Screening Assessment
Petroleum Sector Stream Approach

Gas Oil
[Site-Restricted]

Chemical Abstracts Service Registry Number
68333-25-5

Environment Canada
Health Canada

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Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment of a site-restricted gas oil, Distillates (petroleum), hydrodesulfurized light catalytic cracked, Chemical Abstracts Service Registry Number[1] (CAS RN) 68333-25-5.

This substance was identified as a high priority for action during the categorization of the Domestic List (DSL), as it was determined to present the greatest potential or intermediate potential for exposure of individuals in Canada and was considered to present a high hazard to human health. Some components of this substance also met the ecological categorization criteria for bioaccumulation and inherent toxicity to non-human organisms. This substance was included in the Petroleum Sector Stream Approach (PSSA) because it is related to the petroleum sector and is a complex mixture.

Gas oils are a group of complex petroleum mixtures that serve as blending stocks in the production of fuels that are used in diesel engines and for both industrial and domestic heating. Some of these substances may also be blended into solvents. The composition and physical and chemical properties of gas oils vary with the sources of crude oils or bitumen and the processing steps involved. As such, gas oils are considered to be of Unknown or Variable composition, Complex reaction products or Biological materials (UVCBs). CAS RN 68333-25-5, which is a complex mixture of aromatic and aliphatic hydrocarbons, mainly in the carbon range of C_9 to C_{25}, is a hydrodesulfurized light catalytically cracked distillate with a typical boiling point range of 185–391°C. In order to predict overall behaviour of this complex substance for purposes of assessing the potential for ecological effects, representative structures have been selected from each chemical class in the mixture.

Based on the available information, only a small proportion of the components of this gas oil (C_{20}–C_{25} two-ring alkyl cycloalkanes) are considered to be persistent according to criteria in the *Persistence and Bioaccumulation Regulations* of CEPA 1999 (Canada 2000). Based on the combined evidence of empirical and modelled bioaccumulation potential, the gas oil assessed in this report likely contains a large proportion of C_9 to C_{15} components that are bioaccumulative according to the criteria in the *Persistence and Bioaccumulation Regulations*. No components of this gas oil were found to be both persistent and bioaccumulative based on the criteria in the *Persistence and Bioaccumulation Regulations.*

Site-restricted gas oil was identified as a high priority for action because it was considered to present a high hazard to human health. A critical effect for the initial categorization of the site-restricted gas oil substance was carcinogenicity, based primarily on classifications by international agencies. Several studies conducted in mice reported development of skin tumours following repeated dermal application of gas oil substances. Gas oils demonstrated

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genotoxicity in *in vivo* and *in vitro* assays but appear to have limited potential to adversely affect reproduction and development. As data pertaining specifically to the site-restricted gas oil CAS 68333-25-5 were not found for characterization of human health effects, information on additional gas oil substances in the PSSA that are similar from a processing and physical-chemical perspective was considered.

The gas oil considered in this screening assessment has been identified as site-restricted (i.e., it is a subset of gas oils that are not expected to be transported off refinery or upgrader facility sites). According to information submitted under section 71 of CEPA 1999 and other sources of information, this gas oil is consumed on-site or blended into substances leaving the site under different CAS RNs. In addition, a number of regulatory and non-regulatory measures are already in place in Canada, which limit releases of site-restricted petroleum sector substances, including provincial/territorial operating permit requirements, and best practices and guidelines put in place by the petroleum industry at refinery and upgrader facilities. Accordingly, environmental and general population exposure to this substance is not expected. As such, harm to the environment or human health is not expected.

Therefore, it is concluded that this site restricted gas oil is not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity, or that constitute or may constitute a danger to the environment on which life depends, or that constitute or may constitute a danger in Canada to human life or health.

Based on the information available, it is concluded that the site-restricted gas oil listed under CAS RN 68333-25-5 does not meet any of the criteria set out in section 64 of CEPA 1999.

Because this substance is listed on the Domestic List, its import and manufacture in Canada are not subject to notification under subsection 81(1) of CEPA 1999. Given the potential hazardous properties of this substance, there is concern that new activities that have not been identified or assessed could lead to this substance meeting the criteria set out in section 64 of the Act. Therefore, application of the Significant New Activity provisions of the Act to this substance is being considered, so that any proposed new manufacture, import or use of this substance outside a petroleum refinery or upgrader facility is subject to further assessment, to determine if the new activity requires further risk management consideration.

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that have met the categorization criteria set out in the Act to determine whether these substances present or may present a risk to the environment or to human health.

Based on the information obtained through the categorization process, the Ministers identified a number of substances as high priorities for action. These include substances that

- met all of the ecological categorization criteria, including persistence (P), bioaccumulation potential (B) and inherent toxicity to aquatic organisms (iT), and were believed to be in commerce in Canada; and/or
- met the categorization criteria for greatest potential for exposure (GPE) or presented an intermediate potential for exposure (IPE), and had been identified as posing a high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity.

A key element of the Government of Canada's Chemicals Management Plan (CMP) is the Petroleum Sector Stream Approach (PSSA), which involves the assessment of approximately 160 petroleum substances that are considered high priorities for action. These substances are primarily related to the petroleum sector and are considered to be of Unknown or Variable composition, Complex reaction products or Biological materials (UVCBs).

Screening assessments focus on information critical to determining whether a substance meets the criteria as set out in section 64 of CEPA 1999. Screening assessments examine scientific information and develop conclusions by incorporating a weight of evidence approach and precaution.[2]

Grouping of Petroleum Substances

The high priority petroleum substances fall into nine groups of substances based on similarities in production, toxicity and physical-chemical properties (Table A1.1 in Appendix 1). In order to conduct the screening assessments, each high priority petroleum substance was

[2] A determination of whether one or more of the criteria of section 64 are met is based upon an assessment of potential risks to the environment and/or to human health associated with exposures in the general environment. For humans, this includes, but is not limited to, exposures from ambient and indoor air, drinking water, foodstuffs, and the use of consumer products. A conclusion under CEPA 1999 on the petroleum substances in the Chemicals Management Plan (CMP) is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the *Controlled Products Regulations*, which is part of the regulatory framework for the Workplace Hazardous Materials Information System (WHMIS) for products intended for workplace use. Similarly, a conclusion based on the criteria contained in section 64 of CEPA 1999 does not preclude actions being undertaken in other sections of CEPA 1999 or other Acts.

placed into one of five categories ("streams") depending on its production and uses in Canada:

0. substances concluded not to be relevant to the petroleum sector and/or not in commerce;
1. site-restricted substances, which are substances that are not expected to be transported off refinery, upgrader or natural gas processing facility sites[3];
2. industry-restricted substances, which are substances that may leave a petroleum-sector facility and be transported to other industrial facilities (for example, for use as a feedstock, fuel, or a blending component), but that do not reach the public market in the form originally acquired;
3. substances that are primarily used by industries and consumers as fuels;
4. substances that may be present in products available to the consumer.

An analysis of the available data determined that approximately 70 high priority petroleum substances are site-restricted under stream 1, as described above. These occur within four of nine substance groups: heavy fuel oils, gas oils, petroleum and refinery gases, and low boiling point naphthas.

These site-restricted substances were identified as GPE or IPE during the categorization exercise based on their production volumes reported in the Domestic Substances List (DSL). However, according to information submitted under section 71 of CEPA 1999, voluntary submissions, an in-depth literature review, and a search of material safety data sheets, these substances are consumed on-site or are blended into substances leaving the site under different Chemical Abstracts Service Registry Numbers (CAS RNs) (which will also be addressed under the CMP).

This screening assessment addresses one site-restricted gas oil described under CAS RN 68333-25-5. The remaining high priority gas oils (under 15 different CAS RNs) will be assessed separately, as they belong to streams 2, 3 or 4 (as described above). Health effects were assessed using toxicological data pooled across all 16 gas oil CAS RNs.

Included in this screening assessment is the consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under section 71 of CEPA 1999. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches, up to August 2010 for ecological sections, July 2009 for the exposure section of the document and up to October 2009 for the health effects section. Key studies were critically evaluated; modelling results may have been used to reach conclusions.

Characterization of risk to the environment involves consideration of data relevant to environmental behaviour, persistence, bioaccumulation and toxicity, combined with an estimation of exposure to potentially affected non-human organisms from the major sources

[3] For the purposes of the screening assessment of PSSA substances, a site is defined as the boundaries of the property where a facility is located. In these cases, facilities are either petroleum refineries or upgraders.

of release to the environment. Conclusions about the risk to the environment are based in part on an estimation of environmental concentrations resulting from releases and the potential for these concentrations to have a negative impact on non-human organisms. As well, other lines of evidence of environmental hazard are taken into account. The ecological portion of the screening assessment summarizes the most pertinent data on environmental behaviour and effects, and does not represent an exhaustive or critical review of all available data. Environmental models and comparisons with similar petroleum mixtures may assist in the assessment.

Evaluation of risk to human health involves consideration of data relevant to estimation of exposure (non-occupational) of the general population, as well as information on health hazards (based principally on the weight of evidence assessments of other agencies that were used for prioritization of the substance). Decisions for human health are based on the nature of the critical effect and/or margins between conservative effect levels and estimates of exposure, taking into account confidence in the completeness of the identified databases on both exposure and effects, within a screening context. The screening assessment does not represent an exhaustive or critical review of all available data. Rather, it presents a summary of the critical information upon which the conclusion is based.

This screening assessment was prepared by staff in the Existing Substances programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. The human health and ecological portions of this assessment have undergone external written peer review/consultation. Comments on the technical portions relevant to human health were received from scientific experts selected and directed by Equilibrium Environmental Inc., including Anthony Knafla (Equilibrium Environmental Inc.) and Ross Wilson (Wilson Scientific Consulting Inc.).

Additionally, the draft of this screening assessment was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Health Canada and Environment Canada.

The critical information and considerations upon which the screening assessment is based are summarized below.

Substance Identity

Gas oils are a category of petroleum mixtures that are used primarily in the production of fuels that are used in diesel engines and for both industrial and domestic heating. In addition, some gas oil substances may also be used as solvents (CONCAWE 1996). Gas oils in general are complex hydrocarbon mixtures that contain hydrocarbons in the C_9–C_{25} carbon range and boil between 185 and 391°C (ECB 2000) (Table A3.1 in Appendix 3). The boiling point range will be smaller for individual gas oils depending on their degree and type of refining.

Physical and Chemical Properties

Typical properties of gas oils vary over a wide range, as composition depends on the source of crude oil (CONCAWE 1996) or bitumen from which they are derived and the types of refinery or upgrader processes that they undergo.

Typically, gas oils contain C_9–C_{25} straight and branched alkanes, cycloalkanes, aromatic hydrocarbons and mixed aromatic cycloalkanes. Those that undergo cracking processes (including CAS RN 68333-25-5) generally contain some unsaturated hydrocarbons (alkenes) (CONCAWE 1996), although the proportion of alkenes in this CAS RN makes up less than 4% of the overall mixture. As well, the boiling point range determines the size and type of hydrocarbons in the mixture. While no data on boiling point range were found for this CAS RN, a similar light catalytic cracked gas oil (64741-59-9) has a boiling point range of 185–391°C (API 2003a).

In order to predict the overall behaviour of this complex petroleum substance in the environment, representative structures were chosen from each chemical class within the mixture. Chemical components were selected (Table A3.2 in Appendix 3) based in part on data availability, those with the maximum number of available data, including an identifiable CAS RN, being preferred. As the precise composition of this gas oil is not well defined, there was no effort made to choose representative structures based on the proportions in the mixture. Where there was a range of substances with the same carbon number listed in the database, within the boiling point range and molecular type, a middle value was chosen as the best representative of that subclass.

Table 1 contains physical and chemical property data estimated for this site-restricted gas oil using nonane (a C_9 alkane) and a C_{20} polycyclic aromatic hydrocarbon (PAH). Many of the representative structures are poorly soluble in water and hydrophobic, except for the smallest ring structures. All of the C_9–C_{15} representative structures are moderately to highly volatile while the C_{20} and C_{25} substances have low to moderate volatility (Table A3.3 in Appendix 3). Solubility generally decreases with increasing carbon number (i.e., increasing molecular size). Aromatic compounds tend to exhibit greater solubility when compared to aliphatics of the same carbon number (Gustafson et al. 1997).

Henry's Law constants (HLCs) all increase with increasing molecular size. Evaporation from water will occur for some of the representative structures: the alkanes, isoalkanes, alkenes, cycloalkanes and mono-aromatics will evaporate readily from water, as they all have high to very high HLCs, while the two- and three-ring aromatics will evaporate from water more slowly, as they have moderate HLCs. Fugacity modelling predicts little evaporation from water due to the competing forces of water solubility and increasing K_{ow} and K_{oc} values. The C_{20} and C_{25} compounds are more likely to bind to suspended sediments than they are to evaporate from water.

Table 1. General physical and chemical properties for the site-restricted gas oil

Property	Type	Value	Temperature (°C)	Reference
Melting point (ºC)	Experimental	-15 to -12	-	CONCAWE 1996
Boiling point (ºC)	Experimental	185–391[1]	-	ECB 2000
Density (kg/m^3)	Experimental	840–970	15	CONCAWE 1996
Vapour pressure (Pa)	Experimental/ Modelled*	0–400	40	CONCAWE 1996; MPBPWIN 2008
Henry's Law constant (Pa·m^3/mol)	Modelled	1.2 x 10^{-6} - 1.3 x 10^2	25	HENRYWIN 2008
Log K_{ow} (dimensionless)	Experimental	3.9–> 6.0	-	CONCAWE 1996
Log K_{oc} (dimensionless)	Modelled	4.79–5.28	-	KOCWIN 2009
Water solubility (mg/L)	Modelled	0.0004–0.22	25	WSKOWWIN 2008

***** Estimated using a C_9 alkane and a C_{20} PAH.
[1] From CAS RN 64741-59-9, a similar light catalytic cracked gas oil (API 2003a).

Abbreviations: K_{oc}, organic carbon–water partition coefficient; K_{ow}, octanol–water partition coefficient.

Sources

The site-restricted gas oil CAS RN 68333-25-5 is produced in Canadian refineries and upgraders. The CAS RN description (NCI 2007), typical process flow diagrams (Figures A2.1a and b in Appendix 2) (Hopkinson 2008), and information collected under section 71 of CEPA 1999 (Environment Canada 2008, 2009) indicate that this substance is part of an intermediate stream within both refineries or upgraders, or is blended to make other products under a new CAS RN. As such, this gas oil is not expected to be transported off facility sites. Consequently, the quantities produced are not relevant to this screening assessment since the potential for releases to the environment is negligible.

CAS RN 68333-25-5 represents a bottom fraction derived from a distillation column treated with a hydrodesulfurized light cracked distillate after a catalytic cracking process (Figures A2.1a and b in Appendix 2).

Uses

According to the information collected through the *Notice with respect to certain high priority petroleum substances* (Environment Canada 2008) and the *Notice with respect to potentially industry-limited high priority petroleum substances* (Environment Canada 2009), published under section 71 of CEPA 1999, the gas oil addressed in this screening assessment was identified as being consumed at the facility or blended into substances leaving the site under different CAS RNs. Although the substance was identified by multiple use codes established during the development of the DSL, it has been determined from information submitted under section 71 of CEPA 1999 (Environment Canada 2008, 2009), voluntary submissions from industry, an in-depth literature review and a search of material safety data sheets that this site-restricted gas oil is not expected to be transported off refinery or upgrader facility sites.

Releases to the Environment

Potential releases of gas oil substances from refineries or upgraders can be characterized as either controlled or unintentional releases. Controlled releases are planned releases from pressure relief valves, venting valves and drain systems that occur for safety purposes or maintenance, are considered part of routine operations and occur under controlled conditions. Unintentional releases are typically characterized as unplanned releases due to spills or leaks from various equipment, valves, piping or flanges resulting from equipment failure, poor maintenance, lack of proper operating practices, adverse weather conditions or other unforeseen factors. Refinery and upgrader operations are highly regulated and regulatory requirements are established under various jurisdictions. As well, voluntary non-regulatory measures implemented by the petroleum industry are in place to manage these releases (SENES 2009).

Controlled Releases

The site-restricted gas oil CAS RN in this screening assessment originates as a distillate (e.g., sidestream) or a bottom product from a distillation column in a refinery or an upgrader. Thus, the potential locations for the controlled release of this site-restricted gas oil include relief valves, venting valves or drain valves on the piping or (e.g., vessels) in the vicinity of the equipment.

Under typical operating conditions, controlled releases of this site-restricted gas oil would be captured in a closed system,[4] according to defined procedures, and then returned to the processing facility. In cases where the amount of the substance is small or its concentration is dilute, the site-restricted gas oil is sent to the facility wastewater treatment plant. In both cases, exposure to the general population or the environment is not expected from this site-restricted gas oil under the CAS RN identified in this screening assessment, as it is not expected to be transported off refinery or upgrader facility sites.

Unintentional Releases

Unintentional releases (including fugitive releases) occur from equipment (e.g., pumps, storage tanks), seals, valves, piping, flanges, etc. during processing and handling of petroleum substances, and can be greater in situations of poor maintenance or operating practice. Regulatory and non-regulatory measures are in place to reduce these events at petroleum refineries and upgraders (SENES 2009). Rather than being specific to one substance, these measures are developed in a more generic way in order to reduce unintentional releases of all substances in the petroleum sector.

For the Canadian petroleum industry, requirements at the provincial/territorial level typically prevent or manage the unintentional releases of petroleum substances and streams within a facility (through the use of operating permits) (SENES 2009).

At the federal level, unintentional releases of some petroleum substances are addressed under the *Fisheries Act*; the *Petroleum Refinery Liquid Effluent Regulations and Guidelines* set the discharge limits of oil and grease, phenol, sulphides, ammonia nitrogen and total suspended matter, as well as testing requirements for acute toxicity in the final petroleum effluents entering Canadian waters.

Additionally, existing occupational health and safety legislation specify measures to reduce occupational exposures of employees, and some of these measures also serve to reduce unintentional releases (CanLII 2009).

Non-regulatory measures (e.g., guidelines, best practices) to reduce unintentional releases from petroleum sector facilities include appropriate material selection during the design and setup processes, regular inspection and maintenance of storage tanks, piping and other process equipment, the implementation of leak detection and repair or other equivalent programs, the use of floating roofs in above-ground storage tanks to reduce the internal gaseous zone, and the minimal use of underground tanks (which can lead to undetected leaks) (SENES 2009).

[4] For the purposes of the screening assessment of PSSA substances, a closed system is defined as a system within a facility that does not have any releases to the environment, and in which losses are collected and either recirculated or destroyed.

Environmental Fate

Given that this is a site-restricted gas oil that is not expected to be transported off refinery or upgrader sites, only general data on the environmental behaviour of this CAS RN are presented in the screening assessment.

Persistence and Bioaccumulation Potential

Environmental Persistence

No empirical data on this site-restricted gas oil as a whole are available. A quantitative structure-activity relationship (QSAR)-based weight of evidence approach (Environment Canada 2007) was therefore applied using the BioHCwin (2008), BIOWIN (2008) and AOPWIN (2008) degradation models. Table A3.2 (Appendix 3) presents representative structures of this complex mixture. Modelling was based on the various representative structures of this gas oil. In addition, persistence in the environment was estimated with a series of models specific to different environmental compartments (Tables A3.4 and A3.5 in Appendix 3).

Based on the atmospheric degradation model AOPWIN (2008), all of the representative structures of gas oils are expected to degrade readily by interactions with hydroxyl radicals in air (Table A3.4 in Appendix 3).

Representative structures such as alkanes, alkenes, alkylated benzenes, alkylated biphenyls, PAHs and heterocyclic PAHs are all known to be resistant to hydrolysis, so hydrolysis half-lives in water could not be calculated (Lyman et al. 1990; EPI Suite 2008).

Bacterial primary degradation was estimated using BioHCwin (2008) and ultimate degradation was estimated with BIOWIN (2008). Most of the C_9–C_{20} representative structures would readily undergo primary and ultimate degradation. Some of the higher-molecular-weight representative structures of gas oils (C_{20}–C_{25} two-ring cycloalkanes) would be persistent in water (Table A3.5 in Appendix 3). Using an extrapolation ratio of 1:1:4 for water:soil:sediment biodegradation half-lives (Boethling et al. 1995), the half-lives of C_{20}–C_{25} two-ring cycloalkanes in soil and sediment can be extrapolated from the half-life estimations in water. This extrapolation indicates that these components would also be persistent in soil and sediment.

A small proportion of CAS RN 68333-25-5 is represented by these alkylated cycloalkanes (CONCAWE 1996), as the total cycloalkane component is 8–10% of a typical gas oil (API 1987a).

Based on the modelled data, only the C_{20}–C_{25} two-ring cycloalkanes in this gas oil are persistent (half-life in soil and water $\geq$ 182 days and half-life in sediment $\geq$ 365 days) based on the criteria in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

Since no experimental bioaccumulation or bioconcentration data for this gas oil as a mixture were available, empirical data for the representative structures found in gas oils and a predictive approach were applied using a bioconcentration factor (BCF) model (BCFBAF 2008a). This model incorporates the generic QSAR model of Arnot and Gobas (2003).

Uptake and depuration of various petroleum hydrocarbons (PHCs) by molluscs and fishes has been shown in numerous studies (Stegeman and Teal 1973; Hardy et al. 1974; Fong 1976; Roubal et al. 1978; McCain et al. 1978; Nunes and Benville 1978; Cravedi and Tulliez 1983; Niimi and Palazzo 1986; Niimi and Dookhran 1989; Hellou et al. 1994; Burkhard and Lukasewycz 2000; Wetzel and van Vleet 2004; Colombo et al. 2007; Zhou et al. 1997). Aromatic and aliphatic components are readily taken up, primarily in adipose tissue. Moderate concentrations have been found in muscle, gall bladder, gill and brain of exposed fish, but once these fish were removed to a clean environment, depuration occurs. However, tissue levels can remain relatively constant for a period of time. It may take weeks to months in order to reach undetectable levels. After a spill, the pollution load may remain for some time in the natural environment; therefore, the time for depuration in fish will be longer than that reported in laboratory-controlled studies.

Due to the lack of a rapid detoxification system, molluscs are unable to metabolize aromatic hydrocarbons readily. Moderate accumulation of petroleum hydrocarbons (PHCs) can occur in stable tissue compartment(s) with low hydrocarbon turnover and are not readily exchangeable (Stegeman and Teal 1973; Neff et al. 1976).

It is reported that bioaccumulation of PHCs in higher-chain organisms, such as fish, is found to be low due to their metabolic elimination and detoxification mechanisms (Varanasi et al. 1989; Jonsson et al. 2004). There is no evidence that PHCs biomagnify up food chains (Broman et al. 1990; Wan et al. 2007; Takeuchi et al. 2009).

Only three studies on bioaccumulation factors (BAFs) of PAHs in aquatic organisms (fish and clams) were found (Neff et al. 1976; Zhou et al. 1997; Burkhard and Lukasewyez 2000). Selected PAHs studied were one-ring C_6 to C_9, two-ring C_{10} to C_{13} and three-ring C_{14} to C_{18}. In concert with the findings of Niimi and Dookhran (1989) and Niimi and Palazzo (1986), PAHs were not accumulated by fish through dietary exposure because of the combined effects of poor absorption efficiencies and rapid elimination rates. Hence, none of the measured BAFs for one-ring aromatics and PAHs in the carbon range C_6 to C_{18} are considered to be high.

For bioaccumulation, the derivation of a BAF is preferred over a BCF, where chemical exposure through the diet is not included in the latter (BCFBAF 2008b). However, due to the scarcity of measured BAFs available, BCFs from various published works were compiled to provide further evidence for bioaccumulation and BAFs were predicted using kinetic mass-balance modeling (Arnot and Gobas 2003).

A suite of BCFs for components of gas oils (C_6 to C_{18}) were found (Table A3.7 in Appendix 3), namely, alkanes, isoalkanes, two-ring cycloalkanes, monoaromatics, cycloalkane monoaromatics, cycloalkane diaromatic and polyaromatics (Carlson et al. 1979; CITI 1992; Tolls and van Dijk 2002; Jonsson et al. 2004; Yakata et al. 2006; EMBSI 2004, 2005a, 2005b, 2006, 2007, 2008, 2009; JNITE 2010). Of the 31 components studied, only a C_{13} two-ring aromatic, 2-isopropyl naphthalene had a BCF > 5000. However, this isopropyl functional group was considered to be atypical of petroleum hydrocarbons (Lampi et al. 2010). The remaining measured BCF show that this fraction is not expected to highly bioconcentrate in fish via water borne exposures (Table A3.7 Appendix 3).

The BCF and BAF model estimates for the C_9 to C_{15} linear and cyclic representative structures range from 98–880 000 (Table A3.6 in Appendix 3). For the carbon ranges C_{11} to $<C_{15}$, the modeled values generally agree with the measured BCF data (Table A3.7 in Appendix 3). Only the C_{15} two-ring cycloalkanes were predicted to have a BCF greater than 5000 suggesting a lower potential for uptake from the water for this carbon range in general. However, the carbon range around C_{15} appears to be highly bioaccumulative via the diet as most of the BAFs predicted for the C_{15} linear and cyclic components exceed 5000 (Table A3.6 in Appendix 3). The BCF and BAF predictions for the C_9 to C_{15} fraction are within the parametric, mechanistic and metabolic domains of the model and so are considered reliable.

In Arnot and Gobas (2006a), at a log K_{ow} of 8.0, the empirical distribution of "acceptable" fish BCF data shows that there are very few chemicals with fish BCFs exceeding 5000. Examination of Environment Canada's empirical BCF/BAF database for DSL and non-DSL chemicals developed by Arnot and Gobas (2003b) and further by Arnot (2005, 2006b) shows that these are only highly chlorinated substances (i.e., decachlorobiphenyl, nonachlorobiphenyl, heptachlorobiphenyl), which have BCFs in the 10^5 range noting that octachloronaphthalene has a measured BCF of <1000 (Fox et al. 1994, Gobas et al. 1989, Oliver and Niimi 1988) and all have log K_{ow} values less than 9.0. The log K_{ow} of the C_{20} cyclo alkane fraction and $>C_{20}$ fractions is ~9.0 or greater than 9.0. At this log K_{ow} there are no empirically observed BCF (laboratory) or BAF values recorded for any species of invertebrates or vertebrates. This is most likely a result of very low bioavailability (and thus poor dietary assimilation efficiency). Therefore, the predicted BCF and BAF values for the C_{20} cycloalkane fraction and $>C_{20}$ fraction are considered to be out of the parametric domain of the Arnot-Gobas model (2003) and considered as being highly uncertain and not reliable values. The bioaccumulation potential of the C_{20} cycloalkane and $>C_{20}$ fractions is thus expected to be very low which means the BCF and BAF for these fractions is also very likely ≤ 5000.

Based on reported data, aquatic organisms readily take up PHCs, primarily into lipids. Moderate concentrations can be found in muscle and internal organs of fish, based on chronic concentration of PHCs and the distribution of fatty tissues. Once these fish are no longer exposed, depuration occurs quickly. Observed decreases in tissue burdens of hydrocarbons with increasing exposure time indicate biotransformation in fish. The tendency for specific types of PHCs to bioaccumulate in tissues suggests that these PHC compounds could be transferred at low concentrations into the food chain, although they do not bioaccumulate to

high levels or biomagnify in food chains. This pattern of uptake and depuration also indicates that pulsed exposures likely would not result in bioaccumulation over the long term.

Based on the combined evidence of empirical and modeled BAFs, the gas oil assessed in this report likely contains a large proportion of C_9 to C_{15} components that are bioaccumulative based on the criteria defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

No components of this gas oil were found to meet both both the persistence and bioaccumulation criteria in the *Persistence and Bioaccumulation Regulations.*

Potential to Cause Ecological Harm

Ecological Effects Assessment

Aquatic Compartment

No experimental data on the aquatic toxicity of this gas oil were available; therefore, modelled data were used to estimate the potential of gas oil mixtures for aquatic toxicity.

CONservation of Clean Air and Water in Europe (CONCAWE) developed an aquatic toxicity model specific to PHC mixtures, called PetroTox. It assumes toxicological action via narcosis and therefore accounts for additive effects according to the toxic unit approach (PetroTox 2009). It models the toxicity of C_5–C_{41} PHCs dissolved in the water fraction. The model considers compounds smaller than C_5 to be too volatile to remain in water long enough to impart any significant toxicity, and compounds larger than C_{41} to be too hydrophobic and immobile to impart any significant aquatic toxicity. PetroTox (2009) generates estimates of toxicity with a median lethal loading concentration (LL_{50}) rather than the median lethal concentration (LC_{50}), due to the insolubility of petroleum substances in water. The LL_{50} value is not a measure of the concentration of the petroleum constituents in the water-accommodated fraction (WAF), but rather the amount of petroleum substances needed to generate a WAF that is toxic to 50% of the test organisms.

The modelled aquatic toxicity data indicates that this gas oil may be harmful to aquatic organisms at relatively low concentrations (< 1 mg/L). The modelled freshwater toxicity values were 0.6 to 3.8 mg/L, and the modelled marine toxicity values were 0.2 to 6.6 (Table 3.8 in Appendix 3).

To determine whether the modelling data from PetroTox are suitable to use, a read-across approach was also conducted to compare the modelled toxicity of this gas oil with Fuel Oil No. 2 and diesel fuel oil. Fuel Oil No. 2 is a distillate light fuel oil, also referred to as home heating oil, with a boiling point range of 160–360°C (IARC 1989a). Diesel fuels are petroleum distillate fractions consisting primarily of C_9 to C_{20} hydrocarbons, and have a typical boiling point range of 282–338°C (Coast Guard 1985). The acute aquatic toxicity

values of Fuel Oil No. 2 and diesel fuel are presented in tables A3.9a and A3.9b in Appendix 3.

Aquatic LC_{50} values for Fuel Oil No.2 (Anderson et al. 1974; MacLean et al. 1989; Lee et al. 1978; and Rossi et al. 1976) and diesel fuel (Lockhart et al. 1987; MacLean and Doe 1989) range from 0.9 to 23.7 mg/L. The modelled aquatic LL_{50}s from PetroTox (0.2 to 6.6 mg/L) fall within the low end of this range, indicating that this gas oil may be somewhat more harmful than commercial fuels. The modelled data from PetroTox are within the appropriate range of measured toxicity values for similar commercial products.

This gas oil is potentially hazardous to a variety of aquatic organisms. Modelled toxicity values are generally in the range of similar commercial fuels; however, due to the lack of available empirical toxicity data on this gas oil, these results cannot be further substantiated.

Other Environmental Compartments

There are limited empirical ecological effects studies and no suitable models found for this gas oil in media other than water. In this screening assessment, only the aquatic compartment was considered.

Ecological Exposure Assessment

The gas oil considered in this report has been identified as site-restricted, indicating that it is not expected to be transported off refinery or upgrader facility sites, and thus release to the ecosystem is expected to be negligible. As there is no significant release to the environment, ecological exposure is not expected and exposure assessments are not considered.

Characterization of Ecological Risk

Based on the available information, only a small proportion of components of this gas oil (C_{20}–C_{25} two-ring alkyl cycloalkanes) are considered to be persistent based on criteria in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Based on the combined evidence of empirical and modelled BAFs, the gas oil assessed in this report likely contains a large proportion of C_9–C_{15} components that are bioaccumulative based on the criteria in the *Persistence and Bioaccumulation Regulations*.

No components of this gas oil were found to be both persistent and bioaccumulative based on criteria in the *Persistence and Bioaccumulation Regulations.*

Based on information obtained from a variety of sources (voluntary industry submissions, an in-depth literature review, and a search of material safety data sheets), the gas oil considered in this screening assessment has been identified as site-restricted - i.e., it is not expected to be transported off refinery or upgrader facility sites. This gas oil is consumed on-site or is blended into other substances leaving the site under different CAS RNs. Measures (including provincial/territorial operating permit requirements, and best practices and guidelines put in place by the petroleum industry) are in place to minimize releases from refineries and

upgrader facilities. As a result of these factors, the likelihood of exposure, and potential for risk, of organisms in the environment to this gas oil is considered to be low.

Uncertainties in Evaluation of Ecological Risk

As the site-restricted gas oil is considered to be a UVCB, its specific chemical composition is not well defined. Gas oil streams under the same CAS RN can vary significantly in the number, identity and proportion of constituent compounds, depending on operating conditions, feedstocks and processing units.

All modelling of a substance's physical and chemical properties, persistence and bioaccumulation, and toxicity characteristics is based on representative structures. Given that a variety of representative structures may be derived from the same gas oil, it is recognized that structure-related uncertainties exist for these substances. The physical and chemical properties of 22 representative structures were used to estimate the overall behaviour of this gas oil, in order to represent the expected range in physical and chemical characteristics. Given the large number of potential permutations of the type and percentages of the structures in gas oils, there is uncertainty in the results associated with modelling.

As this substance is classified as site-restricted, environmental releases and exposures are expected to be negligible. However, monitoring data for specific CAS RN were not identified to verify this assumption.

Potential to Cause Harm to Human Health

Health Effects Assessment

No toxicological data were found for CAS RN 68333-25-5. Therefore, in order to characterize the toxicity of this site-restricted substance, additional gas oils in the PSSA that are similar from both a process and a physical-chemical perspective were evaluated for their toxicological effects. Because the site-restricted and the additional PSSA high-priority gas oil substances have similar physical-chemical properties and toxicological properties, the toxicological data were pooled across CAS RNs to construct a toxicological profile to represent all gas oils.

Appendix 4 contains a summary of available health effects information for this site-restricted gas oil substance and the lowest-observed-adverse-effect levels/concentrations (LOAELs/LOAECs) observed from the pooled toxicological data representing distillate fuels and the refinery or upgrader streams used in the production of these fuels. As such, the complete gas oils dataset can be considered a continuum delimited by substances that are largely composed of either saturated or aromatic hydrocarbons. This approach was taken in order to represent the toxicity of gas oils as a group.

Although no information regarding acute toxicity was available for the site-restricted gas oil CAS RN 68333-25-5, oral median lethal doses (LD_{50}s) for the gas oil substances were noted to range from 3200 to 17 838 mg/kg-body weight (kg-bw) in rats. Inhalation median lethal concentrations (LC_{50}s) ranged from 3350 to 7640 mg/m^3 in rats. Dermal LD_{50}s were noted to be > 40 000 mg/kg-bw in mice and range between > 2000 and > 4207 mg/kg-bw in rabbits (CONCAWE 1996; API 2003a, b). Moderate to severe skin irritation was observed in all cases of acute dermal exposure.

Multiple short-term and subchronic dermal toxicity studies have been conducted for gas oil substances. Doses ranged from 8 to 40 000 mg/kg-bw per day for exposure periods ranging from approximately 2 to 60 weeks in rats, mice and rabbits. Again, moderate to severe skin irritation was observed at various doses. Selected dermal effects observed in the short-term and subchronic dermal toxicity studies include: erythema, flaking, scabbing and thickening of the skin, inflammation, epidermal hyperplasia, parakeratosis, hyperkeratosis, ulceration, alopecia and necrosis of the hair follicles at the application site (API 1980a, 1985a; Easley et al. 1982; Beck et al. 1984; IITRI 1984; NTP 1986; UBTL 1986; Mobil 1985, 1988a, b, 1991; Freeman et al. 1990; Feuston et al. 1994; Ingram et al. 1993; Nessel et al. 1998; Walborg et al. 1998). The highly irritating nature of these substances, however, may act as a self-limiting factor for exposure. Selected systemic effects observed in these dermal studies include: increased mortality, decreased body weight gain and body weight, changes in liver, kidney and spleen weights, hematological and clinical chemistry variation, renal lesions, karyomegaly in the liver, and increased lymphocytes (Schultz et al. 1981; Easley et al. 1982; IITRI 1984; NTP 1986; Mobil 1988b, 1991; Feuston et al. 1994). A short-term LOAEL of 50 mg/kg-bw per day was established based on decreased body weight gain, body weight and food consumption following exposure of pregnant rats to CAS RN 64741-59-9 at doses of 25, 50, 125, 250, 500 or 1000 mg/kg-bw per day from gestational days 0 to 19 (Mobil 1988b). A subchronic LOAEL of 30 mg/kg-bw per day was established based on increased lymphocytes and decreased thymus weight following exposure of male and female rats to CAS RN 64741-82-8 at doses of 30, 125, 500 or 2000 mg/kg-bw per day for 13 weeks (Mobil 1991).

Short-term and subchronic inhalation studies were conducted over periods of five days to 13 weeks. Of the six studies available, no data were obtained for the site-restricted gas oil substance. Selected systemic effects observed in studies assessing representative gas oil substances include: increased mortality, decreased body weight gain and body weight, increased response time (startle reflex), histological lesions in the lungs, increased macrophages and other free pulmonary cells, and decreased red blood cells (Cowan and Jenkins 1981; Lock et al. 1984; Dalbey et al. 1987). A short-term LOAEC of 25 mg/m^3 was established based on microscopic changes in the nasal tissue, including subacute inflammation of the respiratory mucosa, of rats exposed to CAS RN 64742-80-9 at a single concentration of 25 mg/m^3 for four weeks (API 1986a). An increased leukocyte count (~ 30%) was also noted, but no corresponding macroscopic changes were observed at necropsy. A subchronic LOAEC of 250 mg/m^3 was established based on decreased body weight and increased response time, using the startle reflex assay following exposure of rats to CAS RN 68334-30-5 (diesel fuel) at concentrations of 250, 750 or 1500 mg/m^3 for 13

weeks, however, no corresponding histological changes in the nervous system were noted (Lock et al. 1984).

Only one oral study was conducted. Increased liver enzyme activity was observed in male rats following administration of CAS RN 68476-34-6 (commercial diesel fuel #2) at a dose of 1013 mg/kg-bw via gavage on days 1, 3, 5 and 8 (Khan et al. 2001).

The genotoxicity of gas oils has been evaluated through both *in vivo* and *in vitro* assays. Results from *in vivo* genotoxicity testing with gas oil substances were mixed. While no studies have been conducted using the site-restricted gas oil, positive results were observed following administration of additional representative gas oil substances for bone marrow chromosomal aberration in rats. One positive sister chromatid exchange assay conducted in mice was noted following administration of a light catalytic cracked distillate (API 1978, 1979a, 1989a; Conaway et al. 1984). Negative results were observed for bone marrow micronuclei induction, dominant lethal mutation and one sister chromatid exchange assay conducted in mice for five gas oil substances. Negative results were also obtained for bone marrow chromosomal aberrations in two studies assessing light and middles distillates, respectively, in rats (API 1980b, 1984, 1985b, c, 1986b, 1988a; McKee et al. 1994).

The genotoxicity of gas oils evaluated through *in vitro* assays also exhibited mixed results. Positive results were observed for Ames, mouse lymphoma and sister chromatid exchange assays (API 1979a, 1984, 1985c, d, e, 1986c, 1987b; Ellenton and Hallett 1981; Blackburn et al. 1984, 1986; Conaway et al. 1984; DGMK 1991; McKee et al. 1994; Nessel et al. 1998). Negative results were observed for Ames and mouse lymphoma assays, as well as for morphological transformation (API 1978, 1987c; Henderson et al. 1981; Schultz et al. 1981; Blakeslee et al. 1983; Blackburn et al. 1984, 1986; Conaway et al. 1984; NTP 1986; McKee et al. 1989, 1994; DGMK 1991; Przygoda et al. 1994; Nessel et al. 1998). Equivocal results were observed *in vitro* for sister chromatid exchange (API 1988b, c).

The overall genotoxicity database indicates that while the results were variable depending on the substance tested and the assay used, gas oils display genotoxic potential as evidenced by consistently positive *in vivo* results for the induction of chromosomal aberrations by the three gas oils tested and from positive Ames assay results observed for various gas oil substances.

Gas oils were classified by the European Commission as Category 2 (*may cause cancer*) and Category 3 (*limited evidence of a carcinogenic effect*) carcinogens. Specifically, the site-restricted gas oil substance CAS RN 68333-25-5 was classified as a Category 2 carcinogen (European Commission 1994; ESIS 2008). The International Agency for Research on Cancer (IARC) has also classified gas oils as Group 2A carcinogens (*probably carcinogenic to humans*) for "occupational exposures in petroleum refining"; Group 2B carcinogens (*possibly carcinogenic to humans*) for residual (heavy) fuel oils and marine diesel fuel; Group 3 carcinogens (*not classifiable as to their carcinogenicity to humans*) for distillate (light) fuel oils and distillate (light) diesel fuels (IARC 1989a, b, c).

A number of studies were conducted in laboratory animals to investigate the carcinogenicity of gas oils. All studies were conducted through dermal exposure (skin painting) in mice, with

the exception of one study that tested inhalation exposure in rats. The lone inhalation study (Bruner 1984) resulted in no increase of renal tumours in Fischer 344 rats after a continuous 90-day exposure and lifetime observation; a no-observed-effect concentration (NOEC) of 300 mg/m^3 was noted. ATSDR (1995) notes, however, that this study is of limited use, as it was not designed to evaluate a carcinogenic response (Bruner 1984). In contrast, substances tested by the dermal route have consistently resulted in the development of skin tumours. Durations of dermal exposure for chronic studies ranged from 17 weeks to the lifetime of the animal. Significant skin tumour development was observed in the majority of these studies and both malignant and benign tumours were identified (Easley et al. 1982; IITRI 1985; McKee et al. 1986; NTP 1986; Witschi et al. 1987; Biles et al. 1988; Gerhart et al. 1988; API 1989b, c; Freeman et al. 1993; Skisak et al. 1994; Broddle et al. 1996; Nessel et al. 1998). For example, in a chronic study, male mice were dermally treated with CAS RN 64741-59-9 at doses of 343 mg/kg-bw (seven times per week), 601 mg/kg-bw (four times per week) or 1203 mg/kg-bw (two times per week) for up to 104 weeks. Significant skin tumour formation was observed at all doses in a dose-response fashion (Nessel et al. 1998). Six gas oil substances were examined for tumour initiating/promoting activity. Durations of dermal exposure for initiation/promotion studies in mice ranged from 25 to 52 weeks. Combined results from these studies illustrate that gas oils are skin tumour promoters but do not appear to initiate tumour formation (Gerhart et al. 1988; McKee et al. 1989; DGMK 1993; Skisak et al. 1994; Nessel et al. 1999). In summary, the gas oil substances examined exhibit tumour-promoting activity and are skin carcinogens when applied chronically to the skin of laboratory animals.

Gas oils have also been investigated for their developmental and reproductive effects. The only reproductive and developmental effects that were noted occurred at 1000 mg/kg-bw per day following dermal exposure of pregnant rats to CAS RN 64741-59-9 at doses of 25, 50, 125, 250, 500 or 1000 mg/kg-bw per day. The substance was applied from gestational days 6 to 15 for the reproductive study and days 0 to 6 and 6 to 15 for the developmental study. The observed toxic effects were an increased incidence of resorptions and decreased fetal body weight, respectively (Feuston et al. 1994; Mobil 1988b). All other studies, when administered dermally or via inhalation, however, were noted to have negative results at all doses/concentrations tested. The overall evidence indicates that while results may vary depending on the substance tested, gas oils generally do not appear to affect the reproductive capacity of laboratory animals or alter fetal development.

Insufficient human epidemiological data were available for gas oils. Although some case-control studies have investigated the potential for increased cancer risk, as well as other health effects following exposure to CAS RN 68334-30-5, the identified reports are inadequate for hazard identification, due to limitations in study design. The available studies provide few details, exposures were not quantified and were based on self-reported exposure, co-exposure to other chemicals was not considered, and in some instances the specific compounds to which individuals were exposed were not clearly identified (Crisp et al. 1979; Spiegelman and Wegman 1985; Siemiatycki et al. 1987; Ahrens et al. 1991; Lindquist et al. 1991; Partanen et al. 1991; De Roos et al. 2001).

Characterization of Risk to Human Health

Site-restricted gas oil was identified as a high priority for action because it was considered to present a high hazard to human health. Based on the classification of gas oils by the European Commission as Category 2 and 3 carcinogens (European Commission 1994; ESIS 2008) and by IARC as Group 2A, Group 2B and Group 3 carcinogens (IARC 1989a, b, c), the critical effect for the initial categorization of gas oils for human health hazard was carcinogenicity. However, the gas oil considered in this screening assessment has been identified as site-restricted (i.e., indicating that it is not expected to be transported off refinery or upgrader facility sites), and therefore general population exposure is not expected. Accordingly, the likelihood of exposure to Canadians is considered to be low; hence, the risk to human health is likewise considered to be low.

Uncertainties in Evaluation of Risk to Human Health

As the site-restricted gas oil is considered to be a UVCB, its specific chemical composition is not well defined. Gas oil streams under the same CAS RN can vary significantly in the number, identity and proportion of constituent compounds, depending on operating conditions, feedstocks and processing units. Consequently, it is difficult to obtain a truly representative toxicological dataset for individual CAS RNs. For this reason, all available toxicological data for substances with similar processing and physical-chemical properties were pooled across multiple CAS RNs to develop a comprehensive toxicity profile by including the available data for all gas oils. Specific physical-chemical properties of some gas oil substances were not available; therefore, properties of representative gas oils were used as needed.

The scope of this screening assessment does not involve full investigation of the mode of induction of effects.

The PSSA screening assessments evaluate substances that are complex mixtures (UVCBs) composed of a number of substances in various proportions due to the source of the crude oil and its subsequent processing. Monitoring information or provincial release limits from petroleum facilities target broad releases (such as oils and greases) to water or air. These widely encompassing release categories do not allow for detection of individual complex mixtures or production streams. As such, the monitoring of broad releases cannot provide sufficient data to associate a detected release with a specific substance identified by a CAS RN, nor can the proportion of releases attributed to individual CAS RNs be defined.

Conclusion

Based on the available information, only a small proportion of the components of this gas oil (C_{20}–C_{25} two-ring alkyl cycloalkanes) are considered to be persistent based on criteria in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Based on the combined evidence of empirical and modelled bioaccumulation potential, the gas oil assessed in this report likely contains a large proportion of C_9–C_{15} components that are bioaccumulative based on the criteria in the *Persistence and Bioaccumulation Regulations*.

No components of this gas oil were found to be both persistent and bioaccumulative based on the criteria in the *Persistence and Bioaccumulation Regulations.*

Based on the information presented in this screening assessment, the basis for categorization for human health hazard was carcinogenicity. Gas oil substances also exhibit properties of genetic toxicity but appear to have limited potential to adversely affect reproduction and development.

The gas oil listed in this screening assessment (CAS RN 68333-25-5) is restricted to petroleum refineries and upgrader facilities; therefore, exposure of the general population or the environment is not expected. It is concluded that this site-restricted gas oil is not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity; that constitute or may constitute a danger to the environment on which life depends; or that constitute or may constitute a danger in Canada to human life or health.

It is therefore concluded that this site-restricted gas oil does not meet any of the criteria set out in section 64 of CEPA 1999.

Because this substance is listed on the Domestic List, its import and manufacture in Canada is not subject to notification under subsection 81(1) of CEPA 1999. Given the potential hazardous properties of this substance, there is concern that new activities that have not been identified or assessed could lead to this substance meeting the criteria set out in section 64 of the Act. Therefore, application of the Significant New Activity provisions of the Act to this substance is being considered, so that any proposed new manufacture, import or use of this substance outside a petroleum refinery or upgrader facility is subject to further assessment, to determine if the new activity requires further risk management consideration.

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Appendix 1: Description of the Nine Groups of Petroleum Substances

Table A1.1: Description of the nine groups of petroleum substances

Group[1]	Description	Example
Crude oil	Mixture of aliphatic and aromatic hydrocarbons and small amounts of inorganic compounds, naturally occurring under the earth's surface or under the sea floor	Crude oil
Petroleum and refinery gases	Mixture of light hydrocarbons primarily from C_1 to C_5	Propane
Low boiling point naphthas	Mixture of hydrocarbons primarily from C_4 to C_{12}	Gasoline
Gas oils	Mixture of hydrocarbons primarily from C_9 to C_{25}	Diesel
Heavy fuel oils	Mixture of heavy hydrocarbons primarily from C_{20} to C_{50}	Fuel Oil No. 6
Base oils	Mixture of hydrocarbons primarily from C_{15} to C_{50}	Lubricating oils
Aromatic extracts	Mixture of primarily aromatic hydrocarbons from C_{15} to C_{50}	Feedstock for benzene production
Waxes, slack waxes and petrolatum	Mixture of primarily aliphatic hydrocarbons from C_{12} to C_{85}	Petrolatum
Bitumen or vacuum residues	Mixture of heavy hydrocarbons having carbon numbers greater than C_{25}	Asphalt

[1] Groupings were based on classifications developed by CONCAWE and a contractor's report commissioned by the Canadian Petroleum Products Institute (CPPI) (Simpson 2005).

Appendix 2: Engineering Process Flow Diagrams for Gas Oils

Red dotted line indicates the process relevant to the particular CAS RN.
FCCU: Fluid Catalytic Cracking Unit
LPG: Liquified Petroleum Gas

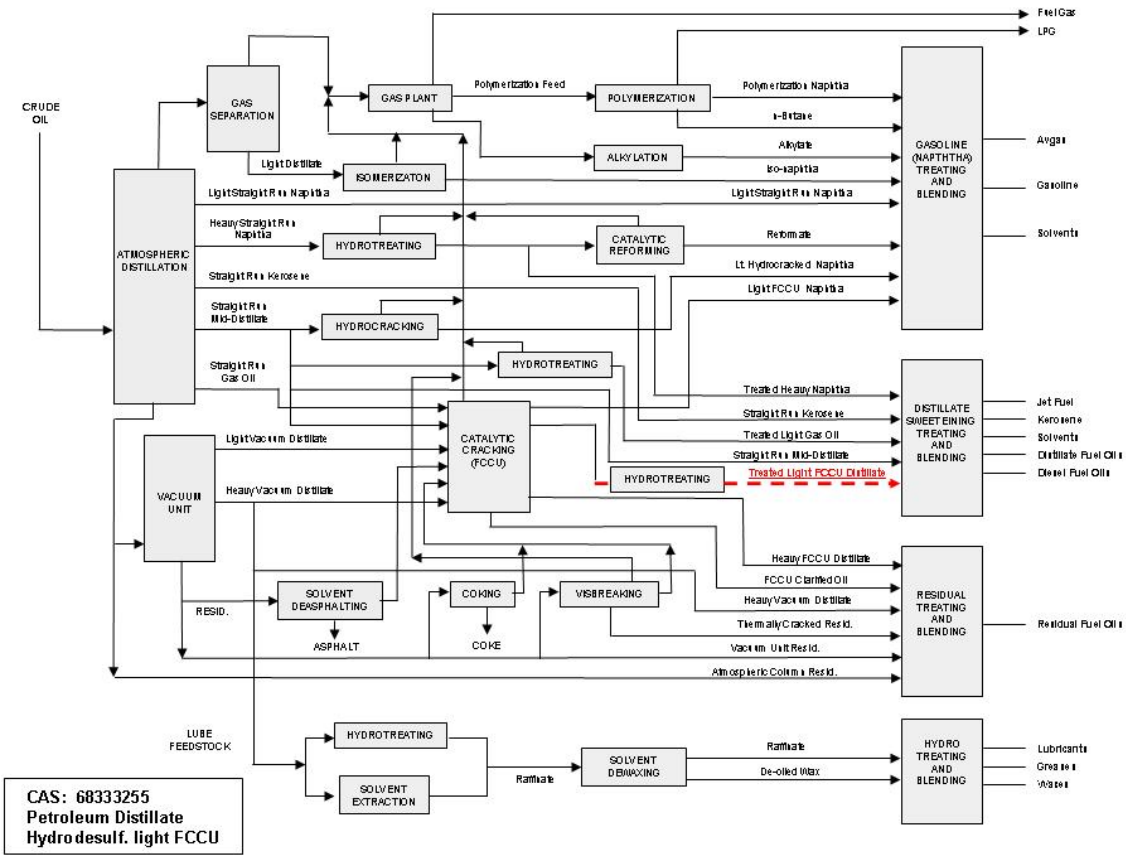

Figure A2.1a. Process flow diagram for CAS RN 68333-25-5 in a refinery (Hopkinson 2008)

CAS RN 68333-25-5 is shown to be a processing intermediate formed after hydrotreating in a refinery.

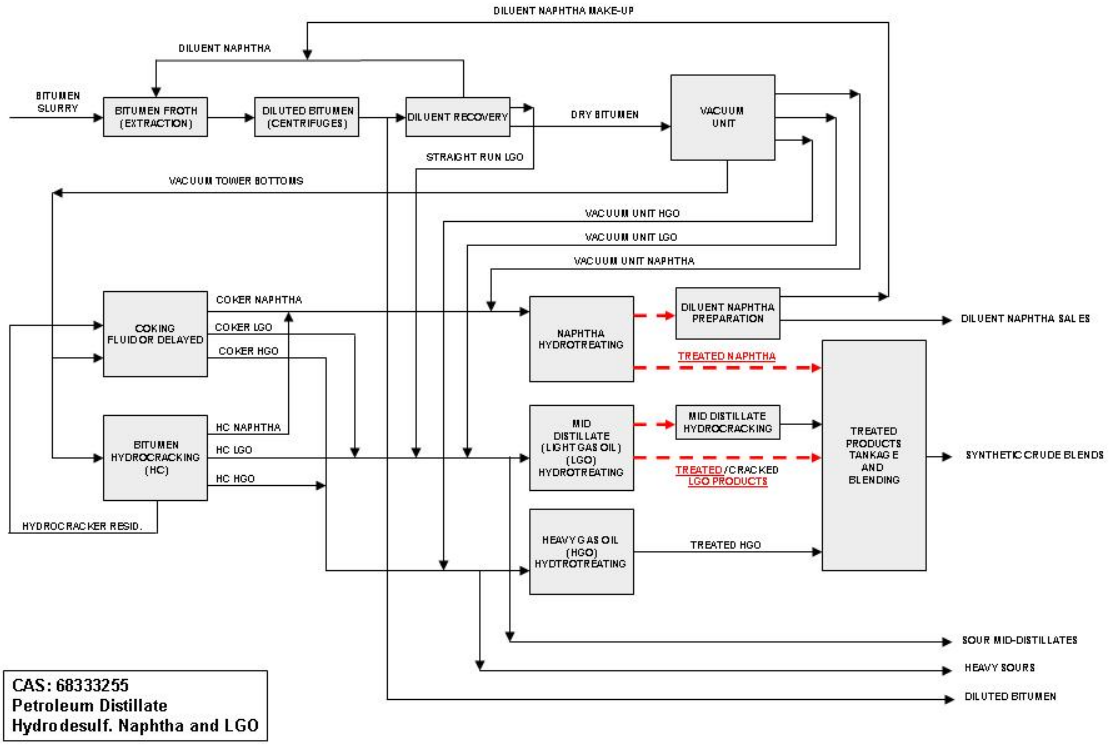

Figure A2.1b. Process flow diagram for CAS RN 68333-25-5 in an upgrader (Hopkinson 2008)

CAS RN 68333-25-5 is shown to be a processing intermediate formed after naphtha and mid-distillate hydrotreating at an upgrader.

Appendix 3: Data Tables for Site-Restricted Gas Oil

Table A3.1. Substance identity

CAS RN	**68333-25-5**
DSL name	Distillates (petroleum), hydrodesulfurized light catalytic cracked
NCI	Distillates (petroleum), hydrodesulfurized light catalytic cracked
Chemical group (DSL stream)	UVCB-organic
Major chemical class or use	Refinery streams
Major chemical subclass [1]	Complex mixture of alkanes, cycloalkanes, alkenes and aromatics
Carbon range[2]	C_9–C_{25}
Aromatic content (%)[3]	48–60
Aliphatic content (%)[3]	31–48
Alkene content (%)[3]	4–7
Boiling point range (°C)	150–450[4] 185–391[5]

Abbreviations: NCI, National Chemical Inventories; UVCB, Unknown or Variable composition, Complex reaction products or Biological materials.

[1] This substance is a UVCB; that is, it is not a discrete chemical and thus may be characterized by a variety of structures.

[2] CONCAWE 1996.

[3] From a similar light catalytic cracked gas oil (64741-59-9).

[4] BP range for gas oils in general (API 2003a).

[5] BP range for a similar light catalytic cracked gas oil (64741-59-9) (ECB 2000).

Table A3.2. Representative structures

Chemical class	Name	CAS RN
Alkanes		
C_{10}	Decane	124-18-5
C_{15}	Pentadecane	629-62-9
C_{20}	Eicosane	112-95-8
Isoalkanes		
C_{10}	4-Methylnonane	17301-94-9
C_{15}	2-Methyl tetradecane	1560-95-8
C_{20}	3-Methyl nonadecane	6418-45-7
Alkenes		
C_{10}	Decene	872-05-9
C_{15}	Pentamethyl decene	
C_{20}	Eicosene	3452-07-1
One-ring cycloalkanes		
C_{10}	Butyl cyclohexane	1678-93-9
C_{15}	Nonyl cyclohexane	2883-02-5
C_{20}	Tetradecyl cyclohexane	1795-18-2
Two-ring cycloalkanes		
C_9	*cis*-Bicyclononane	4551-51-3
C_{15}	Pentamethyl decalin	
C_{20}	2,4-Dimethyl octyl-2-decalin	
C_{25}	2,4,6-Trimethyl dodecyl-2-decalin	
One-ring aromatics		
C_9	Ethylmethyl benzene	25550-14-5
C_{15}	*n*-Nonyl benzene	1081-77-2
C_{20}	Tetradecyl benzene	
Two-ring aromatics		
C_{10}	Naphthalene	91-20-3
C_{15}	4-Isopropyl biphenyl	
C_{20}	2-Isodecyl naphthalene	
Three-ring aromatics		
C_{15}	2-Methyl phenanthrene	2531-84-2

Table A3.3. Physical and chemical properties of representative substances (EPI Suite 2008)[a]

Chemical class, name and CAS RN	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]	Sub-cooled liquid vapour pressure (Pa)[c]
Alkanes				
C_{10} Decane (124-18-5)	174.1 (e)	−29.7 (e)	191 (e)	
C_{15} Pentadecane (629-62-9)	270.6 (e)	9.9 (e)	0.5 (e)	
C_{20} Eicosane (112-95-8)	343.0 (e)	36.8 (e)	6.2E−4 (e)	8.1E−4
Isoalkanes				
C_{10} 4-Methylnonane (17301-94-9)	165.7 (e)	−99 (e)	339	
C_{15} 2-Methyl tetradecane (1560-95-8)	250.2	1.5	5.8	
C_{20} 3-Methyl nonadecane (6418-45-7)	326.3	39.5	0.09	0.13
Alkenes				
C_{10} Decene (872-05-9)	170.5 (e)	-66.3 (e)	223 (e)	
C_{15} Pentamethyl decene	215.7	-31.9	32.4	
C_{20} Eicosene (3452-07-1)	341.0 (e)	28.5 (e)	1.41E-3 (e)	

Chemical class, name and CAS RN	**Boiling point (°C)**	**Melting point (°C)**	**Vapour pressure (Pa)[b]**	**Sub-cooled liquid vapour pressure (Pa)[c]**
One-ring cycloalkanes				
C_{10} Butyl cyclohexane (1678-93-9)	180.9 (e)	−74.7 (e)	180 (e)	
C_{15} Nonyl cyclohexane (2883-02-5)	282 (e)	−10 (e)	1.2 (e)	
C_{20} Tetradecyl cyclohexane (1795-18-2)	339.4	58.2	0.02	
Two-ring cycloalkanes				
C_9 *cis*-Bicyclononane (4551-51-3)	167 (e)	−53 (e)	320.0	
C_{15} Pentamethyl decalin	248	8.6	6.6	
C_{20} 2,4-Dimethyl octyl-2-decalin	329	78	0.03	0.03
C_{25} 2,4,6-Trimethyl dodecyl-2-decalin	376.3	79.7	0.003	0.009
One-ring aromatics				
C_9 Ethylmethyl benzene (25550-14-5)	165.2 (e)	−80.8 (e)	384 (e)	

Chemical class, name and CAS RN	**Boiling point (°C)**	**Melting point (°C)**	**Vapour pressure (Pa)[b]**	**Sub-cooled liquid vapour pressure (Pa)[c]**
C_{15} n-Nonyl benzene (1081-77-2)	280.5 (e)	−24 (e)	0.76 (e)	
C_{20} Tetradecyl benzene	349.0	79.25	0.01	
Two-ring aromatics				
C_{10} Naphthalene (91-20-3)	217.9 (e)	80.2 (e)	11.3 (e)	
C_{15} 4-Isopropyl biphenyl	309.0	43.7	0.1	
C_{20} 2-Isodecyl naphthalene	366.44	99.47	0.001	
Three-ring aromatics				
C_{15} 4-Methyl phenanthrene (2531-84-2)	340	94	0.02	0.004

Table A3.3 cont. Physical and chemical properties of representative substances (EPI Suite 2008)[a]

Chemical class, name and CAS RN	**Henry's Law constant ($Pa \cdot m^3/mol$)[d]**	**Log K_{ow}**	**Log K_{oc}**	**Aqueous solubility (mg/L)[e]**	**Sub-cooled liquid solubility (mg/L)[f]**
Alkanes					
C_{10} Decane (124-18-5)	5.2E5 (e)	5.01 (e)	2.2E4	0.052 (e)	

Chemical class, name and CAS RN	Henry's Law constant ($Pa \cdot m^3/mol$)[d]	Log K_{ow}	Log K_{oc}	Aqueous solubility (mg/L)[e]	Sub-cooled liquid solubility (mg/L)[f]
C_{15} Pentadecane (629-62-9)	1.3E6 (e)	7.7	6.7	7.6E−5 (e)	
C_{20} Eicosane (112-95-8)	5.3E6	10.2	5.9	0.002 (e)	0.002
Isoalkanes					
C_{10} 4-Methylnonane (17301-94-9)	5E4	5.2	3E4	0.087	
C_{15} 2-Methyl tetradecane (1560-95-8)	3.7E5	7.6	6.6	0.003	
C_{20} 3-Methyl nonadecane (6418-45-7)	2.4E6	10*	8.8	1.1E−5	0.004
Alkenes					
C_{10} Decene (872-05-9)	2.16E5	5.7 (e)	4.9	0.57 (e)	
C_{15} Pentamethyl decene	2.5E6	7.3	6.3	0.007	
C_{20} Eicosene (3452-07-1)	6.8E6	10.0	8.7	1.4E−5	
One-ring cycloalkanes					
C_{10} Butyl cyclohexane (1678-93-9)	2E4	5.1	4.4	1.2	
C_{15} Nonyl cyclohexane	5.8E4	7.5	4.6	0.004 (e)	

Chemical class, name and CAS RN	**Henry's Law constant ($Pa \cdot m^3/mol$)[d]**	**Log K_{ow}**	**Log K_{oc}**	**Aqueous solubility (mg/L)[e]**	**Sub-cooled liquid solubility (mg/L)[f]**
(2883-02-5)					
C_{20} Tetradecyl cyclohexane (1795-18-2)	3.0E6	10.0	8.7	1.4E–5	
Two-ring cycloalkanes					
C_9 *cis*-Bicyclononane (4551-51-3)	2100	3.7	3.0	19.3	
C_{15} Pentamethyl decalin	2.8E4	6.3	5.5	0.05	
C_{20} 2,4-Dimethyl octyl-2-decalin	8.2E4	8.9	7.7	1.1E−4	0.03
C_{25} 2,4,6-Trimethyl dodecyl-2-decalin	4.8E6	11.3	9.8	4.4E-7	
One-ring aromatics					
C_9 Ethylmethyl benzene (25550-14-5)	324.2	3.6 (e)	2.93	74.6 (e)	
C_{15} n-Nonyl benzene (1081-77-2)	4200	7.1 (e)	4.4	0.04	
C_{20} Tetradecyl benzene	5.7E4	8.9	7.7	0.0004	
Two-ring aromatics					
C_{10} Naphthalene (91-20-3)	44.6 (e)	3.3 (e)	731	31 (e)	

Chemical class, name and CAS RN	Henry's Law constant ($Pa \cdot m^3/mol$)[d]	Log K_{ow}	Log K_{oc}	Aqueous solubility (mg/L)[e]	Sub-cooled liquid solubility (mg/L)[f]
C_{15} 4-Isopropyl biphenyl	23.8	5.5 (e)	4.63	0.9	
C_{20} 2-Isodecyl naphthalene	1190	8.1	7.0	0.002	
Three-ring aromatics					
C_{15} 4-Methyl phenanthrene (2531-84-2)	5 (e)	4.9	2.6E4	1.7	

[a] All values are modelled unless denoted with an (e) for experimental data. Models used were: MPBPWIN (Version 1.43) for melting point, boiling point and vapour pressure, AEROWIN (Version 1.01) for sub-cooled liquid vapour pressure, HENRYWIN (Version 3.20) for Henry's Law constants, KOWWIN (Version 1.67a) for log K_{ow}, KOCWIN (Version 2.0) for log K_{oc}, WSKOW (Version 1.41) for water solubility, and CONCAWE 1462 for sub-cooled liquid solubility.

[b] This is the maximum vapour pressure of the representative substance; the actual vapour pressure as a component of a mixture will be lower due to Raoult's Law (the total vapour pressure of an ideal mixture is proportional to the sum of the vapour pressures of the mole fractions of each individual component). The lightest C_{15} representative substances were chosen to estimate a range of vapour pressures from the minimum to maximum values.

[c] Estimated sub-cooled liquid vapour pressures were obtained from AEROWIN (Version 1.01) in EPI Suite (2008). Sub-cooled liquid vapour pressures were only estimated for representative substances determined to be solid at 25°C (i.e., $\geq C_{20}$).

[d] Henry's Law constants for C_{20} representative substances were calculated with HENRYWIN Version 3.10 from EPI Suite (2008), using both sub-cooled liquid solubility and sub-cooled liquid vapour pressure. Solubility data gave anomalously high values for substances that have negligible solubility and volatility.

[e] Maximum water solubility was estimated for each representative substance based on its individual physical and chemical properties. The actual water solubility of a component in a mixture will decrease, as the total water solubility of an ideal mixture is proportional to the sum of the water solubilities of the mole fractions of each individual component (Banerjee 1984).

[f] Estimated sub-cooled liquid solubilities were obtained from the CONCAWE 1462 database within PetroTox (2009). The estimates contained within the database were calculated using the SPARC Performs Automated Reasoning in Chemistry (SPARC 2007). Sub-cooled liquid solubility values were only estimated for representative substances determined to be solid at 25°C (i.e., $\geq C_{20}$). See the Environmental Fate section for a discussion of sub-cooled liquid solubility.

[g] n.a.: not applicable.

Table A3.4. Modelled atmospheric degradation of representative structures via reaction with hydroxyl radicals (AOPWIN 2008)

Representative Structure	Half-lives (days)[a]
Alkanes	
C_{10}	1
C_{15}	0.6
C_{20}	0.4
Isoalkanes	
C_{10}	0.9
C_{15}	0.6
C_{20}	0.4
Alkenes	
C_{10}	0.3
C_{15}	0.2
C_{20}	0.2
One-ring cycloalkanes	
C_{10}	0.7
C_{15}	0.4
C_{20}	0.4
Two-ring cycloalkanes	
C_9	0.8
C_{15}	0.4
C_{20}	0.3
C_{25}	0.3
One-ring aromatics	
C_9	1.4
C_{15}	0.7
C_{20}	0.5
Two-ring aromatics	
C_{10}	0.5
C_{15}	1.1
C_{20}	0.2
Three-ring aromatics	
C_{15}	0.3

[a] Half-life estimations are for non-specific media (i.e., water, soil and sediment).

Table A3.5. Modelled data for primary (BioHCwin 2008) and ultimate (BIOWIN 2008) biodegradation of representative structures of gas oils[1]

	Primary half-life (days) (BioHCWIN)	Ultimate biodegradation result (BioWin)	Half-life compared to criteria (days)
Alkanes			
C_{10}	8.6	Days–weeks	< 182
C_{15}	19	Days–weeks	< 182
C_{20}	40	Weeks	< 182
Isoalkanes			
C_{10}	7.7	Weeks	< 182
C_{15}	17	Weeks	< 182
C_{20}	36	Weeks	< 182
Alkenes			
C_{10}	7	Weeks	< 182
C_{15}	26	Weeks–months	< 182
C_{20}	32	Weeks	< 182
One-ring cycloalkanes			
C_{10}	11.6	Weeks	< 182
C_{15}	25	Weeks	< 182
C_{20}	53	Weeks	< 182
Two-ring cycloalkanes			
C_9	56	Weeks	< 182
C_{15}	88	Weeks–months	< 182
C_{20}	250	Weeks–months	≥ 182
C_{25}	618	Weeks–months	≥ 182
One-ring aromatics			
C_9	4.9	Weeks	< 182
C_{15}	14	Weeks	< 182
C_{20}	31	Weeks	< 182
Two-ring aromatics			
C_{15}	73	Weeks–months	< 182
C_{20}	24	Weeks	< 182
Three-ring aromatics			
C_{15}	24	Weeks–months	< 182

[1] Half-life estimations are not media-specific (i.e., they are based on combined data from water studies).

Table A3.6. Fish BCF and BAF predictions for representative structures of gas oils using BCFBAF (2008a) with metabolism

	log K_{ow}	k_M[a] (/day)	BCF (L/kg)	BAF (L/kg)
Alkanes*				
C_{10}	5	0.28	1 146	1 333
C_{15}	7.7	0.34-0.45[b]	37-48[b]	456-753[b]

Isoalkanes*				
C_{10}	5.2	0.27	1 255	1 572
C_{15}	7.6	0.05	680	100 000
Alkenes*				
C_{10}	5.7	0.17	2113	5057
C_{15}	7.3	0.07	1101	84 400
One-ring cycloalkanes*				
C_{10}	5.1	0.22	1447	1794
C_{15}	7.5	0.04	1000	160 000
Two-ring cycloalkanes*				
C_9	3.7	0.15	300	310
C_{15}	6.5	0.005	18 000	880 000
One-ring aromatics				
C_9	3.6	0.28-0.38[b]	219[b]	219[b]
C_{15}	7.1	0.14	770	25 000
Two-ring aromatics				
C_{10}	3.3	0.06[b]	98[b]	98[b]
C_{15}	5.5	0.07	3569	6961
Three-ring aromatics				
C_{15}	4.5	0.36	1813	2399

[a] Biotransformation rate constant for 10 g fish.
[b] Representative structures that were remodelled using BAF-QSAR v1.5 based on similar structures with experimental data.
* Alkanes C_{20}, isoalkanes C_{20}, alkenes C_{20}, one-ring cycloalkanes C_{20}, two-ring cycloalkanes C_{25}, all having values of log K_{ow} > 9, were excluded from this comparison, as model predictions may be highly uncertain for chemicals that have estimated log K_{ow} values > 9 (Arnot and Gobas 2003).

Table A3.7. Comparisons of experimental BCFs and modeled BCFs (BCFBAF 2008) on some representative structures of gas oils.

	Reference; Species tested	**Log K_{ow}**	**BCF[a] Measured (L/kg)**	**BCF[b] Modeled (L/kg)**
Alkanes*				
C_8 n-parafins Octane	JNITE; Carp	5.18 (e)	530	1480
C_{12} n-parafins n-dodecane	Tolls and v Dijk, 2002 cited Lampi et al. (2010) – unpublished; fathead minnow	6.10 (e)	400	901
C_{15} n-parafins n-pentadecane	CITI 1992; Carp	7.71	20	723
C_{15} n-parafins n-pentadecane	JNITE; Carp	7.71	26	723
C_{16} n-parafins n-hexadecane	CITI 1992; Carp	8.20	46	494
C_{16} n-parafins n-hexadecane	JNITE; Carp	3.15 (e)	20.2	494
Isoalkanes*				
C_{15}	EMBSI 2004b; 2005c; rainbow	7.49	291/817	1 646

2,6,10-trimethyl dodecane	trout			
One-ring cycloalkanes*				
C_6 Cyclohexane	CITI 1992; Carp	3.44 (e)	77	76
C_7 1-methylcyclohexane	CITI 1992; Carp	3.61 (e)	240	220
C_8 ethylcyclohexane	CITI 1992; Carp	4.56 (e)	2 529	839
Two-ring cycloalkanes*				
C_{10} Trans-decalin	CITI 1992; Carp	4.20	2 200	884
C_{10} Cis-decalin	CITI 1992; Carp	4.20	2 500	884
One-ring aromatics*				
C_9 1,2,3-trimethylbenzene	CITI 1992; Carp	3.66 (e)	125/141	159
C_{10} 1,2-diethylbenzene	CITI 1992; Carp	3.72 (e)	478/556	221
C_{11} 1-methyl-4-tert-butylbenzene	JNITE; Carp	3.66 (e)	<1.0	890
Cycloalkanes monoaromatic*				
C_{10} Tetralin	CITI 1992; Carp	3.49 (e)	230	176
C_{18} dodecahydrochrysene	EMBSI 2008c; rainbow trout	6.00	4 588	2 234
Two-ring aromatics*				
C_{10} Naphthalene	JNITE; Carp	3.30 (e)	94	112
	CITI 1992; Carp	3.30 (e)	95/91	112
C_{11} 2-methylnaphthalene	Jonsson et al. 2004 (cited in Lampi et al. 2010); sheepshead minnow	3.86 (e)	1 871	405
C_{12} 1,3-dimethylnaphthalene	Jonsson et al. 2004 (cited in Lampi et al. 2010); sheepshead minnow	4.42 (e)	2 051	1 021
C_{13} 2-iso-Propylnaphthalene	Jonsson et al. 2004 (cited in Lampi et al. 2010); sheepshead minnow	4.63	12 298[c]	1 745
C_{14} 4-ethylbiphenyl	Yakata et al. 2006 (cited in Lampi et al. 2010); carp	4.80	1 039	611
Cycloalkanes diaromatic*				
C_{12} acenaphthene	CITI 1992; Carp	3.92 (e)	979/1 003	122
C_{18} hexahydro terphenyl	EMBSI 2008c, 2009c; rainbow trout	6.44	1 646	713
Four-ring aromatics*				
C_{12} acenaphthylene	Yankata 2006; Carp	3.94 (e)	579/596	415
C_{13} fluorene	CITI 1992; Carp	4.18 (e)	672/780	698
C_{14}	Carlson et al. 1979; fathead	4.46 (e)	2 927/3 546	1 096

phenanthrene	minnow			
C_{16} fluoranthene	EMBSI 2007b, 2009c; rainbow trout	5.16 (e)	435	560
C_{18} chrysene	EMBSI 2006b, 2009c; rainbow trout	5.81 (e)	153	2 010
C_{18} Triphenylene	JNITE; Carp	5.49 (e)	61	489

[a] Experimental BCFs from various sources.
[b] Modeled BCFs using BCFBAF (2008); BCF of a lower trophic fish were chosen to match the lipid content of fish in the Janpanese database.
[c] C_{13} 2-iso-Propylnaphthalene: The only measured BCF found >5000 out of the thirty-one data points; it is greater than the modeled value by an order of magnitude.

Table A3.8. Modelled acute toxicity data of CAS RN 68333-25-5 (Distillates (petroleum), hydrodesulfurized light catalytic cracked) (PetroTox 2009)*

Test organism	Common name	LL_{50} (mg/L)
Pseudokirchneriella capricornutum	Green algae	3.8
Daphnia magna	Water flea	1.3
Palaemonetes pugio	Grass shrimp	0.5
Rhepoxynius abronius	Marine amphipod	0.2
Neanthes arenaceodentata	Marine worm	2.7
Onchorhynchus mykiss	Rainbow trout	0.6
Menidia beryllina	Inland silverside	6.6

* Low-resolution mode run with a 10% headspace.

Table A3.9a. Aquatic toxicity of Fuel Oil No. 2

Organism	Common name	Duration	Endpoint		Value (mg/L)	Reference
Fundulus similis	Longnose Killifish	48 hours (acute)	Mediane lethal concentration (LC_{50}) LC_{50}	Water soluble fraction (WSF)	4.7	Anderson et al. 1974
Cyprinodon variegatus	Sheepshead Minnow	48 hours (acute)	LC_{50}	WSF	> 6.9	Anderson et al. 1974
Menidia beryllina	Inland Silverside	48 hours (acute)	LC_{50}	WSF	5.2	Anderson et al. 1974
Daphnia magna	Water Flea	48 hours	LC_{50}	WSF	2.2	MacLean

Organism	Common name	Duration	Endpoint		Value (mg/L)	Reference
		(acute)				et al. 1989
Artemia spp.	Brine shrimp	48 hours (acute)	LC_{50}	WSF	11.2	MacLean et al. 1989
Lucifer faxoni	Planktonic shrimp	48 hours (acute)	Mediane lethal dose (LD_{50})	WSF	4.6	Lee et al. 1978
Mysidopsis almyra	Mysid shrimp	48 hours (acute)	LC_{50}	WSF	0.9	Anderson et al. 1974
Palaemonetes pugio	Grass Shrimp	48 hours (acute)	LD_{50}	WSF	4.1	Anderson et al. 1974
Neanthes arenaceodentata	Marine Worm	48 hours (acute)	LC_{50}	WSF	3.2	Rossi et al. 1976
Capitella capitata	Marine Worm	48 hours (acute)	LC_{50}	WSF	3.5	Rossi et al. 1976

Table A3.9b. Aquatic toxicity of diesel fuel

Organism	Common name	Duration	Endpoint		Value (mg/L)	Reference
Oncorhynchus mykiss	Rainbow Trout	48 hours (acute)	Median lethal loading concentration (LL_{50})	WAF	2.4	Lockhart et al. 1987
Artemia spp.	Brine Shrimp	48 hours (acute)	LC_{50}	WSF	23.7	MacLean and Doe 1989
Daphnia magna	Water Flea	48 hours (acute)	LC_{50}	WSF	7.16	MacLean and Doe 1989

Appendix 4: Summary of Health Effects Information from Pooled Toxicological Data for Gas Oil Substances

Endpoints	CAS RNs[1]	Effect levels[2]/Results
Acute toxicity	**68333-25-5**	No studies identified.
	64741-59-9	**Lowest oral LD_{50}** (rat) = 3200 mg/kg-bw for samples API 83-07 (female) (API 2003a, b).
	64741-59-9 64742-80-9 68334-30-5 68476-30-2	**Other oral LD_{50}s** (rat) = 4660–17 838 mg/kg-bw (21.2 ml/kg-bw = 17 838 mg/kg-bw[3]) for four CAS RNs tested (CONCAWE 1996; API 2003a, b).
	64741-59-9	**Lowest inhalation LC_{50}** (rat) = 3350 mg/m^3 (3.35 mg/l)[4] for sample API 83-07 (male) (API 2003a).
	64741-59-9 64742-80-9	**Other inhalation LC_{50}s** (rat) = 4600–7640 mg/m^3 for two CAS RNs tested (CONCAWE 1996; API 2003a).
	64741-59-9 64742-80-9	**Lowest dermal LD_{50}** (rabbit) = > 2000 mg/kg-bw for samples API 83-07, API 83-08, API 81-09 and API 81-10 (API 2003a, b).
	68476-31-3	**Other dermal LD_{50}** (mice) = > 40 000 mg/kg-bw (CONCAWE 1996).
Short-term repeated-dose toxicity	64741-59-9	**Lowest dermal LOAEL =** 50 mg/kg-bw per day for decreased body weight gain and body weight. Pregnant Sprague-Dawley rats were exposed via dermal application to the shorn dorsal skin to a dose of 25, 50, 125, 250, 500 or 1000 mg/kg-bw, once per day from gestation days 0 to 19. Increased cholesterol and triglycerides were observed at doses ≥ 250 mg/kg-bw, and severe sensory irritation was noted at doses ≥ 500 mg/kg-bw (Mobil 1988b).
	68476-34-6	**Other dermal LOAEL** = 200 mg/kg-bw per day based on hematological changes (decreased mean corpuscular hemoglobin concentration). Male and female New Zealand White rabbits (10 animals per sex per dose) exposed dermally to *Diesel fuel LF-7765 RI* at a dose of 200, 670 or 2000 mg/kg-bw per day on 5 days/week for 3 weeks. Decreased body weight gain and severe dermal irritation were also observed at 200 mg/kg-bw per day. Decreased alkaline phosphatase and increased glucose and white blood cell counts were observed following exposure to doses ≥670 mg/kg-bw per day. Death

		occurred in 2/10 female and 1/10 male rabbits in the group exposed to 2000 mg/kg-bw per day. Clinical chemistry changes for albumin, serum glutamate–oxaloacetate transaminase (SGOT), hematocrit and neutrophil counts were also noted at the highest dose tested (IITRI 1984).
	64742-80-9	**Inhalation LOAEC** = 25 mg/m^3 for microscopic changes in nasal tissue, including subacute inflammation of the respiratory mucosa. Male and female Sprague-Dawley rats (20 animals per sex) were exposed to a concentration of 25 mg/m^3 for 6 h/day, 5 days/week for 4 weeks. An increased leukocyte count (~ 30%) was also noted, but no macroscopic changes were observed at necropsy; may be stress-related. Test substance was atomized into an atomization chamber, then diluted with chamber air to achieve the desired concentration (API 1986a).
	68476-34-6	**Oral LOAEL** = 1013 mg/kg-bw for biochemical changes. Male Sprague-Dawley rats (six animals) were administered 1013 mg/kg-bw (1.25 ml/kg-bw^3) of *commercial diesel fuel #2* via gavage on days 1, 3, 5 and 8 of the study. Observed effects included an increase in liver somatic index, increased activity in hepatic enzymes, including 7-ethoxyresorufin *O*-deethylase (EROD), 7-ethoxycoumarin *O*-deethylase (ECOD), glutathione transferase and aryl hydrocarbon hydroxylase. Increased activity was also noted in renal enzymes, including ECOD (Khan et al. 2001).
Subchronic toxicity	64741-82-8	**Lowest dermal LOAEL** = 30 mg/kg-bw per day based on increased lymphocytes in female rats and decreased thymus weight by 10% in male rats. Sprague-Dawley rats (10 animals per sex per group) were exposed on 5 days/week for 13 weeks to 30, 125, 500 or 2000 mg/kg-bw per day via application of the substance to the shaved skin. At doses ≥ 125 mg/kg-bw per day, changes in megakaryocytes, increased lymphocytes and decreased body weight in male rats were observed. Additional effects were observed at doses of ≥ 500 mg/kg-bw per day, including severe skin irritation and decreased body weight in females. Exposure to the highest dose tested, 2000 mg/kg-bw per day, resulted in increased leukocytes (white blood cells) and segmented neutrophils, as well as a reduction in erythropoietic cells and megakaryocytes. Basophilia in the renal tubular cortex was also observed in male rats (Mobil 1991). **Other dermal LOAEL** = 125 mg/kg-bw per day for

		increased relative liver weights in male and female rats. Sprague-Dawley rats were exposed on 5 days/week for 13 weeks to 30, 125, 500 or 2000 mg/kg-bw per day. Additional effects noted (doses unspecified) included decreased body and thymus weights, skin irritation and altered serum chemistry and hematology (it was not indicated by the study authors if the aforementioned effects were all observed for this specific substance, as the study examined several substances) (Feuston et al. 1994).
	68334-30-5	**Inhalation LOAEC =** 250 mg/m^3 based on decreased body weight and increased response time in a startle reflex assay (no histological changes in the nervous system were noted, however) in rats. Male and female Sprague-Dawley rats (24 animals per sex per concentration) were exposed to *diesel fuel* at 250, 750 or 1500 mg/m^3 for 4 hours per day, 2 days per week for 13 weeks. The effects noted at 250 mg/m^3 were also observed at the higher concentrations. Increased relative right lung lobe weight was observed following exposure to 1500 mg/m^3, but no histopathological changes or effects on pulmonary function were noted. Decreased blood cholesterol in females was also noted at this concentration, but was not considered to be treatment-related. Test substance was flash vaporized using a Vycor heater attached to the end of a stainless steel tube. The aerosol was subsequently carried into the exposure chamber and diluted with chamber air to achieve the desired concentrations (Lock et al. 1984). (A LOAEC was not identified in an additional inhalation study [API 1979b]). **Oral studies:** No oral studies were identified.
Carcinogenicity	64741-59-9	**Lowest dermal effect level** = 343 mg/kg-bw for MD-7 light cycle oil (50 microlitres [µL] at 28.5%). Groups of male C3H mice (50 animals per dose) were treated with 50 µL of MD-7 light cycle oil at 28.5% (343 mg/kg-bw)[5,6,7,8] (7 times/week), 50% (601 mg/kg-bw)[5,6,7,8] (4 times/week) and 100% (1203 mg/kg-bw)[5,6,7] (2 times/week) (in mineral oil), for up to 104 weeks. The test substance was applied to the back skin. Observed significant increase in skin tumour incidence for 28.5% MD-7 LCO light cycle oil (7/50 exposed mice developed tumours after 301 days). Observed significant increase in skin tumour incidence for 50% MD-7 light cycle oil LCO (17/50 exposed mice developed tumours after 266 days). Observed insignificant increase in skin tumour

		incidence for 100% MD-7 LCO light cycle oil (1/50 exposed mice developed tumours after 651 days). Exposure to the negative control (mineral oil) resulted in 0 mice developing tumours. Exposure to the positive control (5% heavy clarified oil) resulted in 47/50 mice developing skin tumours after 217 days (Nessel et al. 1998).
	64742-30-9	**Dermal Exposure** *Initiation/promotion study* ***Initiation*:** Groups of male CD-1 mice (30/group) were treated with 25 µL of lightly refined paraffinic oil (LRPO) (neat) (573 mg/kg-bw)[5,6,7], 3 times/week, for 2 weeks. Starting on day 14, 2.5 micrograms (µg) of the promoter 12-*O*-tetradecanoylphorbol-13-acetate (TPA) was applied 3 times/week, for 48 weeks. Observed insignificant increase in skin tumour incidence (papillomas) (3/30 exposed mice developed tumours after 50 weeks). Exposure to the negative control (acetone/TPA) resulted in 9/30 mice developing skin tumours after 50 weeks. Exposure to the positive control 7,12-dimethylbenz[*a*]anthracene (DMBA) / TPA resulted in 30/30 mice developing skin tumours after 50 weeks. ***Promotion*:** Groups of male CD-1 mice (30/group) were treated with a single application of 50 µg of the initiator DMBA. After a 2-week rest period, 25 µL of LRPO was applied (neat) (573 mg/kg-bw)[5,6,7], 3 times/week, for ~ 25 weeks. Observed significant increase in skin tumour incidence (5/30 exposed mice developed papillomas after ~ 27 weeks). Exposure to the negative control (DMBA/acetone) resulted in 0 mice developing tumours. Exposure to the positive control (DMBA/TPA) resulted in 30/30 mice developing skin tumours after ~ 27 weeks (McKee et al. 1989). No oral studies were identified. One inhalation study was identified but was of limited use, as it was not designed to evaluate a carcinogenic response (Bruner 1984).
Developmental and reproductive toxicity	68334-30-5	**Inhalation NOAEC** = 3777 mg/m^3 for developmental toxicity. A concentration of 3777 mg/m^3 (401.5 ppm)[9,10] of *diesel fuel* was administered to pregnant rats from gestational days 6 to 15. No developmental effects were noted (Beliles and Mecler 1983).
	68476-34-6	**Dermal NOAEL** = 4050 mg/kg-bw per day for reproductive toxicity. Doses of 405, 1620 or 4050 mg/kg-bw per day (0.5, 2 or 5 ml/kg per day)[3,11] of *Diesel Fuel No. 2* were applied to Sprague-Dawley rats (10 animals per sex per dose), 5 days per week for 4

	64741-59-9	weeks. No effects on testes or ovaries were observed (UBTL 1986). **Dermal LOAEL =** 1000 mg/kg-bw per day for reproductive toxicity based on an increased incidence of resorptions following dermal application of 25, 50, 125, 250 or 500 mg/kg-bw per day to pregnant Sprague-Dawley rats from gestational days 0 to 19 and 1000 mg/kg-bw per day from gestational days 6 to 15 (Feuston et al. 1994). **Dermal LOAEL =** 1000 mg/kg-bw per day for developmental toxicity based on decreased fetal body weight following dermal application of 25, 50, 125, 250 or 500 mg/kg-bw per day to the shorn dorsal skin of pregnant Sprague-Dawley rats from gestational days 0-19 and 1000 mg/kg-bw per day from gestational days 0-6 and 6-15. No developmental malformations or reproductive effects were noted (Mobil 1988b). **Oral Studies:** No oral studies were identified.
Genotoxicity: *in vivo*	**68333-25-5** 68476-34-6 68476-30-2 68334-30-5 64742-80-9	No studies identified. **Chromosomal aberration assay** ***Positive*:** Groups of male rats (five animals per dose) were exposed to *No.2-DA* by intraperitoneal injection to 486, 1620 or 4860 mg/kg-bw (0.6, 2.0 or 6.0 ml/kg-bw[3,11]) for up to 48 h or for 5 days. An increased percentage of aberrations was observed in bone marrow of rats exposed to 2.0 and 6.0 ml/kg-bw (API 1978). ***Positive*:** Groups of Sprague-Dawley rats were orally administered 125, 417 or 1250 mg/kg-bw per day for 5 days. Increases in cells with chromatid breaks and in aberrant cells in the bone marrow were observed (Conaway et al. 1984). ***Positive*:** Groups of Sprague-Dawley rats were exposed by intraperitoneal injection to *diesel fuel* at concentrations of 0.6, 2.0 and 6.0 ml/kg (493, 1644 and 4933 mg/kg bw)[3,12] for 1 or 5 days. Increased number of aberrant cells reported in bone marrow at the highest dose level (Conaway et al. 1984). **Sister chromatid exchange assay** ***Positive*:** Mice were exposed by intraperitoneal injection to API 83-07 at 340, 1700 or 3400 mg/kg-bw (API 1989a).

	68476-30-2 64742-46-7 64742-30-9	**Micronuclei induction** ***Negative*:** Groups of CD-1 mice (15 per sex per dose) were exposed once via oral gavage to 0, 1000, 2500 or 5000 mg/kg-bw. No increase in frequency of micronuclei induction in bone marrow cells was observed (McKee et al. 1994).
	68476-34-6	**Dominant lethal mutations** ***Negative*:** Groups of male CD-1 mice (12 per group) were exposed to *No.2-DA* by inhalation to 777 or 3108 mg/m^3 (100 or 400 ppm[9,13]) for 6 h/day, 5 days/week, for 8 weeks. No effect on the frequency of dominant lethal mutations was reported (API 1980b).
Genotoxicity: *in vitro*	64741-82-8	**Mutagenicity** ***Positive for reverse mutations*:** Modified Ames assay. *S. typhimurium* TA98 exposed to DGMK No. 8 with S9 metabolic activation. Mutagenic index of 2.1 polynuclear aromatic compounds content of 8% (Blackburn et al. 1984, 1986; DGMK 1991). ***Positive for reverse mutations*:** *S. typhimurium* TA98 and TA100 exposed to concentrations of 0.26 to 42 mg/plate, with and without S9 metabolic activation (Conaway et al. 1984).
	68476-30-2	**Mouse lymphoma assay** ***Positive*:** L5178Y TK$^{+/-}$ cells exposed to 1.2 µg/ml. Mutation frequency 17.1 times higher than controls, without metabolic activation (Conaway et al. 1984). ***Positive*:** L5178Y TK$^{+/-}$ cells exposed to 1.2 µg/ml. Mutation frequency 17.1 times higher than controls, without metabolic activation (Conaway et al. 1984). **Sister Chromatid Exchange** ***Positive*:** Fractions of Fuel Oil No. 2, containing 1-3 ring PAHs, in Chinese Hamster ovary cells, with metabolic activation (Ellenton and Hallett 1981).
Human studies	**68333-25-5**	No studies identified.

[1] Site-restricted gas oil substance is indicated in bold.
[2] LC_{50}, median lethal concentration; LD_{50}, median lethal dose; LOAEC, lowest-observed-adverse-effect concentration; LOAEL, lowest-observed-adverse-effect level; NOAEC, no-observed-adverse-effect concentration; NOAEL, no-observed-adverse-effect level.
[3] The following formula was used for conversion of provided values into mg/kg-bw: *x* ml/kg-bw × ρ.
[4] 1m^3 = 1000L
[5] Body weight (bw) not provided; thus, laboratory standards from Salem and Katz (2006) were used.
[6] The following formula was used for conversion of provided values into mg/kg-bw: (% of dilution × *x* ml × ρ)/bw.
[7] Density (ρ) not provided; thus, a density from ECB (2000) was used.
[8] A volume/volume dilution was assumed.
[9] The following formula was used for conversion of provided values into mg/m^3: (*x* in parts per million (ppm) × molecular mass (MM))/24.45.

[10] MM of diesel fuel estimated to be 230 grams per mole (g/mol) (http://www.epa.gov/athens/learn2model/part-two/onsite/es.html).
[11] Density (ρ) not provided; thus, a density from Khan et al. (2001) was used.
[12] Density (ρ) not provided; thus, a density from API (2003b) was used.
[13] MM of Diesel Fuel No. 2 reported to be 190 g/mol (Henderson and Willwerth 2001).