544	3.01	0.3	2.1	0.6	0.0	0.0	0.0	0.0	25.4	22.4	3.0
Wyoming	5545	4.78	0.4	2.9	1.4	0.0	0.0	0.0	0.0	27.8	22.1	5.7
Wyoming	5546	4.41	0.2	2.6	1.3	0.0	0.0	0.0	0.0	28.4	22.5	5.9
Illinois	5547	7.14	0.6	5.0	1.4	0.0	0.0	0.0	0.0	34.2	26.6	7.6
Illinois	5548	5.16	0.5	3.6	1.0	0.0	0.0	0.0	0.0	31.5	24.4	7.1
Ohio	5550	4.09	0.4	3.3	0.4	0.0	0.0	0.0	0.0	29.0	25.0	4.0
Colorado	5551	2.15	0.2	1.5	0.4	0.0	0.0	0.0	0.0	17.9	16.1	1.8
Colorado	5552	4.11	0.4	2.5	0.8	0.0	0.0	0.0	0.0	28.4	23.9	4.5
Michigan	5553	3.47	0.3	2.4	0.7	0.0	0.0	0.0	0.0	27.3	23.1	4.2
Michigan	5554	4.00	0.3	2.8	0.8	0.0	0.0	0.0	0.0	28.2	23.7	4.5
Missouri	5555	2.58	0.3	1.8	0.5	0.0	0.0	0.0	0.0	25.5	18.9	2.5
Missouri	5556	4.02	0.3	3.2	0.4	0.0	0.0	0.0	0.0	31.5	20.9	4.6
Nevada	5557	4.87	1.0	3.4	0.5	0.0	0.0	0.0	0.0	28.5	26.4	4.6
Nevada	5558	4.07	0.4	2.8	0.4	0.0	0.0	0.0	0.0	21.2	24.2	4.3
California	5560	2.47	0.2	1.7	0.5	0.0	0.0	0.0	0.0	27.6	18.5	2.7
Tennessee	5561	4.30	0.4	2.6	1.3	0.1	0.0	0.0	0.0	27.1	22.7	4.9
Tennessee	5562	4.24	0.4	2.5	1.3	0.1	0.0	0.0	0.0	31.6	22.3	4.8
Florida	5563	4.70	0.9	3.3	0.5	0.0	0.0	0.0	0.0	32.3	27.1	4.5
Florida	5564	4.92	1.0	3.4	0.5	0.0	0.0	0.0	0.0	23.3	27.2	5.1
Minnesota	5565	2.41	0.2	1.9	0.2	0.0	0.0	0.0	0.0	25.3	21.3	2.0
Minnesota	5566	2.81	0.2	1.7	0.8	0.0	0.0	0.0	0.0	30.5	21.1	4.2
New York	5567	4.15	0.4	2.9	0.8	0.0	0.0	0.0	0.0	30.5	25.7	4.8
New York	5568	3.88	0.3	2.7	0.8	0.0	0.0	0.0	0.0	27.7	26.0	4.5
Pennsylvania	5569	5.16	0.4	3.6	1.5	0.0	0.0	0.0	0.0	26.5	21.0	6.7
Pennsylvania	5570	5.27	0.5	3.2	1.6	0.0	0.0	0.0	0.0	22.1	19.6	6.9
Texas	5571	2.51	0.2	2.0	0.5	0.0	0.0	0.0	0.0	23.0	19.3	2.8
Texas	5572	3.09	0.3	2.2	0.3	0.0	0.0	0.0	0.0	23.7	20.1	2.9

Washington	5573	2.49	0.2	1.7	0.5	0.0	0.0	0.0	0.0	22.8	20.6	3.1
Washington	5574	2.74	0.2	1.6	0.8	0.0	0.0	0.0	0.0	24.6	19.3	3.5
Missouri	5575	2.89	0.3	2.3	0.3	0.0	0.0	0.0	0.0	24.6	22.1	2.5
Missouri	5576	3.27	0.3	2.3	0.3	0.0	0.0	0.0	0.0	25.9	23.1	2.8

The fuels and streams in the Gas Oil Category are characterized by alkylated 1 and 2 ring compounds with small percentages of 3 ring and virtually no 4-ring aromatics. The majority of gas oil streams and fuels have lower aromatic content than heavier fuels (See Heavy Fuel Oils CAD) in the 1-15% DMSO extractable range. However catalytic cracked stocks [e.g. CAS RN 64741-59-9, CAS RN 64741-60-2] may contain up to 80% aromatics with the highest concentrations of 2-3 ring PAC in this category.

2.0 CATEGORY DEFINITION AND JUSTIFICATION

The Gas Oil Category contains 29 gas oil petroleum substances, of which 4 are finished distillate fuels and 25 are the refinery streams from which the fuels are blended. These hydrocarbon streams comprising a carbon range of approximately C9-C30 are manufactured by different refinery processes to produce distillate fuels. A list of category members by CAS RN and full substance definition is provided in Appendix A. The fuels have physical and chemical specifications which limit the types of molecules which can be used for fuel blending fairly tightly in the C10-C25 range. Distinguishing characteristics are levels of aromatics and boiling points. Physical properties, process history and product use specifications rather than composition define gas oils streams (ASTM, 2003) and provide the rationale for the composition of this category

- The materials included in the Gas Oils category are related from both process and physical-chemical perspectives;
- The saturated and aromatic hydrocarbon content of the category members forms a continuum from high saturate content to high aromatic content;
- Key parameters when analyzing this category for environmental hazards are the distribution of aromatic and saturated hydrocarbons, and for some mammalian endpoints (repeated-dose, developmental, and mutagenic) the content and distribution of 1-3 ring PAC are important

The carbon number range of Gas Oils determines the volatility, water solubility, and viscosity of these substances. These properties in turn determine their environmental fate and potential for environmental hazard. Due to the diversity of constituents in the Gas Oils category, it is not feasible to model the physicochemical and environmental fate endpoints for each substance. Where modeling was necessary to fulfill an endpoint, such estimates were made for common hydrocarbon structures (e.g., saturated, aromatic) and range of molecular weight hydrocarbons (i.e., number of carbon atoms) known to be represented in Gas Oil substances. Since molecular weight and structural conformation determine in large part many of the physico-chemical and fate processes, the modeled estimates for these isomeric structures are expected to represent potential ranges of values for all substances in the Gas Oil Category.

The ecotoxicological hazard evaluation of the gas oil category is described on the basis of the water accommodated fractions (WAFs) that are used in tests of aquatic organisms. WAFs are the preferred means of exposing aquatic organisms to complex substances having limited solubility.

Thus, substances can be compared on the basis of the amount of test substance applied during test medium preparation that caused the observed effect (Girling et al., 1992; OECD, 2000a).

Mammalian toxicity has been evaluated using measured data. In addition to previously available data, two recent sets of animal studies [repeated dose and developmental toxicity tests] have been performed to explore the association of aromatic content to toxicity. These studies employed an ultralow sulfur diesel fuel [CAS RN 68334-30-5] with a very low DMSO extractable aromatic content which proved to be essentially non-toxic and a light catalytically cracked light cycle oil [CAS RN 64741-59-9] containing higher levels of aromatics (C1 - C3 ring PAC) which produced both systemic and developmental toxicity. Results of these and other studies identify the range of mammalian toxicity resulting from exposure to members of the Gas Oil Category. The DMSO extractable PAC content and distribution profile for samples used in animal studies and described in robust summaries are provided in Appendix D, Table D-1

Statistical models have been explored to determine the association between polycyclic aromatic compounds (ARC profiles) in gas oils and certain repeated dose, developmental and genetic toxicity endpoints in order to predict toxicity where measured data are unavailable (API, 2008; Nicolich et al., 2012) The repeated dose and developmental toxicity results are located in Appendices D and E for completeness. However, the preponderance of low molecular weight aromatics in most gas oils limits the utility of the modeling procedure in its present form for this category of petroleum compounds.

3. PHYSICAL-CHEMICAL PROPERTIES

Substances in the gas oil category have carbon number distributions in the range of C_9 to C_{30}. Although their compositions are highly variable, the streams and finished products consist of components from the principal classes of hydrocarbon types which vary in relative proportions but fall within the cited range of carbon numbers. This similarity among the streams in this category allows the characterization of physical-chemical properties to be given as ranges of values for the different endpoints. When the physical-chemical properties are compared across the various substances that are characterized and described in the robust summaries, it is evident that these attributes are similar across the category.

3.1 Physical-Chemical Endpoints

The physical-chemical endpoints in the HPV chemicals program include the following:

Melting Point
Boiling Point
Vapor Pressure
Octanol/Water Partition Coefficient
Water Solubility

For complex substances such as gas oils, it is not possible to measure or calculate a single numerical value for some of the physicochemical properties. For example, a complex substance does not have a single boiling point. Instead, the boiling point is described as a range of values reflective of the values of the individual components as described in Section 3.1.2.

Although some measured physical-chemical data for category members exist, not all of these endpoints are defined and a consensus database for chemicals that represent products in this

category does not exist. For the physical-chemical properties that cannot be provided as single values, ranges of endpoint values were reported for constituent hydrocarbons covering the principal hydrocarbon types and molecular weight ranges in these streams. When available, measured data were reported. In the absence of measured data, physical-chemical properties were estimated using the EPI-Suite^{TM} computer subroutines (US EPA, 2000).

When estimated data were provided, the individual compounds were chosen from detailed hydrocarbon analyses of representative gas oil streams. Since molecular weight and structural conformation determine in large part the solubility and vapor pressure characteristics of the hydrocarbons, representative isomeric structures of the lower (C_9) and higher molecular weight (C_{30}) hydrocarbons of each group of the chemical species found in these materials (paraffinic, naphthenic, olefinic and aromatic) were modeled for relevant physicochemical and fate processes. This provided a range of values that were considered to encompass the majority of the compounds in the gas oil category.

3.1.1 Melting Point

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 material is observed under prescribed conditions of the test (ASTM, 1999). The pour point temperature increases as the viscosity increases. The pour points of two samples of light catalytic cracked gas oil (60.8% - 79.8% aromatic hydrocarbons) were measured by API (1987d) to be –15°C and –12°C. The maximum pour points of three types of distillate fuels, an automotive gas oil (diesel), a heating oil, and a marine distillate fuel were reported by CONCAWE (1996) to range from -6°C to 0°C. The pour point values for four commercial diesel fuels (Alaska, Canada, and Southern USA) reported by Jokuty et al. (2002) ranged from –50°C to -14°C. The wide range in pour point values for commercial fuels may be attributed to fuel additives (e.g., flow improvers) to meet market specifications for particular regions.

Conclusion: The pour point values of gas oils fall within the approximate range of -50°C to 0°C.

3.1.2 Boiling Point

Gas oils do not have a single numerical value for boiling point, but rather a boiling or distillation range that reflects the individual components in the complex hydrocarbon substance. CONCAWE (1996) provided a boiling range of 150°C to 450°C (302° F to 842° F) as a general distribution for this category. Ranges for specific streams or products vary depending on the refinery processes used and sources of the feedstocks. CONCAWE (1996) listed representative ranges for three fuel types, an automotive gas oil (160°C to 390°C), a heating oil (160°C to 400°C), and a distillate marine fuel (170°C to 420°C). Jokuty et al. (2002) also provided boiling point ranges for several fuels from commercial retailers from different geographical region in Canada and the U.S. They reported boiling point distributions for samples taken from the southern U.S., Alaska, and Canada of 174°C to 355°C, 141°C to 320°C, and 246°C to 388°C, respectively. Some variability in the ranges was attributed to the manner in which these values were reported. Some of the boiling point limits were given as initial and final values, while others were reported for a given weight percent, typically 5% and 90-95%.

With respect to several individual gas oil streams, API (1987d) reported low end and high end distillation temperatures for a hydrodesulfurized middle distillate (172 to 344°C), a straight-run middle distillate (185°C to 391°C), and a light catalytic cracked distillate (185°C and 372°C). No

substantial differences in boiling ranges were apparent for gas oils with high concentrations of either aromatic (catalytic cracked stock) or saturated hydrocarbons (straight run stock).

Conclusion: The boiling point distributions of gas oils can be expected to fall approximately within the range 150°C to 450°C (302° F to 842° F).

3.1.3 Vapor Pressure

Gas oils are expected to have low but measurable vapor pressure due to their boiling range (150 to 450°C) and the molecular weights of the constituent hydrocarbons (C_9 – C_{30} carbon atoms). Measured values according to ASTM Method D2889 for an automotive gas oil (diesel fuel) and a heating oil were approximately 0.4 kPa at 40°C (CONCAWE, 1996), while the vapor pressure of a No. 2 fuel oil and a diesel oil measured according to the Reid Method (ASTM, D323) were reported as 2 kPa at 38°C (Jokuty et al., 2002). Because the physical-chemical characteristics of distillate fuels reflect the gas oil streams from which they were produced, these vapor pressure measurements are expected to approximate the vapor pressures of individual gas oils. However, estimated vapor pressure values of constituent hydrocarbons in gas oil streams were made using EPI-Suite™ (EPA, 2000). These estimates were determined for representative low (C_9), middle (C_{15}, and high (C_{30}) molecular weight hydrocarbon constituents in gas oils. Because the vapor pressure of a mixture is dependent on the vapor pressure of each chemical component and the mole fraction of each of the components present (Raoult's law) and gas oils typically contain small amounts of large numbers of constituents, no single constituent would be expected to contribute substantially to the overall vapor pressure. Vapor pressure estimates of low molecular weight hydrocarbons (e.g. C9) of varying isomeric structures fell within a range of 0.03 to 0.8 kPa, with higher molecular weight hydrocarbons (e.g. C30) showing very low vapor pressures (e.g., 10^{-8} to 10^{-10} kPa).

Conclusion: The vapor pressures of gas oils can be expected to approximate the range of 0.4 kPa to 2 kPa when measured at approximately 40°C.

3.1.4 Partition Coefficient

Standard tests for partition coefficient are intended for mono-constituent substances and are not appropriate for complex substances such as gas oils. Therefore it is not possible to determine a single log K_{ow} value for these substances. Instead, partition coefficients have been calculated for individual component hydrocarbons with known hydrocarbon composition (CONCAWE, 1996). The percent distribution of the hydrocarbon groups (i.e., paraffins, olefins, naphthenes, and aromatics) and the carbon chain lengths of hydrocarbon constituents in gas oils 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). The calculated range reported by CONCAWE (1996) for hydrodesulfurized middle distillates, straight-run middle distillates, and catalytic cracked middle distillates fell within the range of 3.9 to >6.0. That range is in agreement with a range of log K_{ow} values of 3.3 to >6 determined by the Testing Group using EPI-Suite™ (EPA, 2000) for various C_9 to C_{30} hydrocarbon components in gas oils. There are no apparent differences in the range of K_{ow} values determined for gas oils with high concentrations of either aromatic or saturated hydrocarbons.

Conclusion: The partition coefficients of individual constituent hydrocarbons found in gas oils can be expected to fall within the range of 3.3 to >6.

3.1.5 Water Solubility

Individual components of complex petroleum substances have specific and differing water solubility characteristics that are related to their molecular weights and hydrocarbon structures. For example, solubility decreases with increasing molecular weight, and aromatic hydrocarbons typically are more water soluble than saturated hydrocarbons of equal molecular weight. When addressing the aqueous solubility of complex and variable composition of petroleum substances, the amount dissolving in the aqueous phase is a function of: 1) the loading rate (i.e., ratio of petroleum substance to water), 2) log K_{ow} of the component hydrocarbons, 3) the amount of component present, and 4) the maximum water solubility of each component. Initially, as the complex petroleum substance is added to water in amounts below the solubility limit of the least soluble component, the aqueous concentration increases proportionally until the least soluble component reaches its saturation concentration. As more of the test substance is added to water, only the more soluble components continue to dissolve until they reach their own solubility limits, resulting in a two phase system. Further addition of the complex petroleum substance results in an aqueous concentration that is a non-linear function of the amount added.

The gas oils are complex substances that follow this pattern of component dissolution in an aqueous medium, which has been shown by analysis of hydrocarbon components in the dissolved phase. Shiu et al. (1990) demonstrated the effect of loading rate required to maximize the amount of total hydrocarbons in the aqueous phase for a variety of petroleum fractions. It was shown that the water-to-oil ratio should be ≤40 to create a consistent saturated solution. For a No. 2 fuel oil (density: 0.862 g/cm^3 @ 20°C, viscosity: 3.64 cp @ 20°C), Shiu et al. (1990) measured the total dissolved hydrocarbons by purge-and-trap GC for water-to-oil loading rates of 5-10:1. Measurements were taken at two temperatures (5 and 20°C) and for distilled and salt water (3% NaCl). Under those conditions, the solubility levels of the No. 2 fuel oil in distilled water at 5 and 20°C were 2.7 and 3.2 mg/L, respectively. For saltwater, at the same two temperatures, the solubility levels were 2.05 and 2.5 mg/L, respectively. Anderson et al. (1974) measured the aqueous fraction of a 10:1 ratio of seawater to No. 2 fuel oil using infrared analysis. The total amount of petroleum hydrocarbons in the aqueous fraction was 8.7 mg/L.

For individual hydrocarbon constituents in gas oils, water solubility values vary by orders of magnitude. Water solubilities of component hydrocarbon molecules were estimated using the WSKOW V1.40 subroutine of the EPI-Suite^{TM} computer model (EPA, 2000). Water solubility values ranged from essentially insoluble (approximately 10^{-8} mg/L) for the higher molecular weight fractions (e.g., C_{30} paraffin) within gas oil to approximately 52 mg/L for a C_9 alkylbenzene (propylbenzene).

Conclusions: Precise measurements of water solubility for complex substances such as gas oils are complicated by factors such as the sensitivity of the analytical method and the water-to-oil ratio. When the ratio is optimized to achieve maximum hydrocarbon concentrations, measurements have ranged from 2.05 mg/L to 8.7 mg/L. Solubility values of individual constituents in gas oils vary widely due to the wide range of molecular weights. Individual water solubility values may range from essentially insoluble (e.g., <0.001 mg/L) to 52 mg/L, depending on the specific molecular structures considered.

3.2 Assessment Summary for Physical-Chemical Endpoints

Gas oils are complex substances with variable hydrocarbon compositions predominantly having carbon chains from C_9 to C_{30}, and boiling over the temperature range of 150°C to 450°C. Vapor pressures are within a measurable range, with values of 0.4 kPa and 2 kPa being reported. Partition coefficients of constituent hydrocarbons range from 3.3 to >6. Water solubility values for these substances have been reported from 2.0 mg/L to 8.7 mg/L for dissolved hydrocarbons.

4.0 ENVIRONMENTAL FATE

4.1 Environmental Fate Endpoints

To assess the environmental fate properties for the HPV program, the U.S. EPA has selected the fate endpoints by which these substances may be characterized. The environmental fate endpoints include the following:

- Photodegradation
- Stability in water [Hydrolysis]
- Transport Between Environmental Compartments [Fugacity/Distribution]
- Biodegradation

In determining these fate characteristics for constituents in gas oils, the US EPA's collection of physical-chemical and environmental fate models in EPI-Suite™ (US EPA, 2000) were used to estimate the properties of photodegradation, stability in water, and environmental distribution. Measured data, when available, were included in the assessment. Biodegradation was examined for these substances in light of their physical-chemical properties and the capacities of the constituent compounds to be used for microbial metabolism.

4.1.1 Photodegradation

4.1.1.1 Direct

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 750 nm can result in photochemical transformations in the environment, although absorption is not always sufficient for a chemical to undergo photochemical degradation (Harris, 1982a). 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. Polycyclic aromatic hydrocarbons, on the other hand, have shown absorbance of the 290 to 800 nm range of light energy and could potentially undergo photolysis reactions (Fasnacht and Blough, 2002). The degree and rate at which these compounds photodegrade depends upon whether conditions allow penetration of light with sufficient energy to effect a change.

4.1.1.2 Indirect

Constituents of gas oils that volatilize to the troposphere have the potential to undergo gas-phase oxidation reactions with photochemically produced hydroxyl radicals (OH) as well as other oxygen containing radicals (e.g., NO_3) and ozone (O_3). Atmospheric oxidation as a result of these types of reactions is not direct photochemical degradation but indirect photodegradation (Schwarzenbach et al, 2003). The importance of the different atmospheric reactants to degradation depends on the structure of the compound. For example, Atkinson (1990) reports that reactions with OH and NO_3 radicals can be important for alkanes, whereas reactions with O_3 are negligible. Additionally, nighttime reactions with NO_3 occur at rates approximately two orders of magnitude less than

daytime OH radical reactions. Olefins may react with OH and NO_3 radicals and O_3, with OH and O_3 being the most important. Of the latter two, OH reaction rates are faster. For aromatic compounds, interaction with the OH radical is the only important removal process.

The potential to undergo indirect photodegradation was estimated using the atmospheric oxidation potential (AOP) model subroutine (AOPWIN V1.90) of the EPI-Suite™ computer models (EPA, 2000). This model calculates a chemical half-life and an overall OH radical reaction rate constant based on a 12-hour day and a given OH radical concentration. This program also estimates the reaction rates and half-lives for the reaction of olefins with O_3, but as described by Atkinson (1990), these rates tend to be substantially less than for those for the OH radical. For this reason, only the half-lives for the reaction with the OH radical are reported for the series of olefinic hydrocarbons selected for the AOP model. It should be understood that these reactions have been worked out only for gaseous phase compounds in the troposphere. Reactions occurring for particulate, aerosol, and surface particle-adsorbed interactions are beyond the scope of the model. The half-life values estimated for the heterocyclic compounds should be qualified by adding that these substances have not been fully investigated as to their involvement in OH radical reactions. It is presumed that these substances also undergo similar reactions since it is the aromatic structure that is susceptible to OH radical addition. The AOPWIN routine also provides reaction rate constants and half-life data for heterocyclic compounds.

Atmospheric oxidation half-lives were calculated by the AOPWIN model for the various molecular weight and isomeric structures representing constituent hydrocarbon (paraffins, naphthenes, olefins, aromatics) compounds in gas oils. Structures and molecular weights of selected constituents were chosen on the basis of carbon number as identified in the description of the category substances and known hydrocarbon composition of gas oils. Therefore, the estimated values identify a potential range of half-lives for substances in the gas oil category. The half-lives for representative constituents of gas oils were determined to range from 0.1 days to approximately 1.5 days. This range spans isomeric structures for representative paraffinic, olefinic, naphthenic, and aromatic compounds in gas oils that cover the molecular weights of C_9 to C_{30} carbon chain lengths. For the majority of the thousands of compounds constituting gas oils, the low vapor pressures of the majority of the compounds would preclude them from entering the troposphere where these reactions take place. However, the half life values determined for these substances indicate that should any of the lighter fractions of these streams enter the atmosphere, they would degrade and not persist.

Conclusion: Direct photodegradation is not likely to be an important fate process for gas oils due to their relatively low concentrations of photosensitive constituents. However, indirect photodegradation will be an important degradation pathway for constituents that volatilize to the atmosphere. Reaction rates calculated for indirect photodegradation ranged from 0.1 days to approximately 1.5 days for a variety of hydrocarbon and heterocyclic compounds covering carbon numbers from C_9 to C_{30} and show that these substances would not persist in the atmosphere.

4.1.2 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, 1982b). Because gas oils do not contain significant levels of these functional groups, materials in the gas oils category are not subject to hydrolysis.

Conclusion: Gas oils will be stable and not react with water. Constituent compounds do not contain chemical moieties that undergo hydrolysis.

4.1.3 Transport and Distribution in the Environment (Fugacity)

Fugacity-based multimedia modeling provides basic information on the relative distribution of chemicals between selected environmental compartments (e.g., air, water, soil, sediment, suspended sediment and biota). The US 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 (Mackay et al., 1996, 1997). 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 regional environment. 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. EPA cites the use of this model in its document "Determining the Adequacy of Existing Data" that was prepared as guidance for the HPV chemicals program (US EPA, 1999).

Results of Level I models are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition in the environment. One drawback of these and higher level models is their inability to predict the environmental distribution of all the constituents comprising complex petroleum streams. To gain an understanding of the potential environmental distribution for these complex substances, modeling was performed on a representative range of molecular weight compounds covering the different isomeric hydrocarbon structures. Specific compounds were selected on the basis of carbon number and hydrocarbon type as identified in the description of the category substances and detailed hydrocarbon analyses. The resulting distribution characteristics represent the potential ranges of distribution to environmental media for those hydrocarbon constituents found in these streams.

The range of properties of gas oil components is such that the components cannot be considered as a single group with respect to environmental distribution. Because of the varied properties of the individual constituents, if a gas oil enters the environment, the individual compounds will distribute independently of one another according to their own physical-chemical characteristics. Therefore, it is useful to consider a representative range of molecular weight compounds and isomeric structures to assess how the various fractions of gas oil can potentially distribute. To gain an understanding of the potential distribution of the constituent compounds in gas oil, the EQC model was used to characterize the environmental distribution of representative hydrocarbon and heterocyclic compounds in gas oils for different molecular weight ranges and isomeric structures. Compounds selected for modeling were chosen on the basis of carbon number as identified in the description of the category substances and known and estimated hydrocarbon composition of gas oils (Potter and Simmons, 1998). In so doing, an understanding of the potential environmental distribution of components in gas oil may be gained. Distribution patterns determined by the EQC model for the different constituents are shown in Table 6

Table 6. Estimated Percent Distribution of Constituent Compounds Represented in Gas Oils.

Compound Type/ Carbon Chain	Air	Water	Soil	Sediment	Suspended Sediment	Biota

n-alkanes						
C9	99	<0.1	1	<0.1	<0.1	<0.1
C15	13	<0.1	85	2	<0.1	<0.1
C30	<0.1	<0.1	98	2	<0.1	<0.1
iso-alkanes						
C9	99	<0.1	0.5	<0.1	<0.1	<0.1
C15	68	<0.1	31	0.7	<0.1	<0.1
C30	0.1	<0.1	98	2	<0.1	<0.1
straight olefins						
C9	99	<0.1	0.7	<0.1	<0.1	<0.1
C15	17	<0.1	81	2	<0.1	<0.1
C30	<0.1	<0.1	98	2	<0.1	<0.1
cyclic olefins						
C9	99	<0.1	0.7	<0.1	<0.1	<0.1
C15	49	<0.1	50	1	<0.1	<0.1
C30	<0.1	<0.1	98	2	<0.1	<0.1
1-ring naphthenes						
C9	99	<0.1	0.9	<0.1	<0.1	<0.1
C15	0.4	<0.1	97	2	<0.1	<0.1
C30	0.1	<0.1	98	2	<0.1	<0.1
2-ring naphthenes						
C9	99	0.2	1	<0.1	<0.1	<0.1
C15	51	<0.1	48	1	<0.1	<0.1
C30	0.1	<0.1	98	2		
1-ring aromatics						
C9	97	1	2	<0.1	<0.1	<0.1
C15	18	<0.1	79	2	<0.1	<0.1
C30	<0.1	<0.1	98	2	<0.1	<0.1
2-ring aromatics						
C10	77	8	15	0.3	<0.1	<0.1
C15	0.7	0.2	97	2	<0.1	<0.1
C30	<0.1	<0.1	98	2	<0.1	<0.1

Regardless of chemical structure, hydrocarbons having nine carbon atoms showed a tendency to partition to air (up to 99%). As molecular weight increases, partitioning shifts to soil, accounting for 98% of the distribution of the C_{30} components. Few of the representative structures partitioned to water or other environmental compartments.

Conclusion: The low molecular weight constituents in gas oils will tend to partition to the air. As molecular weight increases, partitioning shifts to the soil compartment.

4.1.4 Biodegradation

On the basis of the biodegradability characteristics of other petroleum substances such as kerosene and lubricating oil basestocks, gas oils are not likely to pass the criteria for ready biodegradability. However, most hydrocarbon species present in gas oils are known to be ultimately degraded by aerobic microorganisms (Connell and Miller, 1980; CONCAWE, 1996). Lower molecular weight compounds may be expected to be degraded relatively quickly in aerobic conditions, while higher molecular weight compounds, particularly polycyclic aromatics, will degrade more slowly. Much of this evidence is based on bioremediation studies of contaminated

soils, which have shown that hydrocarbon components in gas oils are degraded in the presence of oxygen (Hoeppel et al., 1991; Miethe et al., 1994). Bioremediation of a diesel fuel spill also has been demonstrated under Arctic conditions (Liddell et al., 1994).

Biodegradation data was available for a solvent-refined gas oil (CAS no. 64741-90-8; Exxon, 1994) and two samples of a blended diesel fuel appear to bear this out (Clark, et al., 2003; Mobil, 1999). The data show that these substances are inherently biodegradable. A fourth study was cited in CONCAWE (1996) for an undisclosed gas oil sample. For the solvent-refined gas oil, an inherent biodegradability study (method ISO 14593) using adapted inoculum achieved 36% biodegradation by day 7 of the test. However, degradation could not be prolonged, as a maximum of only 41% was attained between day 7 and day 28 (Exxon, 1994). In a ready biodegradability test following the manometric respirometry method (OECD 301F), Clark et al. (2003) measured 60% biodegradation at the end of 28 days for a commercial diesel fuel. This test did not attain the 60% biodegradation level within the 10-day window criterion that is applied to pure chemicals. However, for ready biodegradability classification of complex substances containing structurally similar constituents such as petroleum substances, the 10-day window should not be applied. For such substances where the 60% biodegradation level is achieved by day 28, then the substance may be considered readily biodegradable (OECD, 2006). Following the same respirometry method, Mobil (1999) achieved a similar biodegradation rate of 57.5% for a commercial diesel fuel. CONCAWE (1996) reported on a study by Battersby et al. (1992), who observed approximately 40% biodegradation for a gas oil in a 28-day modified Sturm procedure.

New ready biodegradability test data was developed for two gas oil streams, one containing 82% saturated and 17% aromatic hydrocarbons (CAS 64741-77-1) and one containing 18% saturated and 75% aromatic hydrocarbons (CAS 64741-59-9). Testing of these two streams with widely differing saturate/aromatic percent composition provides a suitable basis for characterization of the entire category. Using the OECD 301F method for manometric respirometry measurement of ready biodegradability, EMBSI (2011a,b) reported 56% biodegradation of the high aromatic sample and 64% biodegradation of the high saturate sample. Collectively, these studies show that gas oils may not pass ready biodegradability status, but biodegradation does occur and these substances are considered inherently biodegradable. Some individual gas oil samples may meet the criterion for ready biodegradability.

While the studies cited above indicate gas oils can undergo biodegradation under aerobic conditions, in many spill situations, anaerobic conditions prevail. When gas oil substances are combined with anoxic sediments, rates of biodegradation are negligible and these substances may persist under those conditions for some time (CONCAWE 1996; Brown 1989). Standard 275-day anaerobic tests designed to measure ultimate biodegradation, such as ISO 11734 (ISO 1995), indicated diesel fuel to have limited potential to biodegrade (0 – 3% biodegradation) (ACC 2006). However, when single electron-acceptor systems were made available to the microbes (e.g., sulfate, nitrate, methanogenic), significant biodegradation of diesel was demonstrated over systems using natural attenuation (Boopathy 2004). Further enhancement of anaerobic biodegradation of diesel and crude oil was achieved over single electron-acceptor systems when mixed electron acceptors were used (Boopathy 2004; Boopathy et al 2012). While these studies offer insight into augmenting anaerobic biodegradation of these substances, natural biodegradation rates are expected to be low, and degradation then will be dependent on bioturbation or re-suspension to provide microbes access to oxygen.

Conclusion: Rates of biodegradation of gas oils can be high, and these substances are considered to be inherently biodegradable. Biodegradation rates for some individual gas oil samples may be sufficient to pass the criterion for ready biodegradability in 28-day tests

4.2 Assessment Summary for Environmental Fate

If gas oils are released to the environment, individual components will disperse and partition according to their individual physical-chemical properties. Their final disposition is shaped by both abiotic and biotic processes. Based on modeling individual structures encompassing the different types and molecular weights of hydrocarbons, volatilization to the atmosphere is an important process for the low molecular weight fractions. 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 these reactions. Components in gas oils will biodegrade, and moderate to rapid rates of biodegradation were measured in standard tests. Gas oils are considered to be inherently biodegradable, and for some individual gas oil samples, biodegradation rates may be high enough to achieve ready biodegradability classification. Anaerobic biodegradation is expected to be low unless sufficient electron-acceptor conditions are made available.

5.0 ENVIRONMENTAL EFFECTS

The environmental effects endpoints in the HPV Challenge program include:

- Acute Toxicity to Fish,
- Acute toxicity to Aquatic Invertebrates, and
- Toxicity to Algae (Growth Inhibition).

For the assessment of environmental toxicity of poorly water soluble substances such as petroleum products, the generally accepted procedure is to report results expressed in terms of the "loading rate" (OECD, 2000a). The loading rate is defined as the amount of the substance that is equilibrated with the aqueous test medium, and the aqueous phase at equilibrium is termed the water-accommodated fraction (WAF) for the specific loading rate. Toxicological endpoints such as the LL_{50} or EL_{50} define the loading rate of the test substance lethal to or producing a specific effect in 50% of the test organisms. Tests may be conducted as oil-water dispersions (OWDs), where the insoluble petroleum fractions remain in the exposure solutions. This method also results in an expression of the concentration of the applied substance (i.e., mg test substance/l), but the methodology does not prevent potential adverse effects to the organisms due to physical entrapment. Water-soluble fractions (WSFs) and their dilutions also may be reported in ecotoxicity studies. These preparations are commonly expressed in terms of the percent dilution of a WSF. Occasionally, the measured concentrations of hydrocarbons in solution may be reported. Expressing toxicity as percent dilutions of water soluble fractions has fallen out of favor because this practice does not allow the ecotoxicity of the test substance to be expressed in terms of the amount of that test substance required to produce a particular effect (OECD, 2000). Such results are not comparable to results obtained under WAF or OWD preparation methods.

Acute and chronic endpoints developed by the HPV Testing Group for the HPV program are reported as recommended by OECD (2000a) on the basis of loading rate and measured concentrations. In these new studies, concentrations of dissolved hydrocarbons in the WAFs were

quantified against gas oil standards using automated static headspace gas chromatography with flame ionization detection (HS GC-FID). The total peak area for eluted hydrocarbon components from WAF headspace analysis was summed for quantification. The distribution and percentage of gas oil components measured in the WAFs differed from the parent gas oil owing to the differing solubilities of individual gas oil hydrocarbons. Therefore, measured concentrations do not represent all hydrocarbons constituting the test substance. Due to the complex nature of the test substance, no attempt was made to identify and quantify specific hydrocarbons solubilized in the WAFs.

5.1 Aquatic Toxicity

Hydrocarbon constituents in gas oils elicit acute aquatic toxicity through non-polar narcosis, a mode of action involving disruption of biological membrane function (van Wezel and Opperhuizen, 1995). Therefore, hydrocarbon constituents in gas oil streams share a common mode of action, and their acute toxicities would be expected to fall within a relatively narrow range. Any differences between toxicities (i.e., LC/LL_{50}, EC/EL_{50}) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals (Verbruggen et al., 2000). For example, the existing fish toxicity database for hydrophobic neutral chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of approximately 2-8 mmol/kg fish (wet weight) (McCarty and Mackay, 1993; McCarty et al., 1991). When normalized to lipid content, the CBR is approximately 50 µmol/g of lipid for most organisms (Di Toro et al., 2000). On the basis of a common mode of action, the acute toxicity of complex petroleum mixtures may be predicted using the hydrocarbon block method (CONCAWE 1996). This method utilizes detailed hydrocarbon analysis and knowledge of the partitioning behaviour of hydrocarbons together with the Target Lipid Model (TLM) to calculate acute toxicity (Di Toro et al. 2000). PETROTOX was developed as a spreadsheet-based program designed to calculate the toxicity of petroleum products to aquatic organisms using hydrocarbon blocking and TLM (CONCAWE 2007). This program was used in conjunction with detailed 2D-GC-MS analyses (Appendix C) to calculate predicted EL/LL_{50} values for two gas oil streams.

5.1.1 Aquatic Endpoints – Acute Toxicity

The acute aquatic toxicity of gas oils to fish, invertebrates, and algae is described below, and an overall range of acute toxicity values is provided for each trophic level. The referenced data are studies conducted using the WAF or OWD methods of preparing exposure solutions. Other studies using dilutions of WSFs are also discussed, although these are not considered reliable studies for characterizing aquatic hazard.

The Petroleum HPV Testing Group recognized that aquatic hazard data based on blended fuels may not represent the hazard of the category as a whole given compositional diversity of the wide spectrum of hydrocarbon types shown by the individual gas oil substances (see Figure 3). Therefore, the Testing Group proposed in its Test Plan (API, 2005) to conduct additional aquatic toxicity testing on two gas oils that represented the widest possible boundaries of the aromatic/saturate hydrocarbon range. Test samples were selected on the basis of their saturated and aromatic hydrocarbon content. A light catalytic cracked gas oil (CAS 64741-59-9) having a high proportion of aromatic hydrocarbons (75 v% aromatics, 18 v% saturates) and a hydrocracked gas oil (CAS 64741-77-1) having a high proportion of saturated hydrocarbons (17 v% aromatics, 82 v% saturates) were selected for testing. These new data are presented as key endpoint studies for acute toxicity to fish and invertebrates, toxicity to aquatic plants (algae), and chronic toxicity to invertebrates.

The necessity to conduct toxicity tests has raised concerns regarding the ethical and humane treatment of vertebrate animals used in experimental testing. With respect to ecotoxicology, the recognized need to limit or avoid unnecessary use of fish and other vertebrates has fostered modifications to testing guidelines or new approaches to the testing of vertebrate animals. Standard testing guidelines for fish have been modified to allow a reduction in the number of fish used in acute tests (OECD, 1984, 1992), and new approaches to testing include in vitro assays (Castano et al., 2003), and QSAR estimations (Cronin et al., 2003). One new strategy that can reduce the number of fish used in acute tests is the Upper Threshold Concentration (UTC) Step-Down Approach (Jeram et al., 2005; ECVAM, 2006). The UTC method is based on the observation that for acute aquatic toxicity, fish are in many cases less sensitive than algae and *Daphnia magna* to a variety of toxicants (Weyers et al., 2000). Using this relationship in a testing program can effectively minimize the numbers of fish consumed in testing. As described by Jeram et al (2005) and used here by the Testing Group, tests are first conducted on the invertebrate and algal species. The lowest endpoint in these two toxicity tests is defined as the UTC. Testing of fish in a limit test at the UTC substantially reduces the consumption of fish in cases where the LL/LC_{50} is greater than the UTC. Because hazard classification schemes and risk assessments utilize the lowest endpoint value among the three aquatic test species, the need for a definitive LL/LC_{50} for fish becomes pointless when it is not the most sensitive of the three test species.

5.1.1.1 Acute Toxicity to Aquatic Vertebrates

The results of the studies described in detail in the robust summaries for the hazard of gas oils to fish are provided in the following table.

Table 7. Acute Toxicity Values for Gas Oils to Fish.

Test Substance	Test Species and Type (WAF or OWD)	Toxicity Endpoint	Endpoint Value, mg/L	Reference
CAS No. 64741-59-9, light catalytic cracked gas oil	*Oncorhynchus mykiss* WAF	96-h LL_{50} 96-h LC_{50}[1]	>0.30 >0.21	Key Study EMBSI, 2011c
		96-h LL_{50}[1]	0.18 (PETROTOX model)	Swigert et al. 2011
CAS No. 64741-77-1, light hydrocracked gas oil	*Oncorhynchus mykiss* WAF	96-h LL_{50} 96-h LC_{50}[1]	>2.6 >0.54	Key Study EMBSI, 2011d
		96-h LL_{50}	0.62 (PETROTOX model)	Swigert et al. 2011
CAS No. 68334-30-5, diesel oil	*O. mykiss* WAF	96-h LL_{50} NOELR	21 10	Shell, 1995a
CAS No. 68334-30-5, diesel oil	*O. mykiss* WAF	96-h LL_{50} NOELR	65 10	Shell, 1995b

CAS No. 68476-30-2, No. 2 fuel oil	*O. mykiss* WAF	96-h LL_{50} BPH critical[2]	6.6 155 nmol/mg C	EBSI, 1998a
CAS No. 68476-30-2, no. 2 fuel oil	*Cyprinodon variegatus* WAF	96-h LL_{50} BPH critical[2]	57 202 nmol/mg C	EBSI, 1998b
CAS No. 68476-30-2, no. 2 fuel oil	*Menidia beryllina* WAF	96-h LL_{50} BPH critical[2]	3.2 72 nmol/mg C	EBSI, 1998c
CAS No. 68476-30-2, No. 2 fuel oil	*Pimephales promelas* WAF	96-h LL_{50} BPH critical[2]	57 388 nmol/mg C	EBSI, 1999
No. 2 fuel oil (no CAS No. cited)	*C. variegates* OWD	96-h LL_{50}	93	Anderson, et al., 1974
No. 2 fuel oil (no CAS No. cited)	*M. beryllina* OWD	48-h LL_{50}	125	Anderson, et al., 1974
No. 2 fuel oil (no CAS No. cited)	*Fundulus similis* OWD	96-h LL_{50}	33	Anderson, et al., 1974
No. 2 fuel oil (no CAS No. cited)	*Jordanella floridae* OWD	96-h LL_{50}	51	Hedtke and Puglisi, 1982[3]
No. 2 fuel oil (no CAS No. cited)	*P. promelas* OWD	96-h LL_{50}	33	Hedtke and Puglisi, 1982[3]

[1] Results expressed as LC values represent the concentration of hydrocarbons that solubilized from the test substance into each WAF at its respective loading rate. The distribution and percentage of the test substance components measured in the WAFs differed from the parent substance owing to the differing solubilities of the individual hydrocarbons. The individual hydrocarbons which were solubilized in the WAFs were not identified nor separately quantified, due to the complex nature of the test substances.

[2] The BPH critical represents an estimate of the bioavailable petroleum hydrocarbons (BPH) corresponding to a threshold total body residue in an aquatic organism. Acute toxicity is predicted once the BPH critical is exceeded.

[3] Endpoint values in the Hedtke and Puglisi (1982) study were presented as µL/L. CONCAWE (1996) cited this work and recalculated the endpoints assuming a specific gravity of 0.85 g/cm^3.

Based on the studies cited in Table 7 for WAF exposures, the fish acute LL_{50} values (expressed as loading rates) ranged from >0.30 mg/L for the light catalytic cracked gas oil (CAS No. 64741-59-9) to 65 mg/L for diesel oil (CAS No. 68334-30-5). The OWD studies (Hedtke and Puglisi, 1982) resulted in slightly higher LL_{50} values, which may be expected due to the manner in which these exposure solutions are prepared. The dispersion technique can result in loss of volatile components from the dissolved fraction. Therefore, for gas oils category substances such as No. 2 fuel oil or diesel, the range of toxicity values used for read across to other fuels of this type is >0.3 – 65 mg/L expressed as the loading rate.

Conclusion: The acute toxicity (LL_{50}) of gas oil category substances to fish is expected to fall within the range >0.3 to 65 mg/L based on WAF studies and expressed as the loading rate.

5.1.1.2 Acute Toxicity to Aquatic Invertebrates

The results of the studies described in detail in the robust summaries for the hazard of gas oils to aquatic invertebrates are provided in the following table.

Table 8. Acute Toxicity Values for Gas Oils to Aquatic Invertebrates.

Test Substance	Test Species and Type (WAF or OWD)	Toxicity Endpoint	Endpoint Value, mg/L	Reference
CAS No. 64741-59-9, light catalytic cracked gas oil	*Daphnia magna* WAF	48-h EL_{50} 48-h EC_{50}[1]	0.51 0.45	Key Study EMBSI, 2010a
		48-h EL_{50}	0.35 (PETROTOX model)	Swigert et al. 2011
CAS No. 64741-77-1, light hydrocracked gas oil	*Daphnia magna* WAF	48-h EL_{50} 48-h EC_{50}[1]	5.5 1.0	Key Study EMBSI, 2010b
		48-h EL_{50}	2.3 (PETROTOX model)	Swigert et al. 2011
CAS No. 68334-30-5, diesel oil	*Daphnia magna* WAF	48-h EL_{50} NOELR	13 3	Shell, 1994
CAS No. 68334-30-5, diesel oil	*D. magna* WAF	48-h EL_{50} NOELR	68 46	Shell, 1995c
CAS No. 68334-30-5, diesel oil	*D. magna* WAF	48-h EL_{50} NOELR	210 46	Shell, 1995d
CAS No. 68334-30-5, diesel oil	*D. magna* WAF	48-h EL_{50} NOELR	>100, <300 100	Clark, et al., 2003
CAS No. 68476-30-2, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} BPH critical[2]	2.0 85.3 nmol/mg C	EBSI, 2001
CAS No. 68476-30-2, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} NOELR	7.8 1.25	Fraunhofer-Institut, 2000
CAS No. 68476-30-2, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} NOELR	5.3 1.25	Fraunhofer-Institut, 2000
CAS No. 68476-30-2, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} NOELR	14 1.5	Fraunhofer-Institut, 2000
CAS No. 68476-30-2, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} NOELR	42 7.5	Fraunhofer-Institut, 2000

CAS No. 68476-30-2, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} NOELR	13 <6.25	Fraunhofer-Institut, 2000
CAS No. 68476-34-6, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} NOELR	6.4 <1.9	Fraunhofer-Institut, 2000
CAS No. 68476-34-6, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} NOELR	36 6.25	Fraunhofer-Institut, 2000
CAS No. 68476-34-6, No. 2 fuel oil	*D. magna* WAF	48-h EL_{50} NOELR	9.6 3.1	Fraunhofer-Institut, 2000
No. 2 fuel oil (no CAS No. cited)	*Palaemonetes pugio* OWD	96-h EL_{50}	3.0	Anderson, et al., 1974
No. 2 fuel oil (no CAS No. cited)	*Penaeus aztecus* OWD	96-h EL_{50}	9.4	Anderson, et al., 1974

[1] Results expressed as EC values represent the concentration of hydrocarbons that solubilized from the test substance into each WAF at its respective loading rate. The distribution and percentage of the test substance components measured in the WAFs differed from the parent substance owing to the differing solubilities of the individual hydrocarbons. The individual hydrocarbons which were solubilized in the WAFs were not identified nor separately quantified, due to the complex nature of the test substances

[2] The BPH critical represents an estimate of the bioavailable petroleum hydrocarbons (BPH) corresponding to a threshold total body residue in an aquatic organism. Acute toxicity is predicted once the BPH critical is exceeded.

Based on the tests cited in Table 8 for WAF exposures, the range of EL_{50} values (expressed as loading rates) was 0.51 – 210 mg/L. The study by Clark et al. (2003) only reported the concentration boundaries within which the EC_{50} was expected to fall. The two OWD studies gave EL_{50} values within the range for the WAF studies. Therefore, gas oil streams and blended fuels such as No. 2 fuel oil or diesel, the range of toxicity values used for read across to other fuels of this type is 0.51 – 210 mg/L expressed as the loading rate.

Conclusion: The acute toxicity (EL_{50}) of gas oil category substances to invertebrates is expected to fall within the range 0.51 to 210 mg/L based on WAF studies and expressed as the loading rate.

5.1.1.3 Toxicity to Aquatic Plants

The results of the studies described in detail in the robust summaries for the hazard of gas oils to aquatic plants are provided in the following table.

Table 9. Toxicity Values for Gas Oils to Aquatic Plants.

Test Substance	Test Species and Type (WAF or OWD)	Toxicity Endpoint	Endpoint Value, mg/L	Reference
CAS No. 64741-59-9, light catalytic	*Pseudokirchneriella subcapitata*	72-h E_bL_{50} 72-h E_rL_{50}	0.28 0.53	Key Study EMBSI, 2011e

cracked gas oil	WAF	72-h NOELR 72-h E_bC_{50}[1] 72-h E_rC_{50}[1] 72-h NOEC[1] 96-h E_bL_{50} 96-h E_rL_{50} 96-h NOELR 96-h E_bC_{50}[1] 96-h E_rC_{50}[1] 96-h NOEC[1]	0.10 0.22 0.49 0.07 0.31 0.80 0.10 0.25 0.70 0.07	
		EL_{50}	0.20 (PETROTOX model)	Swigert et al. 2011
CAS No. 64741-77-1, light hydrocracked gas oil	*Pseudokirchneriella subcapitata* WAF	72-h EbL_{50} 72-h ErL_{50} 72-h NOELR 72-h EbC_{50}[1] 72-h ErC_{50}[1] 72-h NOEC[1] 96-h EbL_{50} 96-h ErL_{50} 96-h NOELR 96-h EbC_{50}[1] 96-h ErC_{50}[1] 96-h NOEC[1]	2.57 4.64 <0.10 0.44 0.75 <0.03 3.03 5.29 0.10 0.51 0.85 0.03	Key Study EMBSI, 2011f
		EL_{50}	0.91 (PETROTOX model)	Swigert et al. 2011
CAS No. 68334-30-5, diesel oil	*Raphidocelis subcapitata* *(Selenastrum capricornutum)* WAF	E_bL_{50} E_rL_{50} NOELR	10 22 3	Shell, 1995e
CAS No. 68334-30-5, diesel oil	*Raphidocelis subcapitata* *(Selenastrum capricornutum)* WAF	E_bL_{50} E_rL_{50} NOELR	25 78 3	Shell, 1995f
CAS No. 68334-30-5, diesel oil	*Selenastrum capricornutum* WAF	E_bL_{50} E_rL_{50} NOELR	≥10, ≤22 ≥22, ≤46 <1	Clark et al., 2003

CAS No. 68476-30-2, No. 2 fuel oil	*Selenastrum capricornutum* WAF	E_bL_{50} E_rL_{50} BPH critical[2]	1.9 2.9 63 nmol/mg C	EBSI, 1998e
CAS No. 68476-30-2, No. 2 fuel oil	*Skeletonema costatum* WAF	E_bL_{50} E_rL_{50}	5.8 2.2	EBSI, 1998f

[1] Results expressed as EC and NOEC values represent the concentration of hydrocarbons that solubilized from the test substance into each WAF at its respective loading rate. The distribution and percentage of the test substance components measured in the WAFs differed from the parent substance owing to the differing solubilities of the individual hydrocarbons. The individual hydrocarbons which were solubilized in the WAFs were not identified nor separately quantified, due to the complex nature of the test substances

[2] The BPH critical represents an estimate of the bioavailable petroleum hydrocarbons (BPH) corresponding to a threshold total body residue in an aquatic organism. Acute toxicity is predicted once the BPH critical is exceeded.

For the data in Table 9, endpoints based on algal biomass (E_bL_{50}) ranged from 0.28 – 25 mg/L. The range for the endpoints based on growth rate was somewhat wider, with values of 0.53 to 78 mg/L, expressed as loading rates. For gas oils, the range of toxicity values used for read across to other fuels and streams of this type is 0.28 – 78 mg/L, expressed as the loading rate and based on algal biomass.

Conclusion: The toxicity (EL_{50}) of gas oil category substances to algae, when based on algal biomass, is expected to fall within the approximate range of 0.28 - 25mg/L when expressed as loading rate. When based on algal growth rate, E_rL_{50} values are anticipated to fall within the range 0.53 to 78 mg/L.

5.1.2 Aquatic Endpoints – Chronic Toxicity

5.1.2.1 Chronic Toxicity to Aquatic Vertebrates

The chronic toxicity of a fuel oil No. 2 to rainbow trout (*O. mykiss*) was measured following the OECD 215 guideline (OECD, 2000b). Survival and growth of juvenile trout were measured during a 28-day exposure to WAF preparations of the test substance. The results of this test are shown in the following table.

Table 10. Chronic Toxicity of Gas Oils to Rainbow Trout.

Test Substance	Test Species and Type (WAF or OWD)	Toxicity Endpoint	Endpoint Value, mg/L	Reference
CAS No. 68476-30-2, No. 2 fuel oil	*O. mykiss* WAF	28-d LL_{50} $LOELR_{(growth)}$ $NOELR_{(growth)}$	2.7 3.0 1.2	EMBSI, 2004a
			Endpoint Value (µM/mL PDMS)	
		28-d LC_{50} $LOEC_{(growth)}$ $NOEC_{(growth)}$	24.4 26.4 13.7	

In this study, reduced survival and growth rate were seen at the highest loading rate WAF used in the test (3.0 mg/L). Based on the WAF loading rates used in the test, a 28-d LL_{50} for survival was 2.7 mg/L, with corresponding LOELR and NOELR values of 3.0 and 1.2 mg/L, respectively. Analysis of the exposure solutions involved extraction of the bioavailable petroleum hydrocarbons (BPH) onto solid phase micro-extraction fibers (SPME) that were coated with polydimethylsiloxane (PDMS). Analytical detection of the extracted BPH was by GC/FID. Reporting of the total BPH was in units of µM of hydrocarbons (as 2,3-dimethylnaphthalene)/mL of PDMS.

Conclusion: The no-observed-effect loading rate for chronic toxicity of gas oils to fish is expected to be approximately 1.2 mg/L.

5.1.2.2 Chronic Toxicity to Aquatic Invertebrates

New test data for the chronic toxicity to Daphnia magna for a light catalytic cracked gas oil (CAS 64741-59-9) and a light hydrocracked gas oil (CAS 64741-77-1) are presented in Table 9 together with existing data for fuel oil No. 2. All test procedures followed the OECD 211 guideline (OECD, 1998). Survival and reproduction of daphnids were measured during 21-day exposures to WAF preparations of each test substance. The results of these tests are shown in the following table.

Table 11. Chronic Toxicity of Gas Oils to Aquatic Invertebrates.

Test Substance	Test Species and Type (WAF or OWD)	Toxicity Endpoint	Endpoint Value, mg/L	Reference
CAS No. 64741-59-9, light catalytic cracked gas oil	*D. magna* WAF	21-d EL_{50} $LOELR_{(reproduction)}$ $NOELR_{(reproduction)}$ 21-d EC_{50}[1] $LOEC_{(reproduction)}$[1] $NOEC_{(reproduction)}$[1]	0.24 0.10 0.05 0.18 0.075 0.038	Key Study EMBSI, 2012a
		NOELR	0.06 (PETROTOX model)	Swigert et al. 2011
CAS No. 64741-77-1, light hydrocracked gas oil	*D. magna* WAF	21-d EL_{50} $LOELR_{(reproduction)}$ $NOELR_{(reproduction)}$ 21-d EC_{50}[1] $LOEC_{(reproduction)}$[1] $NOEC_{(reproduction)}$[1]	-- >0.64 0.64 -- >0.13 0.13	Key Study EMBSI, 2012b
		NOELR	0.14 (PETROTOX model)	Swigert et al. 2011
CAS No. 68476-30-2, No. 2 fuel oil	*D. magna* WAF	21-d EL_{50} $LOELR_{(reproduction)}$	>0.5 mg/L 0.5	EMBSI, 2004b

		$NOELR_{(reproduction)}$	0.15	
			Endpoint Value (µM/mL PDMS)	
		21-d EC_{50} $LOELR_{(reproduction)}$ $NOELR_{(reproduction)}$	>7.24 7.24 3.09	
[1] Results expressed as LC, NOEC, and LOEC values represent the concentration of hydrocarbons that solubilized from the test substance into each WAF at its respective loading rate. The distribution and percentage of the test substance components measured in the WAFs differed from the parent substance owing to the differing solubilities of the individual hydrocarbons. The individual hydrocarbons which were solubilized in the WAFs were not identified nor separately quantified, due to the complex nature of the test substances				

For the light catalytic cracked gas oil test the 21-d reproductive EL_{50} was 0.24 mg/L loading. The NOELR for the test was 0.05 mg/L. These values represent new lowest endpoint levels for chronic toxicity in *D. magna* for this category. The new study with light hydrocracked gas oil did not discern any adverse effects at the highest loading rate of 0.64 mg/L. The NOELR for this test was 0.64 mg/L and any effects on survival and reproduction were considered to be >0.64 mg/L. A sample of no. 2 fuel oil was evaluated by EMBSI (2004b) following the same OECD 211 protocol as for the two gas oil streams. In that study, a statistically significant reduction in reproduction was seen at the highest loading rate WAF used in the test (0.5 mg/L), but the reduction was not sufficient to calculate an EL_{50}. Based on the WAF loading rates used in the test, a 21-d LL_{50} for survival and reproduction was >0.5 mg/L, with corresponding LOELR and NOELR values of 0.5 and 0.15 mg/L, respectively. Analysis of the exposure solutions involved extraction of the bioavailable petroleum hydrocarbons (BPH) onto solid phase micro-extraction fibers (SPME) that were coated with polydimethylsiloxane (PDMS). Analytical detection of the extracted BPH was by GC/FID. Reporting of the total BPH were in units of µM of hydrocarbons (as 2,3-dimethylnaphthalene)/mL of PDMS.

Conclusion: The no-observed-effect loading rate for chronic toxicity of gas oils to aquatic invertebrates is expected to be approximately 0.05 mg/L.

5.2 Assessment Summary for Environmental Effects

Multiple ecotoxicological studies on heating and transportation fuels (e.g., No. 2 fuel oil and diesel fuel) were reviewed and new testing of two gas oil streams having a high proportion of aromatic or saturated hydrocarbon content were conducted. Estimated lethal of effect loading toxicity endpoints (LL/EL_{50}s) using the PETROTOX model and detailed 2D-GC-MS hydrocarbon analyses of the two gas oil streams were also calculated. When all LL/EL_{50} experimental data were combined with the modeled endpoints, the acute LL/EL_{50} toxicity values for the three trophic levels ranged from 0.18 mg/L to 125 mg/L for fish, 0.35 mg/L to 210 mg/L for invertebrates, and 0.20 mg/L to 78 mg/L for algae. The light catalytic cracked gas oil (high aromatic stream) was the most acutely toxic to all three trophic levels among the category members.

The chronic effects assessment included a fish growth test with no. 2 fuel oil and *D. magna* reproduction studies of light catalytic cracked gas oil and light hydrocracked gas oil. The LOELR based on reduction in fish growth was 3.0 mg/L while the NOELR was 1.2 mg/L. For invertebrates, reduced reproduction in *D. magna* was observed at the LOELR of 0.10 mg/L. The NOELR was 0.05 mg/L. The NOELR based on the PETROTOX model was 0.06 mg/L for the catalytic cracked gas oil. The NOELR value of 0.05 mg/L for the light catalytic cracked gas oil sample was the

lowest among the chronic effect endpoints and may be used as the chronic NOELR for the category.

6.0 HUMAN HEALTH ENDPOINTS

Reviews of the potential toxicological hazards of this category of fuels have been published by several organizations (ATSDR, 1995, CONCAWE, 1991, 1996, 2001; IARC, 1988; IPCS, 1996). Because fuel oils and transportation fuels of the same grade (e.g. No. 2 home heating oil and No. 2 diesel fuel) are virtually indistinguishable on the basis of their gross physical and chemical properties (IARC, 1988), data generated on either material can be used to characterize the toxicity of both materials. In preparing this document, the approach has been to review the available toxicology studies and in the text, provide summaries of studies by CAS numbers [CAS RN] to each SIDS Level 1 endpoint. Robust summaries contain extensive detail for each study and are provided in a separate document.

This final Category Assessment Document addresses the health effects endpoints by:

- Evaluating the toxicology database for the gas oil related refinery streams and products,
- Using read-across information whenever possible among category members, and other API HPV categories
- Use of an *In vitro* genetic toxicity: model to determine whether or not an tested sample is likely to be a bacterial mutagen based on analytic PAC profile.[see Appendix E]
- Modeled prediction of 10% change in sensitive effects of untested streams [PDR10] based on PAC analytical profile for repeated dose and developmental toxicity are included in Appendix D but has limited utility for this category of compounds.

6.1 Human Health Effects

6.1.1 Acute Toxicity

6.1.1.1 Oral

Table 12. Acute Oral Toxicity

CAS RN/ID/ Composition	LD_{50} value	Species	Observations	Reference
64741-59-9 Light Catalytic Cracked Distillate				
API 83-07 72.4% aromatics 24.3% saturates 3.7% 0lefins	4.7g/kg males 3.2g/kg females	Rat	Hypoactivity, diarrhea, yellow-stained urogenital/abdominal area, hair loss on anal region/abdomen/hind legs, ataxia, red-stained nose and mouth, prostration, lacrimation, catalepsy, dyspnea, possible respiratory congestion, hypothermic to touch, inflamed anal region and death.	API 1982a
API 83-08 60.8% aromatics 31.4% saturates 7.8% 0lefins	7.2g/kg/males 6.8g/kg females	Rat		API 1985d
64741-44-2 Straight run Middle Distillate				
API 83-11 21.2% aromatics	>5.0g/kg	Rat	Hypoactivity, ataxia, diarrhea, lacrimation, oily coat, yellow- or	API 1985e

78.8% saturates			urine-stained abdomen and hair loss on or around the anus, abdomen & hind legs. Animals gained weight in the study.	
64742-80-9 Hydrodesulfurized Middle Distillate				
API 81-09 20.6% aromatics 79.4% saturates	>5.0g/kg	Rat	Hypoactivity, ptosis, diarrhea, urine stained abdomen, oily fur	API 1982b
API 81-10 34.3% aromatics 65.6% saturates	>5.0g/kg	Rat		API 1982c
68476-34-6 Commercial Diesel fuel				
API 79-6 72.6% saturates	9.0ml/kg [95% CI 5.6-14.5]	Rat	No robust summary but clinical signs likely similar to API 83-11 above	API 1980d
68476-30-2 No. 2 fuel oil [Home heating oil[a]				
API 78-02 [83-02] Medium Catalytic cracked stock 30% 22.1% aromatics 73.4% saturates 22.1% 0lefins	19ml/kg [95% CI 16.8 – 21.5]	Rat	No robust summary but clinical signs likely similar to AP 83-11 above.	API 1980a
API 78-03 [83-01] Low Catalytic cracked stock 10% 17.9% aromatics 79.2% saturates 2.9% 0lefins	14.5ml/kg [95% CI 12.3 – 17.0]	Rat	No robust summary but clinical signs likely similar to API 83-11above.	API 1980b
API 78-04 [83-03] High Catalytic cracked stock 50% 26.1% aromatics 67.8% saturates 6.1% 0lefins	21.2ml/kg [95% CI 18.7 – 24.9]	Rat	No robust summary but clinical signs likely similar to API 83-11above.	API 1980c

a- Combination of Straight run Middle Distillate, CAS RN 64741-44-2 and Light Catalytic Cracked Distillate CAS RN 64741-59-9

6.1.1.2 Dermal

Table 13. Acute Dermal Toxicity

CAS RN /ID/Composition[a]	LD_{50} value	Species	Observations	Reference
64741-59-9 Light Catalytic Cracked Distillate				
API 83-07	>2.0g/kg	Rabbit		API 1982a
API 83-08	>2.0g/kg	Rabbit	Irritation from slight to severe for erythema,and edema, slight to moderate atonia, desquamation, coriaceousness, slight to marked for fissuring. Some subcutaneous hemorrhage and blanching	API 1985d
64741-44-2 Straight run Middle Distillate				
API 83-11	>2.0g/kg	Rabbit	Irritation slight to moderate for erythema, edema and atonia, desquamation and fissuring.	API 1985e

			Slight coriaceousness	
64742-80-9 Hydrodesulfurized Middle Distillate				
API 81-09	>2.0g/kg	Rabbit		API 1982b
API 81-10	>2.0g/kg	Rabbit		API 1982c
68476-34-6 Commercial Diesel Fuel				
API 79-6	>5.0ml/kg	Rabbit		API 1980d
68476-30-2 No. 2 fuel oil [Home heating oil[b]				
API 78-02 [83-02] Medium Catalytic cracked stock 30%	>5.0ml/kg	Rabbit		API 1980a
API 78-03 [83-01] Low Catalytic cracked stock 10%	>5.0ml/kg	Rabbit		API 1980b
API 78-04 [83-03] High Catalytic cracked stock 50%	>5.0ml/kg	Rabbit		API 1980c

a- Composition provided in Acute Oral Table 12

b- Combination of Straight run Middle Distillate, CAS RN 64741-44-2 and Light Catalytic Cracked Distillate CAS RN 64741-59-9

6.1.1.3 Inhalation

Table 14. Acute Inhalation

CAS RN/ID /Composition[a]	LC_{50} value	Species	Observations	Reference
64741-59-9 Light Catalytic Cracked Distillate				
API 83-07	5.4mg/L Combined sexes	Rat	Effects similar to API 83-08	API 1986a
API 83-08	4.7mg/L Combined sexes	Rat	Hair coat and some skin abnormalities in exposed animals, at higher exposure levels crust seen around the nose 2 to 4 days post exposure. Some decreased activity/mobility Dark red lungs in animals that died. Lung changes in surviving animals were mild and chronic included interstitial inflammation, focal alveolar histiocytosis and localized emphysema.	API 1986b
64741-44-2 Straight run Middle Distillate				
API 83-11	1.78mg/L combined sexes [95%CL 1.44 – 2.2]	Rat	Decreased activity, wet inguinal area, eyes partially closed, wet coat and oily coat. In the seven days following exposure there were signs of poor condition and respiratory distress. In the second week survivors were considered to be normal. Dark red lungs were observed in all animals that died within a day or two of exposure.	API 1987a
64742-80-9 Hydrodesulfurized Middle Distillate				

API 81-09	4.60 Combined sexes	Rat	-	API, 1983a
API 81-10	7.64 Combined sexes	Rat	-	API, 1983b

a- Composition provided in Acute Oral Table 12

6.1.1.4 Skin Irritation

Table 15. Skin Irritation: 24 hrs occluded

CAS RN/ID/ Composition[a]	Irritation Index PII	Species	Observations	Reference
64741-59-9 Light Catalytic Cracked Distillate				
API 83-07	5.6	Rabbit		API 1982a
API 83-08	6.9	Rabbit	Moderate to severe irritation Blanching in 2 rats at 24 hours, in six rats. at 72 hours. At 96 hours subcutaneous hemorrhaging within the test sites seen in all animals. No differences between abraded, intact skin.	API 1985d
CONCAWE MD-7 69.1% aromatics	-	Rabbit	Moderate to severe erythema in 2/3 rabbits at 60 min. Semi-occluded	Exxon 1996b
64741-44-2 Straight run Middle Distillate				
API 83-11	3.2	Rabbit	Slight to moderate irritation, no differences between abraded, intact skin	API 1985e
CONCAWE MD-6 73.7% saturates	-		Minimal transient irritation Semi-occluded	Exxon 1996b
64742-80-9 Hydrodesulfurized Middle Distillate				
API 81-09	4.3	Rabbit	Blanching, subcutaneous hemorrhage	API 1982b
API 81-10	5.9	Rabbit	Blanching, subcutaneous hemorrhage, severe fissuring, desquamation	API 1982b
68476-34-6 Commercial Diesel Fuel				
API 79-6	-	Rabbit	Extremely irritating	API 1980d
68476-30-2 No. 2 fuel oil [Home heating oil[b]				
API 78-02 [83-02] Medium Catalytic cracked stock 30%	3.37	Rabbit	Moderate irritation	API 1980a
API 78-03 [83-01] Low Catalytic cracked stock 10%	3.98	Rabbit	Moderate irritation	API 1980b
API 78-04 [83-03] High Catalytic cracked stock 50%	3.83	Rabbit	Moderate irritation	API 1980c

a- Composition provided in Acute Oral Table 12

b- Combination of Straight run Middle Distillate, CAS RN 64741-44-2 and Light Catalytic Cracked Distillate CAS RN 64741-59-9

Although skin irritation tended to be moderate to severe, these responses may be exaggerated since the 24 hour exposure period in these studies was significantly longer than the OECD 404 protocol recommended exposure period of 4 hours used for classification purposes.

6.1.1.5 Eye Irritation

Table 16. Eye Irritation: 24 hrs

CAS RN/ID/ Composition	Irritation Indices 24 hr	Species	Observations	Reference
64741-59-9 Light Catalytic Cracked Distillate				
API 83-07	1.7 unwashed; 2.0 washed	Rabbit		API 1982a
API 83-08	3.2 unwashed; 0.0 washed	Rabbit	No corneal irritation	API, 1985d
64741-44-2 Straight run Middle Distillate				
API 83-11	1.0 unwashed; 0.0 washed	Rabbit	No corneal or iridial irritation	API 1985e
64742-80-9 Hydrodesulfurized Middle Distillate				
API 81-09	2.0 unwashed; 0.0 washed	Rabbit		API 1982b
API 81-10	1.0 unwashed; 0.0 washed	Rabbit	Minimal irritation	API 1982c
68476-34-6 Commercial Diesel Fuel				
API 79-6	-	Rabbit	Non-irritating	API 1980d
68476-30-2 No. 2 fuel oil [Home heating oil[b]				
API 78-02 [83-02] Medium Catalytic cracked stock 30%	0.7 unwashed; 0.7 washed	Rabbit	Minimal irritation	API 1980a
API 78-03 [83-01] Low Catalytic cracked stock 10%	1.3 unwashed; 0.0 washed	Rabbit	Minimal irritation	API 1980b
API 78-04 [83-03] High Catalytic cracked stock 50%	0.33 unwashed; 0.0 washed	Rabbit	Non irritation	API 1980c

a- Composition provided in Acute Oral Table 12

b- Combination of Straight Run Middle Distillate, CAS RN 64741-44-2 and Light Catalytic Cracked Distillate CAS RN 64741-59-9

6.1.1.5 Sensitization

Table 17. Sensitization

CAS RN/ID/ Composition	Challenge Response	Species	Observations	Reference
64741-59-9 Light Catalytic Cracked Distillate				
API 83-07	-	Guinea Pig	Non-Sensitizing	API 1982a
API 83-08	0/10	Guinea Pig	Non-Sensitizing	API 1985d
64741-44-2 Straight run Middle Distillate				
API 83-11	0/10	Guinea Pig	Non-Sensitizing	AP! 1985d
64742-80-9 Hydrodesulfurized Middle Distillate				

API 81-09	0/10	Guinea Pig	Non-Sensitizing	API 1984b
API 81-10	-	Guinea Pig	Non-Sensitizing	API 1984c
68476-34-6 Commercial Diesel Fuel				
API 79-6		Guinea Pig	Non-Sensitizing	API 1980d
68476-30-2 No. 2 fuel oil [Home heating oil[b]				
API 78-02 [83-02] Medium Catalytic cracked stock 30%		Guinea Pig	Non-Sensitizing	API 1980a
API 78-03 [83-01] Low Catalytic cracked stock 10%		Guinea Pig	Non-Sensitizing	API 1980b
API 78-04 [83-03] High Catalytic cracked stock 50%		Guinea Pig	Non-Sensitizing	API 1980c

a- Composition provided in Acute Oral Table 12

b- Combination of Straight run Middle Distillate, CAS RN 64741-44-2 and Light Catalytic Cracked Distillate CAS RN 64741-59-9

Conclusions

Gas Oil streams and blended distillate fuels induce minimal acute toxicity by the oral, dermal and inhalation routes. Although skin irritation tended to be moderate to severe, these responses may be exaggerated since the 24 hour exposure period in these studies was significantly longer than the OECD 404 protocol recommended exposure period of 4 hours used for classification purposes. It is suggested that mild to moderate skin irritation is a more realistic assessment. No dermal sensitization was reported. Eye irritation was minimal to slight in unwashed eyes and minimal to unapparent in washed eyes. Existing data are sufficient to characterize acute toxicity for this category.

6.1.2 Repeated Dose Toxicity

Four dermal studies in rats of 13 week, four dermal studies of 4 week duration and two 4 week inhalation studies had been performed with samples in the Gas Oil category and are described below by CAS number [CAS RN]. Two additional recent studies have been conducted to provide additional toxicology information and to explore the association of aromatic content to toxicity by selecting samples approximating the extremes of aromatic content: an ultralow sulfur diesel fuel [CAS RN 68334-30-5] with a very low levels of aromatics of 3 or more rings, and a catalytically cracked light cycle oil [CAS RN 64741-59-9] containing higher levels of aromatics as measured by DMSO extraction (primarily C1-C3 ring PAC). Table 18 summarizes the results of rat dermal repeated dose toxicity studies. Dermal irritation occurred in all studies to varying degrees and though recognized as a possible factor in other expressions of toxic effect was not used alone as an endpoint in establishing LOAEL/NOAEL values. Treatment at very high doses was sometimes terminated due to severe dermal irritation. Repeat dose dermal studies in New Zealand white rabbits and inhalation studies in rats are provided as supplemental information.

13 week Rat Dermal Studies

CAS RN 64741-49-7

Vacuum Tower Overheads (Sample #86270, 8.80% DMSO extractable PAC)was applied undiluted to the shaved backs of Sprague-Dawley rats once daily, five days per week for 13 weeks, at doses of 0, 30, 125 or 500mg/kg/day (Mobil 1989a, Study #62326). Slight decreases in body weight gain [11%] were seen in males at 500mg/kg/day. Small decreases in hematology values and changes in serum chemistry were seen in both sexes at 500 and 125mg/kg day. Liver weight (relative and/or absolute) increased in both sexes at 500 and 125mg/kg. Thymus weight decreased and a mild reduction in thymocytes was observed at 500mg/kg in both sexes. No other effects were seen histologically. Reproductive organ weights and histological evaluations, spermatozoa and spermatid counts and morphology were comparable to untreated controls. Skin irritation was not reported. LOAEL = 125mgkg/day; NOAEL = 30mg/kg day.

CAS RN 64741-59-9

Light cycle oil (Sample #8281, 49.1% DMSO extractable PAC, 79.8% total aromatics) was applied undiluted to the shaved backs of Sprague Dawley rats once daily, five days per week for 13 weeks, at doses of 0, 8, 25,125, 500, or 1250mg/kg/day (Mobil 1985, Study #20535). After 2 weeks of exposure rats dosed at 1250mg/kg/day were terminated due to poor growth and appearance. At 500mg/kg male rats showed marked reduction in body weight and thymus size and weight accompanied by decreased lymphocytes in thymus, and slight decreases at 125mg/kg. Liver weights were increased in both sexes at 500mg/kg. In females, kidney, adrenal, ovary and liver weights (relative and/or absolute) were increased at 500mg/kg. No adverse effects were reported in weights or upon pathological evaluation of reproductive organs Dose related marked persistent skin irritation was seen including severe erythema and edema but was not used to define LOAEL/NOAEL values. LOAELs were 125mg/kg for males and 500mg/kg for females. NOAEL males = 25mg/kg and NOAEL females = 125mg/kg.

Light catalytic cracked oil (Sample # 010903, 32.5% DMSO extractable PAC, 80.9% total aromatics) was applied to the shaved backs of Sprague Dawley rats once daily, five days per week for 13 weeks, at doses of 0, 100, 450 or 750mg/kg/day (WIL 2012, Study #402024). Two control groups: one sham treated and one given the USP mineral oil vehicle were included in the study At the end of 6 hours, test sites were wiped to remove remaining test material. All animals wore Elizabethan collars to prevent oral exposure throughout the study. Two male rats, one each in 450 and 750mg/kg/day groups) died prior to scheduled termination. Body weight gains were reduced and by termination, body weights of males and females in the high dose group were significantly below control values. There were statistically significant reductions in red blood cell counts, hemoglobin content and hematocrit. When differences were found they were often statistically different in the 750 mg/kg/day groups and in some cases significant differences were also apparent at the 450 mg/kg/day treatment levels. The combination of lower RBC counts and lower HGB, HCT, MCV, and MCH values along with higher red cell and hemoglobin distribution width [RDW, HDW] in 450mg/kg males and males and females at 750mg/kg and higher reticulocyte counts in 750mg/kg males indicated the presence of a regenerative anemia. Reductions in eosinophil counts were significantly reduced in both male and female rats in the 450 and 750 mg/kg/day group {absolute and percentages]. At 100mg/kg absolute eosinophil count was statistically significantly reduced in males compared to vehicle controls but not in females. This decrease was not considered toxicologically significant as percentage values were not significantly different at this dose levels and other hematologic parameters showed effects only at 450mg/kg and above. Changes in serum chemistry parameters were small and within historical control values. Increases in adrenal and liver weights and relative weights were seen at 450 and 750mg/kg. No histological changes were seen to correlate with weight differences. No significant pathological changes were seen. With respect to the potential for reproductive effects, it should be noted that there were no changes in weights and no pathological changes in reproductive organs.

LOAEL = 450mg/kg in both sexes based on decreased body weight, increased adrenal and liver weights and hematologic changes NOAEL= 100mg/kg

CAS RN 64741-82-8

Coker light gas oil (Sample # 87213, 56.9% saturated hydrocarbons, 10.5% DMSO extractable PAC,) was applied undiluted to the shaved backs of Sprague Dawley rats once daily, five days per week for 13 weeks, at doses of 0, 30, 125, 500 or 2000mg/kg/day (Mobil 1991a, Study #61996). Animals in the 500 and 2000mg/kg/day were sacrificed in moribund conditions at week 9 and 2 respectively. Perineal staining and dose related skin irritation (generally severe) were seen in all dose groups. Body weights were decreased and changes in hematology and serum chemistry parameters were seen at 125mg/kg and above. Increases in lymphocytes were seen at 125 mg/kg in both sexes and at 30mg/kg in females. Differences in organ weights (absolute and/or relative) were observed at 125mg/kg and above and male thymus weight was decreased at 30mg/kg. Histologically skin irritation and slight effects on kidneys and bone marrow were reported. Bone marrow effects included severe reduction in erythropoietic cells and megakaryocytes at 2000mg/kg and structural changes in megakaryocytes at 2000, 500 and 125mg/kg. No adverse effects were reported in weights or upon pathological evaluation of reproductive organs LOAEL = 30mg/kg based on decreased thymus weight in males and increased lymphocytes in females. NOAEL was not determined, <30mg/kg.

CAS RN 68334-30-5

Ultralow sulfur diesel oil (Sample #120801 2.8% DMSO extractable PAC, 26.4% total aromatics), a blend of 7 diesel fuels, was applied to the shaved backs of Sprague Dawley rats once daily, five days per week for 13 weeks, at doses of 0, 100, 300 or 600mg/kg/day (WIL 2012, Study #402025). At the end of 6 hours, test sites were wiped to remove remaining test material. All animals wore Elizabethan collars throughout the study to prevent oral exposure. All rats survived to study termination. There were no treatment-related effects on body weight or weight gain and no adverse clinical signs. Slight dermal irritation which increased with dose was observed, primarily slight erythema, slight edema and desquamation even at the highest dose. No adverse effects were seen on hematology parameters. In serum chemistry parameters, the only statistically significant effect was an increased albumin/globulin ratio in high dose males which was above the vehicle control values but was not different when compared to untreated controls. There were no treatment related adverse macroscopic changes, no differences in organ weights and no pathological findings other than those associated with dermal application. With respect to the potential for reproductive effects, it should be noted that there were no changes in weights and no pathological changes in reproductive organs The NOAEL for both sexes = 600mg/kg [highest dose tested]

CAS RN 68915-97-9

Heavy atmospheric gas oil (Sample # 86271, 10.5% DMSO extractable PAC) was applied undiluted to the shaved backs of Sprague Dawley rats once daily, five days per week for 13 weeks, at doses of 0, 30, 125, 500 or 2000mg/kg/day (Mobil 1992, Study #63456). At the end of the study the epididymides and testes from the male rats in the control and 500 mg/kg/day groups were given an in-depth histopathology examination, including spermatid (testes) and spermatozoa (epididymides) counts. In general, application of the test material produced only “slight” skin irritation. One of ten high dose males was sacrificed *in extremis*. There were treatment-related changes in a number of serum chemistry and hematological parameters in the rats in the mid- and high dose groups. At necropsy, treatment-related macroscopic findings in both sexes included

increased liver size, decreased thymus size, thickening of the limiting ridge between the non-glandular and glandular sections of the stomach and enlarged and reddened lymph nodes. Organ weight (absolute and relative) differences were seen in the 125 and 500 mg/kg/day groups. Histologically, treatment related changes in the 500mg/kg group included a severe reduction in hematopoiesis in the bone marrow; liver hypertrophy and connective tissue formation; increased areas of hematopoiesis, focal necrosis and individual cell death in the liver; and a reduction in the numbers of lymphocytes in the thymus glands. There were no treatment-related effects on any of the epididymal sperm or testicular spermatid parameters. No adverse effects were reported in weights or upon pathological evaluation of reproductive organs. The investigators concluded the LOAEL was 125 mg/kg/day and the NOAEL was 30mg/kg/day.

4 week Rat Dermal Studies

CAS RN 64741-43-1

F-130, a gas oil intermediate was applied to the shaved backs of Sprague-Dawley rats once daily, five days per week for four weeks, at a dose of 0, 0.01, 0.10 or 0.50 ml/kg/day (9.2, 92, 460 mg/kg/day) (ARCO, 1992b ATX-90-0050). Slight skin irritation was observed at 460mg/kg/day and was very slight at 92mg/kg/day. No adverse effects were observed in terminal body weights, hematology or serum chemistry parameters or organ weights. Histological evaluation indicated treated animals were comparable to controls and reproductive organs were normal. The NOAEL for both sexes excluding slight skin irritation was 460mg/kg the highest dose tested, LOAEL >460mg/kg

CAS RN 64741-77-1

F-188, a light hydrocracked distillate was applied to the shaved backs of Sprague-Dawley rats once daily, five days per week for four weeks, at a dose of 0, 0.05, 0.25 or 1.0 ml/kg/day (41, 205, 820 mg/kg/day) (ARCO, 1992a ATX-91-0094). No adverse effects seen on terminal body weight, organ weights or hematology parameters. Slight changes in globulin level at highest dose in males and A/G ratio in both sexes were not compound related or biologically relevant by study investigators. No abnormal histopathology was seen; reproductive organs were comparable to untreated controls. Skin irritation [very slight to moderate] was observed in all treated animals in a dose related manner but was not used in setting LOAEL/NOAEL;
NOAEL for both sexes = 820mg/kg LOAEL > 820mg/kg [highest dose tested]

CAS RN 64741-86-2

F-233 a sweetened middle distillate [DHHS Stove Oil] was applied to the shaved backs of Sprague-Dawley rats once daily, five days per week for four weeks, at a dose of 0, 0.05, 0.5 or 1.0 ml/kg/day (41, 410, 820 mg/kg/day) (ARCO, 1993a ATX-91-0233). Effects seen at 820mg/kg in both sexes included decreased terminal body weight (9%), increased adrenal weight relative to brain weight and decreased kidney weight relative to brain weight and varying changes in serum chemistry. Absolute liver weight and weight relative to brain weight was decreased in males. Absolute ovary weight and weight relative to brain weight was decreased at 820mg/kg but no abnormalities were seen in ovaries or testes histologically. Skin irritation was slight to moderate increasing in a dose-related manner and was not used in setting LOAEL/NOAEL. Histologically the only changes were hyperplasia of the axillary lymph nodes in both sexes at 820mg/kg/day considered secondary to dermal irritation and inflammation. LOAEL = 820mg/kg/day and NOAEL = 410mg/kg/day.

CAS RN 68476-31-3

F-75-01 Diesel Fuel #2 (60.41% saturate, 39.6% aromatic hydrocarbons) was applied daily, 5days/week for four weeks, to the skin of male and female Sprague-Dawley rats (10/sex/group) at dose levels of 0.5, 2.0 and 5.0 ml/kg day (ARCO, 1986). There were no deaths or any other treatment-related effects observed during the study, with the exception of an effect on body weights and skin irritation. After the second week of the study, the body weights of the mid- and high dose males were less than those of the controls, with the difference persisting throughout the study. At the end of the study the weight gains of the mid and high dose males were 43% and 13% respectively of those of the controls. Skin irritation occurred at all dose levels, ranging from moderate (low dose) to severe (mid and high dose). LOAEL [excluding skin irritation] = 2 ml/kg; NOAEL [excluding skin irritation] = 0.5ml/kg.

4-week Rat Inhalation Studies

Two samples of a hydrosulfurized middle distillate (CAS RN 64742-80-9, API 81-09 79.4% saturated hydrocarbons) and API 81-10, 65.6% saturated hydrocarbons) were administered at nominal concentration of 25mg/m^3, 6 hours/day, 5 days a week for 4 weeks (API, 1986f). No systemic effects were observed except for increased leukocyte counts in rats exposed to API 81-10 and subacute inflammation of the respiratory mucosa lining in animals exposed to API 81-09.

Supplemental data: Repeat dose dermal studies in New Zealand White rabbits.

A light catalytic cracked distillate (CAS RN 64741-59-9, API 83-07, 72.4% aromatic hydrocarbons) was applied undiluted to the shaved skin of rabbits (5/sex/group), at concentrations of 0, 250, 500 or 1000mg/kg, 3 times/week for 4 weeks (API, 1982a). No systemic effects were observed. Treatment related skin irritation ranging up to severe was seen and histologic examination of tissue from high dose animals identified moderate to severe proliferation and inflammatory changes in skin associated with increased granulopoiesis of bone marrow attributed to stress of severe skin irritation.

A diesel fuel was applied to the skin of New Zealand white rabbits 5 days/week for 3 weeks at dose levels of 0.2, 0.67 and 2.0 g/kg /day (IITRI, 1984). Severe skin irritation was seen in all the dosed groups. One of ten males and two of the ten females in the highest dose group died prematurely. A number of compound-related effects were seen.

One, 3 & 10 ml/kg/day of a No. 2 home heating oil (67.8% saturated hydrocarbons) was applied undiluted to the skin of male and female New Zealand white rabbits (API, 1980c). The test material was applied daily for 5 days, the animals were given a two day dose-free rest and then the test material was applied daily for an additional 5 days. Severe skin irritation was seen at all dose levels. Two of eight and 7/8 animals died prematurely in the 3 and 10 ml/kg/day groups, respectively. The only significant histological findings were those associated with the severe skin lesions.

Two additional samples of No. 2 home heating oils (containing 79.2% and 73.4% saturated hydrocarbons) have been tested for repeat-dose toxicity (API, 1980a, b). In these studies, material was applied to the skin of rabbits for two weeks. Doses in the first study were 2.5, 4 and 10 ml/kg/day, while those in the second study 1, 2.5 and 10 ml/kg/day. Both materials produced severe skin irritation at all dose levels. In the first study, 8/8 animals receiving 10/kg/day died prematurely. In the second study, 1/8 and 6/8 animals died prematurely in the 2.5 and 10 ml/kg/day groups, respectively.

The market-place sample of diesel fuel that was summarized in the acute toxicity section was also tested in a two week repeat-dose study (API, 1980d). Applied to the skin of rabbits for two weeks at dose levels of 4 and 8 ml/kg /day, the material produced a 67% mortality rate in the 8 ml/kg/day group.

Conclusions

Among the 13 week rat dermal studies, Vacuum tower overheads [CAS RN 64741-49-7] and Heavy atmospheric gas oils [CAS RN 68915-97-9] had LOAEL = 125mg/kg and NOAEL = 30mg/kg. Both had higher levels of aromatic constituents with 3 or more rings. A light coker gas oil [CAS RN 64741-82-8, C2-C3 PAC distribution 10.5%] had a LOAEL = 30mg/kg the lowest dose tested, effects likely exacerbated by severe skin irritation at all dose levels. Feuston et al, 1994 reported that skin irritation and C2-aromatics are associated. Two samples of catalytically cracked oils [CAS RN 64741-59-9] had lowest observed effect levels of 125mg/kg males and 500mg/kg females for light cycle oil (LCO sample #8281) and 450mg/kg both sexes for light catalytically cracked oil (LCCO sample # 010903), differences related to apparent greater sensitivity to LCO in males and compositional variations within the same CAS RN. These samples had the highest overall aromatic distributions of the tested substances, fairly evenly distributed between C2 and C3 ring constituent. Effects when present were seen in organ weights, primarily liver and thymus with no histopathologic correlates and hematology parameters. Ultralow sulfur diesel fuel [CAS RN 68334-30-5] which contained the lowest distribution of total DMSO extractable aromatics mostly alkylated 1-ring and some 2 ring, and induced very few systemic effects with a NOAEL = 600mg/kg the highest dose tested.

These results suggest that the concentrations and ring distributions of aromatic constituents is associated with the degree of systemic toxicity and where the DMSO extractable content (i.e., aromatics with 2 or more rings) is very low as is the case with ULSD, no systemic toxicity is seen.

Table 18. Comparison of 13 week repeat dermal study results with 1-7 ring PAC content

CAS RN/Name	Sample #	LOAEL	NOAEL	% PAC[a]
68915-97-9 Heavy Atmospheric. gas oil	086271	125	30	0.9% C1-C2 9.2% C3-C7
64741-49-7/ Vacuum Tower overheads	086270	125	30	2.5% C2; 5.2% C3-C7
64741-59-9/ Lt cycle oil	08281	M 125 F 500	M 25 F 125	2.0% C1 30% C2 14% C3
64741-59-9/ Lt cat cracked oil	010913	450	100	17.1% C1-C2 4.6% C3
64741-82-8/ Lt coker gas oil	087213	30	none	4.2% C2 6.3% C3
68334-30-5/ Ultralow Sulfur diesel	120801	none	600	2.3% C1-C2 0.6% C3

a PAC distributions summarized from Appendix Table D-1

The 4 week duration rat dermal studies showed slight to moderate skin irritation for gas oil streams and slight to severe in one study with diesel fuel #2. but minimal systemic toxicity. No significant adverse effects were seen in reproductive organs in any rat dermal study.

The two 4 week inhalation studies with samples of hydrodesulfurized distillates at a single dose of 25mg/m^3 resulted in minimal systemic effects and some inflammation of respiratory tissue. Supplemental studies of rabbit dermal exposure focused on irritation and mortality, more severe for samples with high saturated hydrocarbon content are provided for general information.

Table 19. Gas Oils Dermal Repeat Dose Studies in Rats [28 day and 13 week exposures]

CAS RN/ID	Study: Species/ Route/Duration	Dose/ Frequency	Results	References
64741-43-1 Gas Oil Intermediate (C11-25) straight run				
Gas Oil Intermediate F-130 [64741-43-1]	Rats (10/sex/group) dermal, 4 weeks	0, 9.2, 92, 460mg/kg/d (0, 0.01, 0.10, 0.50ml/kg/d) 5 days/week; 6 hr/day occluded	NOAEL = 460 mg/kg [highest dose] LOAEL > 460mg/kg No systemic effects. No adverse effects on reproductive organs Slight skin irritation at highest dose	ARCO, 1992b ATX-90-0050
64741-49-7 Vacuum Tower Condensate (C11-25)				
Vacuum Tower Overheads Sample # 86270 [64741-49-7]	Rats (10/sex/group) dermal, 13 weeks	0, 30, 125, 500mg/kg/d, 5 days/week Elizabethan collars, weekly wipe off	LOAEL=125mg/kg Based on decreased hematology, changes in serum chemistry parameters, liver weight increases, thymus weight decreases and reduced thymocytes at 500mg/kg. No adverse effects on reproductive organs or spermatozoa, spermatids. NOAEL = 30 mg/kg	Mobil 1989a Study 62326
64741-59-9 Catalytic cracked Distillate Light (C9-C25)				
Light Catalytic Cracked oil Sample # 010903 [64741-59-9]	Rats (10/sex/group) dermal, 13 weeks	0, 100, 450, 750mg/kg/day 5 days/week Elizabethan collars, weekly wipe off	LOAEL = 450mg/kg/; NOAEL = 100mg/kg/day Based on reduced body weight, increased adrenal and liver weighs, changes in hemtology parameters No adverse histologic effects on reproductive or other organs. Slight erythema in treated groups and vehicle controls.	WIL 2012 Study #402024
Light cycle oil Sample #8281 [64741-59-9]	Rats (10/sex/group) dermal, 13 weeks	0, 8, 25, 125, 500, 1250mg/kg/d 1250mg/kg terminated after 2 weeks 5 days/week Elizabethan collars, weekly wipe off	LOAEL male = 125mg/kg; NOAEL =25mg/kg Based on reduced body weight, thymus, testes, adrenal weights, decreased thymocytes, increased liver weights LOAEL females = 500mg/kg; NOAEL = 125mg/kg. Based on increased organ weights – ovary, liver, adrenal, kidney. No adverse histologic effects on reproductive organs. Dose related skin irritation	Mobil 1985 Study 20535

CAS RN/ID	Study: Species/ Route/Duration	Dose/ Frequency	Results	References
64741-77-1 Hydrocracked Distillate light (C10-C18)				
Light Hydrocracked Distillate **F-188** [64741-77-1]	Rats (10/sex/group) dermal, 4 weeks	0, 41, 205,820mg/kg/d (0, 0.05, 0.25, 1.0ml/kg/d) 5 days/week; 6 hr/day occluded	NOAEL = 820mg/kg [highest dose] LOAEL >820mg/kg No systemic effects. No adverse effects on reproductive organs Slight –moderate dose related skin irritation	ARCO 1992a ATX-91-0094
64741-82-8 Thermocracked Distillate, Light (C10-18)				
Coker Light Gas Oil Sample #87213 [64741-82-8]	Rats (10/sex/group) dermal, 13 weeks	0, 30, 125, 500, 2000mg/kg/d 500, 2000mg/kg terminated at wk 9 and 2, respectively 5 days/week Elizabethan collars, weekly wipe off	LOAEL = 30mg/kg Based on decreased body wt (males), changes in serum chemistry, hematology, organ weights, increased lymphocytes in females and decreased thymus wt in males at 30mg/kg, Severe skin irritation, bone marrow effects. NOAEL undetermined, <30mg/kg	Mobil 1991a Study 61996
64741-86-2 Sweetened Distillate (C9-20)				
DHHS Stove Oil F-233 Sample 094629 [64741-86-2]	Rats (10/sex/group) dermal, 4 weeks	0, 41, 410, 820mg/kg/d (0, 0.05, 0.5, 1.0ml/kg/d) 5 days/week; 6 hr/day occluded	LOAEL = 820mg/kg Based on decreased terminal body weight, changes in serum chemistry values, changes in liver, adrenal, kidney and ovary weight not reflected histologically. Dose related slight to moderate skin irritation NOAEL = 410mg/kg	ARCO 1993a ATX-91-0233
68334-30-5 Ultralow Sulfur Diesel				
Ultralow sulfur diesel Sample # 120801 [68334-30-5]	Rats (10/sex/group) dermal, 13 weeks	0, 100, 300, 600mg/kg/day 5 days/week Elizabethan collars, weekly wipe off	NOAEL = 600mg/kg [highest dose tested] No adverse effects on clinical signs, body weight or weigh gain, serum chemistry, organ weights or histopathology. Increased A/G ratio in high dose males not toxicologically significant. Dermal irritation seen as slight erythema, edema and desquamation even at highest dose.	WIL 2012 Study # 40205
68476-31-3 Diesel Fuel #2				
F-75-01 [68476-31-3]	Rats (10/sex/group) dermal, 4 weeks	0, 05, 2.0, 5.0ml/kg 5 days/week	LOAEL [excluding skin irritation] = 2 ml/kg Based on decreased body weight in 2 and 5ml/kg groups. No systemic effects with the exception of	ARCO, 1986

CAS RN/ID	Study: Species/ Route/Duration	Dose/ Frequency	Results	References
			skin irritation increasing from moderate to severe at all doses NOAEL [excluding skin irritation] = 0.5 ml/kg	
68915-97-9 Gas Oil Heavy				
Heavy Atmospheric Gas Oil Sample #86271 [68915-97-9]	Rats (M/F) dermal, 13 weeks	0, 30, 125, 500 mg/kg/d, 5 days/week Elizabethan collars, weekly wipe off	LOAEL = 125 mg/kg Based on serum chemistry, hematology & organ wt changes; Histopathology effects at 500mg/kg in bone marrow, liver, thymus. No adverse effects on epididymal or testicular sperm or reproductive organs at any dose level. Slight skin irritation NOAEL = 30mg/kg	Mobil, 1992 Study #63456

NOAEL and LOAEL were provided by study investigators and appear in robust summaries.
Gas Oil 13 weeks studies were used in developing the PAC Modeling program [see Appendix D].

Modeled data and calculations of PDR10 are not applied to the Gas Oil category because fuels and streams in the Gas Oil Category are characterized by aliphatic constituents and alkylated 1 and 2 ring compounds with small percentages of 3 ring and virtually no 4-ring aromatics. The modeling method described in Appendix D is based on a DMSO extraction procedure (Table D-1) that is most useful for higher molecular weight aromatics and somewhat underestimates lower molecular weight aromatic fractions. The preponderance of low molecular weight C1 and C2 aromatics in most gas oils limits the utility of the modeling procedure in its present form for this category of petroleum compounds. However, the modeled data is included in Appendix D for completeness and variations from results of animal studies are discussed.

6.1.3 Genetic Toxicity *In Vitro*

Table 20. Summary of *In Vitro* Genetic Toxicity Studies

CAS RN/Sample	Assay	Results	Reference
64741-59-9 Catalytic Cracked Distillate, light			
API 83-07 [72.4% aromatic HC]	Mouse Lymphoma	Positive with activation	API, 1985i
	Sister Chromatid Exchange [CHO cells]	Equivocal with and without activation	API, 1988b
API 83-08 [60.8%aromatic HC]	Mouse Lymphoma	Positive with and without activation	API, 1985f
64741-49-7 Vacuum Tower Overheads			
Vacuum Tower Overheads	Chinese Hamster Ovary cells [CHO]	Not clastogenic	Mobil Study 52242
64742-80-9 Hydrodesulfurized Middle distillate			
API 81-09 [79.4% saturated HC]	Mouse Lymphoma	Positive without activation Equivocal with activation	API, 1985h
API 81-10 [65.6% saturated HC]	Mouse Lymphoma 3 trials	Positive with and without activation	API, 1984a, 1986d, 1987e
API 81-10 aromatic fraction	Mouse Lymphoma	Negative	API, 1987b
API 81-10 saturate fraction	Mouse Lymphoma	Negative	API, 1987c
API 81-10	Sister Chromatid Exchange [CHO cells]	Negative without activation Equivocal with activation	API, 1988c
DGMK Middle Distillate Samples			
3 samples [52.4 to 59.8% aromatic HC]	Optimized Ames [a]	Positive with activation MI 7.6 – 9.3	DMGK, 1991
11 samples [52.7 to 79.0% saturated HC]	Optimized Ames [a]	Inactive to positive with activation MI 0.7 – 4.0	DMGK, 1991
Diesel Fuel - 3 samples [59.4 to 76.6% saturated HC]	Optimized Ames [a]	Positive with activation MI 1.7 – 3.9	DMGK, 1991
Distillate Fuels			
68476-34-6 Diesel Fuel No. 2-D [76.1% saturated HC]	Standard Ames	Negative with and without activation	API, 1978
	Mouse Lymphoma	Negative with and without activation	API, 1978
68476-30-2 Home heating oil	Mouse Lymphoma	Positive with and without	API, 1979a

API 78-4 [67.8% saturated HC]		activation	

HC = hydrocarbons
a -Optimized Ames test (previously Modified Ames test) was developed to increase the sensitivity of the Ames *Salmonella* bacteria assay for PAC-rich petroleum streams.

In vitro genetic toxicity studies demonstrate that gas oil streams and distillate fuels induce gene mutation in bacterial and mammalian cells if they contain sufficient levels of the mutagenic polycyclic aromatic constituents. In addition to the standard Ames test (Ames et al, 1975), the Optimized Ames test (previously the Modified Ames test) was developed to enhance exposure of PAC-rich petroleum derived materials to PAC-sensitive *Salmonella* strain TA98. Modifications involved a single step extraction into DMSO, use of hamster liver homogenate, and increased cofactor to maximize metabolic activation. Positive results require a dose responsive increase in mutant colonies compared to negative controls and calculation of a Mutagenicity Index (MI) derived from the dose response curves [see Appendix D]. Table 21 summarizes the results of Optimized Ames tests on 53 samples. Samples selected for testing were those that, based on knowledge of product chemistry and experience with dermal carcinogenesis were considered likely to give a range of gene mutation activity based on PAC content and ring distribution profiles. These data along with data from 189 samples of other high PAC containing petroleum streams with final boiling point ≥ 650 ºF [≥343^{0}C] were used to develop a modeling procedure that employs the PAC analytical profile to predict statistically whether a sample is likely to induce gene mutation in *Salmonella* strain TA98 with metabolic activation. Using this model, the chemical characterization of untested streams compared to the known MI allows prediction of whether a sample will have a mutagenicity index equal to or greater than 1.0 (GE 1) or be non-mutagenic (LT 1) (Nicolich et al, 2010 abst Appendix D, McKee et al., 2011).

Table 21. Gas Oils: Optimized Ames Test Results and Modeled Mutagenicity Indices

CAS RN	CRU Number	1-Ring Weight %	2-Ring Weight %	3-Ring Weight %	4-Ring Weight %	5-Ring Weight %	6-Ring Weight %	7-Ring Weight %	Optimized Ames MI	Modeled MI
64741-44-2 Gas Oil, light										
64741-44-2	87523	0.4	2.5	1.3	0.0	0.0	0.0	0.0	1.0	GE 1
64741-49-7 Vacuum Tower Condensate										
64741-49-7	85242	0.2	1.8	2.4	0.6	0.4	0.1	0.1	5.2	GE 1
64741-49-7	86175	0.0	2.0	3.4	1.3	0.4	0.1	0.1	6.8	GE 1
64741-49-7	86178	0.0	0.8	4.0	1.6	0.8	0.3	0.2	10.6	GE 1
64741-49-7	86186	0.1	2.7	6.2	0.3	0.1	0.1	0.3	6.7	GE 1
64741-49-7	86270	0.9	2.6	3.5	0.9	0.4	0.0	0.4	6.7	GE 1
64741-49-7	86279	0.8	4.8	1.6	0.1	0.0	0.0	0.0	4.6	GE 1
64741-59-9 Catalytic Cracked Distillate, light										
64741-59-9	8281	2.0	29.5	14.7	0.0	0.5	0.5	0.0	28.3	GE 1
64741-59-9	86182	0.0	17.4	11.6	0.0	0.0	0.0	0.0	57.9	GE 1
64741-59-9	86191	0.0	13.2	8.8	0.0	0.0	0.0	0.0	25.1	GE 1
64741-59-9	86195	0.4	25.3	10.9	0.0	0.0	0.0	0.0	34.6	GE 1
64741-59-9	86273	0.4	10.9	5.4	0.2	0.0	0.2	0.0	19.8	GE 1
64741-59-9	86280	0.3	18.1	9.0	0.0	0.0	0.3	0.0	20.1	GE 1
64741-59-9	87524	2.0	16.8	8.4	0.0	0.0	0.0	0.0	13.8	GE 1

CAS RN	CRU Number	1-Ring Weight %	2-Ring Weight %	3-Ring Weight %	4-Ring Weight %	5-Ring Weight %	6-Ring Weight %	7-Ring Weight %	Optimized Ames MI	Modeled MI
64741-59-9	87526	1.1	9.6	6.4	0.2	0.0	0.0	0.0	7.9	GE 1
64741-59-9	87527	0.8	2.0	0.8	0.1	0.0	0.0	0.0	1.2	GE 1
64741-59-9	89295	0.4	42.2	0.0	0.0	0.0	0.0	0.0	0.0	LT 1
64741-59-9	89296	0.0	0.5	0.5	1.0	0.2	0.0	0.0	0.0	LT 1
64741-59-9	89297	0.2	15.2	0.0	0.0	0.0	0.0	0.0	0.0	LT 1
64741-82-8 Thermocracked Distillate, light										
64741-82-8	87213	0.1	4.2	6.3	0.3	0.0	0.0	0.0	13.3	GE 1
64741-86-2 Sweetened Distillate										
64741-86-2	87088	0.0	2.4	0.3	0.0	0.0	0.0	0.0	1.1	LT 1
64741-86-2	87467	0.0	2.3	0.6	0.0	0.0	0.0	0.0	0.0	LT 1
68334-30-5 Diesel Oil and DMGK Middle Distillates										
68334-30-5	85202	0.7	4.1	2.0	0.3	0.0	0.0	0.0	3.8	GE 1
68334-30-5	85203	0.7	4.2	2.1	0.1	0.0	0.0	0.0	3.9	GE 1
68476-30-2	89165	0.1	1.4	1.1	0.1	0.0	0.0	0.0	1.0	GE 1
68476-30-2	89166	0.0	3.2	0.8	0.0	0.0	0.0	0.0	1.2	GE 1
68476-30-2	89167	0.1	0.8	0.6	0.1	0.0	0.0	0.0	0.7	LT 1
68476-30-2	89169	0.0	1.7	2.1	0.1	0.0	0.0	0.0	4.1	GE 1
68476-30-2	89170	0.2	1.6	1.3	0.2	0.0	0.0	0.0	3.8	GE 1
68476-30-2	89175	0.1	4.5	5.7	1.1	0.0	0.0	0.0	9.0	GE 1
68476-30-2	89180	0.4	1.6	2.0	0.1	0.0	0.0	0.0	2.1	GE 1
68476-30-2	89181	0.3	1.3	0.8	0.0	0.0	0.0	0.0	2.8	GE 1
68476-30-2	89182	0.4	1.6	1.6	0.2	0.0	0.0	0.0	4.0	GE 1
68476-30-2	91673	0.3	9.6	4.8	0.0	0.2	0.5	1.0	12.6	GE 1
68476-30-2	92200	0.0	5.5	5.5	0.0	0.0	0.0	0.0	8.2	GE 1
DMGK	89164	0.0	1.1	0.7	0.1	0.0	0.0	0.0	0.8	LT 1
DMGK	89168	0.0	1.5	1.9	0.4	0.0	0.0	0.0	3.1	GE 1
DMGK	89171	0.2	3.3	0.9	0.0	0.0	0.0	0.0	1.4	GE 1
DMGK	89172	0.2	1.6	2.7	0.5	0.0	0.0	0.0	7.6	GE 1
DMGK	89173	0.4	2.1	2.1	0.5	0.0	0.0	0.0	8.4	GE 1
DMGK	89174	0.3	1.6	0.8	0.1	0.0	0.0	0.0	2.0	GE 1
DMGK	89176	0.4	2.4	2.4	0.6	0.0	0.0	0.0	6.5	GE 1
DMGK	89177	0.5	1.4	0.5	0.0	0.0	0.0	0.0	2.3	LT 1
DMGK	89178	0.4	2.6	1.3	0.2	0.0	0.0	0.0	2.7	GE 1
DMGK	89179	0.5	1.9	0.5	0.0	0.0	0.0	0.0	0.0	LT 1
DMGK	89183	0.8	2.5	4.2	1.7	0.1	0.0	0.0	9.3	GE 1
DMGK	89184	0.4	1.5	1.5	0.2	0.0	0.0	0.0	4.0	GE 1
DMGK	89185	0.1	0.7	0.1	0.0	0.0	0.0	0.0	0.7	LT 1
DMGK	89187	0.4	0.8	0.6	0.2	0.0	0.0	0.0	4.2	LT 1
68915-97-9 Gas Oil, heavy										
68915-97-9	86271	0.1	0.8	5.3	3.2	0.4	0.2	0.1	18.3	GE 1

CAS RN	CRU Number	1-Ring Weight %	2-Ring Weight %	3-Ring Weight %	4-Ring Weight %	5-Ring Weight %	6-Ring Weight %	7-Ring Weight %	Optimized Ames MI	Modeled MI
68915-97-9	86190	0.3	3.6	1.0	0.1	0.2	0.0	0.0	2.0	GE 1

GE 1 = modeled MI greater than or equal to 1; predicts that the sample is mutagenic
LT 1 = modeled MI less than 1; predicts that the sample is not mutagenic
DMGK designation identifies distillate fuel oil samples tested in Germany for which CAS RNs were not provided (DGMK, 1993; Jungen et al., 1995).

The results of the Optimized Ames assay confirm the likelihood that many Gas Oils can cause bacterial mutagenicity [MI ≥ 1.0]. The modeled MI determinations were generally in agreement with the test results. CAS RN 64741-59-9 catalytic cracked distillate samples which generally contain higher levels of aromatics with ≥ 3 rings induced higher mutagenicity indices than other CAS RNs. Samples with low levels of aromatics tend to be inactive in *Salmonella* mutagenicity assays or have very low MIs. Levels of activity within a given CAS RN may vary; samples with higher levels of aromatics are mutagenic while others with low aromatic content may be inactive as the result of different crude oil sources and the type and severity of processing.

6.1.4 Genetic Toxicity *In Vivo*

Table 22. Summary of In Vivo Genetic Toxicity Assays

CAS RN/ID	Assay/Species	Route/Dose	Results	Reference
64741-59-9 Catalytic Cracked Distillate, light				
API 83-07 [72.4% aromatic HC]	Chromosome Aberrations Rat [M.F.]	Intraperitoneal, single dose. 0, 0.3, 1.0, 3.0g/kg	Negative	API, 1986e
	Sister Chromatid Exchange Mice [M, F]	Intraperitoneal. 0, 340, 1700, 3400mg/kg	Positive at 1700, 3400mg/kg	API, 1985b
API 83-08 [60.8%aromatic HC]	Chromosome Aberrations Rat [M.F.]	Intraperitoneal, single dose. 0, 0.3, 1.0, 3.0g/kg	Negative	API, 1985b
64742-46-7 Diesel No. 2				
API 79-06 [76.1% saturated HC	Chromosome Aberrations Rat [M.F]	Intraperitoneal, single dose. 0, 2400, 8000, 24000mg/kg	Positive at 8000, 24000mg/kg	API, 1978
	Dominant Lethal Mice [M.F]	Inhalation, 100, 400ppm 8 weeks to males, mated with untreated females at end of exposure	Negative	API, 1980e
Diesel No. 2	Micronucleus Mice [M, F]	Oral gavage, 1-3 days 0, 1.0, 2.5, 5.0g/kg	Negative	McKee et al., 1994
68476-30-2 Home Heating Oil	Micronucleus Mice [M, F]	Oral gavage, 1-3 days 0, 1.0, 2.5, 5.0g/kg	Negative	McKee et al., 1994
64741-82-8 Coker Light Gas Oil	Micronucleus Rat [M,F]	Dermal, 13 weeks, 0, 30, 125, 500, 2000mg/kg	Negative	Mobil, 1988c Study 61997
68915-97-9 Heavy Atmospheric Gas Oil	Micronucleus Rat [M,F]	Dermal, 13 weeks, 0, 30, 125, 500mg/kg	Stat. significant at 125, 500 in females only	Mobil, 1990 Study 63457
64741-49-7 Vacuum Tower Overheads				
Vacuum Tower	Micronucleus Rat [M,F]	Dermal, 13 weeks, 0, 30,	Negative	Mobil, 1988a

CAS RN/ID	Assay/Species	Route/Dose	Results	Reference
Overhead –T		125, 500mg/kg		Study 62327

HC = hydrocarbons

In vivo studies evaluating cytogenetic damage of a selection of gas oils indicate that most of these substances do not induce chromosome damage or statistically significant increases in micronucleus formation in bone marrow of treated animals when administered orally, dermally or by inhalation, the most realistic routes of human exposure. Heavy atmospheric gas oil (CAS RN 68915-97-9) applied dermally for 13 weeks did cause increases in percent of micronucleated polychromatic erythrocytes in female rats based statistically on the total number polychromatic erythrocytes counted in all animals of each sex/group rather than using the animal [5/sex/group] as the investigative unit. The ANOVA results were negative. This occurrence in one sex only and the varying statistical outcomes raise questions about the biological relevance of this finding. Intraperitoneal administration, a severe route of exposure, of diesel Oil No. 2 (CAS RN 64742-46-7) resulted in chromosome damage but inhalation exposure of male mice in a dominant lethal study throughout the spermatogenic cycle did not cause adverse mutational effects on reproductive [failure to impregnate]and developmental activity [i.e. decreased number of fetuses] when males were mated to untreated females. The sister chromatid exchanges were induced by intraperitoneal treatment with a catalytic cracked distillate (CAS RN 64741-59-9; API 83-07), an indication of DNA perturbation. Most likely any DNA lesions were repaired as no chromosome damage was reported at similar doses by the same route.

Conclusions

Overall, the weight of evidence from studies for chromosome damage or micronucleus formation indicates that gas oils are generally not clastogenic in animals. This conclusion is further supported by extensive testing of other PAC category petroleum-derived streams (aromatic extracts, asphalt, crude oils and heavy fuel oils) in bone marrow chromosome and micronucleus assays that demonstrated that these substances did not induce significant cytogenetic damage in these test systems regardless of route of exposure (McKee et al, 2010 abst).

6.1.5. Developmental/Reproductive Toxicity

6.1.5.1, Developmental Toxicity

Developmental toxicity studies are summarized below and listed in Table 23 where studies used in developing the PAC model are identified. Dermal irritation occurred in all studies to varying degrees and was not used in establishing LOAEL/NOAEL. Treatment at very high doses was sometimes terminated due to severe dermal irritation.

CAS RN 64741-43-1 Gas Oil, Intermediate

An intermediate gas oil, F-193 (CAS RN 64741-43-1, ATX 92-0011, ARCO, 1993b) was applied to the shaved backs of presumed pregnant rats at concentrations of 0, 50, 250 and 500mg/kg day from GD 0-19. Animals were sacrificed on GD20. Dose-related increases in skin irritation were observed. Decreased maternal body weights, weight gain and absolute and relative food

consumption were seen in 250 and 500mg/kg groups. Average litter size, number of live fetuses and reduced fetal body weight were seen at 250 and 500mg/kg. At 500mg/kg statistically significant increased resorptions and increased number of dams with resorptions were observed with an increasing trend in resorptions seen in the 250mg/kg group. Other developmental parameters were unaffected by treatment. Fetal aberrations seen at 250 and 500mg/kg included eye malformations, non-dose related cleft palate, increased incidence of hydronephrosis and bifid thoracic vertebral centra. Umbilical hernia and delayed sternal ossification were seen at 500mg/kg. Delayed ossification was also reported at these doses. LOAEL maternal and developmental = 250mg/kg; NOAEL = 50mg/kg.

64741-49-7 Vacuum Tower Condensates

A Vacuum Tower Overheads sample [VTO, CAS RN 64741-49-7, CRU #086270, 8.8% DMSO extractable PAC] was applied to the shaved backs of presumed pregnant rats at dose levels of 0, 30, 125, 500 and 1000mg/kg/day from GD0 – 19 and at a dose of 1000mg/kg/day from GD 10-12 to identify any effects obscured by fetal mortality from longer term exposure and for bioavailability determinations. (Mobil 1989b. study 62328). Animals were sacrificed on GD20. Postnatal groups treated with 0 or 500mg/kg day from GD0-15 were allowed to deliver and litters maintained LD0-4. This group was originally scheduled to be treated from GD 0-19. However treatment was discontinued after day 15 because of a high incidence of resorption noted, and in an attempt to increase the in utero survival of offspring. GD 15 was also the last day of treatment in the standard EPA/FDA teratology studies of that time period. Dose related skin irritation was seen at all doses. Vaginal bleeding, decreased body weight and food consumption, decreased thymus weight were seen at 500 and 1000mg/kg. Histologically thymus size was decreased at 125mg/kg and above. Differences in clinical chemistry parameters were seen at 500 and 1000mg/kg dams treated for GD0-19. For the GD 0-19 groups, treatment at 500 mg/kg/day and higher adversely affected the number and percent of dams with resorptions, the number of resorptions, and litter size. With the exception of litter size, no treatment related differences were noted in other parameters measured including number of pregnant females, duration of gestation, implantation sites, and number of litters with live born. None of the parameters evaluated at GD 10-12 at 1000mg/kg appeared to be adversely affected. Decreased fetal body weight and crown rump length at 500 and 1000mg/kg GD0-19 and increased incidence of soft tissue anomalies including lower spleen weight were observed. Increased urinary anomalies were seen in pups from dams exposed to 125mg/kg GD0-19. For the offspring of the postnatal group, no treatment-related differences were observed between the control and the VTO exposed groups for pup survival, pup body weight or male to female ratio. Maternal LOAEL = 500mg/kg [decreased thymus weights], NOAEL = 125mg/kg. Developmental LOAEL = 125mg/kg [based on urinary anomalies] NOAEL = 30mg/kg.

In the accompanying bioavailability study 5 rats were treated with 1000mg/kg VTO radiolabeled with ^{14}C-carbazole and ^{3}H-benzo(a)pyrene, applied within a protective chamber from GD10-12. On GD13, 24 hours after the last dose, females were sacrificed and maternal blood, fetuses and placental fluid removed. Maternal organs were also examined for distribution of labeled material. Over 72 hours of exposure, 51.2%% of ^{14}C-carbazole and 12.9% ^{3}H-benzo(a)pyrene were measured in maternal tissue and less than 0.01% in fetal tissue. These low levels of radiolabeled material in fetal tissue demonstrated that the placenta is an effective barrier to transport of carbazole and benzo(a)pyrene. No selective accumulation of either material was seen in fetal tissue.

CAS RN 64741-59-9 Catalytic Cracked Distillate, Light

A light catalytic cracked oil (Sample# 010913, 23.9% DMSO extractable,80.9% total aromatics)) was applied to the shaved backs of presumed pregnant Sprague Dawley rats once daily from Gestation days 0-19 for 6 hours/day at doses of 0, 100, 450 or 750mg/kg/day (WIL 2012, Study #402017). Two control groups: one sham treated and one given the USP mineral oil vehicle were included in the study. At the end of 6 hours, test sites were wiped to remove remaining test material. All animals wore Elizabethan collars to prevent oral exposure throughout the study and were sacrificed on GD 20. Two females in the 750mg/kg group died during gestation, one euthanized on GD 13 *in extremis* had 15 normally developing implantations and 1 early resorption *in utero*, the other found dead on GD16 had an entirely resorbed litter [17 early resorptions]. Clinical observations in the 450 and 740mg/kg/day groups included yellow discharge and red material around the urogenital area, red vaginal discharge during the latter part of gestation. Dermal observations in 750mg/kg/day females included slight to moderate erythema, very slight to slight edema and desquamation. There were no dermal effects at 100 or 450mg/kg/day. Significantly lower ($p<0.01$) mean body weight gains were observed in the 450 and 750mg/kg/day groups at various intervals during gestation and for the overall treatment period (gestation days 0-20). A substantial fraction of the overall reduction in maternal weight gain could be attributed to fetal mortality/resorptions but when corrected for uterine weights statistically significant differences are still seen at 450 and 750mg/kg.

	Sham control	Vehicle control	100mg/kg	450mg/kg	750mg/kg
Gravid Uterine Weight	83.0 $\pm$ 22.16	83.0 $\pm$ 11.71	73.3 $\pm$ 18.86	62.0 $\pm$ 18.96**	19.9 $\pm$ 14.96**
Net Extra-Uterine Weight Gain	53.5 $\pm$ 15.77	47.1 $\pm$ 13.40	44.4 $\pm$ 17.81	27.9 $\pm$ 22.60**	12.6 $\pm$ 18.09**

Lower mean food consumption in the 450 and 750mg/kg/day groups corresponded to the changes in body weight and weight gain. For organs examined other than reproductive organs [liver, thymus and brain] only mean thymus weights (absolute and relative to brain weight) were lower in the 450 and 750 mg/kg/day groups compared to the vehicle control group; the differences were significant ($p<0.01$) in the 750 mg/kg/day group. These findings correlated with smaller thymus size in 5 females in the 750mg/kg group at macroscopic examination.

The number of gravid females was similar across groups. There were no differences in numbers of corpora lutea or implantation sites. However, the number of early resorptions was significantly increased, and the number of viable fetuses was significantly decreased in the 750 mg/kg/day group. Fetal weights were significantly decreased in the 450 and 750 mg/kg/day groups. There were no test substance related external or visceral malformations or variations or skeletal malformations. Skeletal variations included reduced ossification at higher incidence and at higher mean litter proportions in the 450 and 750mg/kg groups than in the corresponding control groups and were found at levels outside the historical controls of the testing laboratory. Such delayed ossification and bone maturation can be related to decreased fetal weight. LOAEL maternal and developmental = 450mg/kg based on decreased maternal weight and weight gain and decreased fetal body weight at 450 and 750mg/kg, and maternal mortality and increased resorptions, decreased viable fetuses at 750mg/kg/day. LCCO does not appear to be a “selective” developmental toxicant since fetal toxicity was seen at levels which also produce maternal toxicity. NOAEL maternal and developmental = 100mg/kg.

A light cycle oil [LCO, CAS RN 64741-59-9, Sample # 08281, 49.1% DMSO extractable PAC, 79.8% aromatic hydrocarbons],was applied to the shaved backs of presumed pregnant rats at dose levels of 0, 25, 50, 125, 250 and 500 mg/kg/day from GD0 – 19 (Mobil, 1988b, Study # 50511). At 1000mg/kg day, animals were treated either from GD0-6 or GD6-15 due to severe irritation observed at the onset of treatment. Gestation day 15 was chosen because it is the last day of treatment in standard EPA/FDA teratology studies of that time period. All animals were sacrificed on GD20. In the dams, erythema and flaking of the skin were observed in all gas oil exposed groups. Skin effects were observed in all but the 25 mg/kg group. At doses greater than 25 mg/kg there was a decrease in maternal body weight and body weight gain compared to the controls, with an accompanying reduction in food consumption. There were no treatment-related findings at necropsy. Blood levels of triglycerides were increased in a dose-related manner in the 250, 500 and 1000 mg/kg groups. Fetal body weights were reduced in the 500 and 1000 mg/kg groups, with only the reduction in the 1000 mg/kg group being statistical significant. Resorptions were also increased in the 1000mg/kg GD6-15 group. There were no significant increases in resorptions at 500mg/kg or lower doses and there were similarly no soft tissue variations and malformations, or skeletal malformations in any of the dose groups. As identified by the investigators, maternal LOAEL = 50mg/kg based on decreased body weight, although statistical significance only occurred at the 250 mg/kg/day level and greater; NOAEL = 25mg/kg. Developmental LOAEL = 500mg/kg; NOAEL = 250mg/kg.

A different light cycle oil, F-213 [FCCU light cycle oil, CAS RN 64741-59-9] was applied to the shaved backs of presumed pregnant rats at dose levels of 0, 50, 333, and 1000mg/kg/day from GD0-20 (ARCO 1994a; ATX 91-0262). Litters were maintained to lactation day (LD) 4. One female died at GD20 in the 333mg/kg group. Dose related dermal irritation was observed in all groups. Treatment related decreased body weight and food consumption, vaginal discharge and increased gestation length were observed at 333 and 1000mg/kg groups. Animals delivering pups were 5/9 pregnant in 333mg/kg and 6/9 in 1000mg/kg compared to 11/11 and 15/15 in 50mg/kg groups and control group respectively. Lower total pups and fewer live pups were seen at Lactation day 0 in the 333 and 1000mg/kg groups. Fewer pups survived to LD4 in the 333mg/kg group and decreased pup body weights were observed. In the 1000mg/kg group pup weights were higher at LD0 and 4 likely due to longer gestation and smaller litter sizes. LOAEL maternal and developmental = 333mg/kg; NOAEL = 50mg/kg

CAS RN 64741-82-8 Thermocracked Distillates, Light

A light coker gas oil, light thermal cracked distillate sample [LCGO, CAS RN 64741-82-8, Sample #087213, 10.5% DMSO extractable PAC] was applied to the shaved backs of presumed pregnant rats at dose levels of 0, 15, 60, from GD0 – 19, at 250mg/kg day from GD0-15 due to severe irritation [last treatment day in standard EPA/FDA teratology studies of that time period] and at a dose of 500mg/kg/day from GD 10-12 to identify any effects obscured by fetal mortality from longer term exposure, and for bioavailability determinations. (Mobil 1989c, study 61998). Animals were sacrificed on GD20. Postnatal groups treated with 0 or 60mg/kg day from GD0-15 were allowed to deliver and litters were maintained LD0-4. Moderate to severe skin irritation increased with increasing doses. Dams treated with 250 or 500mg/kg/day LCGO gained significantly less weight than controls and food consumption was lower during gestation. No reproductive parameters were adversely affected in GD0-19 groups or postnatal litters. Mean fetal body weight, crown rump length and pup growth were comparable to controls. No treatment related malformations, soft tissue or skeletal anomalies were observed.

Maternal LOAEL = 250mg/kg; NOAEL = 60mg/kg. Developmental LOAEL >250mg/kg; NOAEL = 250mg/kg.

In the accompanying bioavailability study 5 rats were treated with 60mg/kg LCGO radiolabeled with ^{14}C-carbazole and ^{3}H-benzo(a)pyrene, applied within a protective chamber from GD10-12. Over 72 hours of exposure, dermal penetration of ^{14}C-carbazole occurred more extensively and rapidly than ^{3}H-benzo(a)pyrene in the dam and the amount of radiolabeled material was less than 0.01% in fetal tissue demonstrating that the placenta is an effective barrier to transport of carbazole and benzo(a)pyrene. No selective accumulation of either material was seen in fetal tissue.

Another light coker gas oil, F-199 [CAS RN 64741-82-8] was applied to the shaved backs of presumed pregnant rats at dose levels of 0, 50, and 100mg/kg/day from GD0-19 and at 250mg/kg/day from GD6-11 (ARCO 1993c; ATX 92-0013). Animals were sacrificed on GD20. Skin irritation to varying degrees occurred at all dose levels. Statistically significant incidences of vocalization were observed in animals in the 100 and 250mg/kg groups and in the previous pilot study as well. No significant decreases in body weights were seen but some decreases in weight gain occurred at various times throughout gestation at 100 and 250mg/kg. No adverse effects occurred on pregnancy incidence, duration of gestation or any reproductive parameters (corpora lutea incidence, implantation, litter size, resorptions, live fetuses, fetal body weight or sex ratio. No significant gross external, soft tissue or skeletal effects were seen. Maternal LOAEL = 100mg/kg; NOAEL = 50mg/kg. Developmental NOAEL > 100mg/kg for GD0-19 treatment and 250mg/kg for GD6-11 treatment LOAEL was not determined.

CAS RN 64741-86-2 Sweetened Distillate

DHHS Stove oil, F-233 [CAS RN 64741-86-2] was applied to the shaved backs of presumed pregnant rats at dose levels of 0, 100, and 500mg/kg/day from GD0-20 and at 1000mg/kg/day from GD0-5 (ARCO 1994f; ATX 91-0133). Litters were maintained to lactation day (LD) 4. Dosage at 1000mg/kg was discontinued at GD 5 due to severe dermal irritation and vocalization of the rats and animals retained untreated on study through LD4. Dose related dermal irritation was seen at 100mg/kg and above. Absolute maternal body weight and/or body weight gains and food consumption were significantly lower at doses of 100mg/kg and above at different time intervals throughout the study. No treatment related adverse developmental effects were seen at any dose group. Maternal LOAEL = 100mg/kg; NOAEL not determined, <100mg/kg. Developmental NOAEL = 500mg/kg, highest dose group treated from GD0-20.

CAS RN 68334-30-5 Diesel Oils, C9-20

Ultralow Sulfur Diesel fuel (Sample #1020801 2.8% DMSO extractable PAC, 26.4% total aromatics), a blend of 7 diesel fuels, was applied to the shaved backs of presumed pregnant Sprague Dawley rats once daily from Gestation days 0-19 for 6 hours/day at doses of 0, 100, 300 or 600mg/kg/day (WIL 2012, Study #402014). Two control groups: one sham treated and one treated with USP mineral oil vehicle were included in the study. At the end of 6 hours, test sites were wiped to remove remaining test material. All animals wore Elizabethan collars to prevent oral exposure throughout the study. All of the rats survived to scheduled termination without evidence of test substance-related clinical findings. There were no dermal observations of note, and there were no differences in weight gain during the gestational period. There were no gross findings indicative of treatment-related effects, and weights of the target organs were

similar across the treatment groups. No treatment-related differences were observed in number of gravid dams; numbers of corpora lutea, implantation sites, viable fetuses, early or late resorptions or fetal weights. There were few malformations or developmental variants observed in this study, and no evidence that these variants were treatment-related. NOAEL maternal and developmental = 600mg/kg, the highest dose tested.

A straight run diesel oil, F-195 [SRDO, CAS RN 68334-30-5] was applied to the shaved backs of presumed pregnant rats at dose levels of 0, 50, 150, and 300mg/kg/day from GD0-19 (ARCO 1993d; ATX 92-0156). Animals were sacrificed on GD20. Dose related dermal irritation was seen at all doses and vocalization occurred in rats of 150 and 300mg/kg groups. Maternal body weight gains were reduced at 150 and 300mg/kg various times intervals throughout gestation although absolute body weights were not significantly different from controls in any dose group. Food consumption was decreased at 300mg/kg/day. No significant treatment-related adverse effects or soft tissue or skeletal malformation/anomalies were observed in this study. Maternal LOAEL = 150mg/kg; NOAEL = 50mg/kg. Developmental NOAEL = 300mg/kg, highest dose tested

In another study, F-195 [SRDO, CAS RN 68334-30-5] was applied to the shaved backs of presumed pregnant rats at dose levels of 0, 125, and 250mg/kg day from GD0-20 and at 1000mg/kg/day from GD6-11 (ARCO 1994c; ATX 91-0129). Litters were maintained to lactation day (LD) 4. Dosing adjustment at 1000mg/kg was based on a previous study [data not shown] indicating severe irritation and poor mating performance. Despite short duration of treatment, litters from the 1000mg/kg group were maintained to LD 4. Dose related skin irritation was observed at all dose levels. Decreased maternal body weight, body weight gains and food consumption was seen at 250 and 1000mg/kg. For all dose groups, there were no significant differences in gestation length, number of implantation sites, external pup alterations, proportion of pups dead on lactation day 0, proportion of pups surviving to lactation day 4, or the proportion of males on lactation day 0. Pup body weights were significantly lower ($p<0.01$) at a dose of 250 mg/kg/day on lactation Days 0 and 4. There were no effects on pup body weights at doses of 125 and 1000 mg/kg/day. LOAEL maternal and developmental = 250mg/kg; NOAEL = 125mg/kg.

Results of these studies indicate that maintenance of pregnancy, delivery and survival of fetuses/pups were comparable but that growth of offspring to lactation day 4 in the ARCO 1994c study appeared somewhat affected by *in utero* exposure to SRDO.

CAS RN 68915-97-9 Gas Oil, Heavy

Heavy atmospheric gas oil [CAS RN 68915-97-9, Sample #086271, 10.5% DMSO extractable PAC] was applied daily to the shaved backs of presumed-pregnant rats at concentrations of 0, 8, 30, 125 and 500 mg/kg/day from GD 0-19 (Mobil, 1991b, Study # 64146). Animals were sacrificed on GD20. Signs of maternal toxicity included decreased body weights, body weight gain, food consumption, thymus weights (absolute & relative), increased liver weights (relative), and changes in a number of clinical chemistry and hematological parameters. A red vaginal discharge (normally indicative of litter resorption) was observed in 7/11 animals in the 500 mg/kg/day group and two females dosed with 125 mg/kg/day. The discharge in high dose rats was considered compound related. The significance of 2 rats with vaginal discharge in the 125mg/kg group is questionable as a similar incidence has been seen in untreated control rats in this laboratory. Evaluation of reproductive parameters in the 8 and 30 mg/kg found no

compound-related effects. Statistically non-significant differences in preimplantation losses were seen in both the 125 and 500 mg/kg/day groups. There was a significant increase in the mean number/percent resorptions in the 500 mg/kg/day group. Mean fetal body weights were significantly decreased for all viable fetuses in the 500 mg/kg/day group and in the male pups of the 125 mg/kg group. There was a significant increase in incomplete ossification of a number of skeletal structures (nasal bones, thoracic centra, caudal centra, sternebrae, metatarsal and pubis) in the 125 and 500 mg/kg/day groups. There were no treatment-related abnormalities found in the soft tissues. Exposure to heavy atmospheric gas oil in the 8 and 30mg/kg/day groups did not adversely affect pup survival or development. LOAEL maternal and developmental = 125mg/kg; NOAEL = 30mg/kg.

Supplemental data: Inhalation study

CAS RN 68476-34-6 Diesel Fuel, Market place sample

A developmental toxicity study has been reported on a diesel fuel consisting of 76.1% saturated hydrocarbons (API, 1979b). Groups of presumed-pregnant Sprague-Dawley rats were exposed to nominal atmospheric concentrations of 100 and 400 ppm for 6 hours each day from GD6-15. On day 20 all the animals were sacrificed. One third of the fetuses were fixed for soft tissue examination. The remaining fetuses were examined for skeletal abnormalities. There were no deaths during the study and all animals were normal in appearance throughout. The 400 ppm maternal group had a reduced food intake during days 7-15 of gestation. No treatment-related differences were found in a variety of parameters, including sex ratios of the fetuses, number of implantation sites, resorptions, and live fetuses. With the exception of subcutaneous hematomas that occurred at a higher rate in the test article exposure groups, there were no test article-related abnormalities found in either the soft tissues or skeletons of the fetuses. Developmental NOAEL = 400ppm.

Conclusions

Results of developmental studies with gas oils demonstrate that some gas oils induce developmental effects and others do not. The substances tested in the Gas Oil Category for which treatment began with the onset of presumed pregnancy (Gestation day 0) developmental LOAELs ranging from 125 – 500mg/kg attributed primarily to fewer live fetuses or pups per litter at delivery and lower fetal or pup body weight at delivery or Lactation days 0-4.and NOAELs from 30 – 600mg/kg, Fetal malformations were reported for CAS RN 64741-43-1 [F-193] and CAS RN 64741-49-7 [Vacuum Tower Overheads]. Developmental toxicity was seen only at doses that were maternally toxic [except for VTO urinary anomalies] expressed as decreased body weights and weight gain, and decreased food consumption. Some gas oils showed no developmental toxicity at the highest doses tested [e.g ultralow sulfur diesel] even in the presence of maternal toxicity [two coker gas oils, a sweetened distillate and a straight run diesel oil (treated GD0-19)

Comparison of the result of the developmental studies with the analytical characterization of these gas oils (Table 23) suggests a relationship exists between the content of aromatics and developmental toxicity. The streams with the LOAEL of 125mg/kg, heavy atmospheric gas oil (CAS RN 68915-97-9) and vacuum tower overheads (CAS RN 64741-49-7) have a higher distribution of aromatics of 3-rings or greater. Streams demonstrating virtually no developmental toxicity over the range of doses tested have a very low content of DMSO extractable aromatics (i.e., aromatics with > 2 rings). Other streams with intermediate levels of

toxicity such as the light cycle oils contain a fairly even percentage of C2 and C3 ring aromatic and few if any ring distributions above C3.

Table 23. Comparison of Developmental Results with 1-7 ring PAC Content

CAS RN/Name	Sample No.	Developmental [mg/kg]		% PAC[a]
		LOAEL	NOAEL	
68915-97-9 Heavy Atmospheric. gas oil	086271	125	30	0.9% C1-C2 9.2% C3-C7
64741-49-7/ Vacuum Tower overheads	086270	125	30	2.5% C2; 5.2% C3-C7
64741-43-1/ F193	091646	250	50	2% C2 8.7% C3-C7
64741-82-8/ F277	094628	250	50	na
64741-59-9/ F-213	091679	333	50	20.0% C2 20.4% C3
64741-59-9/ Lt cat cracked oil	010913	450	100	17.1% C1-C2 4.6% C3
64741-59-9/ Lt cycle oil	08281	500	250	30% C2 14% C3
64751-82-8/ F199	091652	none	>100	4.1%C2 10% C3
64751-82-8/ Lt coker gas oil	087213	none	250 [highest dose]	4.2% C2 6.3% C3
68334-30-5/ F-195	091648	none	300	3.1% C1-C2 4.3% C3
64741-86-2/ F-233	094629	none	500	3.0% C1 2.9% C3
68334-30-5/ Ultralow Sulfur diesel	120801	none	600	2.3% C1-C2 0.6% C3

a PAC distributions summarized from Appendix D-1

There are three studies in which females were treated from 7 days premating through mating and gestation, with litters maintained untreated until LD4 [CAS RN 64741-43-1, F-193; CAS RN 64741-82-8, F-199, F-277] that are discussed in Section 7.1.6.2 Reproductive toxicity. Two of the materials F-199 and F-193 showed developmental and maternal toxicity at 250-259mg/kg, NOAEL = 1.0mg/kg respectively while F-277 had a NOAEL = 50mg/kg, a dose which also induced maternal effects. Only F-277 had an intermediate dose between 250 and 1.0mg/kg making the dose range from the other studies too wide to use in setting the category developmental NOAEL. [see Table 24]

Table 24. Developmental Toxicity Studies of Gas Oils in Sprague Dawley Rats by the Dermal Route of Exposure

CAS RN/ID	Sex /Duration	Dose mg/kg/day	Results	References
64741-43-1 Gas Oil, Intermediate				
F-193 [sample # 091646]	Presumed pregnant, (25/group) Treated GD0-19, Sacrificed GD20	0, 50, 250, 500	Decreased maternal body weight, weight gain, food consumption. Decreased fetal body weight, embryo/fetal viability, soft tissue, skeletal alterations LOAEL maternal/developmental = 250mg/kg NOAEL maternal/developmental = 50mg/kg	ARCO, 1993b ATX 92-0011
F-193 [sample # 091646] See Section 6.1.5.2 Reproductive toxicity	Females (15/group treated; 20 controls) Treated 7 days premating, mating, GD0-20. Litters maintained LD0-4	0. 1.0, 259, 1036	Decreased maternal body weights, weight gains, food consumption. No adverse effects on mating, pregnancy, delivery of implantation. At 1036mg/kg, 2/9 delivered and total and live pups decreased at LD0. Pup body weights decreased in 259mg/kg and 1036groups at LD0 and LD4. LOAEL maternal and developmental = 259mg/kg; NOAEL maternal and developmental = 1.0mg/kg	ARCO 1994b, ATX 91-0127
64741-49-7 Vacuum Tower Condensates				
Vacuum Tower Overheads [sample # 86270]	Presumed pregnant, (10/group) Treated GD0-19, Sacrificed GD20	0, 30, 125, 500, 1000 GD0-19; 1000mg/kg GD10-12 0, 500mg/kg GD0-15, litters maintained LD0-4	Decreased maternal body weight, food consumption, vaginal bleeding , decreased thymus weight and Clinical chemistry and Hematology changes at 500, 1000mg/kg Decreased thymus size at greater than 125mg/kg. At 500mg/kg and above, increased number and % of dams with resorptions, number of resorptions, decreased litter size, fetal body weight and length, increased soft tissue anomalies. Increased urinary anomalies at 125mg/kg. Maternal LOAEL = 500mg/kg; NOAEL = 125mg/kg Developmental LOAEL = 125mg/kg; NOAEL = 30mg/kg	Mobil , 1989b Study # 62328
64741-59-9 Catalytic Cracked Distillate, Light				
Light Cycle Oil [sample #08281]	Presumed pregnant, (10/goup) Treated GD0-19, Sacrificed GD20	0, 25, 50, 125, 250, 500 GD0-19 1000mg/kg GD0-6 or GD6-15 (5/subgroup) due to dermal irritation	Decreased maternal body weight, weight gain and food consumption at 50mg/kg and above. Triglycerides increased at 250 and above. Fetal body weight decreased at 500, 1000; resorptions at 1000mg/kg GD6-15; No other adverse developmental effects. LOAEL maternal = 50mg/kg; NOAEL = 25mg/kg LOAEL developmental = 500mg/kg; NOAEL = 250mg/kg	Mobil 1988b Study # 50511
Light catalytic cracked oil [sample #010913]	Presumed pregnant, (25/goup)	0, 100, 450, 750mg/kg GD0-19, 6hours/day,	Maternal mortality at 750mg/kg, decreased maternal weight and weight gain at 450 and 750mg/kg, increased	WIL, 2012 Study # 402017

CAS RN/ID	Sex /Duration	Dose mg/kg/day	Results	References
	Treated GD0-19, Sacrificed GD20	Wiped off Elizabethan collars	resorptions and decreased viable fetuses at 750mg/kg, Decreased fetal body weight at 450 and 750mg/kg and some increased skeletal variations likely associated with decreased fetal weight LOAEL maternal/developmental = 450mg/kg NOAEL maternal/developmental = 100mg/kg	
F-213 [FCCU light cycle oil] [sample # 091679**]**	Presumed pregnant, (12/treated group, 15 controls) Treated GD0-20 Litters maintained to LD 4	0, 50, 333, 1000	Increased gestation length, vaginal discharge, decreased maternal body weight, weight gain and food consumption. Decreased total and live pups/litter, number of litters with live pups, decreased pup body weight on LD0, 4 and decreased pup survival at LD4 LOAEL maternal/developmental = 333mg/kg NOAEL maternal/developmental = 50mg/kg	ARCO, 1994a ATX 91-0262
64741-82-8 Thermocracked Distillates, Light				
Light coker gas oil [sample # 087213]	Presumed pregnant, (10/group) Treated GD0-19, Sacrificed GD20	0, 15, 60, GD0-19; 250mg/kg GD0-15; 500mg/kg GD10-12 0, 60mg/kg GD0-15 litters maintained to LD4	Decreased maternal body weight, weight gain, food consumption. No adverse developmental effects at any dose. Maternal LOAEL = 250mg/kg; NOAEL = 60mg/kg Developmental NOAEL = 250mg/kg	Mobil 1989c Study # 61998
F-199 [sample # 091652]	Presumed pregnant (25/group) Treated GD0-19, Sacrificed GD20	O, 50, 100 GD0-19; 250mg/kg GD6-11	Decreased maternal body weight gain, increased vocalization at 100mg/kg and above. No adverse developmental effects. Maternal LOAEL = 100mg/kg; NOAEL =50mg/kg Developmental NOAEL > 100mg/kg [GD0-19] Developmental NOAEL = 250mg/kg [GD6-11]	ARCO 1993c ATX 92-0013
F-199 [sample # 091652] See Section 6.1.5.2 Reproductive toxicity	Females (15/ treated group, 20 controls) Treated 7 days premating, mating, GD0-20 Litters maintained LD0-4	0, 1.0 premating to GD20; 250mg/kg premating to GD8-11, 1000mg/kg premating days -7 to mating day 4, sacrificed day 5 due to dermal irritation	Decreased maternal body weight, weight gain, food consumption at 250 and 1000mg/kg. Decreased number of implantation sites and decrease in total and live pup numbers on day 0; pup survival and weight comparable at LD4. [dosing at 250mg/kg ended at GD8-11] LOAEL maternal/developmental = 250mg/kg NOAEL maternal/developmental = 1.0mg/kg	ARCO 1994d ATX 91-0133
F-277 [sample # 094628]	Females (15/ treated group, 12 controls) Treated 7 days	0, 1.0, 50, 250	Changes in maternal body weight and weight gain at 250mg/kg and food consumption at 50 and 250mg/kg. Decreased pup body weight on LD0 and 4 at 250mg/kg.	ARCO 1994e ATX 93-0075

CAS RN/ID	Sex /Duration	Dose mg/kg/day	Results	References
See Section 6.1.5.2 Reproductive toxicity	premating, mating, GD0-20 Litters maintained LD0-4		Maternal LOAEL = 50mg/kg; NOAEL =1.0mg/kg Developmental LOAEL = 250mg/kg; NOAEL = 50mg/kg	
64741-86-2 Sweetened Distillate				
F-233 DHHS Stove Oil [sample # 094629]	Presumed pregnant, (12/treated group, 15 controls) Treated GD0-20 Litters maintained to LD 4	0, 100, 500 GD 0-20 1000mg/kg GD0-5 due to vocalization, severe irritation	Decreased maternal body weight, weight gain, food consumption at 100mg/kg and above. No developmental effects seen up to 500mg/kg. 1000mg/kg group not considered since dosing ended at GD5 although maintained to LD4 Maternal LOAEL = 100mg/kg; NOAEL not determined, <100mg/kg Developmental NOAEL = 500mg/kg [highest dose to GD20]	ARCO 1994f ATX 91-0133
68334-30-5 Diesel Oils				
Ultralow Sulfur Diesel Fuel [sample #120801]	Presumed pregnant (25/group) Treated GD0-19, Sacrificed GD20	0, 100, 300, 600mg/kg, 6 hour/day, Wiped off Elizabethan collars	No adverse clinical findings, no effects on maternal body weights or weight gain during gestation, no effect on target organ weights. No treatment-related differences in number of gravid dams; numbers of corpora lutea, implantation sites, viable fetuses, early or late resorptions or fetal weights. Few malformations or developmental variants) and no evidence that these variants were treatment-related. NOAEL maternal/developmental = 600mg/kg , highest dose tested.	Wil, 2012 Study # 402014
F-195 straight run diesel oil [sample # 091648]	Presumed pregnant (25/group) Treated GD0-19, Sacrificed GD20	0. 50, 150, 300	Decreased maternal body weight gains, vocalization at 150 and 300mg/kg. Decreased food consumption at 300mg/kg. No adverse developmental effects Maternal LOAEL = 150mg/kg; NOAEL = 50mg/kg Developmental NOAEL = 300mg/kg [highest dose tested]	ARCO, 1993d ATX 92-0156
F-195 straight run diesel oil [sample # 091648]	Presumed pregnant, (14-15/treated group, 19 controls) Treated GD0-20 Litters maintained to LD 4	0, 125, 250 GD 0-20 1000mg/kg GD 5-9	Decreased maternal body weight, weight gain and food consumption at 250, 1000mg/kg. No adverse developmental effects except decreased pup body weight on LD0 and 4 at 250mg/kg. LOAEL maternal/developmental = 250mg/kg NOAEL maternal/developmental = 125mg/kg	ARCO 1994c ATX 91-0129
68915-97-9 Gas Oil, Heavy				

CAS RN/ID	Sex /Duration	Dose mg/kg/day	Results	References
Heavy Atmospheric Gas oil [sample # 086271]	Presumed pregnant, (12/group) Treated GD0-19 sacrificed GD20	0, 8, 30, 125, 500	Decreased maternal body wt, food consumption at 125, 500mg/kg. Decreased thymus wt, increased liver wt, changes in serum chemistry/hematology at 500mg/kg. Non-significant increased preimplantation loss, decreased mean fetal body wt, incomplete ossification at 125, 500mg/kg. LOAEL maternal/developmental = 125mg/kg NOAEL maternal/developmental = 30mg/kg	Mobil, 1991b Study 64146

a- Only developmental studies with treatment for GD0-19 and sacrifice at GD20 were used for PAC modeling activities [see Appendix D].

6.1.5.2 Reproductive Toxicity

In addition to results of studies which included assessment of reproductive organs after repeated treatment, information on the reproductive effects of gas oils is provided from studies in which female rats were treated dermally for 7 days premating, through mating and gestation to gestation day 20 [GD20] conducted on a sample of CAS RN 64741-43-1 Straight run gas oil [F-193] and 2 samples of CAS RN 64741-82-8 light cycle oil [F-199, F-277] also listed in Table 24 above.

CAS RN 64741-43-1 Straight Run Gas Oils

Test article F-193, (CAS RN 64741-43-1, ATX 91-0127 ARCO, 1994b) was applied to the shaved backs of female rats from one week prior to mating through mating and gestation to GD20 at concentrations of 0, 1.0 259 and 1036 mg/kg/day. Females were mated to untreated males. Litters were maintained to lactation day (LD) 4. One death occurred at 1036mg/kg on LD 1. Dose-related vaginal discharge, decreased maternal body weight and weight gain and food consumption and some skin irritation were reported in 259 and 1036mg/kg groups. At 1036mg/kg only 2/9 pregnant females delivered, total and live pups were decreased at delivery; surviving pup body weights were decreased at LD0 and LD4. No adverse effects were seen on mating capability, gestation length, delivery or number of implantation sites. At 259mg/kg pup body weights were decreased on LD1 and LD4. No adverse effects were seen on proportion of surviving pups at LD4 or male/female pup ratio. LOAEL maternal and developmental = 259mg/kg; NOAEL maternal and developmental = 1.0mg/kg.

CAS RN 64741-82-8 Light Cycle Oils

Test article F-199, Light thermal cracked distillate (CAS RN 64741-82-8, ATX 91-0133 ARCO, 1994d) was applied to the shaved backs of female rats from one week prior to mating through mating and gestation to GD20 at concentrations of 0, 1.0 mg/kg/day, from premating day 7 through GD 8-11 at 250mg/kg/day and from premating day 7 to mating day 4 at 1000mg/kg/day. Females were mated to untreated males. Surviving litters were maintained to lactation day (LD) 4. One female in the 1000mg/kg group died after 1 night of mating and all other females in this group were killed on mating day 5 due to severe skin irritation. Slight to severe skin irritation was observed in the 250mg/kg group resulting in termination of treatment at GD 8 -11 and maintenance of the untreated animals and litters to LD4. Decreased body weight, weight gain and changes in food consumption were observed in the 250 and 1000mg/kg groups. No adverse effects were seen on mating capability, initiation of pregnancy, pup survival to LD4, ratio of male to female pups or appearance of gross malformations were seen at 1.0 or 250mg/kg. Despite termination of test material administration at GD8-11 females in the 250mg/kg group had fewer mean implantation sites and fewer total pups or live pups/litter on LD0. LOAEL maternal and developmental = 250mg/kg; NOAEL maternal and developmental = 1.0mg/kg.

Test article F-277, Light coker gas oil (CAS RN 64741-82-8, ATX 93-0075 ARCO, 1994e) was applied to the shaved backs of female rats from one week prior to mating through mating and gestation to GD20 at concentrations of 0, 1.0, 50 and 250mg/kg/day. Females were mated to untreated males. Litters were maintained to lactation day (LD) 4. Dose related increases in skin irritation were observed. Maternal body weights were lower at 250mg/kg from the last day of premating through LD 4 and body weight gain was lower premating to GD 4, comparable through the remainder of gestation and higher than controls at LD0-4. Changes in relative food

consumption at 50 and 250mg/kg were considered treatment related and use to establish the maternal LOAEL. No treatment related effects were seen on reproductive parameters, number of litters, total number of pups or live pups/litter on LD0, ratio of male pups or malformations. Average pup body weight was lower than controls at LD0 and 4 in the 250mg/kg group. Maternal LOAEL = 50mg/kg; NOAEL = 1.0mg/kg. Developmental LOAEL = 250mg/kg; NOAEL = 50mg/kg.

The reproductive toxicity potential of gas oils can also be evaluated by combining relevant parameters from developmental toxicity studies with histopathological evaluations of reproductive organs in 13 week repeat dose studies as outlined in the EPA HPV guidance document. As documented above, there were 9 repeated dose toxicity studies covering a range of gas oils in which potential toxicity in reproductive organs was assessed. There were no studies in which there were significant differences in reproductive organ weights and there were no pathological changes in these organs which were associated with treatment. These studies provide evidence that reproductive parameters are not affected by gas oil treatment

Conclusions

Reproductive parameters in developmental toxicity studies addressing fertility, successful insemination and implantation demonstrate that in general these endpoints are not adversely affected by treatment with gas oil streams. Evaluation of reproductive organs and sperm morphology and motility from 13-week repeated dose studies consistently demonstrated no adverse effects on ovary or testes weights or abnormal histopathology or sperm at doses ranging up to 500-820mg/kg/day.

The studies in which females were treated for a week prior to mating through mating and gestation to GD20 demonstrated that exposure to high concentrations of several gas oils did not adversely affect mating and establishment of pregnancy but did affect successful completion of pregnancy and pup viability to varying degrees at maternally toxic doses of 250mg/kg and above. The wide range of doses in these three studies makes it difficult to identify an accurate NOAEL value. Of these three studies, only F-277 had an intermediate dose level between 250 and 1.0mg/kg allowing a NOAEL determination of 50mg/kg for that substance, which falls within the range of developmental NOAELs from 30-600mg/kg cited above... The NOAEL for reproductive toxicity is not expected to be lower than the NOAEL for developmental toxicity because the most sensitive endpoints in either developmental or reproductive toxicity studies are expected to be effects on fetal survival and growth resulting from *in utero* exposure (Murray et al., 2012)

6.2 Health Effects - Other

6.2.1 Carcinogenicity - Dermal

In addition to the studies discussed above, a number of dermal carcinogenicity studies have been performed on gas oils and distillate fuels. Although carcinogenicity is not a required endpoint of the HPV program, these results are provided to complete the profile of gas oil toxicity. These studies have been fully summarized and reviewed elsewhere (ATSDR, 1995; CONCAWE, 1996; IARC, 1988). The general conclusions that can be drawn from the animal carcinogenicity studies are:

- Gas oils and distillate fuels are potential skin carcinogens after repeated skin application.
- When applied repeatedly to the skin, carcinogenic gas oils and distillate fuels are associated only with skin tumors and not with an increase in non-metastatic systemic tumors (Freeman and McKee, 1993).
- The skin carcinogenicity of the petroleum streams with high boiling ranges and PAC content correlates with 3-7 ring PAC distribution.
- Skin tumors produced by materials containing low or no PAC is likely due to a non-genotoxic promotion effect and only observed in the presence of sustained severe skin irritation (Nessel et al., 1998).
- Depending on the types and levels of aromatics present, some gas oils can initiate skin tumors whereas others exhibit only promotional activity (Jungen et al. 1995).

Gas Oils Streams

- **Streams Composed Predominantly of Aromatic Hydrocarbons**

A cracked gas oil, CAS RN 64741-59-9 (69.7% aromatic hydrocarbons) was applied to the skins of male C3H mice 2, 4 or 7 days/week for 104 weeks (Exxon, 1996a, Nessel et al., 1998). The test material was applied either undiluted or at 50% or 28.5% dilutions in mineral oil. The concentration and dosing frequencies were adjusted to ensure that each animal received the same total weekly dose of test material irrespective of dosing frequency. Thus, the 100% animals were dosed 2x/week, while the 50% and 28.5% groups were dosed 4x/week and 7x/week respectively. Survival was less in the treated groups compared to the negative controls; at the lower two concentrations (28.5 and 50 %) the difference was statistically significant. Dermal irritation occurred in the groups exposed to the gas oil, scores ranging from 0.0 to 4.0. There were no other treatment-related clinical findings. Treatment related findings at post mortem were limited to dermal irritation. A variety of skin tumors developed in the positive control and gas oil treated groups. Tumor types found included squamous cell carcinomas, fibrosarcomas, melanoma (only 1 treated animal) and papillomas.

Two samples of gas oils with a high aromatic content (48.3% & 55.1% aromatic hydrocarbons) have been tested in an initiation-promotion assay in male CD-1 mice (DGMK, 1993; Jungen et al., 1995). Animal survival was not affected by exposure to the gas oil samples. During both the initiation and promotion phases, the gas oil samples caused slight to moderate skin irritation which was found to be reversible. There were no other treatment-related clinical findings. Of the two samples, both appeared to have weak initiating potentials, while only one showed a weak promoting effect.

- **Streams Composed Predominantly of Saturated Hydrocarbons**

A straight run, hydrotreated gas oil CAS RN 64742-54-7 (73.8% saturated hydrocarbons) was applied to the skins of male C3H mice 2, 4 or 7 days/week for 104 weeks (Exxon, 1996a). The test material was applied either undiluted or at 50% or 28.5% dilutions in mineral oil. The concentration and dosing frequencies were adjusted to ensure that each animal received the same total weekly dose of test material irrespective of dosing frequency. Thus, the 100% animals were dosed 2x /week, while the 50% and 28.5% groups were dosed 4x/week and 7x/week respectively. Survival figures of the gas oil treated groups were comparable to that seen in the negative control group. Dermal irritation scores in the gas oil groups ranged from 0.0 to 4.0. There were no other treatment-related clinical findings. Dermal irritation was the only treatment-related finding at post mortem. A variety of skin tumors developed in the positive control and the 100% and 28.5% gas oil groups. The tumor incidence was highest in the group

in which skin irritation was greatest. The incidence of the tumors in the gas oil groups was much lower than that seen in the study of a cracked gas oil described above.

Three gas oils with high saturated hydrocarbon contents (57.5% - 76.4%) have been tested in an initiation-promotion assay in male CD-1 mice (DGMK, 1993). Animal survival was not affected by exposure to the gas oil samples. During both the initiation and promotion phases, two of the three gas oil samples caused reversible, slight to moderate skin irritation. There were no other treatment-related clinical findings. Of the three samples, two appeared to have weak, if any initiating potentials and one had a very weak, if any promoting potential.

Distillate Fuels

A dermal carcinogenicity study of a diesel fuel (saturate content unknown) in C3H mice has been reported by IITRI (IITRI, 1985). Over the lifetime of the animals, 50µl of undiluted test material was applied 2x /week to the shaved backs of male mice. There was a significant increase in the incidence of malignant skin tumors (squamous cell carcinoma or fibrosarcoma) in the treated mice compared to the controls. Other lesions of the treated skin included sloughing of the skin and lesions resembling infection, both of which were seen more frequently in the treated animals.

A sample of a diesel fuel (76.6% saturated hydrocarbons) has been tested in an initiation-promotion assay in male CD-1 mice (DGMK, 1993). Animal survival was not affected by exposure to the diesel fuel. The study's authors concluded that the diesel fuel sample might be a promoter.

6.3 Assessment Summary for Human Health Effects

Gas Oil streams and distillate fuels demonstrated minimal acute toxicity by the oral, dermal and inhalation routes, minimal eye irritation, moderate to severe skin irritation with 24 hours exposure, and no dermal sensitization.

In vitro genetic toxicity studies demonstrate that some gas oil streams and distillate fuels can induce gene mutation in bacterial assays and some streams are also active in mouse lymphoma tests. In addition to the standard Ames Test (Ames et al, 1975), the Optimized Ames test (previously the Modified Ames test) confirms that some Gas Oils cause bacterial mutagenicity. . Levels of activity within a given CAS RN may vary; samples with higher levels of aromatics are mutagenic while others with low aromatic content can be inactive, variability resulting from different crude oil sources and the type and severity of processing. Results of in vivo studies evaluating chromosome damage or micronucleus formation in bone marrow cells indicate that gas oils are generally not clastogenic in laboratory animals.

The 13-week rat dermal studies on gas oil streams resulted in LOAEL of 125mg/kg with the exception of a light coker gas oil with a LOAEL of 30mg/kg, the lowest dose tested, effects likely exacerbated by severe skin irritation at all dose levels. NOAELs ranged from 25-30mg/kg with the exception of an ultralow sulfur diesel fuel with a NOEL = 600mg/kg, the highest dose tested. This ultralow sulfur diesel fuel had a very low content of DMSO extractable aromatic hydrocarbons. Skin irritation in most studies generally ranged from slight to moderate. Effects when present were seen in organ weights, primarily liver and thymus, and hematologic endpoints. The 4 week duration rat dermal studies showed slight to moderate skin irritation and

minimal systemic toxicity with NOAEL = 400-800mg/kg. No significant adverse effects were seen in reproductive organs in any rat dermal study.

Results of developmental studies with gas oils demonstrate that some gas oils induce developmental effects and others do not. Substances tested in the Gas Oil Category had developmental LOAEL ranging from 125 – 500mg/kg attributed primarily to fewer live fetuses or pups per litter at delivery and lower fetal or pup body weight at delivery or Lactation days 0-4, respectively seen only at doses that were maternally toxic. NOAELs ranged from 30 – 600mg/kg. Fetal malformations were reported for 2 members of the category, CAS RN 64741-43-1 [F-192, intermediate gas oil] and CAS RN 64741-49-7 [Vacuum Tower Overheads]. Ultralow sulfur diesel, a stream with a very low concentration of DMSO extractable aromatic hydrocarbons demonstrated virtually no maternal or developmental toxicity at doses up to 600mg/kg. Other gas oils showed no developmental toxicity at the highest doses tested even in the presence of maternal toxicity.

Reproductive parameters in developmental toxicity studies addressing fertility, successful insemination and implantation demonstrate that in general these endpoints are not adversely affected by treatment with gas oil streams. Evaluation of reproductive organs and sperm morphology and motility in repeated dose studies consistently demonstrated no adverse effects on ovary or testes weights or abnormal histopathology or effects on sperm at doses ranging up to 500-820mg/kg/day. In three studies in which females were treated for a week prior to mating through mating and gestation to GD20, exposure to maternally toxic concentrations of 250mg/kg did not adversely affect mating and establishment of pregnancy but did adversely affect successful completion of pregnancy and pup viability. The NOAEL for reproductive toxicity is not expected to be lower than the NOAEL for developmental toxicity because the most sensitive endpoints in either developmental or reproductive toxicity studies are expected to be effects on fetal survival and growth resulting from *in utero* exposure (Murray et al., 2012).

Overall, for repeated dose and developmental toxicity, effects appear to be related to aromatic content The liver, thymus and hematologic effects seen in repeat dose studies may be more generalized responses to aromatics while developmental effects can be related specifically to higher concentrations of 3-ring and above PAC. Developmental effects may require higher doses than seen in systemic toxicity studies and for some streams developmental effects were not seen even at doses that are systemically toxic to pregnant females.

Dermal carcinogenicity studies indicate that Gas oils and distillate fuels are potential skin carcinogens after repeated skin application but are not associated with the induction of systemic tumors. The skin carcinogenicity of the petroleum streams with high boiling ranges has been demonstrated to correlate with 3-7 ring PAC content. Skin tumors produced by substances in this category which contain low or no PAC are likely due to a non-genotoxic promotion effect and are only observed in the presence of sustained severe skin irritation.

7. HUMAN EXPOSURE SUMMARY

Because the No. 2 distillate fuels have widespread use in transportation and industrial and residential heating applications, both occupational and consumer exposures are possible. Exposure to children is not anticipated. The other substances in the Gas Oil Category are only used in industrial applications.

Very limited information on human exposure to substances in the Gas Oil Category is available in the literature. Dermal exposure is the principle route of exposure because of the low vapor pressure of these substances. A significant effort to develop human exposure data was conducted and published by the European petroleum industry technical organization, CONCAWE (CONCAWE, 2006).

Information on levels of human exposure resulting from the manufacturing, distribution and use of gas oils and blending components was developed for the CONCAWE report. Technical guidance for the collection of exposure information to support EU risk assessment was followed, including direct measurement of exposure levels and indirect, modeling approaches. Exposure estimates were developed for workers and for consumers, but not for the general public. Inhalation exposure data were retrieved and collated from member companies and open literature, and supplemented with new measurements from a dedicated monitoring campaign. Dermal exposure levels were estimated using a simple modeling approach. The collection and collation of exposure information for gas oils vapor from CONCAWE member companies confirmed that worker exposure by inhalation is generally well below the exposure limit of 100 mg/m3 recommended by the American Conference of Governmental Industrial Hygienists (ACGIH); that a wide range of control measures are in place; and that occurrences of elevated exposure appear to be infrequent. Exposures are often simultaneous with other petroleum products, in particular gasoline, making it difficult to characterize those originating from gas oils alone. Inhalation and dermal exposures were estimated to be of the same order of magnitude.

CONCAWE reported conservative estimates of consumer exposure resulting from car refueling with automotive diesel were 1 milligram per day via inhalation and 21 milligram per day as dermal exposure per refueling event. The inhalation estimate was based on measured data, whereas the dermal estimate was derived through modeling. Consumer exposure estimates were considerably lower than worker exposure estimates.

For worker exposures, 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

There are many specific US laws and regulations are in place to limit occupational exposure and environmental release of Gas Oil substances and distillate fuel products. These include;

1. Occupational Safety and Health Act (29 CFR 1910)
2. Marine Occupational Safety and Health Standards (46 CFR 197)
    a. International Convention for the Safety of Life at Sea (74 Fed. Reg. 30, 612 - June 26, 2009)
3. Hazardous Materials Transportation Act (49 CFR 171)
4. Clean Water Act
    a. Oil Spill Prevention, Notification and Cleanup
        i. 30 CFR 250.203, 250.204, 254 Oil Spill Contingency Plan
        ii. 33 CFR Part 153 Control of Pollution by Oil and Hazardous Substances
        iii. 33 CFR Part 154 Facilities Transferring Oil or Hazardous Material in Bulk
        iv. 33 CFR Part 156 Oil and Hazardous Material Transfer Operations
        v. 40 CFR 110 Discharge of Oil
        vi. 40 CFR 112 Oil Pollution Prevention
5. Clean Air Act
    b. National Emission Standards for Hazardous Air Pollutants
        i. 40 CFR Part 63, Subpart Y National Emission Standards for Marine Tank Vessel Loading Operations

8. CATEGORY ANALYSIS CONCLUSIONS

The Gas Oil Category includes 29 members comprised of 4 finished products (distillate fuels) and 25 refinery streams with similar carbon ranges. The category members are complex substances, containing variable amounts of alkanes, cycloalkanes, olefins, and aromatics. The saturated and aromatic hydrocarbon content of the category members form a continuum from high saturate content to high aromatic content. In comparison to gas oil refinery streams and fuel oil No. 4 which do not have product specifications, Fuel Oil No. 2 and the ultralow sulfur diesel (ULSD) fuels must meet stringent ASTM and EPA standards for commercialization. The boiling point specifications for these fuels essentially limit the aromatics to 1and 2- ring compounds with minimal 3-ring PAC and virtually no 4-ring PACs. Physical properties, process history and product use specifications rather than composition define gas oil streams (ASTM, 2003) and provide the rationale for the composition of this category. Key parameters when analyzing this category for environmental hazards are the distribution of aromatic and saturated hydrocarbons, and for some mammalian endpoints (repeated-dose, developmental, and mutagenic) the content and distribution of PACs are important

Physical-Chemical Properties: Gas oils are variable and complex substances of hydrocarbons, predominantly having carbon chains from C_9 to C_{30}, and boiling over the temperature range of 150°C to 450°C. Vapor pressures are within a measurable range, with values of 0.4 kPa and 2 kPa being reported. Partition coefficients of constituent hydrocarbons ranged from 3.3 to >6. Water solubility values for these substances have been reported from 2.0 mg/L to 8.7 mg/L for dissolved hydrocarbons

Environmental Fate: If gas oils are released to the environment, individual components will disperse and partition according to their individual physical-chemical properties. Their final dispositions are shaped by both abiotic and biotic processes. Based on modeling individual structures encompassing the different types and molecular weights of hydrocarbons,

volatilization to the atmosphere is an important process for the low molecular weight fractions. 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 these reactions. Components in gas oils will biodegrade, and moderate to rapid rates of biodegradation were measured in standard tests. It is unlikely that these substances pass ready biodegradability criteria, but available test data proved evidence for inherent biodegradability.

Environmental Effects:
Multiple ecotoxicological studies on heating and transportation fuels (e.g., No. 2 fuel oil and diesel fuel) were reviewed and new testing of two gas oil streams having a high proportion of aromatic or saturated hydrocarbon content were conducted. Estimated lethal of effect loading toxicity endpoints ($LL/EL_{50}s$) using the PETROTOX model and detailed 2D-GC-MS hydrocarbon analyses of the two gas oil streams were also calculated. When all LL/EL_{50} experimental data were combined with the modeled endpoints, the acute LL/EL_{50} toxicity values for the three trophic levels ranged from 0.18 mg/L to 125 mg/L for fish, 0.35 mg/L to 210 mg/L for invertebrates, and 0.20 mg/L to 78 mg/L for algae. The light catalytic cracked gas oil (high aromatic stream) was the most acutely toxic to all three trophic levels among the category members.

The chronic effects assessment included a fish growth test with no. 2 fuel oil and *D. magna* reproduction studies of light catalytic cracked gas oil and light hydrocracked gas oil. The LOELR based on reduction in fish growth was 3.0 mg/L while the NOELR was 1.2 mg/L. For invertebrates, reduced reproduction in *D. magna* was observed at the LOELR of 0.10 mg/L. The NOELR was 0.05 mg/L. The NOELR based on the PETROTOX model was 0.06 mg/L for the catalytic cracked gas oil. The NOELR value of 0.05 mg/L for the light catalytic cracked gas oil sample was the lowest among the chronic effect endpoints and may be used as the chronic NOELR for the category.

Human Health Effects: .
Gas Oil streams and fuels induce minimal acute toxicity by the oral, dermal and inhalation routes. Moderate to severe skin irritation has been reported with 24 hour exposure which is likely to be mild to moderate under 4 hour exposure conditions recommended for classification purposes. No dermal sensitization has been reported. Eye irritation was minimal to slight.

Many but not all Gas Oils can induce gene mutation in bacterial and mammalian cells as demonstrated in both standard *in vitro* assays and the Optimized Ames Test. Compounds with high levels of 1-7 ring PACs are mutagenic while those with very low aromatic content are weakly mutagenic or inactive. Overall, the weight of evidence from studies for chromosome aberrations or micronucleus formation indicate that gas oils generally do not cause cytogenetic damage in animals

The 13-week rat dermal studies on gas oil streams indicate LOAEL of 125mg/kg with the exception of a light coker gas oil with a LOAEL of 30mg/kg, the lowest dose tested, effects likely exacerbated by severe skin irritation at all dose levels. Skin irritation in most studies generally ranged from slight to moderate. NOAELs ranged from 25-30mg/kg with the exception of an ultralow sulfur diesel fuel containing a very low content of DMSO extractable aromatic hydrocarbons and a NOEL = 600mg/kg, the highest dose tested. Effects when present were seen in organ weights primarily liver, thymus with no histopathologic correlates and hematology parameters. The 4 week duration rat dermal studies showed slight to moderate skin irritation

and minimal systemic toxicity with NOAEL = 400-800mg/kg. No significant adverse effects were seen in reproductive organs in any rat dermal study.

Results of developmental studies with gas oils demonstrate that some gas oils induce developmental effects and others do not. Substances tested in the Gas Oil Category had developmental LOAEL ranging from 125 – 500mg/kg attributed primarily to fewer live fetuses or pups per litter at delivery and lower fetal or pup body weight at delivery or Lactation days 0-4, respectively seen only at doses that were maternally toxic. NOAELs ranged from 30 – 600mg/kg. Fetal malformations were reported for 2 members of the category, CAS RN 64741-43-1 [F-192, intermediate gas oil] and CAS RN 64741-49-7 [Vacuum Tower Overheads]. Ultralow sulfur diesel, a stream with a very low concentration of DMSO extractable aromatic hydrocarbons demonstrated virtually no maternal or developmental toxicity at doses up to 600mg/kg. Other gas oils showed no developmental toxicity at the highest doses tested even in the presence of maternal toxicity.

Reproductive parameters in developmental toxicity studies addressing fertility, successful insemination and implantation demonstrate that in general these endpoints are not adversely affected by treatment with gas oil streams. Three studies in which females were treated dermally for a week prior to mating through mating and gestation demonstrated that exposure to high concentrations of several gas oils did not adversely affect mating and establishment of pregnancy but did affect successful completion of pregnancy and pup viability at maternally toxic doses of 250mg/kg and above. Evaluation of reproductive organs and sperm morphology and motility from 13-week repeated dose studies consistently demonstrated no adverse effects on ovary or testes weights, no abnormal histopathology or no effects on sperm at doses ranging up to 500-820mg/kg/day. The NOAEL for reproductive toxicity is not expected to be lower than the NOAEL for developmental toxicity because the most sensitive endpoints in either developmental or reproductive toxicity studies are expected to be effects on fetal survival and growth resulting from *in utero* exposure.

Overall, for dermal repeated dose and developmental toxicity, effects appear to be related to aromatic content. The systemic effects seen in repeated dose studies may be considered generalized responses to total aromatics either adaptive or minimally toxic and reversible while effects in developmental studies are more associated with aromatics containing a higher distribution of 3 or more rings. Effects of developmental toxicity seem to require higher doses than seen in systemic toxicity studies and may not be induced even at doses that are systemically toxic to pregnant females.

The reported repeat dose dermal toxicity and developmental toxicity studies provide a spectrum of effects from virtually non-toxic for streams with minimal DMSO extractable PAC content (e.g. Ultralow sulfur diesel fuel CAS RN 68334-30-5) to streams with higher 1-3+ aromatic ring content which can be characterized as the potentially more hazardous of this category (e.g. light coker gas oil (CAS RN 64741-82-8) or light cycle oils CAS RN 64741-59-9)

Inhalation Studies: Two 4 week repeat dose inhalation studies with samples of hydrodesulfurized distillates and one developmental toxicity study with a marketplace sample of diesel fuel [CAS RN 68476-34-6] did not show any significant substance induced effects. In the inhalation studies with hydrodesulfurized distillates at a single dose of 25mg/m^3, minimal systemic effects and some inflammation of respiratory tissue were seen. In the developmental study presumed-pregnant rats were exposed to nominal atmospheric concentrations of diesel

fuel at 100 and 400 ppm for 6 hours each day from GD6-15. No adverse effects were seen on reproductive or developmental parameters or in soft tissue or skeletons of the fetuses.

Dermal carcinogenesis studies indicate that gas oils and distillate fuels are potential skin carcinogens after repeated skin application but dermal application is not associated with the induction of non-metastatic systemic tumors. The skin carcinogenicity of the petroleum streams with high boiling ranges has been demonstrated to correlate with 3-7 ring PAC content. Skin tumors produced by substances in this category containing low or no PAC are likely due to a non-genotoxic promotion effect and only observed in the presence of sustained severe skin irritation.

Human Exposure

Because the No. 2 distillate fuels have widespread use in transportation and industrial and residential heating applications, both occupational and consumer exposures are possible. Exposure to children is not anticipated. The other substances in the Gas Oil Category are only used in industrial applications.

In conclusion, the information provided in this Gas Oils Category Assessment Document is sufficient to characterize the SIDS endpoints for physiochemical properties, environmental fate, ecotoxicity, and human health hazards of gas oil refinery streams and distillate fuels.

9.0 MATRICES OF GAS OIL CATEGORY DATA

9.1 Data Matrix for Gas Oils: Physical Chemical Properties, Environmental Fate and Environmental Effects

Endpoint		Measured Results	Predicted Results
Physical Chemical Properties			
Melting Point (°C)		No sharply defined melting points	
Pour Point (°C)		approximate range of -50°C to 0°C.	
Freezing Point (°C)		NA	NA
Boiling Point (°C)		approximately within the range 150°C to 450°C (302° F to 842° F).	Gas oils do not have a single numerical value for boiling point, but rather a boiling or distillation range that reflects the individual components in the complex hydrocarbon substance. CONCAWE (1996) provided a boiling range of 150°C to 450°C (302° F to 842° F) as a general distribution for this category. Ranges for specific streams or products vary depending on the refinery processes used and sources of the feedstocks.
Vapor Pressure		approximate range of 0.4 kPa to 2 kPa when measured at approximately 40°C.	
Partition Coefficient Log Kow		The partition coefficients of individual constituent hydrocarbons found in gas oils can be expected to cover the range of 3.3 to >6.	
Water Solubility[1] (mg/L)		Individual water solubility may range from essentially insoluble (e.g., <0.001 mg/L) to 52 mg/L, depending on the molecular structure.	Precise measurements of water solubility for complex substances such as gas oils are complicated by factors such as the sensitivity of the analytical method and the water-to-oil ratio. When the ratio is optimized to achieve maximum hydrocarbon concentrations, measurements have ranged from 2.05 mg/L to 8.7 mg/L. Solubility values of individual constituents in gas oils vary widely due to the wide range of molecular weights.
Environmental Fate			

Endpoint		Measured Results	Predicted Results
Photodegradation, OH^- reaction $T_{1/2}$ (h or d)			Direct photodegradation is not likely to be an important fate process for gas oils due to their relatively low concentrations of photosensitive constituents. Indirect photodegradation will be an important degradation pathway for constituents that volatilize to the atmosphere
Stability in Water			Substances in this category will be stable and not react with water. Constituent compounds do not contain chemical moieties that undergo hydrolysis.
Transport between Environmental Compartments			The low molecular weight constituents in gas oils will tend to partition to the air. As molecular weight increases, partitioning shifts to the soil compartment.
Biodegradation classification		Inherently biodegradable	Although gas oils may not pass criteria for ready biodegradability, current data show that biodegradation rates may be high, and these substances are considered inherently biodegradable. Depending on the sample tested, some gas oils may achieve rates biodegradation rates that pass the criteria for ready biodegradability classification.
Environmental Effects			
Acute Fish LL50 (mg/L WAF loading rate)		>0.3 mg/L – 65 mg/L	The distillate fuels and refinery streams in the gas oil category are expected to elicit acute aquatic toxicity to fish in the range >0.3 mg/L to 65 mg/L on the basis of the loading rates used to prepare WAF exposure solutions. The lowest 96-h LL50 predicted by the PETROTOX model was 0.18 mg/L.
Acute Daphnia EL50 (mg/L WAF loading rate)		0.5 mg/L – 210 mg/L	The distillate fuels and refinery streams in the gas oil category are expected to elicit acute aquatic toxicity to invertebrates in the range 0.5 mg/L to 210 mg/L on the basis of the loading rates used to prepare WAF exposure solutions. The lowest 48-h EL50 predicted by the PETROTOX model was 0.35 mg/L.
Algae E_bL50/E_rL50 (mg/L WAF loading rate) *Pseudokirchneriella subcapitata*		0.28 mg/L – 25 mg/L for biomass-based endpoints 0.53 mg/L – 78 mg/L for growth rate-based endpoints	The distillate fuels and refinery streams in the gas oil category are expected to elicit aquatic toxicity to algae in the range 0.28 mg/L to 25 mg/L on the basis of algal biomass and 0.53 mg/L to 78 mg/L on the basis of algal growth rate when endpoints

Endpoint		Measured Results	Predicted Results
			are expressed as loading rates used to prepare WAF exposure solutions. The lowest 96-h EL50 predicted by the PETROTOX model was 0.35 mg/L.
Chronic Fish LL50 (mg/L WAF loading rate)		CAS No. 68476-30-2, No. 2 fuel oil *O. mykiss WAF* Endpoint value Loading rate 28d LL_{50} = 2.7mg/L LOELR $_{(growth)}$ = 3.0 mg/L NOELR $_{(growth)}$ = 1.2mg/L Endpoint value (uM/mL PDMS) 28d LC50 = 24.4 LOEC $_{(growth)}$ = 26.4 NOEC $_{(growth)}$ = 13.7	The no-observed-effect loading rate for chronic toxicity of blended middle distillate fuels to fish is expected to be approximately 1.2 mg/L.
Chronic Daphnia EL50 (mg/L WAF loading rate)		21d EL_{50} = 0.24mg/L LOELR $_{(reproduction)}$ = 0.10 mg/L $NOELR_{(reproduction)}$ =0.05mg/L Endpoint value (uM/mL PDMS) 21d EC50 > 7.24 LOELR $_{(reproduction)}$ = 7.24 NOELR $_{(reproduction)}$ = 3.09	The no-observed-effect loading rate for chronic toxicity of blended middle distillate fuels to aquatic invertebrates is expected to be approximately 0.05 mg/L. The lowest 21-d $NOELR_{(reproduction)}$ predicted by the PETROTOX model was 0.06 mg/L.

WAF = Water Accommodated fraction

9.2 Data Matrix for Gas Oils: Human Health Effects

CAS RN	Acute Oral Rat (mg/kg)	Acute Dermal Rabbit (mg/kg}	Acute Inhalation Rat (mg/L)	Repeated Dose LOAEL/NOAEL (mg/kg) Rats	Genetic Toxicity *In vitro*	Genetic Toxicity- *In vivo*	Developmental Toxicity Dermal LOAEL/NOAEL (mg/kg) [1]	Reproductive toxicity [2]
Read Across Values for Untested Substances	LD_{50} ≥5000 LD_{50} ≥ 9.0ml/kg	LD_{50} >2000 LD_{50} > 5.0ml/kg	LC_{50} = 1.8 to 7.6	13 week Dermal LOAEL = 30 to 500 NOAEL ≤ 30 to 600	Considered positive with metabolic activation unless composition low in PAC	All CAS RN are considered for negative for cytogenetic effects.	LOAEL = 125 to 500 NOAEL = 30 to 600	Developmental toxicity values can be read across
64741-59-9	[2 samples] LD_{50} ♂ = 4700 to 7200 LD_{50} ♀ = 3200 to 6800	[2 samples] LD_{50} >2000	[2 samples] 4.4 to 5.4	13 week Dermal [2 samples] LOAEL ♂ = 125 NOAEL ♂ = 25 LOAEL ♀ = 500 NOAEL ♀ = 125 LOAEL = 450 NOAEL = 100	Positive Mouse lymphoma Optimized Ames: 9 samples positive; 3 negative	Negative chromosome aberrations	[3 samples] LOAEL = 333 to 500 NOAEL = 50 to 250	
64741-43-1				4 week Dermal LOAEL > 460 NOAEL = 460 [highest dose tested]			LOAEL = 250 NOAEL = 50	
64741-44-2	LD_{50} >5000	LD_{50} >2000	1.78		Positive Optimized Ames			
64741-49-7				13 week Dermal LOAEL = 125 NOAEL = 30	Positive Optimized Ames	Negative micronucleus	LOAEL = 125 NOAEL = 30	
64741-77-1				4 week Dermal LOAEL > 820 NOAEL = 820				

CAS RN	Acute Oral Rat (mg/kg)	Acute Dermal Rabbit (mg/kg}	Acute Inhalation Rat (mg/L)	Repeated Dose LOAEL/NOAEL (mg/kg) Rats	Genetic Toxicity *In vitro*	Genetic Toxicity- *In vivo*	Developmental Toxicity Dermal LOAEL/NOAEL (mg/kg) [1]	Reproductive toxicity [2]
				[highest dose tested]				
64741-82-8				13 week Dermal LOAEL = 30 NOAEL < 30 [lowest dose tested]	Positive Optimized Ames	Negative micronucleus	[2 samples] LOAEL ≥ 250 NOAEL > 100 to 250	
64741-86-2				4 week Dermal LOAEL = 820 NOAEL = 410	Negative Optimized Ames		LOAEL > 500 NOAEL = 500 [highest dose tested	
64742-46-7						Negative, oral chromosomes, dominant lethal; Positive ip chromosomes		
64742-80-9	[2 samples] LD_{50} >5000	[2 samples] LD_{50} >2000	[2 samples] 4.60 – 7.64		Positive			
68334-30-5				13 week Dermal LOAEL **>** 600 NOAEL =600, highest dose tested	Optimized Ames 23 samples positive; 4 negative		[3 samples] LOAEL = 250 to > 600 NOAEL = 125 to 600	
68476-34-6	LD_{50} = 9.0ml/kg	LD_{50} >5.0ml/kg		4 week Inhalation LOAEL = 0.5ml/kg NOAEL < 0.5ml/kg	Negative Ames, mouse lymphoma			
68476-30-2					Positive Optimized Ames, mouse lymphoma	Negative Micronucleus		
68576-30-2	[3 samples]	[3 samples] LD_{50}						

CAS RN	Acute Oral Rat (mg/kg)	Acute Dermal Rabbit (mg/kg}	Acute Inhalation Rat (mg/L)	Repeated Dose LOAEL/NOAEL (mg/kg) Rats	Genetic Toxicity *In vitro*	Genetic Toxicity- *In vivo*	Developmental Toxicity Dermal LOAEL/NOAEL (mg/kg) [1]	Reproductive toxicity [2]
	LD_{50} = 14.5 to 21.2ml/kg	>5.0ml/kg						
68915-97-9				13 week Dermal LOAEL = 125 NOAEL = 30	Positive Optimized Ames		LOAEL = 125 NOAEL = 30	

1-Read across for developmental effects reflects range of developmental LOAEL/NOAEL for studies which include treatment from GD 0-19 or 20, killed on GD20 or maintained untreated to Lactation day 4.

2 -The NOAEL for reproductive toxicity is not expected to be lower than the NOAEL for developmental toxicity because the most sensitive endpoints in either developmental or reproductive toxicity studies are expected to be effects on fetal survival and growth resulting from *in utero* exposure.

10. References

AAM (Alliance of Automobile Manufacturers). 2008. Summer survey diesel samples collected for 2008; fuel quality. Note: AAM analytical results are proprietary and can be purchased directly from AAM. AAM, Washington, DC.

Altgelt, K. and Boduszynski, M. 1994. Composition and Analysis of Heavy Fractions, Marcel Dekker, Inc.

Ames, B.N., McCann, J., and Yamasaki, E. Methods for detecting carcinogens and mutagens with the *Salmonella*/mammalian-microsome mutagenicity test. Mutat Res. 31: 347 –364

Anderson, J.W., J.M. Neff, B.A. Cox, H.E. Tatem, and G.M. Hightower. 1974. Characteristics of dispersions and water-soluble extracts of crude and refined oils and their toxicity to estuarine crustaceans and fish. Mar. Biol. 27:75-88

ACC (American Chemical Council). 2006. A comparison of the environmental performance of olefin and paraffin synthetic base fluids (SBF). Higher Olefins Advocacy Task Group, ACC. November 2006. URL: www.americanchemistry.com

API (American Petroleum Institute). 1978. Mutagenicity evaluation of diesel fuel. API Med. Res. Publ. 26-60102, Washington D.C.

API (American Petroleum Institute). 1979a. In-vitro and in-vivo mutagenicity studies No. 2 home heating oil sample API 78-4. API Med. Res. Publ. 27-30140, Washington D.C.

API (American Petroleum Institute). 1979b. Teratology study in rats, diesel fuel. API Med. Res. Publ. 27-32174, Washington D.C.

API (American Petroleum Institute). 1980a. Acute toxicity tests on API 78-2 No. 2 home heating oil (30% cat) primary dermal irritation, primary eye irritation, skin sensitization, acute dermal toxicity, acute oral toxicity, subacute dermal toxicity. API Report No. 27-32771, Washington D.C.

API (American Petroleum Institute). 1980b. Acute toxicity tests on API 78-3 No. 2 home heating oil (10% cat) primary dermal irritation, primary eye irritation, skin sensitization, acute dermal toxicity, acute oral toxicity, subacute dermal toxicity. API Report No. 27-32773, Washington D.C.

API (American Petroleum Institute). 1980c. Acute toxicity tests on API 78-4 No. 2 home heating oil (50% cat) primary dermal irritation, primary eye irritation, skin sensitization, acute dermal toxicity, acute oral toxicity, subacute dermal toxicity. API Report No. 27-32068, Washington D.C.

API (American Petroleum Institute). 1980d. Acute toxicity tests on API 79-6, diesel fuel (market place sample). API Med. Res. Publ. 27-32817, Washington D.C.

API (American Petroleum Institute). 1980e. Mutagenicity evaluation of diesel fuel in the mouse dominant lethal assay. API Med. Res. Publ. 28-31346, Washington D.C.

API (American Petroleum Institute). 1982a. Acute oral toxicity study in rats, acute dermal study in rabbits, primary dermal irritation study in rabbits, primary eye irritation study in rabbits, dermal sensitization study in guinea pigs API 83-07, light catalytically cracked distillate CAS 64741-59-9. API Med. Res. Publ. 33-30162, Washington D.C.

API (American Petroleum Institute). 1982b. 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 81-09, hydrodesulfurized middle distillate. API Med. Res. Publ. 30-32347, Washington D.C.

API (American Petroleum Institute). 1982c. 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 81-10, hydrodesulfurized middle distillate. API Med. Res. Publ. 30-32348, Washington D.C.

API (American Petroleum Institute). 1983a. LC50 acute inhalation toxicity evaluation of a petroleum derived hydrocarbon in rats, API 81-09, hydrodesulphurized middle distillate. API Med. Res. Publ. 30-32856, Washington D.C.

API (American Petroleum Institute). 1983b. LC50 acute inhalation toxicity evaluation of a petroleum derived hydrocarbon in rats, API 81-10, hydrodesulfurized middle distillate. API Med. Res. Publ. 30-32857, Washington D.C.

API (American Petroleum Institute). 1984a. Mutagenicity evaluation in the rat bone marrow cytogenetic assay and the mouse lymphoma forward mutation assay API 81-10, hydrodesulfurized middle distillate. API Med. Res. Publ. 32-30535, Washington D.C.

API (American Petroleum Institute). 1984b. Dermal sensitization study in guinea pigs, closed patch technique, API 81-09, hydrodesulfurized middle distillate. API Report No. 31-31352, Washington D.C.

API (American Petroleum Institute). 1984c. Dermal sensitization study in guinea pigs, closed patch technique, API 81-10, hydrodesulfurized middle distillate. API Report No. 31-31414, Washington D.C.

API (American Petroleum Institute). 1985a. 28-Day dermal toxicity study in the rabbit, API 83-07 Light catalytically cracked distillate (CAS 64741-59-9). API Med. Res Publ. 32-32751, Washington D.C.

API (American Petroleum Institute). 1985b. Activity of API 83-08 in the acute in-vivo cytogenetic assay in male and female rats, TEM CAS No. 51-18-3. API Med. Res. Publ. 33-30493, Washington D.C.

API (American Petroleum Institute). 1985c. Acute in-vivo cytogenetics assay in male and female rats of API 83-11. API Med. Res. Publ. 32-32408, Washington D.C.

API (American Petroleum Institute). 1985d. 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 83-08 Light catalytically cracked distillate (CAS 64741-59-9). API Med. Res. Publ. 32-32859, Washington D.C.

API (American Petroleum Institute). 1985e. 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 83-11, straight run middle distillate. API Med. Res. Publ. 32-32857, Washington D.C.

API (American Petroleum Institute). 1985f. L5158Y TK+/- Mouse lymphoma mutagenesis assay of API 83-08. API Med. Res. Publ. 32-31709, Washington D.C.

API (American Petroleum Institute). 1985g. L5178Y TK+/- Mouse lymphoma mutagenesis assay of API 83-11. API Med. Res. Publ. 32-31768, Washington DC.

API (American Petroleum Institute). 1985h. Mutagenicity evaluation in the rat bone marrow cytogenetic assay and the mouse lymphoma forward mutation assay API 81-09, hyrodesulfurized middle distillate. API Med. Res. Publ. 32-30965, Washington D.C.

API (American Petroleum Institute). 1985i. Mutagenicity evaluation of API 83-07 in the mouse lymphoma forward mutation assay. API Med. Res. Publ. 32-32167, Washington D.C.

API (American Petroleum Institute). 1985j. Mutagenicity evaluation of API 83-11 in the mouse lymphoma forward mutation assay. API Med. Res. Publ. 32-32166, Washington D.C.

API (American Petroleum Institute). 1986a. Acute inhalation toxicity evaluation in rats, API 83-07, light catalytic cracked distillate CAS No. 64741-59-9. API Med. Res. Publ. 33-30549, Washington D.C.

API (American Petroleum Institute). 1986b. Acute inhalation toxicity evaluation in rats, API 83-08, light catalytic cracked distillate CAS No. 64741-59-9. API Med. Res. Publ. 33-30444, Washington D.C.

API (American Petroleum Institute). 1986c. Mutagenicity evaluation in the rat bone marrow cytogenetic assay API 83-11, Straight run middle distillate (CAS 64741-44-2). API Med. Res. Publ. 33-30930, Washington D.C.

API (American Petroleum Institute). 1986d. Mutagenicity in a mouse lymphoma mutation assay API 81-10, hydrodesulfurized middle distillate CAS No. 64742-80-9. API Med. Res. Publ. 33-31224, Washington D.C.

API (American Petroleum Institute). 1986e. Mutagenic evaluation in the rat bone marrow cytogenetic assay, API 83-07 Light catalytically cracked distillate (CAS 64741-59-9). API Med. Res. Publ. 33-30929, Washington D.C.

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

API (American Petroleum Institute). 1987a. Acute inhalation toxicity evaluation of a petroleum derived hydrocarbon in rats, API 83-11 Straight run middle distillate (CAS 64741-44-02). API Med. Res. Publ. 34-30635, Washington D.C.

API (American Petroleum Institute). 1987b. Mutagenicity of API 81-10 ARO. aromatic fraction of hydrodesulfurized middle distillate (CAS 64742-80-9) (coded as API 86-10 ARO) in a mouse lymphoma mutation assay. API Med. Res. Publ. 34-32644, Washington D.C.

API (American Petroleum Institute). 1987c. Mutagenicity of API 81-10 SAT. saturated fraction of hydrodesulfurized middle distillate (CAS 64742-80-9) (coded as API 86-10 SAT) in a mouse lymphoma mutation assay. API Med. Res. Publ. 34-32645, Washington D.C.

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

API (American Petroleum Institute). 1987e. Mutagenicity of API 81-10, hydrodesulfurized middle distillate CAS No. 64742-80-9. API Med. Res. Publ. 34-32643, Washington D.C.

API (American Petroleum Institute). 1988a. In-vivo sister chromatid exchange assay, API 81-10 hydrodesulfurized middle distillate. API Med. Res. Publ. 35-32479, Washington D.C.

API (American Petroleum Institute). 1988b. Sister chromatid exchange assay in Chinese hamster ovary (CHO) cells with API 83-07: Light catalytic cracked distillate. API Med. Res. Publ. 35-32432, Washington D.C.

API (American Petroleum Institute). 1988c. Sister chromatid exchange assay in Chinese hamster Ovary (CHO) cells with API 81-10 hydrodesulfurized middle distillate: Final Report. API Med. Res. Publ. 35-32433, Washington D.C.

API (American Petroleum Institute). 1989. In vivo sister chromatid exchange assay with API 83-07 (light catalytic cracked distillate). API Med. Res. Publ. 36-31429, Washington D.C.

API (American Petroleum Institute). 2005. Test Plan – Gas Oils Category. Test Plan Submitted to the EPA by the Petroleum HPV Testing Group, December 16, 2005. Consortium Number 1100997, API, Washington, DC.

API (American Petroleum Institute). 2008. PAC Analysis Task group. The relationship between the aromatic ring class content and selected endpoints of repeat-dose and developmental toxicity of high-boiling petroleum substances. http://www.petroleumhpv.org.

ARCO, 1986. Twenty-eight day dermal toxicity study in rat on Watson Cherry Point diesel fuel number 2. (F-75-01). Study No. 60764. UBTL Inc. Salt Lake City, USA. Performed at UBTL Inc. Study No. 60764, Salt Lake City, UT

ARCO 1992a. Twenty-eight (28) day dermal toxicity study in rats administered test article F-188. Report No ATX -91-0094. performed at UBTL Inc. Study No. 66197, Salt Lake City, UT

ARCO 1992b. Twenty-eight (28) day dermal toxicity study in rats administered test article F-130. Report No ATX -90-0050. performed at UBTL Inc. Salt Lake City, UT

ARCO 1993a. Twenty-eight (28) day dermal toxicity study in rats administered test article F-233. Report No ATX -91-0233 performed at UBTL Inc. Salt Lake City, USA.

ARCO. 1993b. Developmental Toxicity (Embryo-Fetal Toxicity and Teratogenic Potential) Study of F-193 Administered Percutaneously to Crl:CD®BRK VAF/Plus® Presumed Pregnant Rats. 1993. Report ATX-92-0011.

ARCO. 1993c. Developmental Toxicity (Embryo-Fetal Toxicity and Teratogenic Potential) Study of F-199 Administered Percutaneously to Crl:CD®BRK VAF/Plus® Presumed Pregnant Rats. 1993. Report ATX-92-0013.

ARCO. 1993d. Developmental Toxicity (Embryo-Fetal Toxicity and Teratogenic Potential) Study of F-195 Administered Percutaneously to Crl:CD®BRK VAF/Plus® Presumed Pregnant Rats. Report ATX-92-0156.

ARCO. 1994a. A Developmental Toxicity Screen in Female Sprague-Dawley Rats Administered F-213 Dermally During GD 0 to 20. Report ATX-91-0262

ARCO. 1994b. A Developmental Toxicity Screen in Female Sprague-Dawley Rats Administered F-193 Dermally During Gestation Days -7 to 20. 1994. Report ATX-91-0127

ARCO. 1994c. A Developmental Toxicity Screen in Female Sprague-Dawley Rats Administered F-195 Dermally During Gestation Days 0 to 20. 1994. Report ATX-91-0129.

ARCO. 1994d. A Developmental Toxicity Screen in Female Sprague-Dawley Rats Administered F-199 Dermally During Gestation Days -7 to 20. 1994. Report ATX-91-0133.

ARCO. 1994e. A Developmental Toxicity Screen in Female Rats Administered F-277 Dermally During GD -7 to 20. 1994. Report ATX-93-0075.

ARCO. 1994f. A Developmental Toxicity Screen in Female Rats Administered F-233 Dermally During GD 0 to 20. 1994. Report ATX-91-0133.

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). 2001. 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.

ASTM (American Society for Testing and Materials) Standard D2889-95. 2010. "Standard test method for calculation of true vapor pressures of petroleum distillate fuels," ASTM International, West Conshohocken, PA, www.astm.org.

ASTM (American Society for Testing and Materials) Standard D323-08, “Standard test method for vapor pressure of petroleum products (Reid Method),” ASTM International, West Conshohocken, PA, www.astm.org.

Atkinson, R. 1990. Gas-phase tropospheric chemistry of organic compounds: A review. Atmos. Environ. 24A(1):1-41.

ATSDR (Agency for Toxic Substances and Disease Registry). 1995. Toxicological Profile for Fuel Oils

Battersby, N.S., et al. 1992. A correlation between the biodegradability of oil products in the CEC L-33-T-82 and modified Sturm tests. Chemosphere. 24:1989-2000. (As cited in CONCAWE, 1996).

Boopathy, R. 2004. Anaerobic biodegradation of no. 2 diesel fuel in soil: a soil column study. Biorsour Technol 94:143-151.

Boopthy, R., S. Shields, and S. Nunna. 2012. Biodegradaton of crude oil from the BP oil spill in the marsh sediments of Southeast Louisiana, USA. Appl Biochem Biotechnol [Epub ahead of print]

Brown, M. 1989. Biodegradation of oil in freshwater. In: The Fate and Effects of Oil in Freshwater. Green and Trett, eds. Elsevier, London.

Castano, A., N. Bols, T. Braunbeck, P. Dierick, M. Halder, B. Isomaa, K. Kawahara, L.E.J. Lee, C. Mothersill, P. Part, G. Repetto, J. Riego Sintes, H. Rufli, R. Smith, C. Wood, and H. Segner. 2003. The use of fish cells in ecotoxicology. Altern. Lab. Anim. 31:317-351.

Clark, R.H., Battersby, N. S., Louis, J.J.J., Palmer, A.P., Stradling, R.J and Whale, G.F. 2003. The Environmental Benefits of Shell GTL Diesel: Proceedings of the 4th Int. Colloquium, "Fuels". Tech. Akad. Esslingen, Ostfilern, Germany, January 15-16.

ChevronTexaco. 2003. A schematic layout of a modern, fully integrated refinery, http://www.chevron.com/prodserv/fuels/bulletin/diesel/L2_4_2_fs.htm.

CONCAWE. 1991. Middle distillates - a review of the results of a CONCAWE programme of short-term biological studies. CONCAWE, Brussels.

CONCAWE. 1996. Gas oils (diesel fuels/heating oils). Product Dossier No. 95/107. CONCAWE, Brussels.

CONCAWE. 1996. Environmental risk assessment of petroleum substances: the hydrocarbon block method. Report no. 96/52. CONCAWE, Brussels, Belgium.

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

CONCAWE, 2006. Human exposure information for EU substance risk assessment of gas oils. Prepared for the CONCAWE Health Management Group by its Special Task Force H/STF-29. Report No. 01/06. CONCAWE, Brussels.

CONCAWE. 2007. PETRORISK users guide, version 3.01. CONCAWE, Brussels, Belgium.

Connell, D.W., and G.J. Miller. 1980. Petroleum Hydrocarbons in Aquatic Ecosystems – Behavior and Effects of Sublethal Concentrations: Part I in: Critical Reviews in Environmental Control. pp. 37 – 104. C.P. Straub, ed. CRC Press, Boca Raton, Florida.

Cronin, M.T.D., J.D. Walker, J.S. Jaworska, M.H.I. Comber, C.D. Watts, and A.P. Worth. 2003. Use of AWARs in international decision-making frameworks to predict ecologic effects and environmental fate of chemical

Crump, K. 1984. A new method for determining allowable daily intakes. Fund. Appl. Toxicol. 4: 854-871.

Di Toro, D.M., J.A. McGrath, and D.J. Hansen. 2000. Technical basis for narcotic chemicals and polycyclic aromatic hydrocarbon criteria. I. Water and tissue. Environmental Toxicology and Chemistry 19: 1951-1970.

DGMK (Deutsche Wissenschaftliche Gesellschaft fur Erdol, Erdgas und Kohle -German Research Organization for Oil, Gas and Coal). 1991. Middle distillates: Analytical investigations and mutagenicity studies. Research Report 412-1. DGMK, Hamburg, Germany.

DGMK (Deutsche Wissenschaftliche Gesellschaft fur Erdol, Erdgas und Kohle (German Research Organization for Oil, Gas and Coal). 1993. Middle distillates: Dermal Initiation // Promotion study. Research Report 412-2 DGMK. Hamburg, Germany.

ECVAM (European Centre for the Validation of Alternative Methods. 2006. Statement on the scientific validity of the upper threshold concentration (UTC) step-down approach – a new testing strategy to reduce the use of fish in acute aquatic toxicity testing. European Commission, Joint Research Centre, Institute for Health and Consumer Protection, ECVAM. 24th Meeting, 20-21 March 2006.

EPA (U.S. Environmental Protection Agency). 1999. Guidance for Assessing Adequacy of Existing Data, http://www.epa.gov/chemrtk/guidocs.htm

EPA (U.S. Environmental Protection Agency.) 1999. Determining the Adequacy of Existing Data. http://www.epa.gov/chemrtk/datadfin/htm

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

Exxon (Exxon Biomedical Sciences, Inc.). 1994. Internal test summary for Water Insoluble Biodegradation Test Method Development Using Concawe Reference Gas Oil:Phase III.

Exxon (Exxon Biomedical Sciences Inc.). 1996a. Two year dermal carcinogenicity study of middle distillates in mice: Final report. Project No. 117811A.

Exxon (Exxon Biomedical Sciences, Inc.). 1996b. Primary dermal irritation study in the rabbit, test materials MD-6 and MD-7: Final report. Project No. 117904A. Study performed for CONCAWE.

Exxon (Exxon Biomedical Sciences Inc.). 1998a. Acute toxicity of water accommodated fractions to Skeletonema costatum. Study #142967SK.

Exxon (Exxon Biomedical Sciences, Inc.). 1998b. Acute Fish Toxicity Test with *Menidia beryllina*. Study #142940MB.

Exxon (Exxon Biomedical Sciences, Inc.). 1998c. Rainbow Trout Acute Fish Toxicity Test. Study #142958.

Exxon (Exxon Biomedical Sciences, Inc.). 1998d. Sheepshead Minnow Acute Fish Toxicity Test. Study #142961.

Exxon (Exxon Biomedical Sciences Inc.). 1998e. Acute toxicity of water accommodated fractions to *Selenastrum capricornutem*. Study #142967

Exxon Biomedical Sciences Inc. (EBSI). 1998e. Acute toxicity of water accomodated fractions to *Skeletonema costatum*. Study #142967SK

Exxon (Exxon Biomedical Sciences, Inc.). 1999. Fathead Minnow Acute Fish Toxicity Test. Study #142940FHM.

Exxon (Exxon Biomedical Sciences, Inc.). 2001. Static Daphnid Acute Toxicity Test . Study #146342A.

ExxonMobil Biomedical Sciences Inc. (EMBSI). 2004a. Fish Juvenile Growth Test. Study #146365.

ExxonMobil Biomedical Sciences Inc. (EMBSI). 2004b. *Daphnia magna* Reproduction Test. Study # 146346.

ExxonMobil Biomedical Sciences Inc. (EMBSI) 2010a. *Daphnia magna*, Acute Immobilisation Test on Water Accommodated Fractions of a Light Hydrocracked Gas Oil. Final Report, Study No. 1057742, EMBSI, Annandale, NJ USA.

ExxonMobil Biomedical Sciences Inc .(EMBSI). 2010b. *Daphnia magna*, Acute Immobilisation Test on Water Accommodated Fractions of a Light Catalytic Cracked Gas Oil. Final Report, Study No. 1057642, EMBSI, Annandale, NJ USA.

ExxonMobil Biomedical Sciences Inc (EMBSI) 2011a. Ready biodegradability: OECD 301F manometric respirometry test of light catalytic cracked gas oil. Final report, study no. 1057679, EMBSI, Annandale, NJ.

ExxonMobil Biomedical Sciences Inc (EMBS) 2011b. Ready biodegradability: OECD 301F manometric respirometry test of light hydrocracked gas oil. Final report, study no. 1057779, EMBSI, Annandale, NJ.

ExxonMobil Biomedical Sciences Inc. (EMBSI) 2011c. *Oncorhynchus mykiss*, Fish Acute Toxicity Test on Water Accommodated Fractions of a Light Hydrocracked Gas Oil. Final Report, Study No. 1057658, EMBSI, Annandale, NJ USA.

ExxonMobil Biomedical Sciences Inc. (EMBSI) 2011d. *Oncorhynchus mykiss*, Fish Acute Toxicity Test on Water Accommodated Fractions of a Light Hydrocracked Gas Oil. Final Report, Study No. 1057758, EMBSI, Annandale, NJ USA

ExxonMobil Biomedical Sciences Inc. .(EMBSI) 2011e. Alga, Growth inhibition test on water accommodated fractions of a light hydrocracked gas oil. Final Report, Study No. 1057767, EMBSI, Annandale, NJ USA.

ExxonMobil Biomedical Sciences Inc. .(EMBSI) 2011f. Alga, Growth inhibition test on water accommodated fractions of a light catalytic gas oil. Final Report, Study No. 1057667, EMBSI, Annandale, NJ USA.

ExxonMobil Biomedical Sciences Inc. (EMBSI) 2012a. Daphnia magna, Reproduction test on water accommodated fractions of a light hydrocracked gas oil. Final Report, Study No. 1057746, EMBSI, Annandale, NJ USA.

ExxonMobil Biomedical Sciences Inc. .(EMBSI) 2012b. Daphnia magna, Reproduction test on water accommodated fractions of a light catalytic cracked gas oil. Final Report, Study No. 1057646, EMBSI, Annandale, NJ USA.

Fasnacht, M.P. and Blough, N.V. 2002. Aqueous photodegradation of polycyclic aromatic hydrocarbons. Environ. Sci. Technol. 36:4364-4369.

Feuston, M. H., Low, L. K., Hamilton, C. E and Mackerer, C.R. 1994. Correlation of systemic and developmental toxicities with chemical component classes of refinery streams. Fund. Appl. Toxicol. Vol 22, pp 622-630.

Fraunhofer-Institut, Umweltchemie und Okotoxikologie. 2000. *Daphnia magna*, Acute Immobiliation Test with Gas oil WAFs. GLP-Code: DGM-001/4-20.

Freeman, J., and McKee, R. (1993). The objectives and goals of dermal carcinogenicity testing of petroleum liquids. In: Health Risk Assessment. Dermal and Inhalation Exposure and Absorption of Toxicants. R. Wang, J. Knaak and H. Maibach, eds., CRC Press, Boca Raton, Fl. pp. 283-290.

Girling, A.E., Markarian, R.K., and Bennett, D.. 1992. Aquatic toxicity testing of oil products – some recommendations. Chemosphere 24(10):1469-1472.

Gift, J., Howard, A., and Zhao, J. 2011. Benchmark dose modeling and its use in Risk Assessment. http://www.epa.gov/ncea/bmds/training/capitivate/bmd-intro/bmd-intro.html. , updated on Tuesday, September 13, 2011. Accessed September 26, 2011.

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

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

Hedtke, S.F., and F.A. Puglisi. 1982. Short-term toxicity of five oils to four freshwater species. Arch. Environ. Contam. Toxicol. 11:425-430.

Hoeppel, R.E. et al. 1991. Bioventing soils contaminated with petroleum hydrocarbons. J. Indust. Microbiol. 8:141-146.

IARC (International Agency for Research on Cancer). 1988. IARC Monographs on the evaluation of the carcinogenic risk of chemicals to humans, Volume 45: Occupational Exposures in Petroleum Refining; Crude Oil and Major Petroleum Fuels. Lyon, France.

IITRI (IIT Research Institute). 1984. Three week percutaneous toxicity study of diesel fuel in rabbits: Final Report. IITRI project No. L8100. Study sponsored by Standard Oil Co. (Ind). IIT Research Institute, Chicago.

IITRI (IIT Research Institute). 1985. Lifetime dermal tumorigenesis study of premier diesel fuel in male mice. Study No. 134 IITRI Project No. L8100. IIT Research Institute, Chicago.

ISO (International Organization for Standardization). 1995. Evaluation of the "ultimate" anaerobic biodegradability of organic compounds in digested sludge – Method by measurement of the biogas production. ISO 11734:1995. Geneva, Switzerland. URL: www.iso.org

IPCS, 1996. Diesel Fuel and Exhaust Emissions, IPCS Environmental Health Criteria 171. World Health Organization, Geneva, Switzerland.

Jeram, S., J.M. Riego Sintes, Mk. Halder, J. Baraibar Fentanes, B. Sokull-Klüttgen, and T.H. Hutchinson. 2005. A strategy to reduce the use of fish in acute ecotoxicity testing of new chemical substances notified in the European Union. Regulatory Toxicology and Pharmacology 42:218-224.

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.

Jungen, H., Mellert, W., and Wenzel-Hartung, R. (1995). Studies on the tumor initiation/promotion potential of six middle distillates (MDs) in mouse skin. Fundamental and Applied Toxicology 27:114-120.

Liddell, B.V., et al. 1994. Arctic bioremediation – a case study. SPE Prod. Facil. 9:132-136.

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

Mackay, D., DiGuardo, A. Paterson, S., and Cowan, C. 1997. EQC Model, Version. 1.01, 1997, available from the Environmental Modeling Centre, Trent University, Canada.

McCarty, L.S. and Mackay, D. 1993. Enhancing ecotoxicological modeling and assessment. Environmental Science and Technology 27:1719-1728.

McCarty, L.S. et al. 1991. Interpreting aquatic toxicity QSARs: the significance of toxic body residues at the pharmacologic endpoint. In: Hermens, J.L.M. and Opperhuizen, A. (Eds). QSAR in environmental toxicology. Volume IV, p. 515-525. Amsterdam: Elsevier.

McKee, R., Amoruso, M., Freeman, J., and Przygoda. 1994. Evaluation of the genetic toxicity of middle distillate fuels. Environ Mol Mutag 23: 234-238.

McKee, R.H., Schreiner, C.A., Nicolich, M.J., and Gray, T.M. 2010. Assessment of the *in vivo* cytogenetic potential of petroleum-derived substances. 49th Annual Meeting of the Society of Toxicology, Salt Lake City, Utah, March 7-11. The Toxicologist, Suppl to Toxicological Sciences 114 (1). Abst 1122.

Miethe, D., et al. 1994. The relationship between the microbial activity of the autochthonous microorganisms of pristine and contaminated soils and their potential for the degradation of mineral oil hydrocarbons. Act. Biotechnmo. 14:131-140.

Mobil. 1985. Thirteen week dermal administration of light cycle oil to rats. Study No. 20535. Mobil Environmental and Health Science Laboratory, Princeton, New Jersey.

Mobil, 1987. Chinese hamster ovary cells cytogenetics Vacuum Tower Overheads [Beaumont]. Study No. 52242. Mobil Environmental and Health Science Laboratory, Princeton, New Jersey.

Mobil, 1988a. Micronucleus assay of bone marrow red blood cells from rats treated via dermal administration of Vacuum Tower Overheads [Torrance]. Study No. 62327. Mobil Environmental and Health Science Laboratory, Princeton, New Jersey.

Mobil. 1988b. Light cycle oil developmental toxicity screen in rats. Study No. 50511. Mobil Environmental and Health Science Laboratory, Princeton, New Jersey.

Mobil. 1988c. Micronucleus assay of bone marrow red blood cells from rats treated via dermal administration of Coker Light Gas Oil. Study No 61997. Mobil Environmental and Health Science Laboratory, Princeton, New Jersey

Mobil. 1989a. Thirteen week dermal administration of Vacuum Tower Overheads to Rats. Study No. 62326. Mobil Environmental and Health Sciences laboratory, Princeton, New Jersey.

Mobil. 1989b. Developmental Toxicity Study in Rats Exposed Dermally to Vacuum Tower Overheads. Mobil Environmental and Health Sciences Laboratory Report 62328.

Mobil. 1989c. Developmental Toxicity Study in Rats Exposed Dermally to Light Coker Gas Oil. Mobil Environmental and Health Sciences Laboratory Report 61998

Mobil. 1990. Micronucleus assay of bone marrow red blood cells from rats treated via dermal administration of Heavy Atmospheric Gas Oil. Study No. 63457. Mobil Environmental and Health Science Laboratory, Princeton, New Jersey.

Mobil 1991a. Thirteen week dermal administration of Beaumont coker light gas oil to rats: Study No. 61996. Mobil Environmental and Health Sciences laboratory, Princeton, New Jersey.

Mobil. 1991b. Developmental Toxicity Study in Rats Exposed Dermally to Heavy Atmospheric Gas Oil. Mobil Environmental and Health Sciences Laboratory Report 64146.

Mobil. 1992. Thirteen-week dermal administration of heavy atmospheric gas oil to rats. Study No. 63456. Mobil Oil Corporation Environmental and Health Sciences Laboratory, Princeton, New Jersey.

Mobil, 1999. Determination of the aerobic ready biodegradability of Nigerian diesel fuel using the OECD 301F manometric respirometry test method. Mobil Business Resources Corp., Ecotoxicology Laboratory, Paulsboro, NJ.

Myers, L.E., Sexton, N.H., Southerland, L.I., and T.J. Wolff. 1981. Regression analysis of Ames test data. Environmental Mutagenesis 3:575-586.

Nicolich, M.T., McKee, R.H., Schreiner, C.A. and Gray, T.M. 2010. Predicting the outcome of Optimized Salmonella Assays. 49th Annual Meeting of the Society of Toxicology, Salt Lake City, Utah, March 7-11. The Toxicologist, Suppl to Toxicological Sciences 114 (1). Abst. 698.

Nessel, C., Priston, R., McKee, R., Cruzan, G., Riley, A., Hageman, R., Plutnick, R., and Simpson, B (1998). A comprehensive evaluation of the mechanism of skin tumorigenesis by straight-run and cracked petroleum distillates. Toxicological Sciences 44:22-31.

OECD (Organization for Economic Cooperation and Development). 1984. OECD Guideline 203: Fish, Acute Toxicity Test, Adopted 4 April 1984. OECD Guidelines for Testing of Chemicals, Paris, France.

OECD (Organization for Economic Cooperation and Development). 1992. OECD Guideline 203: Fish, Acute Toxicity Test, Adopted 17 July 1992. OECD Guidelines for Testing of Chemicals, Paris, France.

OECD (Organization for Economic Cooperation and Development). 1998. OECD Guideline No. 211, *Daphnia magna* Reproduction Test. Adopted 21 September 1998. OECD, Paris, France.

OECD (Organization for Economic Cooperation and Development). 2000a. Guidance document on aquatic toxicity testing of difficult substances and mixtures. OECD Environmental Health and Safety Publications, Series on Testing and Assessment No. 23. OECD, Paris, France.

OECD (Organization for Economic Cooperation and Development). 2000b. OECD Guideline No. 215, Fish, Juvenile Growth Test. Adopted 21 January 2000. OECD, Paris, France.

OECD (Organisation for Economic Cooperation and Development). 2003. OECD guidelines for testing of chemicals, Section 3, Part 1: Principles and strategies related to the testing of degradation of organic chemicals. OECD, Paris, France.

OECD (Organization for Economic Cooperation and Development). 2006. OECD Guidelines for Testing of Chemicals, Section 3, Part I: Principles and strategies related to the testing of degradation of organic chemicals. Adopted 23 March 2006, OECD, Paris, France.

Potter, T.L. and Simmons K.E. 1998. Total petroleum hydrocarbon criteria working group series, Volume 2. Composition of petroleum mixtures. Amherst Scientific Publishers, Amherst, Massachusetts. 114 pp.

Roth, R., Simpson, B., Nicolich, M., Murray, F.J. and Gray, T. 2012 [in press] The relationship between repeat –dose toxicity and aromatic-ring class content of high-boiling petroleum substances. Reg Toxicol Pharm**.**

Schwarzenbach, R.P., Gschwend, P.M., and Imboden, D.M., eds. 2003. Chapter 16: Indirect Photolysis: Reactions with Photooxidants in Natural Waters and in the Atmosphere. In: Environmental Organic Chemistry, 2nd Edition. John Wiley and Sons, Inc.

Shell (Shell Research Limited.). 1994. Acute toxicity of water accommodated fractions (WAFs) to Daphnia magna. Study #6167.

Shell (Shell Research Limited.). 1995a. Acute toxicity of water accommodated fractions to *Oncorhynchus mykiss*. Study #6304.

Shell (Shell Research Limited.). 1995b. Acute toxicity of water accommodated fractions to *Oncorhynchus mykiss*. Study #6303.

Shell (Shell Research Limited.). 1995c. Acute toxicity of water accomodated fractions to *Daphnia magna*. Study #6304.

Shell (Shell Research Limited.). 1995d. Acute toxicity of water accommodated fractions to *Daphnia magna*. Study #6303.

Shell (Shell Research Limited.). 1995e. Acute toxicity of water accommodated fractions to *Raphidocelis subcapitata*. Study #6304.

Shell (Shell Research Limited.). 1995f. Acute toxicity of water accommodated fractions to *Raphidocelis subcapitata*. Study #6303.

Shiu, W.Y., M. Bobra, A.M. Bobra, A. Maijanen, L. Suntio, and D. Mackay. 1990. The water solubility of crude oils and petroleum products. Oil & Chemical Pollution. 7:57-84.

Speight, J.G. 1998. Petroleum Chemistry and Refining. Applied Energy Technology Series. Taylor and Francis, Washington, D.C.

Speight, J. 2007. The Chemistry and Technology of Petroleum, 4th ed., CRC Press, Taylor & Francis Group, Boca Raton,

Swigert, J.P., C. Lee, D.C.L. Wong, and P. Podhasky. 2011. Environmental hazard assessment of petroleum distillates. Poster presentation, Society of Environmental Toxicology and Chemistry North America 32nd Annual Meeting, 13-17 November 2011, Boston, MA.

Van Wezel, A.P. and A. Opperhuizen. 1995. Narcosis Due to Environmental Pollutants in Aquatic Organisms: Residue-Based Toxicity, Mechanisms, and Membrane Burdens. Critical Reviews in Toxicology 25:255-279.

Verbruggen, E.M.J., W.H.J. Vaes, T.F. Parkerton, and J.L.M. Hermens. 2000. Polyacrylate-Coated SPME Fibers as a Tool To Simulate Body Residues and Target Concentrations of Complex Organic Mixtures for Estimation of Baseline Toxicity. Environ. Sci. Technol. 34: 324-331.

Weyers, A., B. Sokull-Klüttgen, J. Baraibar-Fentanes, and G. Vollmer. 2000. Acute toxicity data: a comprehensive comparison of results of fish, *Daphnia* and algae tests with new substances notified in the EU. Environ. Toxicol. Chem. 19:1931-1933.

WIL Laboratories 2012. A 90-day Repeat-Dose Dermal Toxicity Study Utilizing Ultra-Low Sulfur Diesel Fuel in Sprague Dawley Rats. WIL Study # 402025. WIL Research Laboratories, LLC. 1407 George Road, Ashland, OH 44805-8946

WIL Laboratories 2012. A 90-day Repeat-Dose Dermal Toxicity Study Utilizing Distillates (Petroleum), Light Catalytic Cracked in Sprague Dawley Rats. WIL Study # 402024. WIL Research Laboratories, LLC. 1407 George Road, Ashland, OH 44805-8946

WIL Laboratories 2012. A Dermal Prenatal Developmental Toxicity Study of Distillates (Petroleum), Light Catalytic Cracked in Rats. WIL Study # 402017. WIL Research Laboratories, LLC. 1407 George Road, Ashland, OH 44805-8946

WIL Laboratories 2012. A Dermal Prenatal Developmental Toxicity Study of Ultralow Sulfur Diesel Fuel in Rats. WIL Study # 402014. WIL Research Laboratories, LLC. 1407 George Road, Ashland, OH 44805-8946

11. LIST OF APPREVIATIONS AND ACRONYMS

API – American Petroleum Institute
BOD – biological oxygen demand
AUGC – area under the growth curve
CAS RN/CAS #/CAS No. - Chemical Abstract Service Registry Number
^{o}C – degrees Celsius
CIR – Cosmetics Ingredients Review Panel
CONCAWE – Conservation of Clean Air and Water in Europe
d - day
DMSO – Dimethyl sulfoxide
EINECS – European Inventory of Existing Commercial Chemical Substances
EL_{50} – effective loading rate lethal to 50% of the test population
E_bL_{50} – effective loading rate that causes 50% reduction in algal cell biomass
E_rL_{50} – effective loading rate that causes 50% reduction in algal growth rate
EPA/US EPA – United States Environmental Protection Agency
g/cm^3 – grams per cubic centimeter
h - hour
HLS – Huntingdon Life Sciences
HPV – High Production Volume
HSDB – Hazardous Substances Data Bank
IRDC – International Research and Development Corporation
^{o}K – degrees Kelvin
kPa - kilopascal
LC_{50} – lethal concentration for 50% of the test population
LC_{50}– lethal dose level for 50% of the test population
LL_{50} – 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^3 – 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
NTP – National Toxicology Program
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
UNEP – United Nations Environment Program
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

12. GLOSSARY

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

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.

Alga, Growth Inhibition Test: In a three-day exposure, growth inhibition is defined by the EC_{50}, 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.

ARC: Aromatic ring class that reflects the weight percent of PACs that have a given number of aromatic rings (1 through 7) within the total analyzed sample.

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 which is available for uptake by organisms. (AIHA, 2000)

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.

BMD: The Benchmark Dose is the dose producing a predetermined change in response and is calculated from a dose-response model statistically fitted to experimental data. (Gephart, et al, 2001)

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)

***Daphnia* sp., Acute Immobilization Test:** In a one or two-day exposure, acute toxicity is defined by the EC_{50}, 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.

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)

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 an 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)

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)

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)

Fish, Acute Toxicity Test: In a four-day exposure, acute toxicity is defined by the LC_{50}, 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.

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 studies in cultured cells using methods described in OECD Guideline 476, in OECD Guidelines for the Testing of Chemicals.

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 studies in the whole animal using methods described in OECD Guideline 475, in OECD Guidelines for the Testing of Chemicals.

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

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).

Health Effects: all endpoints (OECD definitions, unless otherwise specified)

Highly Refined: a descriptor for those lubricant oil basestocks that are not expected to be mutagenic or dermally carcinogenic based on knowledge of refining history or results from tests such as the optimized Ames assay, IP346 assay, skin-painting tests in mice, and analysis of PAC content by GC (such as PAC-2 method).

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).

Modified Ames Test: A modification of the Ames test used for petroleum materials and designed to facilitate physical contact between the test substance and the bacteria as well as enhance the reactions among the bacteria. Also referred to as the Optimized Ames test.

Mutagenicity Index: The primary endpoint in the modified Ames test indicating the slope for the linear portion of the dose-response curve (number of revertant colonies vs dose of test substance per plate).

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).

Optimized Ames Test: See Modified Ames test.

PAC Profile: The listing of the weight percent of each of the DMSO-extractable 1- through 7-ring polycyclic aromatic compounds from a test material. (API, 2008)

PAC 2: A single analytical method that involves solvent extraction (DMSO) and an analysis of the DMSO-extracted concentrate of PACs by gas chromatography with an FID or MS detector. The DMSO extraction procedure is selective for the less polar PAC species, so that highly alkylated PACs are excluded from measurement. (API, 2008)

PDR_{10}: The Predicted Dose for a Response that is a 10% change from control. The prediction is based on models developed from a series of exposure-response studies. (API, 2008)

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.

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, 1994).

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)

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)

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.

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).

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.

APPENDIX A. CAS Numbers and Definitions of Category Members

The CAS numbers and definitions of refinery streams, including gas oils and distillate fuels, 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.

The Petroleum HPV Testing Group has included in its listing of CAS numbers an indication of the corresponding category adopted by the European Union (EU) in their legislation (Official Journal of the European Communities, L84 Volume 36, 5 April 1993, *Council Regulation (EEC) No 793/93 of 23 March 1993 on the evaluation and control of risks of existing substances*) and updated by CONCAWE [*Classification and labeling of petroleum substances according to EU dangerous substances directive (CONCAWE recommendations – July 2005)*, Report No. 6/05]. The EU category information is being included in this test plan to facilitate the international harmonization of classification and the coordination of efforts to summarize existing data and develop new hazard data that will be appropriate for hazard and risk characterization worldwide. In doing so, it will help avoid unnecessary duplication of testing.

Distillate Fuels

68334-30-5

Diesel Oil ..C9-20 325F-675F

Petroleum products, diesel oil

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 C20 and boiling in the range of approximately 163 degrees C to 357 degrees C (325 degrees F to 675 degrees F).
[EU Category: Other Gas Oils - Distillate Fuel Oils]
CONCAWE Vacuum Gas Oil, hydrocracked gas oils and distillate fuels

68476-30-2

Fuel Oil No. 2 ..32.6 To 37.9 SSU
A distillate oil having a minimum viscosity of 32.6 SUS at 37.7 degrees C (100 degrees F) to a maximum of 37.9 SUS at 37.7 degrees C (100 degrees F).
[EU Category: Other Gas Oils - Distillate Fuel Oils]
CONCAWE Vacuum Gas Oil, hydrocracked gas oils and distillate fuels

68476-31-3

Fuel Oil No. 4 ..45 To 125 SSU
A distillate oil having a minimum viscosity of 45 SUS at 37.7 degrees C (100 degrees F) to a maximum of 125 SUS at 37.7 degrees C (100 degrees F).
[EU Category: Other Gas Oils - Distillate Fuel Oils]
CONCAWE Vacuum Gas Oil, hydrocracked gas oils and distillate fuels

68476-34-6

Diesel Fuel No. 2 ..32.6 To 40.1 SSU

Fuels diesel, no. 2
The distillate oil having a minimum viscosity of 32.6 SUS at 37.7 degrees C (100 degrees F) to a maximum of 40.1 SUS at 37.7 degrees C (100 degrees F).
[EU Category: Other Gas Oils - Distillate Fuel Oils]
CONCAWE Vacuum Gas Oil, hydrocracked gas oils and distillate fuels

Refinery Streams

64741-43-1

Gas Oil, Intermediate ..C11-25 401F-752F

Gas oils (petroleum), straight-run
A complex combination of hydrocarbons produced by the distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C11 through C25 and boiling in the range of approximately 205 degrees C to 400 degrees C (401 degrees F to 752 degrees F).
[EU Category: Straight Run Gas Oils]
CONCAWE Straight run gas oils

64741-44-2

Gas Oil, Light ..C11-20 401F-653F

Distillates (petroleum), straight- run middle
A complex combination of hydrocarbons produced by the distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C11 through C20 and boiling in the range of 205 degrees C to 345 degrees C (401 degrees F to 653 degrees F).
[EU Category: Straight Run Gas Oils]
CONCAWE Straight run gas oils

64741-49-7

Vacuum Tower Condensate ..C11-25 401F-752F

Condensates (petroleum), vacuum tower

A complex combination of hydrocarbons produced as the lowest boiling stream in the vacuum distillation of the residuum from atmospheric distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C11 through C25 and boiling in the range of approximately 205 degrees C to 400 degrees C (401 degrees F to 752 degrees F).
[EU Category: Vacuum Gas Oils]
CONCAWE Vacuum Gas Oil, hydrocracked gas oils and distillate fuels

64741-58-8

Vacuum Distillate, Light Paraffin ..C13-30 446F-842F

Gas Oils (petroleum), light vacuum

A complex combination of hydrocarbons produced by the vacuum distillation of the residuum from atmospheric distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C13 through C30 and boiling in the range of approximately 230 degrees C to 450 degrees C (446 degrees F to 842 degrees F).
[EU Category: Vacuum Gas Oils]
CONCAWE Vacuum Gas Oil, hydrocracked gas oils and distillate fuels

64741-59-9

Cat Cracked Distillate, Light ..C9-25 302F-752F

Distillates (petroleum), light catalytic cracked

A complex combination of hydrocarbons produced by the distillation of products from a catalytic cracking process. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C25 and boiling in the range of approximately 150 degrees C to 400 degrees C (302 degrees F to 752 degrees F). It contains a relatively large proportion of bicyclic aromatic hydrocarbons.
[EU Category: Cracked Gas Oils [excluding hydrocracked gas oils)]
CONCAWE Cracked gas oils

64741-60-2

Cat Cracked Distillate, Intermediate ..C11-30 401F-842F

Distillates (petroleum),intermediate catalytic cracked
A complex combination of hydrocarbons produced by the distillation of products from a catalytic cracking process. It consists of hydrocarbons having carbon numbers predominantly in the range of C11 through C 30 and boiling in the range of approximately 205 degrees C to 450 degrees C (401degrees F to 842 degrees F). It contains a relatively large proportion of tricyclic aromatic hydrocarbons.
[EU Category: Cracked Gas Oils [excluding hydrocracked gas oils)]
CONCAWE Cracked gas oils

64741-77-1

Hydrocracked Distillate, Light ..C10-18 320F-608F

Light Hydrocracked Distillate (Petroleum)
A complex combination of hydrocarbons from distillation of the products from a hydrocracking process. It consists predominantly of saturated hydrocarbons having carbon numbers predominantly in the range of C10 through C18, and boiling in the range of approximately 160 degrees C to 320 degrees C (320 degrees F to 608 degrees F).
[EU Category: Hydrocracked Gas Oils]
CONCAWE Vacuum Gas Oil, hydrocracked gas oils and distillate fuels

64741-82-8[1]

Thermocracked Distillate, Light ..C10-18 320F-698F

Distillates (petroleum), light thermal cracked
A complex combination of hydrocarbons from the distillation of the products from a thermal cracking process. It consists predominantly of unsaturated hydrocarbons having carbon numbers predominantly in the range of C10 through C22 and boiling in the range of approximately 160 degrees C to 370 degrees C (320 degrees F to 698 degrees F).
[EU Category: Cracked Gas Oils [excluding hydrocracked gas oils)]
CONCAWE Cracked gas oils

64741-86-2

Sweetened Distillate ..C9-20 302F-653F

Distillates (petroleum), sweetened middle
A complex combination of hydrocarbons obtained by subjecting a petroleum distillate to a sweetening process to convert mercaptans or to remove acidic impurities. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C20 and boiling in the range of approximately 150 degrees C to 345 degrees C (302 degrees F to 653 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

[1] Overlaps with ICCA C10 - C12 Aromatic Hydrocarbon Solvents and OECD C10+ Aromatics Hydrocarbon Solvents

64741-90-8

Solvent Refined Gas Oils..C11-25 401F-752F

Gas oils (petroleum), solvent refined

A complex combination of hydrocarbons obtained as the raffinate from a solvent extraction process. It consists predominantly of aliphatic hydrocarbons having carbon numbers predominantly in the range of C11 through C25 and boiling in the range of approximately 205 degrees C to 400 degrees C (401 degrees F to 752 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

64741-91-9[2]

Solvent Refined Distillate, Middle..C9-20 302F-653F

Distillates (petroleum), solvent-refined middle

A complex combination of hydrocarbons obtained as the raffinate from a solvent extraction process. It consists predominantly of aliphatic hydrocarbons having carbon numbers predominantly in the range of C9 through C20 and boiling in the range of approximately 150 degrees C to 345 degrees C (302 degrees F to 653 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

64742-29-6

Neutralized Gas Oils..C13-25 446F-752F

Gas oils (petroleum), chemically neutralized

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 C13 through C25 and boiling in the range of approximately 230 degrees C to 400 degrees C (446 degrees F to 752 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

64742-30-9

Neutralized Distillate, Middle ..C11-20 401F-653F

Distillates (petroleum) chemically neutralized middle

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 C11 through C20 and boiling in the range of approximately 205 degrees C to 345 degree C (401 degrees F to 653 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

64742-38-7

Clay Treated Distillate ..C9-20 302F-653F

Distillates (petroleum), clay-treated

A complex combination of hydrocarbons resulting from treatment of a petroleum fraction with natural or modified clay, usually in a percolation process to remove the trace amounts of polar compounds and impurities present. It consists of hydrocarbons having carbon numbers predominantly in the range of C9

[2] Overlaps with ICCA C14 - C20 Aliphatics (2% aromatics or less) and OECD C14+ Aliphatic Hydrocarbons Solvents (<2% aromatics)

through C20 and boiling in the range of approximately 150 degrees C to 345 degrees C (302 degrees F to 653 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

64742-46-7[3]

Hydrotreated Distillate, Middle ..C11-25 401F-752F

Distillates (petroleum), hydrotreated middle
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 C11 through C25 and boiling in the range of approximately 205 degrees C to 400 degrees C (401 degrees F to 752 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

64742-72-9

Distillates (petroleum), catalytic dewaxed middle ..C9-20 302F 653F

Distillates, petroleum, catalytic dewaxed middle
A complex combination of hydrocarbons obtained from a catalytic dewaxing process. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C20 and boiling in the range of approximately 150.degree.C to 345.degree.C (302.degree.F to 653.degree.F).
[EU Category: none] CONCAWE none

64742-79-6

Hydrodesulfurized Gas Oil ..C13-25 446F-752F

Gas oils (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 predominantly of hydrocarbons having carbon numbers predominantly in the range of C13 through C25 and boiling in the range of approximately 230 degrees C to 400 degrees C (446 degrees F to 752 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

64742-80-9[4]

Hydrodesulfurized Distillate, Middle ..C11-25 401F-752F

Distillates (petroleum), hydrodesulfurized middle

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 C11 through C25 and boiling in the range of approximately 205 degrees C to 400 degrees C (401 degrees F to 752 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

64742-87-6

[3] Overlaps with ICCA C14 - C20 Aliphatics (2% aromatics or less) and OECD C14+ Aliphatic Hydrocarbons Solvents (<2% aromatics)

[4] Overlaps with ICCA C14 - C20 Aliphatics (2-35% aromatics)

Hydrodesulfurized Gas Oil, Light Vacuum ..C13-30 446F-842F

Gas oils (petroleum), hydrodesulfurized light vacuum

A complex combination of hydrocarbons obtained from a catalytic hydrodesulfurization process. It consists of hydrocarbons having carbon numbers predominantly in the range of C13 through C30 and boiling in the range of approximately 230 degrees C to 450 degrees C (446 degrees F to 842 degrees F).
[EU Category: Vacuum Gas Oils]
CONCAWE Vacuum Gas Oil, hydrocracked gas oils and distillate fuels

68333-25-5

Hydrodesulfurized Distillate, Light Cat Cracked ..C9-25 302F-752F

Distillates (petroleum), hydrodesulfurized light catalytic cracked

A complex combination of hydrocarbons obtained by treating light catalytic cracked distillates 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 C25 and boiling in the range of approximately 150 degrees C to 400 degrees C (302 degrees F to 752 degrees F). It contains a relatively large proportion of bicyclic aromatic hydrocarbons.
[EU Category: Cracked Gas Oils (excluding hydrocracked gas oils)]
CONCAWE Cracked gas oils

68333-88-0[5]

Aromatic Hydrocarbons, C9-17
No description
[EU Category: none] CONCAWE none

68477-31-6

Reformate Still Bottoms, Light ..To 550F

Distillates (petroleum), catalytic, reformer fractionator residue, low-boiling

The complex combination of hydrocarbons from the distillation of catalytic reformer fractionator residue. It boils approximately below 288 degrees C (550 degrees F).
[EU Category: Other Gas Oils]
CONCAWE Other gas oils

68814-87-9

Gas Oil, Intermediate ..C9-25 320F-752F

Distillates (petroleum), full-range straight-run middle

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 C25 and boiling in the range of approximately 150 degrees C to 400 degrees C (302 degrees F to 752 degrees F).
[EU Category: Straight Run Gas Oils]
CONCAWE Straight run gas oils

68915-96-8

Gas Oil Heavy ..550F-880F

Distillates (petroleum), straight-run, b. 557-880 degrees F.
[EU Category: Straight Run Gas Oils]
CONCAWE Straight run gas oils

68915-97-9

[5] Overlaps with ACC Low Benzene Naphthas

Gas Oil, Heavy ..540F-660F

Gas oils (petroleum), straight-run, high-boiling

A complex combination of hydrocarbons produced by the atmospheric distillation of crude oil. It boils in the range of approximately 282 degrees C to 349 degrees C (540 degrees F to 660 degrees F).
[EU Category: Straight Run Gas Oils]
CONCAWE Straight run gas oils

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 Analyses of 2 Gas Oil samples used in Biodegradation and Aquatic Toxicity Studies

Product Composition/Monitoring	
Test Substance Category Name: GAS OILS CATEGORY	
Category Chemical	Light Hydrocracked Gas Oil, CAS No. 64741-77-1
Test Substance	Light Hydrocracked Gas Oil, CAS No. 64741-77-1
Test Substance Purity/Composition and other Test Substance Comments	Density (ASTM D4052) @ 15°C/59°F ..... 0.8244 g/mL Relative Density @ 60°F ..... 0.8248 g/mL API Gravity @ 60°F ..... 40.1 °API Boiling Range (ASTM D2887): initial ..... 134.4 °C final ..... 290.4 °C Hydrocarbon Types by FIA (ASTM D1319): Aromatics ..... 16.7 vol % Olefins ..... 1.5 vol % Saturates ..... 81.8 vol % Determination of aromatic content by supercritical fluid chromatography (ASTM D5186): Monoaromatics ..... 20.8 Wt % Polynuclear aromatics ..... <0.5 Wt % Total aromatics ..... 21.0 Wt %
Reference	ExxonMobil Research and Engineering Co. 2010. Analysis report, Reference No. 2011AN 02. Annandale, NJ, USA. Intertek. 2009. Report of analysis, Reference no. US785-0017157. Intertek, Deer Park, Texas.
Description	The results field provides an attachment containing high resolution two dimensional gas chromatography (2D-GC) with flame ionization detection of a sample of light hydrocracked gas oil (CAS No. 64741-77-1). This sample was used in aquatic toxicity testing for complete data gaps for biodegradability, fish acute toxicity, invertebrate acute toxicity, invertebrate chronic toxicity, and algal toxicity. **GCxGC Chromatographic Conditions** The sample was analyzed directly by GCxGC using the conditions shown below: Instrument: Agilent Technologies 6890 Series GC Injector: Split/Splitless in Split Mode Initial Temp 60°C Ramp 3°C/sec Final Temp 330°C Column flow at 1 mL/min in constant flow mode Split ratio at 1:50 Sample injection: Agilent ALS- Injection volume 0.2 µL

	Modulator: Cryogenic modulator, single jet loop type (ZOEX Corporation) Modulation time 10 sec Pulse width 400 ms N2 Flow rate approx 5L/min, controlled by a flow meter Detector: Flame-ionization Temperature at 300°C Makeup gas He Makeup flow 20 mL/min Hydrogen flow 40 mL/min Air flow 450 mL/min Column 1: 30 m x 0.25 mm i.d. 5% phenyldimethylpolysiloxane column (BPX-5) with film thickness of 1.0 μm Column 2: 3m x 0.25 mm i.d. polysilphenylene-siloxane column (BPX-50) with film thickness of 0.25 μm (One end of 2nd Dim column forms loop modulation, and the other end direct into FID) Carrier gas: Helium Oven temperature: 60°C (0 min isothermal) then 3.0°C/min to 240°C Hot Jet: 180°C offset from Oven: 240°C (0 min temperature isothermal) then 3.0°C/min to 390°C (50 min isothermal) **Data Analysis** GCxGC data is processed and visualized with in-house developed software. A mixture of normal paraffin from C10 to C28 has been used for qualitative analysis purpose to locate the retention position (both X-axis and Y-axis retention times) in the GCxGC. Based on the position of the normal paraffins; all other compound classes have been identified based on their relative position to normal paraffins. The peak area for each component or component group identified was directly integrated with the assumption of a universal unit response factor to all hydrocarbons by the flame ionization detector Having acquired the raw GCxGC data on the sample, the profile was examined and templates constructed to group individual components into the appropriate carbon number (C5 to C30) and chemical functionalities shown below: • n-paraffins • iso-paraffins • n-alkane substituted cyclohexane and cyclopentane • mono-naphthenics • di-naphthenics • mono-aromatics • N-mono-aromatics

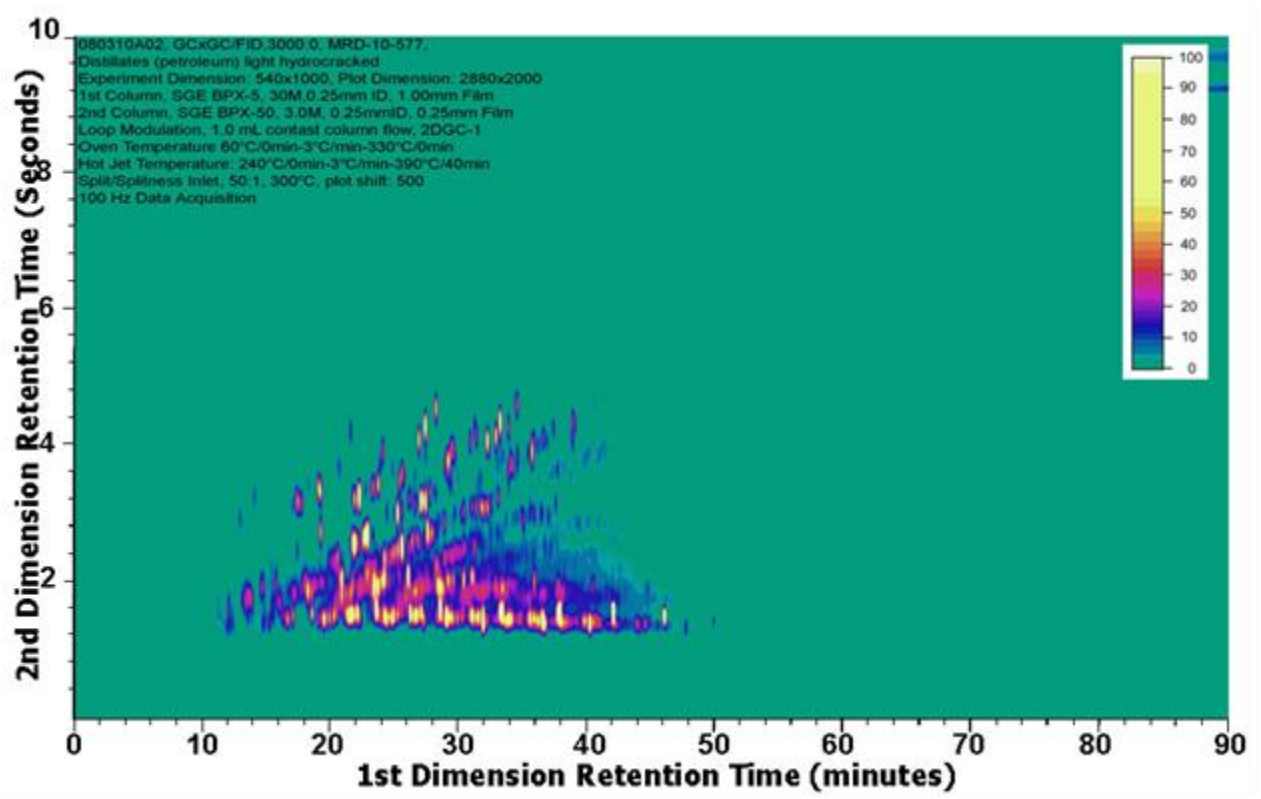
	• di-aromatics • N-di-aromatics • Tri-aromatics • N-tri-aromatics • tetra-aromatics • N-tetra-aromatics • penta-aromatics
Results	Results are tabulated for the sample as shown in the spreadsheet. Numbers are reported in wt%. The peak area for each component or component group identified was directly integrated with the assumption of a universal unit response factor to all hydrocarbons by the flame ionization detector. The components found in the sample has been determined and tabulated in compound classes and carbon number order, as shown in the spreadsheet. The corresponding GCxGC chromatogram of the sample is also attached for reference purpose. Please note the 2DGC method does not differentiate olefins from naphthenes.
Conclusions	The two independent analyses gave good agreement for the percentage of aromatic and saturate components. As determined by 2DGC analyses, the saturate and aromatic components of CAS No. 64741-77-1 totaled 75.2 wt% and 24.8 wt%, respectively. Analyses by Intertek using ASTM D1319 showed 81.8 vol% and 16.7 vol% as saturates and aromatic, respectively. ASTM D5186 measured total aromatics as 21.0 wt%.

2D-GC Analysis Results for light hydrocracked gas oil, CAS No. 64741-77-1.

C-num	nP	isoP	N	diN	triN	tetraN	pentaN		mono-A	N-mono-A	Di-A	N-Di-A	tri-A	N-tri-A	trtea-A	N-tetra-A	penta-A	
5	0.00								0									
6	0.00	0.00	0.00	0.00					0									
7	0.00	0.00	0.00	0.00					0.00									
8	0.01	0.00	0.83	0.00					0.19									
9	0.39	0.57	2.98	0.00					1.19	0.21								
10	0.87	1.50	6.79	6.70					1.86	2.10	0.00							
11	1.67	4.28	5.41	2.69					2.90	3.51	0.05							
12	1.77	4.74	4.95	1.66					2.09	2.25	0.12	0.00						
13	1.83	4.67	2.95	1.24					1.18	1.65	0.17	0.02						
14	2.31	3.90	1.86	0.67					0.56	0.54	0.11	0.02	0.00					
15	1.49	2.54	0.90	0.20					0.29	0.22	0.02	0.00	0.01					
16	0.63	1.25	0.22	0.02					0.07	0.04	0.01	0.01	0.01	0.05				
17	0.06	0.30	0.01	0.00					0.01	0.00	0.01	0.01	0.01	0.03	0.32			
18	0.00	0.01	0.00	0.00					0.00	0.02	0.01	0.01	0.01	0.02	0.21			
19	0.00	0.00	0.00	0.01					0.01	0.01	0.00	0.00	0.01	0.02	0.22	0.22		
20	0.00	0.00	0.01	0.00					0.00	0.00	0.00	0.01	0.01	0.01	0.14	0.35		
21	0.00	0.01	0.01	0.00					0.00	0.01	0.01	0.01	0.01	0.01	0.03	0.56		
22	0.00	0.02	0.00	0.00					0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.59		
23	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.01	0.01	0.01	0.02	0.01	0.00			
24	0.00	0.01	0.00	0.00	0.00	0.00			0.01	0.01	0.01	0.01	0.02	0.01				
25	0.00	0.01	0.01	0.00	0.00	0.00			0.00	0.01	0.00	0.02	0.03	0.01				
26	0.00	0.01	0.01	0.00	0.00	0.00			0.00	0.01	0.02	0.02	0.02	0.00				
27	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.01	0.01	0.01	0.00					
28	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.02	0.01	0.00						
29	0.00	0.01	0.01	0.01	0.00	0.00			0.01	0.03								
30	0.01	0.01	0.01	0.01	0.00	0.00			0.01	0.03								
Total	11.06	23.89	26.98	13.24	0.02	0.02	0.00		10.39	10.69	0.58	0.16	0.16	0.18	0.92	1.72	0.00	100.00

Heading Codes:
C-num = number of carbon atoms in group; nP = normal paraffins; isoP = iso-paraffins; N = naphthenes; diN = di-naphthenes; triN = tri-naphthenes; tetraN = tetra-naphthenes; pentaN = penta-naphthenes; mono-A = monoaromatics; N-mono-A = napthenic-mono-aromiatics; Di-A = di-aromatics; N-Di-A = naphthenic-di-aromatics; tri-A = tria-aromatics; N-tri-A = naphthenic-tri-aromatics; tetra-A = tetra-aromatics; N-tetra-A = naphthenic-tetra-aromatics; penta-A = penta-aromatics.

2d-GC chromatogram of distillates (petroleum) light hydrocracked gas oil, CAS No. 64741-77-1



Product Composition/Monitoring	
Test Substance Category Name: GAS OILS CATEGORY	
Category Chemical	Distillates (Petroleum), light catalytic cracked gas oil, CAS No. 64741-59-9
Test Substance	Distillates (Petroleum), light catalytic cracked gas oil, CAS No. 64741-59-9
Test Substance Purity/Composition and Other Test Substance Comments	Relative Density (ASTM D4052) @ 60/60°F ..... 0.9618 g/mL API Gravity @ 60°F ..... 15.6 °API Boiling Range (ASTM D2887): initial ..... 142.7 °C final ..... 357.7 °C Hydrocarbon Types by FIA (ASTM D1319): Aromatics ..... 75.3 vol % Olefins ..... 7.2 vol % Saturates..... 17.5 vol % Determination of aromatic content by supercritical fluid chromatography (ASTM D5186): Monoaromatics ..... 24.0 Wt % Polynuclear aromatics..... >50.0 Wt % Total aromatics..... 83.5 Wt %
Reference	ExxonMobil Research and Engineering Co. 2010. Analysis report, Reference No. 2011AN 02. Annandale, NJ, USA. Intertek. 2009. Report of analysis, Reference no. US785-0016408. Intertek, Deer Park, Texas.
Description	The results field provides an attachment containing high resolution two dimensional gas chromatography (2D-GC) with flame ionization detection of a sample of light catalytic cracked gas oil (CAS No. 64741-59-9). This sample was used in aquatic toxicity testing for complete data gaps for biodegradability, fish acute toxicity, invertebrate acute toxicity, invertebrate chronic toxicity, and algal toxicity. **GCxGC Chromatographic Conditions** The sample was analyzed directly by GCxGC using the conditions shown below: Instrument: Agilent Technologies 6890 Series GC Injector: Split/Splitless in Split Mode Initial Temp 60°C Ramp 3°C/sec Final Temp 330°C Column flow at 1 mL/min in constant flow mode Split ratio at 1:50 Sample injection: Agilent ALS- Injection volume 0.2 µL Modulator: Cryogenic modulator, single jet loop type (ZOEX Corporation) Modulation time 10 sec Pulse width 400 ms

N2 Flow rate approx 5L/min, controlled by a flow meter
Detector: Flame-ionization
Temperature at 300°C
Makeup gas He
Makeup flow 20 mL/min
Hydrogen flow 40 mL/min
Air flow 450 mL/min
Column 1: 30 m x 0.25 mm i.d. 5% phenyldimethylpolysiloxane column (BPX-5) with film thickness of 1.0 μm
Column 2: 3m x 0.25 mm i.d. polysilphenylene-siloxane column (BPX-50) with film thickness of 0.25 μm
(One end of 2nd Dim column forms loop modulation, and the other end direct into FID)
Carrier gas: Helium
Oven temperature: 60°C (0 min isothermal) then 3.0°C/min to 240°C
Hot Jet: 180°C offset from Oven: 240°C (0 min temperature isothermal) then 3.0°C/min to 390°C (50 min isothermal)

Data Analysis
GCxGC data is processed and visualized with in-house developed software.

A mixture of normal paraffin from C10 to C28 has been used for qualitative analysis purpose to locate the retention position (both X-axis and Y-axis retention times) in the GCxGC. Based on the position of the normal paraffins; all other compound classes have been identified based on their relative position to normal paraffins.

The peak area for each component or component group identified was directly integrated with the assumption of a universal unit response factor to all hydrocarbons by the flame ionization detector

Having acquired the raw GCxGC data on the sample, the profile was examined and templates constructed to group individual components into the appropriate carbon number (C5 to C30) and chemical functionalities shown below:

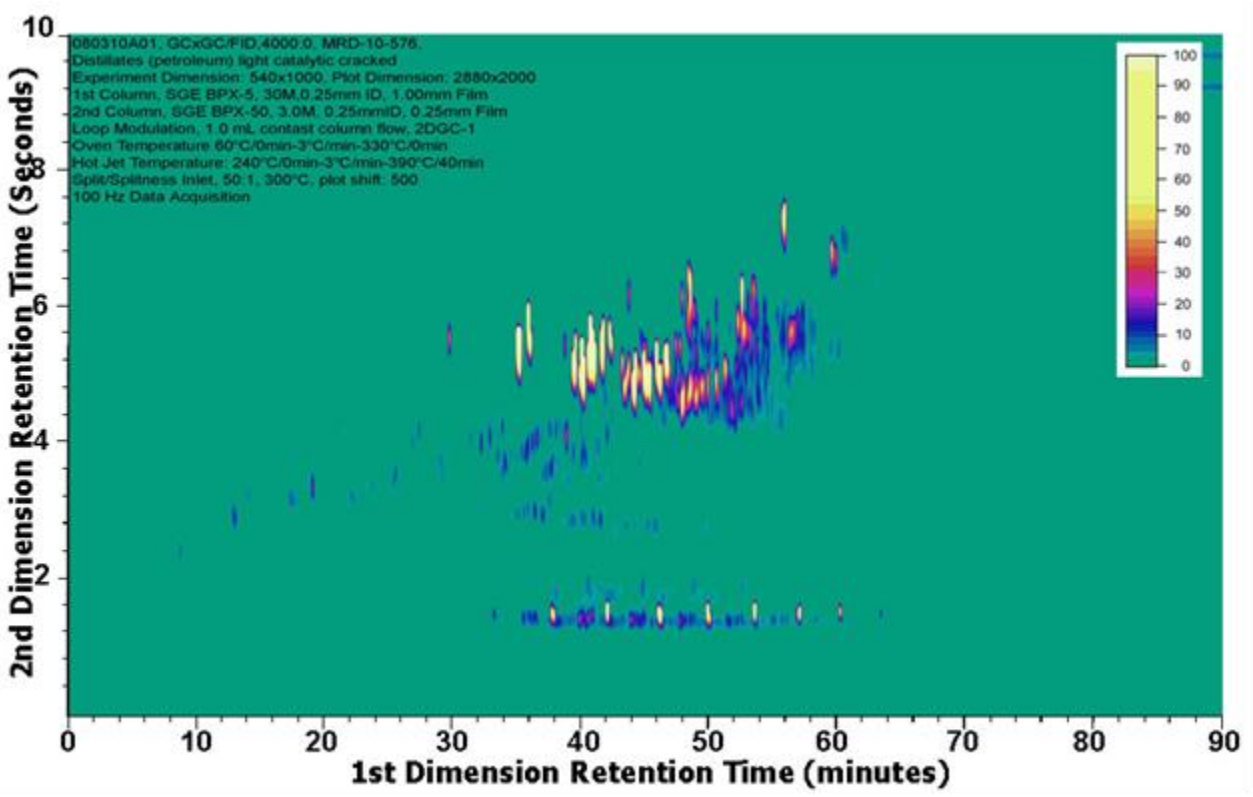
- n-paraffins
- iso-paraffins
- n-alkane substituted cyclohexane and cyclopentane
- mono-naphthenics
- di-naphthenics
- mono-aromatics
- N-mono-aromatics
- di-aromatics
- N-di-aromatics
- Tri-aromatics

	• N-tri-aromatics • tetra-aromatics • N-tetra-aromatics • penta-aromatics
Results	Results are tabulated for the sample as shown in the spreadsheet. Numbers are reported in wt%. The peak area for each component or component group identified was directly integrated with the assumption of a universal unit response factor to all hydrocarbons by the flame ionization detector. The components found in the sample has been determined and tabulated in compound classes and carbon number order, as shown in the spreadsheet. The corresponding GCxGC chromatogram of the sample is also attached for reference purpose. Please note the 2DGC method does not differentiate olefins from naphthenes.
Conclusions	The two independent analyses gave good agreement for the percentage of aromatic and saturate components. As determined by 2DGC analyses, the saturate and aromatic components of CAS No. 64741-59-9 totaled 15.2 wt% and 84.8 wt%, respectively. Analyses by Intertek using ASTM D1319 showed 17.5 vol% and 75.3 vol% as saturates and aromatic, respectively. ASTM D5186 measured total aromatics as 83.5 wt%.

2D-GC Analysis Results for Light Catalytic Cracked Gas Oil, CAS No. 64741-59-9.																		
	nP	iso P	N	diN	triN	tetraN	pentaN		mono-A	N-mono-A	Di-A	N-Di-A	tri-A	N-tri-A	trtea-A	N-tetra-A	penta-A	
5	0.00								0									
6	0.00	0.00	0.01	0.00					0									
7	0.01	0.01	0.01	0.00					0.06									
8	0.01	0.02	0.03	0.00					0.23									
9	0.01	0.04	0.03	0.00					0.35	0.08								
10	0.01	0.04	0.03	0.01					0.23	0.31	0.27							
11	0.01	0.04	0.03	0.02					0.18	0.76	7.14							
12	0.02	0.06	0.08	0.09					0.20	1.49	20.23	0.73						
13	0.10	0.11	0.30	0.29					0.57	2.17	14.93	3.91						
14	0.67	0.54	0.58	0.39					0.63	0.91	6.61	6.63	1.32					
15	0.91	0.99	0.61	0.31					0.48	0.44	2.92	3.39	1.05					
16	0.93	0.94	0.50	0.25					0.31	0.22	0.79	0.70	0.21	0.07				
17	0.88	0.72	0.40	0.24					0.28	0.17	0.20	0.09	0.04	0.04	0.29			
18	0.74	0.53	0.32	0.20					0.20	0.15	0.03	0.01	0.01	0.01	0.20			
19	0.52	0.38	0.19	0.09					0.12	0.06	0.01	0.01	0.01	0.02	0.18	0.20		
20	0.24	0.23	0.07	0.02					0.04	0.02	0.01	0.01	0.01	0.02	0.11	0.33		
21	0.05	0.10	0.02	0.01					0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.48		
22	0.01	0.04	0.01	0.01					0.00	0.01	0.01	0.00	0.02	0.01	0.01	0.49		
23	0.00	0.02	0.01	0.00	0.00	0.00			0.00	0.01	0.01	0.01	0.01	0.00	0.00			
24	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.01	0.01	0.02	0.00	0.00				
25	0.00	0.01	0.01	0.00	0.00	0.00			0.00	0.01	0.01	0.01	0.00	0.00				
26	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.01	0.01	0.00	0.00	0.00				
27	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.02	0.00	0.00	0.00					
28	0.00	0.01	0.01	0.00	0.00	0.00			0.01	0.02	0.00	0.00						
29	0.00	0.02	0.01	0.00	0.00	0.00			0.01	0.01								
30	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.01								
Total	5.16	4.86	3.24	1.95	0.01	0.02	0.00		3.92	6.90	53.21	15.54	2.71	0.18	0.81	1.50	0.00	100.00

Heading Codes:
C-num = number of carbon atoms in group; nP = normal paraffins; isoP = iso-paraffins; N = naphthenes; diN = di-naphthenes; triN = tri-naphthenes; tetraN = tetra-naphthenes; pentaN = penta-naphthenes; mono-A = monoaromatics; N-mono-A = napthenic-mono-aromatics; Di-A = di-aromatics; N-Di-A = naphthenic-di-aromatics; tri-A = tria-aromatics; N-tri-A = naphthenic-tri-aromatics; tetra-A = tetra-aromatics; N-tetra-A = naphthenic-tetra-aromatics; penta-A = penta-aromatics.

2d-GC chromatogram of distillates (petroleum) light catalytic cracked gas oil, CAS No. 64741-59-9



APPENDIX D. Repeat Dose and Developmental Toxicity Statistical Modeling

The development of these models began with the observation that the more biologically significant effects of several types of refinery streams with high final boiling points in both repeated-dose and developmental studies appeared to be related to the total amount of 3-7 ring polycyclic aromatic compounds (PACs) (Feuston et al, 1994). The relationship was qualitative and not predictive for individual samples.

The statistical models, developed by the Petroleum High Production Volume Testing Group (HPVTG), quantitatively predict effects by individual samples on selected sensitive endpoints based on the PAC profile in each sample (API, 2008). The models are empirically based on a number of toxicity studies on petroleum substances for which there are also analyses of PAC content profile using PAC-2 method or simply Method II. Method II analyses provided the weight percent of each DMSO extractable aromatic ring class that served as a basis for the models (the ARC in Table D-1). This analytical data set also characterizes the DMSO extractable PAC distribution for samples tested in animal studies and summarized in the Robust Summaries (separate document).

Table D-1. PAC Analytical Profile of Gas Oils

CAS RN/ Sample No.	DMSO wt %[1]	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
Distillate Fuels								
68334-30-5 Diesel Oils Ultralow sulfur Diesel								
080801	4.9	1.0	3.4	0.5	0.0	0.0	0.0	0.0
080802	4.1	0.4	2.9	0.4	0.0	0.0	0.0	0.0
080803	2.5	0.2	1.7	0.5	0.0	0.0	0.0	0.0
080804	2.7	0.2	1.6	0.8	0.0	0.0	0.0	0.0
080805	2.5	0.2	2.0	0.5	0.0	0.0	0.0	0.0
080806	3.1	0.3	2.2	0.3	0.0	0.0	0.0	0.0
080807	4.7	0.9	3.3	0.5	0.0	0.0	0.0	0.0
080808	4.9	1.0	3.4	0.5	0.0	0.0	0.0	0.0
080809	2.4	0.2	1.7	0.5	0.0	0.0	0.0	0.0
080810	2.5	0.2	2.0	0.3	0.0	0.0	0.0	0.0
080811	4.3	0.4	2.6	1.3	0.1	0.0	0.0	0.0
080812	4.2	0.4	2.5	1.3	0.1	0.0	0.0	0.0
080813	4.0	0.3	3.2	0.4	0.0	0.0	0.0	0.0
080814	2.6	0.3	1.8	0.5	0.0	0.0	0.0	0.0
080815	4.1	0.4	2.5	0.8	0.0	0.0	0.0	0.0
080816	2.2	0.2	1.5	0.4	0.0	0.0	0.0	0.0
080817	2.9	0.3	2.3	0.3	0.0	0.0	0.0	0.0
080818	3.3	0.3	2.3	0.3	0.0	0.0	0.0	0.0
080819	2.4	0.2	1.9	0.2	0.0	0.0	0.0	0.0
080820	2.8	0.2	1.7	0.8	0.0	0.0	0.0	0.0
080821	4.4	0.2	2.7	1.3	0.0	0.0	0.0	0.0
080822	4.8	0.4	2.9	1.4	0.0	0.0	0.0	0.0
080823	4.2	0.4	2.9	0.8	0.0	0.0	0.0	0.0
080824	3.9	0.3	2.7	0.8	0.0	0.0	0.0	0.0
080825	3.2	0.3	2.2	0.6	0.0	0.0	0.0	0.0
080826	3.0	0.3	2.1	0.6	0.0	0.0	0.0	0.0
080827	6.4	0.5	3.8	1.9	0.1	0.0	0.0	0.0
080828	4.1	0.4	3.3	0.4	0.0	0.0	0.0	0.0
080829	5.2	0.5	3.6	1.0	0.0	0.0	0.0	0.0
080830	7.1	0.6	5.0	1.4	0.0	0.0	0.0	0.0

CAS RN/ Sample No.	DMSO wt %[1]	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
080831	5.2	0.4	3.6	1.6	0.0	0.0	0.0	0.0
080832	5.3	0.5	3.2	1.6	0.0	0.0	0.0	0.0
080833	4.4	0.4	3.1	0.9	0.0	0.0	0.0	0.0
080834	4.3	0.4	3.0	0.9	0.0	0.0	0.0	0.0
080835	3.5	0.3	2.4	0.7	0.0	0.0	0.0	0.0
080836	4.0	0.3	2.8	0.8	0.0	0.0	0.0	0.0
080837	1.3	0.1	1.1	0.3	0.0	0.0	0.0	0.0
080838	2.5	0.2	1.7	0.5	0.0	0.0	0.0	0.0
080839	3.7	0.3	2.2	1.1	0.0	0.0	0.0	0.0
080840	4.3	0.4	3.0	0.9	0.0	0.0	0.0	0.0
120801	2.8	0.1	2.2	0.6	0.0	0.0	0.0	0.0
060812	1.3	0.1	1.0	0.1	0.0	0.0	0.0	0.0
081001	3.4	0.2	2.7	0.3	0.0	0.0	0.0	0.0
081003	2.5	0.2	1.8	0.5	0.0	0.0	0.0	0.0
091648		0.1	3.0	4.0	0.1	0.1	0.1	0.0
094523	2.4	0.0	0.7	1.2	0.5	0.0	0.1	0.0
085202	6.8	0.7	4.1	2.0	0.3	0.0	0.0	0.0
085203	7.0	0.7	4.2	2.1	0.1	0.0	0.0	0.0
68476-30-2 No 2 Fuel Oil								
089164	1.8	0.0	1.1	0.7	0.1	0.0	0.0	0.0
089165	2.8	0.1	1.4	1.1	0.1	0.0	0.0	0.0
089166	4.0	0.0	3.2	0.8	0.0	0.0	0.0	0.0
089167	1.4	0.1	0.8	0.6	0.1	0.0	0.0	0.0
089169	4.2	0.0	1.7	2.1	0.1	0.0	0.0	0.0
089170	3.2	0.2	1.6	1.3	0.2	0.0	0.0	0.0
089175	11.3	0.1	4.5	5.7	1.1	0.0	0.0	0.0
089180	4.0	0.4	1.6	2.0	0.1	0.0	0.0	0.0
089181	2.5	0.3	1.3	0.8	0.0	0.0	0.0	0.0
089182	4.0	0.4	1.6	1.6	0.2	0.0	0.0	0.0
089183	8.3	0.8	2.5	4.2	1.7	0.1	0.0	0.0
091022	3.4	0.3	2.4	0.6	0.0	0.0	0.0	0.0
091023	3.6	0.1	2.9	0.6	0.0	0.0	0.0	0.0
091024	4.0	0.2	3.2	0.6	0.0	0.0	0.0	0.0
091025	3.6	0.3	2.9	0.5	0.0	0.0	0.0	0.0
091026	3.8	0.2	3.0	0.6	0.0	0.0	0.0	0.0
091027	3.6	0.2	2.9	0.5	0.0	0.0	0.0	0.0
091675	15.2	0.3	6.1	4.6	1.5	0.8	1.5	0.9
089172	5.4	0.2	1.6	2.7	0.5	0.0	0.0	0.0
DGMK Middle Distillate Fuel Oil Samples (no CAS number)								
091673[6]	16.0	0.3	9.6	4.8	0.0	0.2	0.5	1.0
089168[6]	3.7	0.0	1.5	1.9	0.4	0.0	0.0	0.0
089171[6]	4.7	0.2	3.3	0.9	0.1	0.0	0.0	0.0
089173[6]	5.3	0.4	2.1	2.1	0.5	0.0	0.0	0.0
089174[6]	2.7	0.3	1.6	0.8	0.1	0.0	0.0	0.0
089176[6]	6.0	0.4	2.4	2.4	0.6	0.0	0.0	0.0
089177[6]	2.4	0.5	1.4	0.5	0.0	0.0	0.0	0.0
089178[6]	4.4	0.4	2.6	1.3	0.2	0.0	0.0	0.0
089179[6]	2.7	0.5	1.9	0.5	0.0	0.0	0.0	0.0
089184[6]	3.8	0.4	1.5	1.5	0.2	0.0	0.0	0.0
089185[6]	1.0	0.1	0.7	0.1	0.0	0.0	0.0	0.0
089186[6]	2.0	0.6	1.2	0.2	0.0	0.0	0.0	0.0
089187[6]	2.1	0.4	0.8	0.6	0.2	0.0	0.0	0.0
Refinery Streams								
64741-43-1 Gas Oil Intermediate C11-C25								
085288	8.8	0.0	2.6	5.3	0.2	0.3	0.4	0.3
091646		0.0	2.0	4.0	2.0	0.7	2.0	0.0
090901	5.1	0.1	2.1	2.6	0.2	0.0	0.0	0.0
090903	4.8	0.1	2.4	1.9	0.1	0.0	0.0	0.0
090904	7.1	0.0	0.6	6.4	0.2	0.0	0.0	0.0

CAS RN/ Sample No.	DMSO wt %[1]	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
64741-58-8 Vacuum Distillate, Light Paraffin C13-C30								
030917	4.6	0.0	0.1	4.4	0.1	0.0	0.0	0.0
64741-60-2 Catalytic Cracked Distillate, Intermediate C11-C30								
060948	41.0	0.4	28.7	12.3	0.0	0.0	0.0	0.0
060939	48.0	0.0	0.5	33.6	14.4	1.0	0.0	0.0
64741-77-1 Hydrocracked Distillate, light C10–C18								
030922	4.8	1.4	3.4	0.0	0.0	0.0	0.0	0.0
030923	2.1	0.6	1.5	0.0	0.0	0.0	0.0	0.0
087525	3.4	1.4	2.0	0.1	0.0	0.0	0.0	0.0
64741-82-8 Thermocracked Distillate, light C10-C18								
010919	9.8	0.5	7.9	1.0	0.0	0.0	0.0	0.0
060928	12.0	0.1	6.0	6.0	0.0	0.0	0.0	0.0
060931	8.6	0.2	5.2	3.4	0.3	0.0	0.0	0.0
060942	9.8	0.9	6.9	2.0	0.0	0.0	0.0	0.0
087213	10.5	0.1	4.2	6.3	0.3	0.0	0.0	0.0
091652		0.1	4.0	10.0	0.0	0.0	0.0	0.0
091037	10.4	0.6	5.7	3.8	0.3	0.0	0.0	0.0
091038	10.3	0.5	5.7	3.9	0.3	0.0	0.0	0.0
091039	10.2	0.6	6.2	3.3	0.2	0.0	0.0	0.0
094628		7.0	4.0	0.0	0.0	0.0	0.0	0.0
64742-80-9 Hydrodesulfurized Distillate Middle, C11-C25								
010908	3.4	0.0	2.4	1.0	0.0	0.0	0.0	0.0
010916	2.5	0.2	2.0	0.5	0.0	0.0	0.0	0.0
010917	7.4	0.2	3.7	3.7	0.0	0.0	0.0	0.0
086413	3.3	0.0	3.0	0.3	0.0	0.0	0.0	0.0
086414	10.5	0.8	6.3	3.2	0.0	0.0	0.0	0.0
64742-38-7 Clay treated distillate C9-C20								
060950	3.6	0.7	2.9	0.0	0.0	0.0	0.0	0.0
68333-25-5 Hydrodesulfurized distillate , light catalytic cracked C9-C25								
030925	9.4	0.5	6.6	2.8	0.0	0.0	0.0	0.0
030926	2.1	0.0	1.5	0.4	0.0	0.0	0.0	0.0
68333-88-0 Aromatic hydrocarbons								
010921	12.0	3.6	4.8	3.6	0.0	0.0	0.0	0.0
080903	31.0	9.3	18.6	0.6	0.0	0.0	0.0	0.0
080904	8.8	4.4	3.5	0.3	0.0	0.0	0.0	0.0
094628		7.0	4.0	0.0	0.0	0.0	0.0	0.0
68477-31-6 Reformed Bottoms								
080906	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
080907	1.4	1.3	0.1	0.0	0.0	0.0	0.0	0.0
68915-96-8 Gas Oil, Heavy [straight run distillate]								
060911	5.7	0.0	0.5	2.3	2.9	0.2	0.0	0.0
060924	5.4	0.2	1.6	2.2	1.1	0.5	0.1	0.0
060929	4.7	0.0	0.9	1.9	0.9	0.5	0.2	0.0
060941	5.0	0.1	1.0	2.0	1.0	0.5	0.1	0.0
64741-44-2 Gas Oil, light C11-C20								
087523	4.2	0.4	2.5	1.3	0.0	0.0	0.0	0.0
088773	0.9	0.0	0.7	0.2	0.0	0.0	0.0	0.0
64741-49-7 Vacuum Tower Condensate C11-C25								
085242	6.0	0.2	1.8	2.4	0.6	0.4	0.1	0.1
086175	6.7	0.0	2.0	3.4	1.3	0.4	0.1	0.1
086178	8.0	0.0	0.8	4.0	1.6	0.8	0.3	0.2
086186	8.9	0.1	2.7	6.2	0.3	0.1	0.1	0.3
086270	8.8	0.9	2.6	3.5	0.9	0.4	0.0	0.4
081005	7.7	0.0	4.6	3.1	0.0	0.0	0.0	0.0
086279	8.0	0.8	4.8	1.6	0.1	0.0	0.0	0.0
64741-59-9 Catalytic Cracked Distillate, light C9-C25								
008281	49.1	2.0	29.5	14.7	0.0	0.5	0.5	0.0
010912	39.8	0.4	27.9	8.0	0.0	0.0	0.0	0.0
010915	31.5	0.0	22.1	9.5	0.0	0.0	0.0	0.0

CAS RN/ Sample No.	DMSO wt %[1]	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
086182	29.0	0.0	17.4	11.6	0.0	0.0	0.0	0.0
086191	22.0	0.0	13.2	8.8	0.0	0.0	0.0	0.0
086195	36.2	0.4	25.3	10.9	0.0	0.0	0.0	0.0
086280	30.1	0.3	18.1	9.0	0.0	0.0	0.3	0.0
087524	28.0	2.0	16.8	8.4	0.0	0.0	0.0	0.0
087527	4.0	0.8	2.0	0.8	0.1	0.0	0.0	0.0
091679		0.4	20.0	20.0	0.4	0.0	0.0	0.0
010903	32.5	3.3	19.5	9.8	0.0	0.0	0.0	0.0
010913	23.9	2.4	16.7	4.8	0.0	0.0	0.0	0.0
010914	38.2	0.0	34.4	3.8	0.0	0.0	0.0	0.0
086273	18.1	0.4	10.9	5.4	0.2	0.0	0.2	0.0
089295	42.2	0.4	42.2	0.0	0.0	0.0	0.0	0.0
097526	16.0	1.1	9.6	6.4	0.2	0.0	0.0	0.0
64741-86-2 Sweetened Distillate C9-C20								
087088	2.7	0.0	2.4	0.3	0.0	0.0	0.0	0.0
094629		3.0	0.0	2.3	0.6	0.0	0.0	0.0
087467	2.9	0.0	2.3	0.6	0.0	0.0	0.0	0.0
64742-46-7 Hydrotreated Distillate, Middle C11-C25								
060809	4.3	0.3	3.0	1.3	0.0	0.0	0.0	0.0
060811	3.2	0.3	2.6	0.3	0.0	0.0	0.0	0.0
081004	0.3	0.0	0.2	0.1	0.0	0.0	0.0	0.0
64742-87-6 HYdrodesulfurized Gas Oil, light vacuum C13-C30								
081008	9.5	0.0	3.8	4.8	0.3	0.0	0.0	0.0
68814-87-9 Gas Oil, Intermediate C9-C25								
081002	4.3	0.1	2.6	1.7	0.1	0.0	0.0	0.0
081006	9.6	0.5	5.8	2.9	0.1	0.0	0.0	0.0
081007	14.0	0.7	9.8	4.2	0.0	0.0	0.0	0.0
68915-97-9 Gas Oil, Heavy								
086174	5.8	0.0	0.3	4.6	0.6	0.1	0.1	0.1
086183	6.2	0.0	0.4	4.3	1.2	0.2	0.1	0.1
086190	5.2	0.3	3.6	1.0	0.1	0.2	0.0	0.0
086271	10.5	0.1	0.8	5.3	3.2	0.4	0.2	0.1
Gas Oil Stream Blends No CAS RN								
060806	3.8	0.3	3.0	0.4	0.0	0.0	0.0	0.0
060807	3.6	0.2	2.9	0.7	0.0	0.0	0.0	0.0
060808	2.1	0.4	1.5	0.2	0.0	0.0	0.0	0.0
060810	4.4	0.4	3.1	0.9	0.0	0.0	0.0	0.0
10% 64741-59-9 and 90% 64741-44-2 088415	5.1	0.3	4.1	1.0	0.0	0.0	0.0	0.0
30% 64741-59-9 and 70% 64741-44-2 088416	7.4	0.7	5.2	1.5	0.0	0.0	0.0	0.0
50% 64741-59-9 and 50% 64741-44-2 088416	8.7	0.9	5.2	2.6	0.0	0.0	0.0	0.0

1 – Percent of DMSO-extractable PACs as determined by PAC-2 Method.

2 – ARC is "aromatic ring class". ARC 1 (%) is the weight percent of PACs that have 1 aromatic ring within the total sample; "ARC 2 (%) is the percent of PACs with 2 aromatic rings, and so forth to 7 aromatic rings determined by the PAC-2 method.

DMGK designation identifies distillate fuel oil samples tested in Germany for which CAS RNs are not available.

The systemic endpoints used in the models were selected by an extensive analysis to determine the most sensitive endpoints among studies of both repeated-dose toxicity and developmental toxicity. The test material samples included crude oils, gas oils, heavy fuel oils, a lubricating oil basestock, a heavy paraffinic distillate aromatic extract, and one waste stream. Modeling is only appropriate for petroleum streams that have a final boiling point ≥ 650ºF [≥343^{0}C] and for which toxicity is related to polycyclic aromatic carbon content.

The methods by which the modeling procedures were developed are reported in publications by Roth et al., 2012 and Nicolich et al., 2012. Application of these modeling procedures for repeated dose toxicity endpoints are described by Simpson et al 2012 and for developmental and reproductive toxicity by Murray et al., 2012.

The DMSO extraction procedure employed in Method II concentrates non-polar potentially bioactive aromatics which are analyzed by gas chromatography with flame ionization detection (GC/FID) or mass spectrometry (GC/MS) and the percentage of each ring distribution in the extract is calculated. The method is particularly definitive for higher molecular weight aromatics of 3-ring and above, generally representing the upper bounds of these fractions but tends to underestimate the lower molecular ring aromatics of 1 and 2 rings.

The fuels and streams in the Gas Oil Category are characterized by aliphatic constituents and alkylated 1 and 2 ring compounds with small percentages of 3 ring and virtually no 4-ring aromatics. The preponderance of low molecular weight aromatics in most gas oils limits the utility of the modeling procedure in its present form for this category of petroleum compounds.

However the modeled data for repeated dose and developmental toxicity endpoints are presented here for completeness.

Repeated Dose Modeling

Values in Table D-2 are the modeled PDR_{10} values and where appropriate BMD_{10}s. The PDR_{10} identifies a change of 10% from control value for a given sensitive endpoint but is not necessarily an indicator of adverse effect. The most sensitive endpoints for systemic effects in repeat dose studies are liver weight, thymus weight, platelet counts and hemoglobin concentration. The lowest value of all the endpoints for each sample constitutes the overall sample PDR_{10} (highlighted in Table D-2). A common measure of relative toxicity from a standard toxicity study is the Benchmark Dose. Values are calculated employing the methods of Crump, 1984 and Gift et al., 2011. The study BMD_{10} is also the lowest of the original BMD_{10} endpoint values. The BMD_{10} calculations from 13 week dermal rat studies that meet the criteria for the modeling domain give similar values to the PDR_{10}s.

Table D-2. Repeated-dose PDR_{10} and BMD_{10} for Gas Oils by Endpoint

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day								Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Thymus Wt.		Platelet Count		Hemaglobin Count		Relative liver wt.			
	Male	Female	Male	Female	Male	Female	Male	Female		
68334-30-5 Diesel Oils C9-C20 Ultralow Sulfur Diesel										
080801	422	372	E	E	2000	2000	-	-	372 thymus, F	na
080802	751	663	91	92	2000	2000	-	-	91	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day								Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Thymus Wt.		Platelet Count		Hemaglobin Count		Relative liver wt.			
	Male	Female	Male	Female	Male	Female	Male	Female		
									Platelets M	
080803	1685	1486	179	182	2000	2000	-	-	179 Platelets, M	na
080804	2000	2000	240	244	2000	2000	2000	2000	240 Platelets, M	na
080805	1454	1282	145	148	2000	2000	-	-	145 Platelets, M	na
080806	994	877	120	122	2000	2000	-	-	120 Platelets, M	na
080807	458	404	E	E	2000	2000	-	-	404 Thymus, F	na
080808	422	372	E	E	2000	2000	-	-	372 Thymus, F	na
080809	1685	1486	179	182	2000	2000	-	-	179 Platelets, M	na
080810	1269	1120	132	135	2000	2000	-	-	132 Platelets, M	na
080811	841	742	134	136	2000	2000	2000	2000	134 Platelets, M	na
080812	864	762	142	145	2000	2000	2000	2000	142 Platelets, M	na
080813	788	695	81	82	2000	2000	-	-	81 Platelets, M	na
080814	1282	1131	168	171	2000	2000	-	-	168 Platelets, M	na
080815	995	878	126	128	2000	2000	-	-	126 Platelets, M	na
080816	1722	1519	198	201	2000	2000	-	-	198 Platelets, M	na
080817	964	850	114	116	2000	2000	-	-	114 Platelets, M	na
080818	964	850	114	116	2000	2000	-	-	114 Platelets, M	na
080819	1240	1094	134	137	2000	2000	-	-	134 Platelets, M	na
080820	2000	1989	217	221	2000	2000	2000	2000	217 Platelets, M	na
080821	1971	1739	137	139	2000	2000	2000	2000	137 Platelets, M	na
080822	1204	1062	E	E	2000	2000	2000	2000	1062 Thymus, F	na
080823	885	780	E	E	2000	2000	-	-	780 Thymus, F	na
080824	1096	966	113	114	2000	2000	-	-	113 Platelets, M	na
080825	1169	1031	136	138	2000	2000	-	-	136 Platelets, M	na
080826	1213	1070	144	147	2000	2000	-	-	144 Platelets, M	na
080827	E	E	E	E	E	E	E	E	E	
080828	687	606	E	E	2000	2000	-	-	606 Thymus, F	na
080829	711	627	E	E	2000	2000	-	-	627 Thymus, F	na
080830	555	490	E	E	2000	2000	-	-	490 Thymus, F	na
080831	1053	928	E	E	2000	2000	2000	2000	928 Thymus, F	na
080832	1021	900	E	E	2000	2000	2000	2000	900 Thymus, F	na
080833	875	771	E	E	2000	2000	-	-	771 Thymus, F	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day								Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Thymus Wt.		Platelet Count		Hemaglobin Count		Relative liver wt.			
	Male	Female	Male	Female	Male	Female	Male	Female		
080834	899	793	E	E	2000	2000	-	-	793 Thymus, F	na
080835	1152	1016	126	129	2000	2000	-	-	126 Platelets, M	na
080836	1059	934	107	109	2000	2000	-	-	107 Platelets, M	na
080837	2000	2000	270	274	2000	2000	-	-	270 Platelets, M	na
080838	1685	1486	179	182	2000	2000	-	-	179 Platelets, M	na
080839	1638	1456	175	178	2000	2000	2000	2000	175 Platelets, M	na
080840	899	793	E	E	2000	2000	-	-	793 Thymus, F	na
120801	1834	1617	133	136	2000	2000	-	-	133 Platelets, M	NOAEL=600
060812	2000	2000	254	259	2000	2000	-	-	254 Platelets, M	na
081001	993	875	94	96	2000	2000	-	-	94 Platelets, M	na
081003	1600	1411	166	169	2000	2000	-	-	166 Platelets, M	na
091648	2000	2000	2000	2000	2000	2000	252	249	249 Rel. Liver, F	na
094523	1020	900	420	428	1277	1275	717	709	420 Platelets, M	na
085202	E	E	E	E	E	E	E	E	E	
085203	E	E	E	E	E	E	E	E	E	
68476-30-2 No 2 Fuel Oil										
089164	2000	2000	315	320	2000	2000	2000	2000	315 Platelets, M	na
089165	2000	1974	323	328	2000	2000	1391	1377	323 Platelets, M	na
089166	1656	1460	89	90	2000	2000-	-	-	89 Platelets, M	na
089167	1966	1734	467	475	2000	2000	2000	2000	467 Platelets, M	na
089169	2000	2000	847	861	2000	2000	549	543	543 Rel Liver, F	na
089170	1034	912	253	257	2000	2000	1087	1075	253 Platelets, M	na
089175	318	280	117	119	740	738	186	184	117 Platelets, M	na
089180	1905	1680	1219	1239	2000	2000	561	555	555 Rel. liver, F	na
089181	2000	1864	356	362	2000	2000	2000	2000	356 Platelets, M	na
089182	887	782	352	358	2000	2000	759	751	352 Platelets, M	na
089183	E	E	E	E	E	E	E	E	E	
091022	1089	960	121	123	2000	2000	-	-	121 Platelets, M	na
091023	1307	1153	95	96	2000	2000	-	-	95 Platelets, M	na
091024	986	869	85	86	2000	2000	-	-	85 Platelets, M	na
091025	889	784	93	95	2000	2000	-	-	93 Platelets, M	na
091026	1051	927	92	93	2000	2000	-	-	92 Platelets, M	na
091027	1031	909	92	94	2000	2000	-	-	92	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day								Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Thymus Wt.		Platelet Count		Hemaglobin Count		Relative liver wt.			
	Male	Female	Male	Female	Male	Female	Male	Female		
									Platelets, M	
091675	E	E	E	E	E	E	E	E	E	
089172	678	598	666	678	1522	1519	353	350	350 Rel liver, F	na
DGMK Middle Distillate Samples (no CAS number)										
091673	E	E	E	E	E	E	E	E	E	
089168	884	780	322	327	2000	2000	554	548	322 Platelets, M	na
089171	E	E	E	E	E	E	E	E	E	
089173	446	393	182	185	1582	1579	548	543	182 Platelets, M	na
089174	1031	909	207	211	2000	2000	2000	2000	207 Platelets, M	na
089176	386	340	153	156	1352	1349	478	473	153 Platelets, M	na
089177	1036	914	244	248	2000	2000	-	-	244 Platelets, M	na
089178	628	554	122	124	2000	2000	2000	2000	122 Platelets, M	na
089179	891	786	160	162	2000	2000	-	-	160 Platelets, M	na
089184	872	769	365	371	2000	2000	805	796	365 Platelets, M	na
089185	2000	2000	380	386	2000	2000	-	-	380 Platelets, M	na
089186	828	730	241	245	2000	2000	-	-	241 Platelets, M	na
089187	726	640	376	382	2000	2000	2000	2000	376 Platelets, M	na
64741-43-1										
085288	-	-	E	E	1419	1416	153	151	151 Rel liver, F	na
091646	226	199	E	E	261	260	109	108	108 Rel liver, F	na
090901	2000	2000	521	530	2000	2000	434	430	430 Rel liver, F	na
090903	2000	2000	208	212	2000	2000	819	816	208 Thymus, M	na
090904	-	-	-	-	1546	1542	126	125	125 Rel. Liver, F	na
64741-58-8 030917	-	-	-	-	2000	2000	179	177	177 Rel liver, F	na
64741-60-2										
060948	287	253	E	E	2000	2000	1417	1402	253 Thymus , F	na
060939	E	E	E	E	E	E	E	E	E	
64741-77-1										
030922	308	272	E	E	2000	2000	-	-	272 Thymus, F	na
030923	713	629	164	166	2000	2000	-	-	164 Platelet, M	na
087525	363	320	E	E	2000	2000	-	-	320 Thymus, F	na
64741-82-8										
010919	363	320	E	E	2000	2000	-	-	320 Thymus, F	na
060928	2000	2000	E	E	2000	2000	222	220	220	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day								Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Thymus Wt.		Platelet Count		Hemaglobin Count		Relative liver wt.			
	Male	Female	Male	Female	Male	Female	Male	Female		
									Rel liver, F	
060931	E	E	E	E	E	E	E	E	E	na
060942	390	344	E	E	2000	2000	-	-	344 Thymus, F	na
087213	2000	2000	2000	2000	1506	1503	168	166	166 Rel liver, F	
087213BMD	-	-	-	-	>125	>125	>30<125	>30<125		>30<125 Rel Liver, M,F
091652	-	-	E	E	1500	1497	94	93	93 Rel liver, F	na
091037	E	E	E	E	E	E	E	E	E	
091038	E	E	E	E	E	E	E	E	E	
091039	E	E	E	E	E	E	E	E	E	
094628	E	E	E	E	E	E	E	E	E	
64742-80-9										
010908	2000	2000	141	143	2000	2000	2000	2000	141 Platelet, M	na
010916	1454	1282	145	148	2000	2000	-	-	145 Platelet, M	na
010917	2000	2000	267	271	2000	2000	359	355	267 Platelet, M	na
086413	1264	1115	83	84	2000	2000	-	-	83 Platelet, M	na
086414	818	545	E	E	2000	2000	1179	1167	545 Thymus, F	na
64742-38-7 060950	501	442	82	84	2000	2000	-	-	82 Platelet, M	na
68333-25-5										
030925	691	610	E	E	2000	2000	2000	2000	610 Thymus, F	na
030926	2000	2000	193	196	2000	2000	-	-	193 Platelet, M	na
68333-88-0										
010921	E	E	E	E	E	E	E	E	E	
080903	E	E	E	E	E	E	E	E	E	
080904	E	E	E	E	E	E	E	E	E	
094628	E	E	E	E	E	E	E	E	E	
68477-31-6										
080906	2000	2000	2000	2000	2000	2000	2000	-	2000 Non-toxic	na
080907	488	430	E	E	2000	2000	2000	2000	430 Thymus, F	na
68915-96-8										
060911	81	71	65	67	404	404	208	204	65 Platelet, M	na
060924	143	126	146	148	1404	1402	223	221	126 Thymus, F	na
060929	172	152	303	308	2000	2000	226	224	152 Thymus, F	na
060941	157	138	239	243	2000	2000	225	223	138 Thymus, F	na
64741-44-2										
087523	1325	1168	159	161	2000	2000	2000	2000	159 Platelet, M	na
088773	2000	2000	422	429	2000	2000	-	-	422 Platelet, M	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day								Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Thymus Wt.		Platelet Count		Hemaglobin Count		Relative liver wt.			
	Male	Female	Male	Female	Male	Female	Male	Female		
64741-49-7										
085242	E	E	E	E	E	E	E	E	E	
086175	117	102	143	145	2000	2000	173	171	102 Thymus, F	na
086178	105	93	1360	1383	2000	2000	117	116	93 Thymus, F	na
086186	E	E	E	E	E	E	E	E	E	
086270	281	247	204	209	482	481	228	226	204 Platelet, M	na
086270BMD	>30<125	>30<125	>125 <500	>125 <500	>125 <500	>125 <500	>30<125	>30<125		>30<125 Thymus, Rel Liver
081005	2000	2000	102	104	2000	2000	650	643	102 Platelet, M	na
086279	E	E	E	E	E	E	E	E	E	na
64741-59-9										
008281	200	176	E	E	950	948	184	182	176 Thymus, F	
008281BMD	82	146	-	-	>500	>500	150	189		82 Thymus, M
010912	186	164	E	E	2000	2000	-	-	164 Thymus, F	na
010915	458	404	E	E	2000	2000	1805	1786	404 Thymus, F	na
086182	2000	2000	E	E	2000	2000	176	174	174 Rel liver, F	na
086191	2000	2000	E	E	2000	2000	232	230	230 Rel liver, F	na
086195	321	283	E	E	2000	2000	1431	1416	283 Thymus, F	na
086280	2000	2000	E	E	961	959	480	475	475 Rel liver, F	na
087524	239	211	E	E	1828	1824	480	475	211 Thymus, F	na
087527	534	471	160	163	2000	2000	2000	2000	160 Platelet, M	na
091679	E	E	E	E	E	E	E	E	E	
089295	E	E	E	E	E	E	E	E	E	
097526	E	E	E	E	E	E	E	E	E	
010903	E	E	E	E	E	E	E	E	E	
010913	E	E	E	E	E	E	E	E	E	
010914	E	E	E	E	E	E	E	E	E	
086273	E	E	E	E	E	E	E	E	E	
097526	E	E	E	E	E	E	E	E	E	
64741-86-2										
087088	1659	1463	106	108	2000	2000	-	-	106 Platelet, M	na
094629	E	E	E	E	E	E	E	E	E	
087467	2000	2000	125	127	2000	2000	-	-	125 Platelet, M	na
64742-46-7										
060809	1322	1166	117	119	2000	2000	2000	2000	117 Platelet, M	na
060811	884	780	99	101	2000	2000	-	-	99 Platelet, M	na
081004	2000	2000	1864	1896	2000	2000	2000	2000	1864 Platelet, M	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day								Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Thymus Wt.		Platelet Count		Hemaglobin Count		Relative liver wt.			
	Male	Female	Male	Female	Male	Female	Male	Female		
64742-87-6 081008	2000	2000	352	358	1831	1827	235	233	233 Rel liver, F	na
68814-87-9										
081002	1911	1685	158	161	2000	2000	1169	1157	158 Platelet, M	na
081006	E	E	E	E	E	E	E	E	E	
081007	485	428	E	E	2000	2000	2000	2000	428 Thymus, F	na
68915-97-9										
086174	2000	2000	-	-	1101	1099	159	158	158 Rel liver, F	na
086183	289	255	-	-	804	803	154	153	153 Rel liver, F	na
086190	346	305	79	80	2000	2000	2000	2000	79 Platelet, M	na
086271	94	83	129	132	257	256	110	109	83 Thymus, F	
086271BMD	83	44	320	228	162	397	53	94		44 Thymus, F
Gas Oil Stream Blends No CAS RN										
060806	829	731	87	88	2000	2000	-	-	87 Platelet, M	na
060807	1149	1041	99	100	2000	2000	-	-	99 Platelet, M	na
060808	1009	890	179	182	2000	2000	-	-	179 Platelet, M	na
060810	875	771	E	E	2000	2000	-	-	771 Thymus, F	na
088415	799	704	70	71	2000	2000	-	-	70 Platelet, M	na
088416[a]	508	448	E	E	2000	2000	-	-	448 Thymus, F	na
088416[b]	479	510	E	E	2000	2000	1498	1482	510 Thymus, F	na

Highlighted entries indicate definitive value selected for the sample PDR10 or BMD10 as the lowest value causing a 10% change in activity for the most sensitive endpoint

E = Extrapolated, model did not calculate a value

Dash indicates data for this endpoint outside model domain. No reliable predictions can be made for this endpoint.

BMD after the sample number indicates calculation based on repeat dose toxicity study

DMGK designation identifies distillate fuel oil samples tested in Germany for which CAS RNs were not provided (DGMK, 1993; Jungen et al., 1995).

na = not applicable; no BMD_{10} was calculated because no repeated-dose toxicology study was conducted on this sample

a - 30% 64741-59-9 and 70% 64741-44-2
b - 50% 64741-59-9 and 50% 64741-44-2

Table D-3 illustrates the modeled repeat dose data in relation to distribution of 1-7 ring PAC. Given the complex composition of gas oils even when identified by the same CAS RN, individual streams will vary in aromatic ring distribution which may alter the values expressed as PDR_{10}s. Knowledge of the PAC profiles allows ranking of potential toxicity within or between CAS RNs for read-across when animal data are not available. However since most Gas oil PAC profiles are heavily concentrated in the 1-2 ring distribution and models give equal weight to all 1-7 rings, the PDR10s may be inaccurate when overall aromatic content is low as in

ultralow sulfur diesel fuels or toxicity is influenced by irritation [see Table A-3]. Feuston et al, 1994 reported that skin irritation is correlated with skin irritation.

Table D-3. Modeled Repeat Dose PDR10 Values of Gas Oils from Most to Least Severe within each CAS RN

CAS RN	Sample No.	Repeat Dose PDR10 mg/kg	ARC 1 (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
68334-30-5 Diesel Oils Ultralow Sulfur									
68334-30-5	080813	81 Platelets, M	0.3	3.2	0.4	0.0	0.0	0.0	0.0
68334-30-5	080802	91 Platelets M	0.4	2.9	0.4	0.0	0.0	0.0	0.0
68334-30-5	081001	94 Platelets, M	0.2	2.7	0.3	0.0	0.0	0.0	0.0
68334-30-5	80836	107 Platelets, M	0.3	2.8	0.8	0.0	0.0	0.0	0.0
68334-30-5	80824	113 Platelets, M	0.3	2.7	0.8	0.0	0.0	0.0	0.0
68334-30-5	80817	114 Platelets, M	0.3	2.3	0.3	0.0	0.0	0.0	0.0
68334-30-5	80818	114 Platelets, M	0.3	2.3	0.3	0.0	0.0	0.0	0.0
68334-30-5	80806	120 Platelets, M	0.3	2.2	0.3	0.0	0.0	0.0	0.0
68334-30-5	080815	126 Platelets, M	0.4	2.5	0.8	0.0	0.0	0.0	0.0
68334-30-5	080835	126 Platelets, M	0.3	2.4	0.7	0.0	0.0	0.0	0.0
68334-30-5	080810	132 Platelets, M	0.2	2.0	0.3	0.0	0.0	0.0	0.0
68334-30-5	120801 NOEL = 600mg/kg	133 Platelets, M	0.1	2.2	0.6	0.0	0.0	0.0	0.0
68334-30-5	080811	134 Platelets, M	0.4	2.6	1.3	0.1	0.0	0.0	0.0
68334-30-5	080819	134 Platelets, M	0.2	1.9	0.2	0.0	0.0	0.0	0.0
68334-30-5	080825	136 Platelets, M	0.3	2.2	0.6	0.0	0.0	0.0	0.0
68334-30-5	080821	137 Platelets, M	0.2	2.7	1.3	0.0	0.0	0.0	0.0
68334-30-5	080812	142 Platelets, M	0.4	2.5	1.3	0.1	0.0	0.0	0.0
68334-30-5	080826	144 Platelets, M	0.3	2.1	0.6	0.0	0.0	0.0	0.0
68334-30-5	080805	145 Platelets, M	0.2	2.0	0.5	0.0	0.0	0.0	0.0
68334-30-5	081003	166 Platelets, M	0.2	1.8	0.5	0.0	0.0	0.0	0.0
68334-30-5	080814	168 Platelets, M	0.3	1.8	0.5	0.0	0.0	0.0	0.0
68334-30-5	080839	175 Platelets, M	0.3	2.2	1.1	0.0	0.0	0.0	0.0
68334-30-5	080803	179 Platelets, M	0.2	1.7	0.5	0.0	0.0	0.0	0.0
68334-30-5	080809	179 Platelets, M	0.2	1.7	0.5	0.0	0.0	0.0	0.0
68334-30-5	080838	179 Platelets, M	0.2	1.7	0.5	0.0	0.0	0.0	0.0
68334-30-5	080816	198 Platelets, M	0.2	1.5	0.4	0.0	0.0	0.0	0.0
68334-30-5	080820	217	0.2	1.7	0.8	0.0	0.0	0.0	0.0

CAS RN	Sample No.	Repeat Dose PDR10 mg/kg	ARC 1 (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
		Platelets, M							
68334-30-5	080804	240 Platelets, M	0.2	1.6	0.8	0.0	0.0	0.0	0.0
68334-30-5	091648	249 Rel. Liver, F	0.1	3.0	4.0	0.1	0.1	0.1	0.0
68334-30-5	060812	254 Platelets, M	0.1	1.0	0.1	0.0	0.0	0.0	0.0
68334-30-5	080837	270 Platelets, M	0.1	1.1	0.3	0.0	0.0	0.0	0.0
68334-30-5	080801	372 thymus, F	1.0	3.4	0.5	0.0	0.0	0.0	0.0
68334-30-5	080808	372 Thymus, F	1.0	3.4	0.5	0.0	0.0	0.0	0.0
68334-30-5	080807	404 Thymus, F	0.9	3.3	0.5	0.0	0.0	0.0	0.0
68334-30-5	094523	420 Platelets, M	0.0	0.7	1.2	0.5	0.0	0.1	0.0
68334-30-5	080830	490 Thymus, F	0.6	5.0	1.4	0.0	0.0	0.0	0.0
68334-30-5	080828	606 Thymus, F	0.4	3.3	0.4	0.0	0.0	0.0	0.0
68334-30-5	080829	627 Thymus, F	0.5	3.6	1.0	0.0	0.0	0.0	0.0
68334-30-5	080833	771 Thymus, F	0.4	3.1	0.9	0.0	0.0	0.0	0.0
68334-30-5	080823	780 Thymus, F	0.4	2.9	0.8	0.0	0.0	0.0	0.0
68334-30-5	080834	793 Thymus, F	0.4	3.0	0.9	0.0	0.0	0.0	0.0
68334-30-5	080840	793 Thymus, F	0.4	3.0	0.9	0.0	0.0	0.0	0.0
68334-30-5	080832	900 Thymus, F	0.5	3.2	1.6	0.0	0.0	0.0	0.0
68334-30-5	080831	928 Thymus, F	0.4	3.6	1.6	0.0	0.0	0.0	0.0
68334-30-5	080822	1062 Thymus, F	0.4	2.9	1.4	0.0	0.0	0.0	0.0
68334-30-5	080827	E	0.5	3.8	1.9	0.1	0.0	0.0	0.0
68334-30-5	085202	E	0.7	4.1	2.0	0.3	0.0	0.0	0.0
68334-30-5	085203	E	0.7	4.2	2.1	0.1	0.0	0.0	0.0
68476-30-2 No. 2 Fuel Oil									
68476-30-2	091024	85 Platelets, M	0.2	3.2	0.6	0.0	0.0	0.0	0.0
68476-30-2	089166	89 Platelets, M	0.0	3.2	0.8	0.0	0.0	0.0	0.0
68476-30-2	091026	92 Platelets, M	0.2	3.0	0.6	0.0	0.0	0.0	0.0
68476-30-2	091027	92 Platelets, M	0.2	2.9	0.5	0.0	0.0	0.0	0.0
68476-30-2	091025	93 Platelets, M	0.3	2.9	0.5	0.0	0.0	0.0	0.0
68476-30-2	091023	95 Platelets, M	0.1	2.9	0.6	0.0	0.0	0.0	0.0
68476-30-2	089175	117 Platelets, M	0.1	4.5	5.7	1.1	0.0	0.0	0.0
68476-30-2	091022	121 Platelets, M	0.3	2.4	0.6	0.0	0.0	0.0	0.0
68476-30-2	089170	253 Platelets, M	0.2	1.6	1.3	0.2	0.0	0.0	0.0
68476-30-2	089164	315 Platelets, M	0.0	1.1	0.7	0.1	0.0	0.0	0.0
68476-30-2	089165	323 Platelets, M	0.1	1.4	1.1	0.1	0.0	0.0	0.0

CAS RN	Sample No.	Repeat Dose PDR10 mg/kg	ARC 1 (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
68476-30-2	089172	350 Rel liver, F	0.2	1.6	2.7	0.5	0.0	0.0	0.0
68476-30-2	089182	352 Platelets, M	0.4	1.6	1.6	0.2	0.0	0.0	0.0
68476-30-2	089181	356 Platelets, M	0.3	1.3	0.8	0.0	0.0	0.0	0.0
68476-30-2	089167	467 Platelets, M	0.1	0.8	0.6	0.1	0.0	0.0	0.0
68476-30-2	089169	543 Rel Liver, F	0.0	1.7	2.1	0.1	0.0	0.0	0.0
68476-30-2	089180	555 Rel. liver, F	0.4	1.6	2.0	0.1	0.0	0.0	0.0
68476-30-2	089183	E	0.8	2.5	4.2	1.7	0.1	0.0	0.0
68476-30-2	091675	E	0.3	6.1	4.6	1.5	0.8	1.5	0.9
Middle Distillates No CAS RN									
Mid Distillate	089178	122 Platelets, M	0.2	1.6	2.7	0.5	0.0	0.0	0.0
Mid Distillate	089176	153 Platelets, M	0.4	2.4	2.4	0.6	0.0	0.0	0.0
Mid Distillate	089179	160 Platelets, M	0.5	1.9	0.5	0.0	0.0	0.0	0.0
Mid Distillate	089173	182 Platelets, M	0.4	2.1	2.1	0.5	0.0	0.0	0.0
Mid Distillate	089174	207 Platelets, M	0.3	1.6	0.8	0.1	0.0	0.0	0.0
Mid Distillate	089186	241 Platelets, M	0.6	1.2	0.2	0.0	0.0	0.0	0.0
Mid Distillate	089177	244 Platelets, M	0.5	1.4	0.5	0.0	0.0	0.0	0.0
Mid Distillate	089168[6]	322 Platelets, M	0.0	1.5	1.9	0.4	0.0	0.0	0.0
Mid Distillate	089184	365 Platelets, M	0.4	1.5	1.5	0.2	0.0	0.0	0.0
Mid Distillate	089187	376 Platelets, M	0.4	0.8	0.6	0.2	0.0	0.0	0.0
Mid Distillate	089185	380 Platelets, M	0.1	0.7	0.1	0.0	0.0	0.0	0.0
Mid Distillate	091673[6]	E	0.3	9.6	4.8	0.0	0.2	0.5	1.0
Mid Distillate	089171	E	0.2	3.3	0.9	0.1	0.0	0.0	0.0
64741-43-1									
64741-43-1	091646	108 Rel liver, F	0.0	2.0	4.0	2.0	0.7	2.0	0.0
64741-43-1	090904	125 Rel liver, F	0.0	0.6	6.4	0.2	0.0	0.0	0.0
64741-43-1	085288	151 Rel liver, F	0.0	2.6	5.3	0.2	0.3	0.4	0.3
64741-43-1	090903	208 Thymus, M	0.1	2.4	1.9	0.1	0.0	0.0	0.0
64741-43-1	090901	430 Rel liver, F	0.1	2.1	2.6	0.2	0.0	0.0	0.0
64741-58-8	030917	177 Rel liver, F	0.0	0.1	4.4	0.1	0.0	0.0	0.0
64741-60-2									
64741-60-2	060948	253 Thymus , F	0.4	28.7	12.3	0.0	0.0	0.0	0.0
64741-60-2	060939	E	0.0	0.5	33.6	14.4	1.0	0.0	0.0
64741-77-1									
64741-77-1	030923	164 Platelets, M	0.6	1.5	0.0	0.0	0.0	0.0	0.0
64741-77-1	030922	272 Thymus, F	1.4	3.4	0.0	0.0	0.0	0.0	0.0
64741-77-1	087525	320	1.4	2.0	0.1	0.0	0.0	0.0	0.0

CAS RN	Sample No.	Repeat Dose PDR10 mg/kg	ARC 1 (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
		Thymus, F							
64741-82-8									
64741-82-8	091652	93 Rel liver, F	0.1	4.0	10.0	0.0	0.0	0.0	0.0
64741-82-8	087213	166 Rel liver, F	0.1	4.2	6.3	0.3	0.0	0.0	0.0
64741-82-8	060928	220 Rel liver, F	0.1	6.0	6.0	0.0	0.0	0.0	0.0
64741-82-8	010919	320 Thymus, F	0.5	7.9	1.0	0.0	0.0	0.0	0.0
64741-82-8	060942	344 Thymus, F	0.9	6.9	2.0	0.0	0.0	0.0	0.0
64741-82-8	060931	E	0.2	5.2	3.4	0.3	0.0	0.0	0.0
64741-82-8	091037	E	0.6	5.7	3.8	0.3	0.0	0.0	0.0
64741-82-8	091038	E	0.5	5.7	3.9	0.3	0.0	0.0	0.0
64741-82-8	091039	E	0.6	6.2	3.3	0.2	0.0	0.0	0.0
64741-82-8	094628	E	7.0	4.0	0.0	0.0	0.0	0.0	0.0
64742-80-9									
64742-80-9	086413	83 Platelet, M	0.0	3.0	0.3	0.0	0.0	0.0	0.0
64742-80-9	010908	141 Platelet, M	0.0	2.4	1.0	0.0	0.0	0.0	0.0
64742-80-9	010916	145 Platelet, M	0.2	2.0	0.5	0.0	0.0	0.0	0.0
64742-80-9	010917	267 Platelet, M	0.2	3.7	3.7	0.0	0.0	0.0	0.0
64742-80-9	086414	545 Thymus, F	0.8	6.3	3.2	0.0	0.0	0.0	0.0
64742-38-7	060950	82 Platelet, M	0.7	2.9	0.0	0.0	0.0	0.0	0.0
68333-25-5									
68333-25-5	030926	193 Platelet, M	0.0	1.5	0.4	0.0	0.0	0.0	0.0
68333-25-5	030925	610 Thymus, F	0.5	6.6	2.8	0.0	0.0	0.0	0.0
68333-88-0									
68333-88-0	010921	E	3.6	4.8	3.6	0.0	0.0	0.0	0.0
68333-88-0	080903	E	9.3	18.6	0.6	0.0	0.0	0.0	0.0
68333-88-0	080904	E	4.4	3.5	0.3	0.0	0.0	0.0	0.0
68333-88-0	094628	E	7.0	4.0	0.0	0.0	0.0	0.0	0.0
68477-31-6									
68477-31-6	080907	430 Thymus, F	1.3	0.1	0.0	0.0	0.0	0.0	0.0
68477-31-6	080906	2000 Non-toxic	0.0	0.0	0.0	0.0	0.0	0.0	0.0
68915-96-8									
68915-96-8	060911	65 Platelet, M	0.0	0.5	2.3	2.9	0.2	0.0	0.0
68915-96-8	060924	126 Thymus, F	0.2	1.6	2.2	1.1	0.5	0.1	0.0
68915-96-8	060941	138 Thymus, F	0.1	1.0	2.0	1.0	0.5	0.1	0.0
68915-96-8	060929	152 Thymus, F	0.0	0.9	1.9	0.9	0.5	0.2	0.0
64741-44-2									
64741-44-2	087523	159 Platelet, M	0.4	2.5	1.3	0.0	0.0	0.0	0.0
64741-44-2	088773	422 Platelet, M	0.0	0.7	0.2	0.0	0.0	0.0	0.0

CAS RN	Sample No.	Repeat Dose PDR10 mg/kg	ARC 1 (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
64741-49-7									
64741-49-7	086178	93 Thymus, F	0.0	0.8	4.0	1.6	0.8	0.3	0.2
64741-49-7	081005	102 Platelets, M	0.0	4.6	3.1	0.0	0.0	0.0	0.0
64741-49-7	086175	102 Thymus, F	0.0	2.0	3.4	1.3	0.4	0.1	0.1
64741-49-7	086270	204 Platelet, M	0.9	2.6	3.5	0.9	0.4	0.0	0.4
64741-49-7	085242	E	0.2	1.8	2.4	0.6	0.4	0.1	0.1
64741-49-7	086186	E	0.1	2.7	6.2	0.3	0.1	0.1	0.3
64741-49-7	086279	E	0.8	4.8	1.6	0.1	0.0	0.0	0.0
64741-59-9									
64741-59-9	087527	160 Platelet, M	0.8	2.0	0.8	0.1	0.0	0.0	0.0
64741-59-9	010912	164 Thymus, F	0.4	27.9	8.0	0.0	0.0	0.0	0.0
64741-59-9	086182	174 Rel liver, F	0.0	17.4	11.6	0.0	0.0	0.0	0.0
64741-59-9	008281	176 Thymus, F	2.0	29.5	14.7	0.0	0.5	0.5	0.0
64741-59-9	087524	211 Thymus, F	2.0	16.8	8.4	0.0	0.0	0.0	0.0
64741-59-9	086191	230 Rel liver, F	0.0	13.2	8.8	0.0	0.0	0.0	0.0
64741-59-9	086195	283 Thymus, F	0.4	25.3	10.9	0.0	0.0	0.0	0.0
64741-59-9	010915	404 Thymus, F	0.0	22.1	9.5	0.0	0.0	0.0	0.0
64741-59-9	086280	475 Rel liver, F	0.3	18.1	9.0	0.0	0.0	0.3	0.0
64741-59-9	091679	E	0.4	20.0	20.0	0.4	0.0	0.0	0.0
64741-59-9	010903	LOEL = 450mg/kg	3.3	19.5	9.8	0.0	0.0	0.0	0.0
64741-59-9	010913	E	2.4	16.7	4.8	0.0	0.0	0.0	0.0
64741-59-9	010914	E	0.0	34.4	3.8	0.0	0.0	0.0	0.0
64741-59-9	086273	E	0.4	10.9	5.4	0.2	0.0	0.2	0.0
64741-59-9	089295	E	0.4	42.2	0.0	0.0	0.0	0.0	0.0
64741-59-9	087526	E	1.1	9.6	6.4	0.2	0.0	0.0	0.0
64741-86-2									
64741-86-2	094629	E	3.0	0.0	2.3	0.6	0.0	0.0	0.0
64741-86-2	087088	106 Platelets, M	0.0	2.4	0.3	0.0	0.0	0.0	0.0
64741-86-2	087467	125 Platelets. M	0.0	2.3	0.6	0.0	0.0	0.0	0.0
64742-46-7									
64742-46-7	060811	99 Platelet, M	0.3	2.6	0.3	0.0	0.0	0.0	0.0
64742-46-7	060809	117 Platelets, M	0.3	3.0	1.3	0.0	0.0	0.0	0.0
64742-46-7	081004	1864 Platelets, M	0.0	0.2	0.1	0.0	0.0	0.0	0.0
64742-87-6	081008	233 Rel liver, F	0.0	3.8	4.8	0.3	0.0	0.0	0.0
68814-87-9									
68814-87-9	081002	158 Platelet, M	0.1	2.6	1.7	0.1	0.0	0.0	0.0
68814-87-9	081007	428 Thymus, F	0.7	9.8	4.2	0.0	0.0	0.0	0.0
68814-87-9	081006	E	0.5	5.8	2.9	0.1	0.0	0.0	0.0

CAS RN	Sample No.	Repeat Dose PDR10 mg/kg	ARC 1 (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
68915-97-9									
68915-97-9	086190	79 Platelet, M	0.3	3.6	1.0	0.1	0.2	0.0	0.0
68915-97-9	086271	83 Thymus, F	0.1	0.8	5.3	3.2	0.4	0.2	0.1
68915-97-9	086183	153 Rel liver, F	0.0	0.4	4.3	1.2	0.2	0.1	0.1
68915-97-9	086174	158 Rel liver, F	0.0	0.3	4.6	0.6	0.1	0.1	0.1
Gas Oil Blends No CAS RN									
30% 64741-59-9 and 70% 64741-44-2	088416a	448 Thymus, F	0.7	5.2	1.5	0.0	0.0	0.0	0.0
50% 64741-59-9 and 50% 64741-44-2	088416b	510 Thymus, F	0.9	5.2	2.6	0.0	0.0	0.0	0.0
Gas oil blends	060806	87 Platelet, M	0.3	3.0	0.4	0.0	0.0	0.0	0.0
Gas oil blends	060807	99 Platelet, M	0.2	2.9	0.7	0.0	0.0	0.0	0.0
Gas oil blends	060808	179 Platelet, M	0.4	1.5	0.2	0.0	0.0	0.0	0.0
Gas oil blends	060810	771 Thymus, F	0.4	3.1	0.9	0.0	0.0	0.0	0.0

1 – Percent of DMSO-extractable PACs as determined by PAC-2 Method.

2 – ARC is “aromatic ring class”. ARC 1 (%) is the weight percent of PACs that have 1 aromatic ring within the total sample

E = Extrapolated, model did not calculate a value

Dash indicates data for this endpoint outside model domain. No reliable predictions can be made for this endpoint.

DMGK designation identifies distillate fuel oil samples tested in Germany for which CAS RNs were not provided (DGMK, 1993; Jungen et al., 1995).

.

When compared to animal studies PDR_{10} values correlate reasonably well with animal toxicity and BMD10 with the exception of the light coker gas oil where LOAEL was likely related to severe skin irritation and Ultralow sulfur diesel fuel that was not toxic and contained virtually no DMSO extractable aromatics.

Table D-4. Comparison of Repeat Dose 13 week Results with PAC content

CAS RN/Name	Sample #			PDR10	BMD10	% PAC
		LOAEL	NOAEL			
68915-97-9 Heavy Atmospheric. gas oil	086271	125	30	83	44	0.9% C1-C2 9.2% C3-C7
64741-49-7/ Vacuum Tower overheads	086270	125	30	204	>30; <125	2.5% C2; 5.2% C3-C7
64741-59-9/ Lt cycle oil	08281	M 125 F 500	M 25 F 125	176	82	30% C2 14% C3
64741-59-9/ Lt cat cracked oil	010913	450	100	E		17.1% C1-C2 4.6% C3
64751-82-8/ Lt coker gas oil	087213	30	none	166	>30; <125	4.2% C2 6.3% C3
68334-30-5/ Ultralow Sulfur diesel	120801	none	600	133		2.3% C1-C2 0.6% C3

Developmental Toxicity Modeling

Sensitive endpoints for developmental toxicity are fetal body weight, number of live fetuses per litter and resorptions per implantations. For most gas oil samples the most sensitive endpoints were fetal body weight and live fetuses per litter.

Table D-5. Developmental toxicity PDR_{10} and BMD_{10} For Gas Oils by Endpoint

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day			Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Fetal body weight	Live fetuses per litter	Resorptions per Implants		
68334-30-5 Diesel Oils					
080801	335	77	134	77 Live fetuses/litter	na
080802	1403	693	855	693 Live fetuses/litter	na
080803	2000	1691	2000	1691 Live fetuses/litter	na
080804	2000	721	1254	721 Live fetuses/litter	na
080805	2000	2000	2000	2000 all	na
080806	1900	984	1182	984 Live fetuses/litter	na
080807	382	90	156	90 Live fetuses/litter	na
080808	335	77	134	77 Live fetuses/litter	na
080809	2000	1691	2000	1691 Live fetuses/litter	na
080810	2000	2000	-	2000 Fetal wt; live fetuses	na
080811	974	255	443	255 Live fetuses/litter	na
080812	944	239	422	239 Live fetuses/litter	na
080813	2000	-	-	2000 Fetal body wt.	na
080814	1473	409	676	409 Live fetuses/litter	na
080815	1127	311	515	311 Live fetuses/litter	na
080816	2000	1060	1525	1060 Live fetuses/litter	na
080817	2000	1331	1386	1331 Live fetuses/litter	na
080818	2000	1331	1386	1331 Live fetuses/litter	na
080819	2000	2000	2000	2000 all	na
080820	2000	891	1487	891 Live fetuses/litter	na
080821	2000	2000	-	2000 Fetal wt; live fetuses	na
080822	1216	311	542	311 Live fetuses/litter	na
080823	1322	465	696	465 Live fetuses/litter	na
080824	2000	1726	1799	1726 Live fetuses/litter	na
080825	1789	646	955	646 Live fetuses/litter	na
080826	1690	552	854	552 Live fetuses/litter	na
080827	E	E	E	E	
080828	1718	2000	1490	1490	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day			Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Fetal body weight	Live fetuses per litter	Resorptions per Implants		
				Resorptions/implant	
080829	1048	363	545	363 Live fetuses/litter	na
080830	1059	537	677	537 Live fetuses/litter	na
080831	1625	582	912	582 Live fetuses/litter	na
080832	869	204	367	204 Live fetuses/litter	na
080833	1424	556	795	556 Live fetuses/litter	na
080834	1361	484	725	484 Live fetuses/litter	na
080835	1981	837	1151	837 Live fetuses/litter	na
080836	2000	2000	2000	2000 Not toxic	na
080837	2000	2000	-	2000 Fetal wt ; live fetuses	na
080838	2000	1691	2000	1691 Live fetuses/litter	na
080839	1629	409	725	409 Live fetuses/litter	na
080840	1361	484	725	484 Live fetuses/litter	na
120801	2000	-	-	2000 Fetal body wt.	na
060812	2000	2000	-	2000 Fetal wt; live fetuses	na
081001	2000	-	-	2000 Fetal body wt.	na
081003	2000	2000	2000	2000 all	na
091648	2000	258	723	258 Live fetuses/litter	na
091648BMD	>300	-	-	na	>300 Fetal body weight
094523	863	204	392	204 Live fetuses/litter	na
085202	E	E	E	E	
085203	E	E	E	E	
68476-30-2 Middle Distillates					
089164	2000	-	-	2000 Fetal body wt	na
089165	2000	2000	2000	2000 all	na
089166	2000	-	-	2000 Fetal body wt	na
089167	2000	884	1554	884 Live fetuses/litter	na
089169	2000	2000	-	2000 Fetal wt; live fetuses	na
089170	1508	409	738	409 Live fetuses/litter	na
089175	E	E	E	E	
089180	699	128	215	128 Live fetuses/litter	na
089181	1143	233	434	233 Live fetuses/litter	na
089182	665	139	261	139 Live fetuses/litter	na
089183	E	E	E	E	
091022	2000	982	1255	982	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day			Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Fetal body weight	Live fetuses per litter	Resorptions per Implants		
				Live fetuses/litter	
091023	2000	-	-	2000 Fetal wt; live fetuses	na
091024	2000	-	-	2000 Fetal body wt	na
091025	2000	2000	2000	2000 all	na
091026	2000	-	-	2000 Fetal body wt	na
091027	2000	-	-	2000 Fetal body wt	na
091675	E	E	E	E	
089172	855	193	381	193 Live fetuses/litter	na
DGMK Middle Distillate Samples (no CAS number)					
091673	E	E	E	E	
089168	2000	2000	-	2000 Fetal wt; live fetuses	na
089171	E	E	E	E	
089173	572	143	258	143 Live fetuses/litter	na
089174	1118	280	489	280 Live fetuses/litter	na
089176	555	146	262	146 Live fetuses/litter	na
089177	618	130	236	130 Live fetuses/litter	na
089178	873	250	425	250 Live fetuses/litter	na
089179	688	157	275	157 Live fetuses/litter	na
089184	655	137	257	137 Live fetuses/litter	na
089185	2000	2000	2000	2000 all	na
089186	487	102	184	102 Live fetuses/litter	na
089187	604	133	241	133 Live fetuses/litter	na
64741-43-1					
085288	782	84	204	84 Live fetuses/litter	na
091646	70	12	24	12 Live fetuses/litter	na
091646BMD	336	50<BMD<500	62	na	62 Resorptions/implant
090901	2000	758	2000	758 Live fetuses/litter	na
090903	2000	2000	-	2000 Fetal wt; live fetuses	na
090904	1350	100	266	100 Live fetuses/litter	na
64741-58-8 030917	1763	131	343	131 Live fetuses/litter	na
64741-60-2					
060948	-	-	-	-	
060939	E	E	E	E	
64741-77-1					
030922	220	49	86	49 Live fetuses/litter	na
030923	517	115	204	115 Live fetuses/litter	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day			Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Fetal body weight	Live fetuses per litter	Resorptions per Implants		
087525	199	41	74	41 Live fetuses/litter	na
64741-82-8					
010919	2000	-	-	2000 Fetal body wt	na
060928	2000	-	-	2000 Fetal body wt	na
060931	E	E	E	E	
060942	624	238	345	238 Live fetuses/litter	na
087213	2000	416	2000	416 Live fetuses/litter	na
091652	2000	108	357	108 Live fetuses/litter	na
091652BMD	-	-	>100	na	>100 Resorptions/implant
091037	E	E	E	E	
091038	E	E	E	E	
091039	E	E	E	E	
094628	E	E	E	E	
64742-80-9					
010908	2000	-	-	2000 Fetal body wt	na
010916	2000	2000	2000	2000 all	na
010917	2000	1031	2000	1031 Live fetuses/litter	na
086413	2000	-	-	2000 Fetal body wt	na
086414	656	172	301	172 Live fetuses/litter	na
64742-38-7 060950	531	142	232	142 Live fetuses/litter	na
68333-25-5					
030925	2000	-	-	2000 Fetal body wt	na
030926	2000	-	-	2000 Fetal body wt	na
68333-88-0					
010921	E	E	E	E	
080903	E	E	E	E	
080904	E	E	E	E	
094628	E	E	E	E	
68477-31-6					
080906	2000	2000	-	2000 Fetal wt; live fetuses	na
080907	191	37	68	37 Live fetuses/litter	na
68915-96-8					
060911	352	642	430	352 Fetal body wt	na
060924	850	503	663	503 Live fetuses/litter	na
060929	1233	402	683	402 Live fetuses/litter	na
060941	1480	2000	1797	1480 Fetal body wt	na
64741-44-2					
087523	1062	244	441	244 Live fetuses/litter	na

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day			Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Fetal body weight	Live fetuses per litter	Resorptions per Implants		
088773	2000	-	-	2000 Fetal body wt	na
64741-49-7					
085242	E	E	E	E	
086175	1168	1983	1476	1168 Fetal body wt	na
086178	660	182	332	182 Live fetuses/litter	na
086186	E	E	E	E	
086270	371	109	193	109 Live fetuses/litter	na
086270BMD	421	30<BMD<125	67	na	67 Resorptions/implant
081005	-	-	-	-	
086279	E	E	E	E	
64741-59-9					
008281	579	419	665	419 Live fetuses/litter	na
008281BMD	>500	>250; <500	>500	na	>250; <500 Live fetuses/litter
010912	-	-	-	-	
010915	-	-	-	-	
086182	-	-	-	-	
086191	-	-	-	-	
086195	-	-	-	-	
086280	-	-	-	-	
087524	284	80	137	80 Live fetuses/litter	na
087527	359	76	138	76 Live fetuses/litter	na
091679	E	E	E	E	
089295	E	E	E	E	
097526	E	E	E	E	
010903	E	E	E	E	
010913	E	E	E	E	
010914	E	E	E	E	
086273	E	E	E	E	
097526	E	E	E	E	
64741-86-2					
087088	2000	-	-	2000 Fetal body wt	na
094629	E	E	E	E	
087467	2000	-	-	2000 Fetal body wt	na
64742-46-7					
060809	2000	1489	1941	1489 Live fetuses/litter	na
060811	2000	2000	2000	2000 all	na
081004	2000	2000	-	2000 Fetal wt ; live fetuses	na
64742-87-6 081008	2000	-	-	2000 Fetal body wt	na
68814-87-9					
081002	2000	-	-	2000 Fetal body wt	na
081006	E	E	E	E	
081007	2000	-	-	2000 Fetal body wt	na
68915-97-9					

CAS RN/ Sample No	PDR_{10} or BMD_{10} mg/kg/day			Sample PDR_{10} mg/kg/day [Endpoint]	Sample BMD_{10} mg/kg/day [Endpoint]
	Fetal body weight	Live fetuses per litter	Resorptions per Implants		
086174	764	106	244	106 Live fetuses/litter	na
086183	612	134	276	134 Live fetuses/litter	na
086190	E	E	E	E	
086271	222	79	136	79 Live fetuses/litter	na
086271BMD	233	>8; <30	87	na	>8; <30 Live fetuses/litter
Gas Oil Stream Blends No CAS RN					
060806	2000	2000	-	2000 Fetal wt; live fetuses	na
060807	2000	-	-	2000 Fetal wt	na
060808	871	208	359	208 Live fetuses/litter	na
060810	1424	556	795	556 Live fetuses/litter	na
088415	2000	-	-	2000 Fetal body wt	na
088416[a]	773	277	413	277 Live fetuses/litter	na
088416[b]	450	102	184	102 Live fetuses/litter	na

Highlighted entries indicate definitive value selected for the sample PDR10 or BMD10 as the lowest value causing a 10% change in activity for the most sensitive endpoint

E = Extrapolated, model did not calculate a value

Dash indicates data for this endpoint is outside model domain. No reliable predictions can be made for this endpoint.

BMD after the sample number indicates calculation based on repeat dose toxicity study

na = not applicable; no BMD_{10} was calculated because no repeated-dose toxicology study was conducted on this sample

a - 30% 64741-59-9 and 70% 64741-44-2
b - 50% 64741-59-9 and 50% 64741-44-2

Table D-6 presents CAS RN samples in order of average developmental PDR_{10} values organized by severity of effects from lowest PDR_{10} to highest within each CAS RN compared with analytical aromatic ring distribution. These results demonstrate how values can vary within the same CAS RN and highlight the utility of modeling to rank potential effects from untested samples for which analytical data are available.

Table D-6. Modeled Developmental Toxicity PDR10 Values from Most to Least Severe within each CAS RN

CAS RN	Sample No.	Develop PDR10 mg/kg	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
68334-30-5 Diesel Fuels Ultralow Sulfur									
68334-30-5	080801	77 Live fetuses/litter	1.0	3.4	0.5	0.0	0.0	0.0	0.0
68334-30-5	080808	77 Live fetuses/litter	1.0	3.4	0.5	0.0	0.0	0.0	0.0
68334-30-5	080807	90 Live fetuses/litter	0.9	3.3	0.5	0.0	0.0	0.0	0.0
68334-30-5	080832	204 Live fetuses/litter	0.5	3.2	1.6	0.0	0.0	0.0	0.0
68334-30-5	094523	204 Live fetuses/litter	0.0	0.7	1.2	0.5	0.0	0.1	0.0
68334-30-5	080812	239 Live fetuses/litter	0.4	2.5	1.3	0.1	0.0	0.0	0.0

CAS RN	Sample No.	Develop PDR10 mg/kg	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
68334-30-5	080811	255 Live fetuses/litter	0.4	2.6	1.3	0.1	0.0	0.0	0.0
68334-30-5	091648	258 Live fetuses/litter	0.1	3.0	4.0	0.1	0.1	0.1	0.0
68334-30-5	080815	311 Live fetuses/litter	0.4	2.5	0.8	0.0	0.0	0.0	0.0
68334-30-5	080822	311 Live fetuses/litter	0.4	2.9	1.4	0.0	0.0	0.0	0.0
68334-30-5	080829	363 Live fetuses/litter	0.5	3.6	1.0	0.0	0.0	0.0	0.0
68334-30-5	080814	409 Live fetuses/litter	0.3	1.8	0.5	0.0	0.0	0.0	0.0
68334-30-5	080839	409 Live fetuses/litter	0.3	2.2	1.1	0.0	0.0	0.0	0.0
68334-30-5	080823	465 Live fetuses/litter	0.4	2.9	0.8	0.0	0.0	0.0	0.0
68334-30-5	080834	484 Live fetuses/litter	0.4	3.0	0.9	0.0	0.0	0.0	0.0
68334-30-5	080840	484 Live fetuses/litter	0.4	3.0	0.9	0.0	0.0	0.0	0.0
68334-30-5	080830	537 Live fetuses/litter	0.6	5.0	1.4	0.0	0.0	0.0	0.0
68334-30-5	080826	552 Live fetuses/litter	0.3	2.1	0.6	0.0	0.0	0.0	0.0
68334-30-5	080833	556 Live fetuses/litter	0.4	3.1	0.9	0.0	0.0	0.0	0.0
68334-30-5	080831	582 Live fetuses/litter	0.4	3.6	1.6	0.0	0.0	0.0	0.0
68334-30-5	080825	646 Live fetuses/litter	0.3	2.2	0.6	0.0	0.0	0.0	0.0
68334-30-5	080802	693 Live fetuses/litter	0.4	2.9	0.4	0.0	0.0	0.0	0.0
68334-30-5	080804	721 Live fetuses/litter	0.2	1.6	0.8	0.0	0.0	0.0	0.0
68334-30-5	080835	837 Live fetuses/litter	0.3	2.4	0.7	0.0	0.0	0.0	0.0
68334-30-5	080820	891 Live fetuses/litter	0.2	1.7	0.8	0.0	0.0	0.0	0.0
68334-30-5	080806	984 Live fetuses/litter	0.3	2.2	0.3	0.0	0.0	0.0	0.0
68334-30-5	080816	1060 Live fetuses/litter	0.2	1.5	0.4	0.0	0.0	0.0	0.0
68334-30-5	080817	1331 Live fetuses/litter	0.3	2.3	0.3	0.0	0.0	0.0	0.0
68334-30-5	080818	1331 Live fetuses/litter	0.3	2.3	0.3	0.0	0.0	0.0	0.0
68334-30-5	080828	1490 Resorptions/implant	0.4	3.3	0.4	0.0	0.0	0.0	0.0
68334-30-5	080803	1691 Live fetuses/litter	0.2	1.7	0.5	0.0	0.0	0.0	0.0
68334-30-5	080809	1691 Live fetuses/litter	0.2	1.7	0.5	0.0	0.0	0.0	0.0
68334-30-5	080838	1691 Live fetuses/litter	0.2	1.7	0.5	0.0	0.0	0.0	0.0
68334-30-5	080824	1726 Live fetuses/litter	0.3	2.7	0.8	0.0	0.0	0.0	0.0
68334-30-5	080805	2000 all	0.2	2.0	0.5	0.0	0.0	0.0	0.0
68334-30-5	080810	2000 Fetal wt; live fetus	0.2	2.0	0.3	0.0	0.0	0.0	0.0
68334-30-5	080813	2000 Fetal body wt.	0.3	3.2	0.4	0.0	0.0	0.0	0.0
68334-30-5	080819	2000 all	0.2	1.9	0.2	0.0	0.0	0.0	0.0
68334-30-5	080821	2000	0.2	2.7	1.3	0.0	0.0	0.0	0.0

CAS RN	Sample No.	Develop PDR10 mg/kg	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
		Fetal wt; live fetus							
68334-30-5	080836	2000 all	0.3	2.8	0.8	0.0	0.0	0.0	0.0
68334-30-5	080837	2000 Fetal wt ; live fetus	0.1	1.1	0.3	0.0	0.0	0.0	0.0
68334-30-5	120801 NOEL = 600mg/kg	2000 Fetal body wt.	0.1	2.2	0.6	0.0	0.0	0.0	0.0
68334-30-5	060812	2000 Fetal wt; live fetus	0.1	1.0	0.1	0.0	0.0	0.0	0.0
68334-30-5	081001	2000 Fetal body wt.	0.2	2.7	0.3	0.0	0.0	0.0	0.0
68334-30-5	081003	2000 Not toxic	0.2	1.8	0.5	0.0	0.0	0.0	0.0
68334-30-5	080827	E	0.5	3.8	1.9	0.1	0.0	0.0	0.0
68334-30-5	085202	E	0.7	4.1	2.0	0.3	0.0	0.0	0.0
68334-30-5	085203	E	0.7	4.2	2.1	0.1	0.0	0.0	0.0
68476-30-2 No. 2 Fuel Oil									
68476-30-2	089180	128 Live fetuses/litter	0.4	1.6	2.0	0.1	0.0	0.0	0.0
68476-30-2	089182	139 Live fetuses/litter	0.4	1.6	1.6	0.2	0.0	0.0	0.0
68476-30-2	089172	193 Live fetuses/litter	0.2	1.6	2.7	0.5	0.0	0.0	0.0
68476-30-2	089181	233 Live fetuses/litter	0.3	1.3	0.8	0.0	0.0	0.0	0.0
68476-30-2	089170	409 Live fetuses/litter	0.2	1.6	1.3	0.2	0.0	0.0	0.0
68476-30-2	089167	884 Live fetuses/litter	0.1	0.8	0.6	0.1	0.0	0.0	0.0
68476-30-2	091022	982 Live fetuses/litter	0.3	2.4	0.6	0.0	0.0	0.0	0.0
68476-30-2	089164	2000 Fetal body wt	0.0	1.1	0.7	0.1	0.0	0.0	0.0
68476-30-2	089165	2000 all	0.1	1.4	1.1	0.1	0.0	0.0	0.0
68476-30-2	089166	2000 Fetal body wt	0.0	3.2	0.8	0.0	0.0	0.0	0.0
68476-30-2	089169	2000 Fetal wt; live fetus	0.0	1.7	2.1	0.1	0.0	0.0	0.0
68476-30-2	091023	2000 Fetal wt; live fetus	0.1	2.9	0.6	0.0	0.0	0.0	0.0
68476-30-2	091024	2000 Fetal body wt	0.2	3.2	0.6	0.0	0.0	0.0	0.0
68476-30-2	091025	2000 all	0.3	2.9	0.5	0.0	0.0	0.0	0.0
68476-30-2	091026	2000 Fetal body wt	0.2	3.0	0.6	0.0	0.0	0.0	0.0
68476-30-2	091027	2000 Fetal body wt	0.2	2.9	0.5	0.0	0.0	0.0	0.0
68476-30-2	089175	E	0.1	4.5	5.7	1.1	0.0	0.0	0.0
68476-30-2	089183	E	0.8	2.5	4.2	1.7	0.1	0.0	0.0
68476-30-2	091675	E	0.3	6.1	4.6	1.5	0.8	1.5	0.9
Middle Distillates No CAS RN									
Mid distillate	089186[6]	102 Live fetuses/litter	0.6	1.2	0.2	0.0	0.0	0.0	0.0
Mid distillate	089177[6]	130 Live fetuses/litter	0.5	1.4	0.5	0.0	0.0	0.0	0.0
Mid distillate	089187[6]	133 Live fetuses/litter	0.4	0.8	0.6	0.2	0.0	0.0	0.0
Mid distillate	089184[6]	137 Live fetuses/litter	0.4	1.5	1.5	0.2	0.0	0.0	0.0

CAS RN	Sample No.	Develop PDR10 mg/kg	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
Mid distillate	089173[6]	143 Live fetuses/litter	0.4	2.1	2.1	0.5	0.0	0.0	0.0
Mid distillate	089176[6]	146 Live fetuses/litter	0.4	2.4	2.4	0.6	0.0	0.0	0.0
Mid distillate	089179[6]	157 Live fetuses/litter	0.5	1.9	0.5	0.0	0.0	0.0	0.0
Mid distillate	089178[6]	250 Live fetuses/litter	0.4	2.6	1.3	0.2	0.0	0.0	0.0
Mid distillate	089174[6]	280 Live fetuses/litter	0.3	1.6	0.8	0.1	0.0	0.0	0.0
Mid distillates	089168[6]	2000 Fetal wt; live fetus	0.0	1.5	1.9	0.4	0.0	0.0	0.0
Mid distillate	089185[6]	2000 all	0.1	0.7	0.1	0.0	0.0	0.0	0.0
Mid distillate	091673[6]	E	0.3	9.6	4.8	0.0	0.2	0.5	1.0
Mid distillate	089171 [6]	E	0.2	3.3	0.9	0.1	0.0	0.0	0.0
64741-43-1									
64741-43-1	091646	12 Live fetuses/litter	0.0	2.0	4.0	2.0	0.7	2.0	0.0
64741-43-1	085288	84 Live fetuses/litter	0.0	2.6	5.3	0.2	0.3	0.4	0.3
64741-43-1	090904	100 Live fetuses/litter	0.0	0.6	6.4	0.2	0.0	0.0	0.0
64741-43-1	090901	758 Live fetuses/litter	0.1	2.1	2.6	0.2	0.0	0.0	0.0
64741-43-1	090903	2000 Fetal wt; live fetus	0.1	2.4	1.9	0.1	0.0	0.0	0.0
64741-58-8	030917	131 Live fetuses/litter	0.0	0.1	4.4	0.1	0.0	0.0	0.0
64741-60-2									
64741-60-2	060948	-	0.4	28.7	12.3	0.0	0.0	0.0	0.0
64741-60-2	060939	E	0.0	0.5	33.6	14.4	1.0	0.0	0.0
64741-77-1									
64741-77-1	087525	41 Live fetuses/litter	1.4	2.0	0.1	0.0	0.0	0.0	0.0
64741-77-1	030922	49 Live fetuses/litter	1.4	3.4	0.0	0.0	0.0	0.0	0.0
64741-77-1	030923	115 Live fetuses/litter	0.6	1.5	0.0	0.0	0.0	0.0	0.0
64741-82-8									
64741-82-8	091652	108 Live fetuses/litter	0.1	4.0	10.0	0.0	0.0	0.0	0.0
64741-82-8	060942	238 Live fetuses/litter	0.9	6.9	2.0	0.0	0.0	0.0	0.0
64741-82-8	087213	416 Live fetuses/litter	0.1	4.2	6.3	0.3	0.0	0.0	0.0
64741-82-8	010919	2000 Fetal body wt	0.5	7.9	1.0	0.0	0.0	0.0	0.0
64741-82-8	060928	2000 Fetal body wt	0.1	6.0	6.0	0.0	0.0	0.0	0.0
64741-82-8	060931	E	0.2	5.2	3.4	0.3	0.0	0.0	0.0
64741-82-8	091037	E	0.6	5.7	3.8	0.3	0.0	0.0	0.0
64741-82-8	091038	E	0.5	5.7	3.9	0.3	0.0	0.0	0.0
64741-82-8	091039	E	0.6	6.2	3.3	0.2	0.0	0.0	0.0
64741-82-8	094628	E	7.0	4.0	0.0	0.0	0.0	0.0	0.0
64742-80-9									
64742-80-9	086414	172 Live fetuses/litter	0.8	6.3	3.2	0.0	0.0	0.0	0.0
64742-80-9	010917	1031 Live fetuses/litter	0.2	3.7	3.7	0.0	0.0	0.0	0.0
64742-80-9	010908	2000 Fetal body wt	0.0	2.4	1.0	0.0	0.0	0.0	0.0

CAS RN	Sample No.	Develop PDR10 mg/kg	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
64742-80-9	010916	2000 all	0.2	2.0	0.5	0.0	0.0	0.0	0.0
64742-80-9	086413	2000 Fetal body wt	0.0	3.0	0.3	0.0	0.0	0.0	0.0
64742-38-7	060950	142 Live fetuses/litter	0.7	2.9	0.0	0.0	0.0	0.0	0.0
68333-25-5									
68333-25-5	030925	2000 Fetal body wt	0.5	6.6	2.8	0.0	0.0	0.0	0.0
68333-25-5	030926	2000 Fetal body wt	0.0	1.5	0.4	0.0	0.0	0.0	0.0
68333-88-0									
68333-88-0	010921	E	3.6	4.8	3.6	0.0	0.0	0.0	0.0
68333-88-0	080903	E	9.3	18.6	0.6	0.0	0.0	0.0	0.0
68333-88-0	080904	E	4.4	3.5	0.3	0.0	0.0	0.0	0.0
68333-88-0	094628	E	7.0	4.0	0.0	0.0	0.0	0.0	0.0
68477-31-6									
68477-31-6	080907	37 Live fetuses/litter	1.3	0.1	0.0	0.0	0.0	0.0	0.0
68477-31-6	080906	2000 Fetal wt; live fetus	0.0	0.0	0.0	0.0	0.0	0.0	0.0
68915-96-8									
68915-96-8	060911	352 Fetal body wt	0.0	0.5	2.3	2.9	0.2	0.0	0.0
68915-96-8	060929	402 Live fetuses/litter	0.0	0.9	1.9	0.9	0.5	0.2	0.0
68915-96-8	060924	503 Live fetuses/litter	0.2	1.6	2.2	1.1	0.5	0.1	0.0
68915-96-8	060941	1480 Fetal body wt	0.1	1.0	2.0	1.0	0.5	0.1	0.0
64741-44-2									
64741-44-2	087523	244 Live fetuses/litter	0.4	2.5	1.3	0.0	0.0	0.0	0.0
64741-44-2	088773	2000 Fetal body wt	0.0	0.7	0.2	0.0	0.0	0.0	0.0
64741-49-7									
64741-49-7	086270	109 Live fetuses/litter	0.9	2.6	3.5	0.9	0.4	0.0	0.4
64741-49-7	086178	182 Live fetuses/litter	0.0	0.8	4.0	1.6	0.8	0.3	0.2
64741-49-7	086175	1168 Fetal body wt	0.0	2.0	3.4	1.3	0.4	0.1	0.1
64741-49-7	081005	-	0.0	4.6	3.1	0.0	0.0	0.0	0.0
64741-49-7	085242	E	0.2	1.8	2.4	0.6	0.4	0.1	0.1
64741-49-7	086186	E	0.1	2.7	6.2	0.3	0.1	0.1	0.3
64741-49-7	086279	E	0.8	4.8	1.6	0.1	0.0	0.0	0.0
64741-59-9									
64741-59-9	087527	76 Live fetuses/litter	0.8	2.0	0.8	0.1	0.0	0.0	0.0
64741-59-9	087524	80 Live fetuses/litter	2.0	16.8	8.4	0.0	0.0	0.0	0.0
64741-59-9	008281	419 Live fetuses/litter	2.0	29.5	14.7	0.0	0.5	0.5	0.0
64741-59-9	010912	-	0.4	27.9	8.0	0.0	0.0	0.0	0.0
64741-59-9	010915	-	0.0	22.1	9.5	0.0	0.0	0.0	0.0
64741-59-9	086182	-	0.0	17.4	11.6	0.0	0.0	0.0	0.0
64741-59-9	086191	-	0.0	13.2	8.8	0.0	0.0	0.0	0.0
64741-59-9	086195	-	0.4	25.3	10.9	0.0	0.0	0.0	0.0
64741-59-9	086280	-	0.3	18.1	9.0	0.0	0.0	0.3	0.0
64741-59-9	091679	E	0.4	20.0	20.0	0.4	0.0	0.0	0.0
64741-59-9	010903	E	3.3	19.5	9.8	0.0	0.0	0.0	0.0

CAS RN	Sample No.	Develop PDR10 mg/kg	ARC 1[2] (%)	ARC 2 (%)	ARC 3 (%)	ARC 4 (%)	ARC 5 (%)	ARC 6 (%)	≥ARC 7 (%)
64741-59-9	010913	LOEL = 450mg/kg	2.4	16.7	4.8	0.0	0.0	0.0	0.0
64741-59-9	010914	E	0.0	34.4	3.8	0.0	0.0	0.0	0.0
64741-59-9	086273	E	0.4	10.9	5.4	0.2	0.0	0.2	0.0
64741-59-9	089295	E	0.4	42.2	0.0	0.0	0.0	0.0	0.0
64741-59-9	087526	E	1.1	9.6	6.4	0.2	0.0	0.0	0.0
64741-86-2									
64741-86-2	087088	2000 Fetal body wt	0.0	2.4	0.3	0.0	0.0	0.0	0.0
64741-86-2	087467	2000 Fetal body wt	0.0	2.3	0.6	0.0	0.0	0.0	0.0
64741-86-2	094629	E	3.0	0.0	2.3	0.6	0.0	0.0	0.0
64742-46-7									
64742-46-7	060809	1489 Live fetuses/litter	0.3	3.0	1.3	0.0	0.0	0.0	0.0
64742-46-7	060811	2000 all	0.3	2.6	0.3	0.0	0.0	0.0	0.0
64742-46-7	081004	2000 Fetal wt ; live fetus	0.0	0.2	0.1	0.0	0.0	0.0	0.0
64742-87-6	081008	2000 Fetal body wt	0.0	3.8	4.8	0.3	0.0	0.0	0.0
68814-87-9									
68814-87-9	081002	2000 Fetal body wt	0.1	2.6	1.7	0.1	0.0	0.0	0.0
68814-87-9	081007	2000 Fetal body wt	0.7	9.8	4.2	0.0	0.0	0.0	0.0
68814-87-9	081006	E	0.5	5.8	2.9	0.1	0.0	0.0	0.0
68915-97-9									
68915-97-9	086271	79 Live fetuses/litter	0.1	0.8	5.3	3.2	0.4	0.2	0.1
68915-97-9	086174	106 Live fetuses/litter	0.0	0.3	4.6	0.6	0.1	0.1	0.1
68915-97-9	086183	134 Live fetuses/litter	0.0	0.4	4.3	1.2	0.2	0.1	0.1
68915-97-9	086190	E	0.3	3.6	1.0	0.1	0.2	0.0	0.0
Gas Oil Blends No CAS RN									
50% 64741-59-9 and 50% 64741-44-2	088416	102 Live fetuses/litter	0.9	5.2	2.6	0.0	0.0	0.0	0.0
30% 64741-59-9 and 70% 64741-44-2	088416	277 Live fetuses/litter	0.7	5.2	1.5	0.0	0.0	0.0	0.0
10% 64741-59-9 and 90% 64741-44-2	088415	2000 Fetal body wt	0.3	4.1	1.0	0.0	0.0	0.0	0.0
Gas Oil Blends	060808	208 Live fetuses/litter	0.4	1.5	0.2	0.0	0.0	0.0	0.0
Gas Oil Blends	060810	556 Live fetuses/litter	0.4	3.1	0.9	0.0	0.0	0.0	0.0
Gas Oil Blends	060806	2000 Fetal wt; live fetuses	0.3	3.0	0.4	0.0	0.0	0.0	0.0
Gas Oil Blends	060807	2000 Fetal wt	0.2	2.9	0.7	0.0	0.0	0.0	0.0

1 – Percent of DMSO-extractable PACs as determined by PAC-2 Method.

2 – ARC is “aromatic ring class”. ARC 1 (%) is the weight percent of PACs that have 1 aromatic ring within the total

E = Extrapolated, model did not calculate a value

Dash indicates data for this endpoint is outside model domain. No reliable predictions can be made for this endpoint.

Overall, both animal studies and modeling indicate that the main developmental effects of exposure to gas oils affect fetal survival and fetal body weight. Occurrence of malformations is infrequent LOAELs for developmental toxicity may range from 125-500mg/kg and NOAEL = 30-600mg/kg. Effects appear to be related to aromatic content and toxicity is greater where the C3 –C7 distribution is higher (Table D-7). PDR_{10} correlate well with the range of doses seen in animal studies.

Table D-7. Comparison of Developmental Results with PAC content

CAS RN/Name	Sample #	Developmental		PDR10	BMD10	% PAC
		LOAEL	NOAEL			
68915-97-9 Heavy Atmospheric. gas oil	086271	125	30	79	8>BMD>30	0.9% C1-C2 9.2% C3-C7
64741-49-7/ Vacuum Tower overheads	086270	125	30	109	67	2.5% C2; 5.2% C3-C7
64741-43-1/ F193	091646	250	50	12	50>BMD>500	2% C2 8.7% C3-C7
64751-82-8/ F277	094628	250	50			
64741-59-9/ F-213	091679	333	50	E		20.0% C2 20.4% C3
64741-59-9/ Lt cat cracked oil	010913	450	100	E		17.1% C1-C2 4.6% C3
64741-59-9/ Lt cycle oil	08281	500	250	419	250>BMD>500	30% C2 14% C3
64751-82-8/ F199	091652	none	>100	108	>100	4.1%C2 10% C3
64751-82-8/ Lt coker gas oil	087213	none	250 [highest dose]	416		4.2% C2 6.3% C3
68334-30-5/ F-195	091648	none	300	258	>300	3.1% C1-C2 4.3% C3
64741-86-2/ F-233	094629	none	500	E		3.0% C1 2.9% C3
68334-30-5/ Ultralow Sulfur diesel	120801	none	600	2000		2.3% C1-C2 0.6% C3

Appendix E. Optimized Ames Test and Statistical Modeling

The Optimized Ames test was developed to improve the performance of the reverse mutation *Salmonella* assay for detecting mutagenic and potentially carcinogenic lubricant base stocks and related refinery streams (ASTM, 2002). The method involves concentration of polycyclic aromatic compounds (PAC) by extraction, employing the most consistently PAC- sensitive strain of *Salmonella* [TA98] and increasing the metabolic activation system to maximize metabolism of the streams being evaluated. These modifications allowed detection of positive bacterial gene mutation response identified as an increase of mutant colonies in treated groups at least 2-fold that of negative controls as in the Standard Ames Assay and allowed prediction of potential dermal carcinogenesis by calculation of a mutagenicity index (MI).

The mutagenicity index (MI) is the slope of the initial portion of the dose response curve expressed in units of revertants per microliter. The mutagenicity index was highly correlated with dermal carcinogenic potential, suggesting that oils with MI values < 1 were unlikely to be dermally carcinogenic, oils with MI values $\geq$ 1 but < 2 were indeterminate, and oils with MI values $\geq$ 2 would likely produce skin tumors if tested in mice. The test method was refined to provide the greatest predictive value of gene mutagenicity and potential carcinogenicity for the widest range of high boiling [final boiling point approximately >650^{0}F; >343^{0}C (API, 2008)] PAC-containing streams and thus provides a more sensitive general *Salmonella* protocol for this class of petroleum substances. In 1995, the optimized Ames test was standardized as an ASTM method [ASTM E1687-95].

Relation of Mutagenic Activity with PAC Profile

The relationship of the MI with the PAC profile of refinery streams with known dermal carcinogenic potential has been established. The method of quantifying PAC constituents in which the condensed ring aromatics are removed by DMSO extraction and analyzed for 3-7 ring PAC by gas chromatography (GC) was developed by Roy *et al*. (1985; 1988). Having demonstrated a strong correlation between analytical distribution of PAC and mutagenicity in the optimized Ames test for petroleum-derived substances which produce dermal tumors when tested in mice, the utility of this relationship for read-across to untested substances has been expanded by statistical modeling.

Statistical Modeling of Analytical Data with the Optimized Salmonella Assay (Ames Test)

A statistical model has been developed to predict MI scores for untested substances encompassing precision in the critical 0-2 range (McKee, et al., 2010). This model employs the 1-7 ring PAC profile for each sample to predict MI scores. This model separated the data from 193 samples of a range of PAC-rich petroleum streams into those with mutagenicity index values equal to or greater than 1.0 and those with MI values less than 1.0. This model was not designed to quantify mutagenic potency but to identify whether or not a substance had an MI value less than 1 or not; this result can be used as an indication of whether the material has the potential to induce gene mutations in the optimized *Salmonella* assay and thus, to potentially be active in dermal carcinogenesis assays as well.

The statistical model is based on a series of three steps each predicting if the test substance was above or below an MI cut-point using a binary logistic general additive model. Step 1 predicts the probability that the substance has an MI of 5 or larger. The second step used only the substances predicted to have an MI below 5 and tested for a split at an MI of 2 or larger (the

samples from the first step that are predicted to be above 5 were set at 5 and were no longer in the model process). The third step uses only the substances predicted to have an MI below 2 and tested for a split at an MI of 1 or larger (again with the substances from the second step that were predicted to be greater than 2 were set to 2 and were no longer in the modeling process). At each step the probability for a decision is based on a value of 0.50. For example, in the first step, if the probability of the substance having an MI less then 5 was greater than 0.50 the substance was assigned a predicted MI of 'less than 5.' The final result was the combination of the results from the 3 steps with each substance predicted as being either < 1 or ≥ 1.

The model predictions agreed with the experimentally determined results 98% of the time, with the majority of the incorrect predictions being at MI values that were close to 1.0. When the model was tested with 49 hold out samples, 94% of the predictions were in agreement with the experimentally determined values.

From this information it is apparent that the outcome of Optimized Ames tests can be predicted from compositional information with an accuracy that seems comparable to that associated with variability inherent with either the experimental methods or the methods used to calculate mutagenicity index from the experimental data.