Final Screening Assessment
Petroleum Sector Stream Approach

Gas Oils
[Industry-Restricted]

Chemical Abstracts Service Registry Numbers

64741-59-9
64741-82-8

Environment Canada
Health Canada

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Synopsis

The Ministers of the Environment and of Health have conducted a screening assessment of the following industry-restricted gas oils:

CAS RN [a]	DSL [b] name
64741-59-9	Distillates (petroleum), light catalytic cracked
64741-82-8	Distillates (petroleum), light thermal cracked

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[b] DSL, Domestic Substances List

These substances were identified as high priorities for action during the categorization of substances on the *Domestic Substances List* (DSL), as they were determined to present greatest potential for exposure of individuals in Canada, and were considered to present a high hazard to human health. These substances met the ecological categorization criteria for persistence or bioaccumulation potential and inherent toxicity to aquatic organisms. These substances were included in the Petroleum Sector Stream Approach (PSSA) because they are related to the petroleum sector and are considered to be of Unknown or Variable composition, Complex reaction products or Biological materials (UVCBs).

These gas oils are a group of complex combinations of petroleum hydrocarbons 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 the blended products may also be used as solvents. The composition and physical-chemical properties of gas oils vary with the sources of the crude oil or bitumen and the processing steps involved. Chemical Abstracts Service Registry Number (CAS RN) 64741-59-9 is a light, catalytically cracked petroleum distillate with a typical boiling point range of 179–382°C and is a complex combination of aromatic and aliphatic hydrocarbons, mainly in the carbon range of C_9–C_{25}. CAS RN 64741-82-8 is a complex combination of aromatic, aliphatic and cycloalkane hydrocarbons, mainly in the carbon range of C_{10}–C_{22}, with a typical boiling point range from 160–370°C. In order to predict the overall behaviour of these complex substances for the purposes of assessing the potential for ecological effects, representative structures have been selected from each chemical class in the substances.

Both substances considered in this screening assessment have been identified as industry restricted (i.e., they are a subset of gas oils that may leave a petroleum-sector facility and may be transported to other industrial facilities). According to information submitted under section 71 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), and other sources of information, these gas oils are transported from petroleum facilities to other industrial facilities by ship and by truck; therefore, exposure of the environment is possible.

Based on comparison of levels expected to cause harm to organisms with estimated exposure levels and other information, these gas oils have a low risk of harm to aquatic life due to spills in the relatively confined waters around a loading wharf. The estimated frequency of spills of sufficient volume to be of concern to the environment during ship loading is < 1 incident per year; for truck loading, close to zero incidents of concern per year are expected, given the low volumes transported.

Based on the information presented in this screening assessment on the frequency and magnitude of spills, there is low risk of harm to organisms or the broader integrity of the environment from these substances. It is concluded that the industry-restricted gas oils (CAS RN 64741-59-9 and 64741-82-8) do not meet the criteria under paragraphs 64(*a*) or 64(*b*) of the *Canadian Environmental Protection Act, 1999* (CEPA 1999) as they are 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.

A critical effect for the initial categorization of industry-restricted gas oil substances was carcinogenicity, based primarily on classifications by international agencies. Several cancer studies conducted in laboratory animals resulted in the development of skin tumours following repeated dermal application of CAS RN 64741-59-9. Industry-restricted gas oils demonstrated genotoxicity in *in vivo* and *in vitro* assays but do not appear to affect reproduction or development in laboratory animals when applied dermally. There are no carcinogenicity studies by the inhalation route to inform the carcinogenic potential of these substances in the general population following inhalation exposure. Information on additional gas oil substances in the PSSA that are similar from a processing and physical-chemical perspective was considered for characterization of human health effects.

There is potential limited general population exposure via inhalation of ambient air containing gas oil vapours due to evaporative emissions during transportation. A comparison of critical inhalation effect levels and upper-bounding estimates of exposure by the inhalation route results in margins of exposure which are considered adequate to address uncertainties related to health effects and exposure. General population exposure to industry-restricted gas oils via the dermal and oral routes is not expected; therefore, risk to human health from these routes of exposure is not expected.

Based on the information presented in this screening assessment, it is concluded that the industry-restricted gas oils (CAS RNs 64741-59-9 and 64741-82-8) do not meet the criteria under paragraph 64(c) of the *Canadian Environmental Protection Act, 1999* (CEPA 1999) as they are not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

It is therefore concluded that the industry-restricted gas oils listed under CAS RNs 64741-59-9 and 64741-82-8 do not meet any of the criteria set out in section 64 of CEPA 1999.

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 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 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 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.[1]

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

[1] 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 is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the *Controlled Products Regulations*, which are part of the regulatory framework for the Workplace Hazardous Materials Information System 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.

Appendix 1). In order to conduct the screening assessments, each high priority petroleum substance was placed into one of five categories (or "streams") depending on its production and uses in Canada:

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

An analysis of the available data determined that 16 petroleum substances are evaluated under Stream 2, as described above. These occur within five of the nine substance groupings: heavy fuel oils, gas oils, petroleum and refinery gases, low boiling point naphthas and crude oils.

This screening assessment addresses two industry-restricted gas oil substances described under Chemical Abstracts Service Registry Numbers (CAS RNs) 64741-59-9 and 64741-82-8. These substances were identified as GPE during the categorization exercise, and were considered to present a high hazard to human health. These substances met the ecological categorization criteria for persistence or bioaccumulation potential and inherent toxicity to aquatic organisms. According to information submitted under section 71 of CEPA 1999 (Environment Canada 2008, 2009) and other sources of information, these substances can be consumed on-site or transported from petroleum facilities to other industrial facilities, but they are not sold directly to consumers.

One site-restricted gas oil was previously assessed under Stream 1, and an additional eleven gas oils are being assessed separately as they belong to Streams 3 and 4 (as described above). The health effects of the industry-restricted gas oils were assessed primarily using data specific to the two CAS RNs (64741-59-9 and 64741-82-8), but also considered health effects data on additional gas oil substances (i.e., a "pooled" approach).

Included in this screening assessment is the consideration of information on chemical properties, uses, exposure and effects, including additional information submitted under section 71 of CEPA 1999. Data relevant to the screening assessment of these substances were identified in original literature, review and assessment documents and stakeholder research reports and from recent literature searches, up to September 2011 for the environmental, human exposure and health effects sections of the document. Key studies were critically evaluated and used, when available, with modelling results to reach conclusions.

[2] 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 petroleum refineries, upgraders or gas plants.

Characterization of risk to the environment involves consideration of data relevant to environmental behaviour, persistence, bioaccumulation and toxicity, combined with an estimation of exposure of potentially affected non-human organisms from the major sources of release to the environment. To predict the overall environmental behaviour and properties of complex substances such as these industry-restricted gas oils, representative structures were selected from each chemical class contained within the substances. Conclusions regarding risk to the environment are based on an estimation of environmental concentrations resulting from releases and the potential for these concentrations to have harmful effects on non-human organisms. As well, other lines of evidence including fate, temporal/spatial presence in the environment, and hazardous properties of the substance 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. The industry-restricted gas oils are complex and variable, and any approach or model will not fully represent the range of variables found in these substances. Environmental models and comparisons with similar petroleum substances may have assisted 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 effects. Health effects were assessed using toxicological data pooled across high priority gas oil substances. Decisions for risk to human health are based on the nature of the critical effect and 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 final 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 and consultation. Comments on the technical portions relevant to human health were received from scientific experts selected and directed by Toxicology Excellence for Risk Assessment (TERA), including Dr. Thomas Booze (California Environmental Protection Agency, Department of Toxic Substances Control), Dr. Michael Dourson (TERA), Dr. Stephen Embso-Mattingly (NewFields Environmental Forensics Practice, LLC) and Dr. Michael Jayjock (The LifeLine Group). Although 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 draft screening assessment is based are summarized below.

Substance Identity

These gas oils are a category of petroleum substances that are used primarily in the production of fuels used in diesel engines and for both industrial and domestic heating. Some of the blended products may also be used as solvents (CONCAWE 1996). CAS RN 64741-59-9 is a complex combination of petroleum hydrocarbons that boils between 179°C and 382°C with a carbon range of C_9–C_{25} (CONCAWE 1996; ECB 2000; API 2003a) (see Table A2.1 in Appendix 2). CAS RN 64741-59-9 is typically composed largely of aromatic compounds (60–72%), with the remainder being varying proportions of alkanes, cycloalkanes and alkenes. CAS RN 64741-82-8 consists predominantly of unsaturated hydrocarbons (aromatics) in the range of C_{10}–C_{22}, with a boiling point range from 160–370°C (CONCAWE 1996; Shell 2011).

These UVCB substances are complex combinations of hydrocarbon molecules that originate in nature or are the result of chemical reactions and processes that take place during the upgrading and refining process. Given their complex and variable compositions, they could not practicably be formed by simply combining individual constituents.

Physical and Chemical Properties

The composition and physical-chemical properties of gas oils vary, depending on the source of the crude oil or bitumen and the processing steps involved (CONCAWE 1996). The general physical-chemical properties of the industry-restricted gas oils are presented in Table 1.

Table 1. General physical-chemical properties of the industry-restricted gas oils

Property	Type	Values	Temperature (°C)	Reference
Boiling point (ºC)	Experimental	160–382		CONCAWE 1996; ECB 2000; API 2003a
Density (kg/L)	Experimental	0.84–0.97	15	CONCAWE 1996
Vapour pressure (Pa)	Experimental	400	40	CONCAWE 1996
Log K_{ow} (dimensionless)	Experimental	3.9 - >6.0		CONCAWE 1996

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

Typically, gas oils contain C_9–C_{25} straight and branched alkanes, cycloalkanes, aromatic hydrocarbons and mixed aromatic cycloalkanes. Those that undergo cracking processes (processes that break long-chain hydrocarbons into shorter chains), such as those in this report, generally contain some unsaturated alkene hydrocarbons (CONCAWE 1996), although the proportions of these alkenes in these particular CAS RNs typically represent

less than 4% of the substances overall. As well, the boiling point range reflects the size and type of hydrocarbons in the substances.

To predict the environmental behaviour and fate of complex substances such as these industry-restricted gas oils, representative structures were selected from each chemical class contained within the substances. Twenty-seven representative structures were selected (see Table A2.2 in Appendix 2) from the database in PETROTOX (2009). In choosing representative structures, the amount of available data, boiling point ranges and carbon ranges were considered. Structures with a CAS RN were preferred. As the compositions of these gas oils are not well defined and are indeed variable, representative structures are not considered to be proportional with respect to actual concentrations in the substances. The selection process resulted in representative structures for alkanes, isoalkanes, one-ring and two-ring cycloalkanes, polycycloalkanes, cycloalkane monoaromatics and diaromatics, and one- to four-ring aromatics, ranging from C_9–C_{20} (see Table A2.2 in Appendix 2). Physical-chemical data for each representative structure were assembled from scientific literature and from the group of environmental models included in the United States Environmental Protection Agency's (U.S. EPA) Estimation Programs Interface Suite (EPI Suite 2008) (see Table A2.2 in Appendix 2). This process was used to enable the assessment of all gas oils (and other petroleum substances) within the context of the PSSA.

Sources

The industry-restricted gas oils considered in this screening assessment are produced in Canadian refineries and upgraders. The CAS RN descriptions (NCI 2006) and typical process flow diagrams (Hopkinson 2008) indicate the origin of these gas oils. Information submitted under section 71 of CEPA 1999, and other sources of information, indicates that the substances can be intermediate streams consumed within a facility or transported off-site (Environment Canada 2008, 2009).

CAS RN 64741-59-9 is formed from the catalytic cracking of substances from a variety of distillation and extraction (e.g., solvent deasphalting or visbreaking) processes within a refinery.

CAS RN 64741-82-8 refers to a distillate obtained from a thermal cracking unit (e.g., coking or visbreaking process) fed with vacuum distillation residues or bitumen coking and hydrocracking residues.

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, as well as other sources of information,

the industry-restricted gas oils considered in this screening assessment have been identified as being consumed at the facility, blended into substances leaving the site under a different CAS RN or transported to another industrial facility. Although these substances were identified by multiple use codes established during the development of the Domestic Substances List (DSL), it has been determined from information submitted under section 71 of CEPA 1999, voluntary submissions from industry, an in-depth literature review and a search of material safety data sheets that the industry-restricted gas oils identified as CAS RNs 64741-59-9 and 64741-82-8 may leave the petroleum facility and be transported to another industrial facility for use as a feedstock, but do not reach the public market in the form originally acquired.

Releases to the Environment

Potential releases of the industry-restricted gas oils include releases within facilities from activities associated with processing, as well as releases related to transportation of the substances between industrial facilities.

Due to the complex nature of the petroleum industry and transportation industry, as well as the ambiguity in the literature in the use of the terminology that is critical to the understanding of the Stream 2 PSSA assessments, it is important that the definitions specific to the assessment of the industry-restricted petroleum substances are well understood. Table 2 lists the terminology specific to the present assessment.

Table 2. Definitions of terms specific to the PSSA assessments of industry-restricted petroleum substances

Terminology	**Definition**
Release	A generic term to define a leak, spill, vent or other release of a gaseous or liquid substance, including controlled release and unintentional release, as defined below, but not including catastrophic events.
Controlled release	Any **planned** release for safety, maintenance or other purposes that is considered part of routine operations and occurs under controlled conditions.
Unintentional release	Any **unplanned** release of a petroleum substance. Causes can include equipment failure, poor maintenance, lack of proper operating practices, adverse weather-related events or other unforeseen factors, but can also be a routine part of normal operations. The following two categories are included under unintentional releases: (1) unintentional leaks or spills that occur from processing, handling and transport of a petroleum substance—such leaks or spills can be reduced or controlled by the industry; and (2) accidental releases that may not be controllable by the industry. Only unintentional leaks or spills (category 1, defined above) are considered in the assessment of the potential of industry-restricted petroleum substances to cause ecological harm.
Fugitive release	A specific type of unintentional release. It refers to an unintentional release, which occurs under normal operating conditions, of a gaseous

Terminology	Definition
	substance into ambient air and which may occur on a routine basis. Fugitive releases can be reduced but may not be entirely preventable due to the substance's physical-chemical properties, equipment design and operating conditions. Evaporative emission during the transportation of petroleum substances is a fugitive release and is considered in the human exposure analysis for purposes of assessing the potential of the substance to cause harm to human health.

Potential On-site Releases

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 for safety purposes or maintenance. Unintentional releases are typically characterized as spills or leaks from various equipment, valves, piping or flanges. 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 industry-restricted gas oils considered in this screening assessment originate from a distillation column as a distillate. Thus, the potential locations at the facility for the controlled release of these substances include relief and venting valves or drain valves on the piping or vessels where these streams are generated.

Under typical operating conditions, controlled releases of these gas oil substances would be captured in a closed system[3], according to defined procedures, and returned to the processing facility or to the facility's wastewater treatment plant. In both cases, exposure of the general population or the environment to these industry-restricted gas oils is not expected.

Unintentional Releases

Unintentional releases (including fugitive releases) occur from equipment (e.g., pumps, storage tanks), valves, piping, flanges, etc. during the processing and handling of petroleum substances and can be greater in situations of poor maintenance or operating practices. Regulatory and non-regulatory measures are in place to reduce these events at petroleum refineries and upgraders (see Appendix 3) (SENES 2009). Rather than being specific to one substance, these measures are developed to be more generic to limit non-routine releases of all substances in the petroleum sector.

Conclusion for Potential On-site Releases

[3] 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 where losses are collected and recirculated, reused or destroyed.

Based on the information presented in this screening assessment and in the screening assessment of the Stream 1 (site-restricted) gas oils, exposure of the general population or the environment to the on-site releases (controlled or unintentional) of industry-restricted gas oils is not expected.

Potential Releases from Transportation

As these industry-restricted gas oils can be transported between facilities, releases may also occur during transportation. In general, the three operating procedures involved during the process of transportation of petroleum substances are loading, transit and unloading. The transportation modes identified in the information submitted under section 71 of CEPA 1999 (Environment Canada 2009) and other sources of information were ship and truck; however, the volumes transported by truck are so small as to not warrant a release estimation to soil.

The on-site handling of petroleum substances for transportation is often regulated at the federal and provincial/territorial levels through legislation covering loading and unloading (see Appendix 3).

Storage of industry-restricted gas oils may be required before they are transported off-site. However, the general population near the storage area would not be exposed to industry-restricted gas oil vapours *per se*, but rather a complex combination of volatile compounds from all hydrocarbon substances present in the storage area or even in the whole petroleum facility. All relevant releases from storage (e.g., leaks, spills and breathing loss [expulsion of vapour due to changes in temperature and pressure]) are similar to potential on-site releases and are not further addressed in this screening assessment.

Tanks or containers for transferring petroleum substances are typically dedicated vessels; thus, washing or cleaning is not required on a routine basis (U.S. EPA 2008; OECD 2009). As such, the exposure of the general population and the environment around cleaning facilities is expected to be negligible with respect to the industry-restricted gas oils considered in this screening assessment. Cleaning facilities require processing of grey-water to meet local and provincial release standards.

Release Estimation

Information on transportation quantities and relevant transportation modes was collected under section 71 of CEPA 1999 (Environment Canada 2009) and from other sources of information. Ship transportation was the only relevant mode identified, as truck transport was used only for very small volumes.

Two types of releases can potentially occur during transportation and are considered in this screening assessment. These are evaporative emissions and unintentional releases (e.g., spills or leaks) during the handling and transit processes.

Evaporative emissions are similar to breathing loss of organic substances from storage tanks. The quantity lost depends on the volatility of the substances, temperature or pressure changes that occur during transportation and the air-tightness of transport vessels and settings of valves. Ambient air is the receiving medium for the evaporative emissions.

Unintentional releases of gas oil substances due to spills generally enter water or soil, depending on the modes of transportation involved. Due to the relatively low volatility of gas oil substances, as defined by their physical-chemical properties, evaporative emissions into the air from spills would be proportionally less than releases into water and/or soil.

Potential releases associated with ship transport of these gas oils were assessed through analysis of historical spill data (2000–2009) from the Environment Canada Spill Line database (Environment Canada 2011). There are no reported spills of "gas oils" in the database, but there are reported releases of diesel fuel (reported as "diesel" or "diesel fuel"), light fuel or petroleum distillate that could include spills of these industry-restricted gas oils due to their similarity. The extracted data were analyzed to remove duplicate entries, where it was a known diesel fuel or an environmental emergencies training exercise. Spills of less than 10 L were not included in release estimations due to the likelihood that these spills were related to the commercial use of diesel fuel rather than the shipment of gas oils. Spills where collisions, poor road conditions and/or adverse weather-related events were listed as a source or cause of or reason for the spills were not included in the release estimate, as they are not considered preventable with regard to loading/unloading and transport of these gas oils.

Spills data with known volumes were collected from across Canada by the Environment Canada Spill Line database between 2000 and 2009; spills of approximately 2000 litres of light oil, diesel fuel and petroleum distillates in 36 incidents to the marine areas of interest were documented (Environment Canada 2011). Many other reports in the database had no estimate of the volume released into the environment. In order to account for the underestimation of the volume released, the estimated total volume was extrapolated by assuming that the distribution of reported volumes released was representative of all releases (Table A4.1 in Appendix 4). From 2000–2009, the extrapolated total volume of spills of light oil, diesel fuel and petroleum distillates to salt water was 5200 litres from 36 spills.

The Spill Line database did not contain information on releases of light oil, diesel fuel and petroleum distillates to salt water during ship transportation for the marine areas of interest, hence releases during ship transport were not considered for a marine release scenario.

Also, since there is no distinction in the database as to whether the spills occurred during loading, transport or unloading, the average spill volume was used for the loading and unloading scenarios. In the case of ship loading and unloading, the extrapolated total volume spilled of 5168 litres/36 spills = 144 L/spill (122 kg, given an average density of 0.85 kg/L) (CONCAWE 1996) is expected in marine waters.

These numbers of diesel fuel, light oil, and petroleum distillates releases are considered to be a low estimate of actual releases, as not all provinces and territories were reporting their spills to Environment Canada for all years, and some provinces and territories have minimum reportable spill quantities (Table A4.2 in Appendix 4). However, these data would also include spills of petroleum substances other than the two CAS RNs under assessment in this report.

The majority of diesel fuel, light oil, and petroleum distillates releases to marine waters occurred from motor vehicles of unknown kind, representing 85% of the total volume spilled. Industrial plants and other watercraft accounted for the source of 9% of the volume (see Table A4.2a). Unknown spills accounted for the remaining 6% of the volume spilled. Other spill sources included marine terminals, pipelines, tank trucks, marine tankers and others.

The Environment Canada Spill Line data were also analyzed for causes of diesel fuel, light oil, and petroleum distillates spills (Table A4.2b in Appendix 4); it was found that "unknown" and "other" spills accounted for 87% of the volume released, whereas container leaks, discharges and valves accounted for the remaining 13% of the volume.

Analyzing the data on reasons for diesel fuel, light oil, and petroleum distillates spills (Table A4.2c in Appendix 4) identified that the majority of releases had "unknown" or "other" reasons accounting for 90% of spills. Human error and vandalism were responsible for 10% of the volume. Equipment and material failure, corrosion and subsidence were also reasons identified for spills, but represented a small portion of overall volume.

For purposes of assessing the potential exposure of the environment from the transportation of industry-restricted gas oils, the ecological assessment focuses on unintentional releases to water. In comparison, assessment of potential exposure of the general population from transportation of industry-restricted gas oils focuses on evaporative emissions, which occur during regular operating activities. Although spills occur during transit and in loading or unloading operations, such releases are considered to occur on a non-routine or unpredictable basis in distinct locations and are therefore not considered in the assessment of exposure of the general population.

In addition, due to the relatively low volatility of the industry-restricted gas oils (see Table 1), as well as relevant legislation and best practices currently in place for on-site handling of these industry-restricted gas oils (Appendix 3), non-occupational human exposure as a result of loading and unloading is not expected and is not considered in the human exposure assessment.

Environmental Fate

When petroleum substances are released into the environment, four major fate processes will take place, i.e., dissolution in water, volatilization, biodegradation and adsorption.

These processes will cause changes in the composition of these UVCB substances. In the case of spills on land or water surfaces, photodegradation can also be significant.

The rates of dissolution in water or volatilization of individual petroleum components are retarded by the complex nature of these petroleum mixtures. The solubility and volatility of individual components in mixtures are proportional to the solubility or volatility of the components in its pure state and its concentration in the mixture. Solubility and volatility of a component decrease when the component is present in a mixture (Banerjee 1984; Potter and Simmons 1998).

Each of the fate processes affects hydrocarbon families differently. Aromatics tend to be more water soluble than aliphatics of the same carbon number, whereas aliphatics tend to be more volatile (Gustafson et al. 1997). Thus, when a petroleum mixture is released into the environment, the principal water contaminants are likely to be aromatics, while aliphatics will be the principal air contaminants (Potter and Simmons 1998). The trend in volatility by compound class is as follows: alkenes ≈ alkanes > aromatics ≈ cycloalkanes. The most soluble and volatile compounds have the lowest molecular weight; thus, there is a general shift to higher molecular weight compounds in residual materials.

Biodegradation is almost always operative when petroleum mixtures are released into the environment. It has been widely demonstrated that nearly all soils and sediments have populations of bacteria and other organisms capable of degrading petroleum hydrocarbons (Pancirov and Brown 1975). Two key factors that determine degradation rates are oxygen supply and molecular structure. Although degradation occurs both in the presence and absence of oxygen, degradation is more rapid under aerobic conditions. Decreasing trends in degradation rates according to structure are as follows (Potter and Simmons 1998):

(1) *n*-alkanes (especially in the C_{10}–C_{25} range which are degraded readily);
(2) isoalkanes;
(3) alkenes;
(4) benzene, toluene, ethylbenzene and xylenes (BTEX) (when present in concentrations that are not toxic to the microorganisms);
(5) monoaromatics;
(6) polynuclear (polycyclic) aromatic hydrocarbons (PAHs); and
(7) higher molecular weight cycloalkanes (which may degrade very slowly (Pancirov and Brown 1975)).

Level III fugacity modelling of representative structures contained in the gas oils group of substances was performed using EQC (2003) (see Table A5.1 in Appendix 5) based on physical-chemical properties given in Table A2.2 (Appendix 2).

If released solely to air, the majority of C_9–C_{15} representative structures of gas oils will remain in air. Some C_{18}–C_{20} components will also remain primarily in air, except alkanes, two-ring cycloalkanes, polycycloalkanes and cycloalkane monoaromatics. The low volatile C_{20} representative structures will partition primarily to soil and sediments.

If released solely to water, the majority of C_{10} representative structures are expected to remain mostly in water, with minor amounts evaporating. The C_{10} *n*-alkanes will partition evenly between water and sediments (Table A5.1 in Appendix 5). The majority of the C_{15}–C_{20} representative structures are expected to partition mainly to sediments based on their higher range of log K_{oc} values (Table A5.1 in Appendix 5). The exceptions are the C_{15} cycloalkane diaromatics and the two-ring and three-ring aromatics, which will partition evenly between water and sediments if released solely to water (Table A5.1 in Appendix 5). The EQC model predicts little loss from water to air despite the high Henry's Law constants for many of the representative structures.

CAS RN 64741-59-9 is similar to diesel fuel with respect to physical-chemical properties. Fingas (2001) estimated that 60% of a diesel fuel would evaporate from water in 48 hours at 15°C, and this likely approximates the extent of evaporation of CAS RN 64741-59-9 from water.

If released to soil, all components of gas oils are expected to remain primarily in soil. Such behaviour in soil is expected due to high sorption to the point of being relatively immobile for the largest structures, based on the estimated range of log K_{oc} values (Table A2.2 in Appendix 2). Volatilization from moist soil surfaces should be an important fate process for many components, based upon estimated Henry's Law constant values > 100 $Pa \cdot m^3/mol$ (Table A2.2 in Appendix 2); however, the results of the EQC (2003) Level III fugacity estimations indicate that this process does not readily occur for many gas oil components. This is due to the competitive processes of sorption and volatilization.

Fugacity estimations in soil do not take into account situations where large quantities of a hydrocarbon mixture enter the soil compartment. When soil organic matter and other sorption sites in soil are fully saturated, the hydrocarbons will begin to form a separate phase (a non-aqueous phase liquid or NAPL) in the soil. At concentrations below the retention capacity for the hydrocarbon in the soil (Arthurs et al. 1995), the NAPL will be immobile; this is referred to as residual NAPL (Brost and DeVaull 2000). Above the retention capacity, the NAPL becomes mobile and will move within the soil (Arthurs et al. 1995; Brost and DeVaull 2000). According to a study by Brost and DeVaull (2000), the NAPLs of fuel products in the density range of diesel fuel, such as gas oils, will become mobile in the range of 7700–34 000 mg/kg dw depending on the type of soil. Above this range, they can move through the soil due to gravity.

Persistence and Bioaccumulation

Environmental Persistence

In water, hydrolysis half-lives could not be predicted for hydrocarbons with the HYDROWIN (2008) model. Alkanes, alkenes, benzenes, biphenyls, PAHs and heterocyclic PAHs are all known to be resistant to hydrolysis (Lyman et al. 1990).

Since no empirical data were available on the degradation of these gas oils, a QSAR-based weight-of-evidence approach (Environment Canada 2007) was applied using the BioHCWin (2008), BIOWIN 3, 4, 5, and 6 (2009), CATABOL (c2004–2008) and TOPKAT (2004) biodegradation models (Table A5.2 in Appendix 5).

Primary biodegradation (estimated with BIOWIN 4 and BioHCWin) is the transformation of a parent compound to an initial metabolite. Ultimate biodegradation (estimated with BIOWIN 3, 5 and 6, CATABOL and TOPKAT) is the transformation of a parent compound to carbon dioxide and water, mineral oxides of any other elements present in the test compound and new cell material (EPI Suite 2008). BioHCWin (2008) is a biodegradation model specific for petroleum hydrocarbons. Model results are in domain for all MITI-based models (BIOWIN 5 and 6). Modelled results that were out-of-domain were not considered when determining the persistence of components.

For many of the C_9–C_{20} components, both the primary and ultimate biodegradation models agree that these compounds would degrade quickly and would not likely be persistent (Table A5.2 in Appendix 5). The following show persistence in water (half-life ≥ 182 days) based on the *Persistence and Bioaccumulation Regulations* (Canada 2000): C_{15}–C_{20} two-ring cycloalkanes, C_{14}–C_{22} polycycloalkanes, C_{15}–C_{20} cycloalkane monoaromatics, C_{15} two-ring aromatics, C_{12} cycloalkane diaromatics and C_{16} four-ring aromatics.

Using an extrapolation ratio of 1:1:4 for a water : soil : sediment biodegradation half-life (Boethling et al. 1995), the half-life in soil for most heavy (> C_{12}) representative structures is also ≥ 182 days and the half-life in sediments is ≥ 365 days.

The proportion of these gas oils that would be expected to be persistent cannot be accurately determined, as compositional details on these CAS RNs are not available. The limited compositional information on these two CAS RNs indicates that aromatics can account for up to 80% by weight of CAS RN 64741-59-9 and up to 43% by weight of CAS RN 64741-82-8 (API 1987, 2003a). As well, a typical gas oil has a total cycloalkane content of 8–10%.

AOPWIN (2008) is a model that calculates atmospheric oxidation half-lives of compounds in contact with hydroxyl radicals in the troposphere under the influence of sunlight. Atmospheric oxidation rates were calculated for all of the representative structures. According to this model, the components of gas oils will degrade readily by interactions with hydroxyl radicals in air (half-lives < 1 day) (Table A5.3 in Appendix 5).

Persistence Conclusion

Based on results from AOPWIN (2008), there would be a relatively rapid removal process if these gas oils are introduced into the atmosphere, with oxidation half-lives of less than 1 day. With regard to the primary and ultimate biodegradation modelling, the C_{15}–C_{20} two-ring cycloalkanes, C_{14}–C_{22} polycycloalkanes, C_{15}–C_{20} cycloalkane monoaromatics, C_{15} two-ring aromatics, C_{12} cycloalkane diaromatics and C_{16} four-ring aromatics in these gas oils meet the persistence criteria in water, soil and sediment (half-life in soil and water

≥ 182 days and half-life in sediment ≥ 365 days). Cycloalkanes represent a relatively small fraction (8–10%) of gas oils. There is no detailed information on the specific aromatic content of these gas oils; however, CAS RN 64741-59-9 may include up to 80% aromatics. Thus, these gas oils are expected to contain an unknown proportion of components that meet the persistence criteria as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

Bioconcentration Factors (BCF) and Bioaccumulation Factors (BAF)

Experimental Studies

Since no empirical data on the bioaccumulation of gas oils or its components were found, empirical data on the bioaccumulation of components of diesel fuel and Fuel Oil No. 2 were used in a read-across approach. A predictive approach using a bioconcentration/bioaccumulation factor (BAF) model was also applied (Arnot and Gobas 2003, 2004). According to the *Persistence and Bioaccumulation Regulations* (Canada 2000) a substance is bioaccumulative if its BCF or BAF is ≥ 5000; however, measures of BAF are the preferred metric for assessing bioaccumulation potential of substances. This is because BCF may not adequately account for the bioaccumulation potential of substances via the diet, which predominates for substances with log K_{ow} > ~4.5 (Arnot and Gobas 2003).

Neff et al. (1976) exposed clams (*Rangia cuneata*), oysters (*Crassostrea virginica*) and fish (*Fundulus similus*) to the water-soluble fraction of Fuel Oil No. 2 (0.41 kg/L [2 ppm] total naphthalenes) for 2 hours, followed by depuration of hydrocarbons for 366 hours. All organs examined showed rapid accumulation of naphthalenes within the 2-hour exposure period, with the gall bladder and brain of fish accumulating the highest concentrations. BAFs of naphthalenes in clams ranged from 2.3–26.7 L/kg wet weight (ww) (Table A5.4 in Appendix 5). Release of naphthalenes by fish began immediately following transfer to fresh water, reaching undetectable levels after 366 hours (~15 days).

Peterson and Kristensen (1998) exposed eggs and larvae of zebrafish (*Brachydanio rerio*) and larvae of cod (*Gadus morhua*), herring (*Clupea harengus*), and turbot (*Scophthalmus maximus*) to ^{14}C-labeled PAHs (naphthalene and phenanthrene). The experiments were performed in a semistatic test system and steady-state was not reached during the embryonic stage except for naphthalene. High BCFs were found in all cases, indicating that bioaccumulation can occur during early life stages, as fish larvae have higher lipid contents and lower metabolic capabilities than juvenile or adult fish.

Burkhard and Lukasewycz (2000) compiled data on tissue (lake trout *Salvelinus namaycush*), and water and sediment concentrations of PAHs from three published works and used the data to derive BAFs. Bioaccumulation factors for PAHs in these fish were 87 and 1550 L/kg ww for phenanthreneand fluoranthene, respectively (Table A5.4 in Appendix 5). Burkhard and Lukasewycz (2000) note that there is significant uncertainty in

the BAFs for phenanthrene and fluoranthene, as both chemicals were present in the tissues at concentrations just greater than the method detection limit.

Hardy et al. (1974) carried out an experiment giving cod (*Gadus morhua*) single doses of hexadecane (a C_{16} *n*-alkane) in the diet and tracked metabolites. Entirely unchanged hexadecane was found in the liver. Hardy et al. (1974) suggest that such findings do not support high metabolic conversion of hexadecane in the liver of cod; *n*-alkanes were preferentially deposited in liver over flesh of cod. However, the liver is the major site of chemical biotransformation, so higher concentrations in liver would be expected. Cravedi and Tulliez (1981) dosed rainbow trout with dodecyl cyclohexane (a C_{18} alkyl cycloalkane) and studied its elimination and metabolism from the fish. Approximately 75% of the dose was absorbed. A major source of unmodified substance elimination was through the gills. Considerable amounts were also metabolized to a fatty acid and distributed throughout the body and 14% was excreted in urine (Cravedi and Tulliez 1981).

Cravedi and Tulliez (1983) also studied the dietary uptake of 1% C_{13}–C_{22} *n*-alkanes in rainbow trout for 7 months. Trout were dosed with 10 000 ppm total *n*-alkanes in feed, and showed preferential fixation of C_{13}–C_{14} *n*-alkanes in the adipose tissue. The mean accumulated mass of *n*-alkanes was 958 ppm per fish, so that a calculated BCF (diet) was 0.1. Alkanes longer than C_{16} were well retained (over 60% of accumulated *n*-alkanes remained after 8 weeks of depuration), while short-chain (< C_{16}) *n*-alkane concentrations decreased more rapidly (20–50% remained after 8 weeks of depuration).

Colombo et al. (2007) studied the bioaccumulation dynamics of C_{12}–C_{25} *n*-alkanes and aliphatic unresolved complex hydrocarbons (UCM) in a detritivorous fish (*Prochilodus lineatus*) collected from the sewage-impacted Buenos Aires coastal area. Fish muscles contained large amounts of C_{12}–C_{25} *n*-alkanes and aliphatic UCM, reflecting the chronic bioaccumulation of fossil fuels from sewage particulates. The hydrocarbon composition in fish muscles was enriched in C_{15}–C_{17} *n*-alkanes relative to a fresh crude oil and settling particulates. The bioaccumulation factors plotted (BAFs: 0.4–6.4 dry weight or 0.07–0.94 lipid-organic carbon) against K_{ow} showed a parabolic pattern maximizing at C_{14}–C_{18}.

McCain et al. (1978) reported that 1- and 2-methylnaphthalene and 1,2,3,4-tetramethylbenzene were accumulated to a greater extent than other oil components in English sole (*Parophrys vetulus*) from oil-contaminated sediments. Tissue burdens of hydrocarbons decreased with increasing exposure time, such that after 27 days of exposure, only the liver had a detectable hydrocarbon burden. McCain et al. (1978) suggested that induction of the aryl hydrocarbon hydroxylase (AHH) enzyme system eventually resulted in hydrocarbon removal.

Weinstein and Oris (1999) found that 4-day-old fathead minnows (*Pimephales promelas*) bioconcentrated fluoranthene (BCF 9054 L/kg) with only 24 hours exposure and steady-state was reached. They observed that the age of the fish likely impacted the ability to depurate fluoranthene and that older, more mature fish would be unlikely to bioacumulate PAHs. Weinstein and Oris (1999) used a static renewal system which is less preferable to

flow-through designs where consistent exposures can be maintained, thus this study was considered to be of low reliability. However, the study does show that bioaccumulation is important for toxicity in the early life stages (Weinstein and Oris 1999). In contrast, De Maagd (1996) found a BCF of 3388 L/kg ww for fluoranthene in adult fathead minnows.

Guppies (*Poecilia reticulata*) bioconcentrated pyrene, with BCFs in the range of 4786–11 300 L/kg ww (depending on the type of test) after 48 hours of exposure, while lighter-weight PAHs had lower BCFs (1050–2238 L/kg ww for fluorene and 4550–7244 L/kg ww for anthracene) (De Voogt et al. 1991). For fish, only 70% of anthracene depurated within 200 hours and only 20% of fluorene was depurated within 200 hours. The BCF result for anthracene by De Voogt et al. (1991) was not considered reliable in determining the bioconcentration potential of this substance due the lack of evidence that a steady-state had been reached within the 48 hours of exposure.

Mollusc studies have typically found high potentials for the bioconcentration of PAHs. This may be caused by the relatively slow rates of depuration when compared to fish studies coupled with fairly rapid uptake. Other works have shown that BCFs for PAHs in molluscs and some crustaceans are considerably higher than in fish (Table A5.5 in Appendix 5). Unlike fish and some crustaceans, molluscs are unable to rapidly metabolize aromatic hydrocarbons, and accumulation can occur in stable tissue compartments with low hydrocarbon turnover and are not readily exchangeable (Stegeman and Teal 1973; Neff et al. 1976).

McLeese and Burridge (1987) studied the bioaccumulation potential of PAHs by a number of saltwater invertebrates using PAH-seawater solutions or PAH-contaminated sediments. When PAHs were dissolved in water, fluoranthene produced relatively high BCF values in mussels (*Mytilus edulis*) (BCF of 5920 L/kg ww) and clams (*Mya arenaria*) (BCF of 4120 L/kg ww) after short 96-hour exposures. However, when PAHs are present in the sediment, only mussels have a high potential for bioconcentration (BCF of 5950 L/kg ww). Fluoranthene can be depurated from molluscs given time, depuratating faster than heavier PAHs that were also studied (triphenylene and perylene). Shrimps and polychaetes did not readily bioaccumulate PAHs.

Other invertebrates have also been shown to bioaccumulate petroleum hydrocarbons. Muijs and Jonker (2010) studied the bioaccumulation of petroleum hydrocarbons (total and divided into three different carbon ranges) over 49 days by the aquatic worm, *Lumbriculus variegatus,* after exposure to a series of 14 field-contaminated sediments with a known history of oil pollution. A maximum tissue concentration was reached for the C_{11}–C_{16} fraction after 14 days of exposure but then decreased; other fractions did not show any decrease in tissue concentration once a maximum was achieved. After 28 days of exposure, it was estimated that 70–90% of equilibrium was reached, although it was noted that it may take > 90 days for hydrocarbons > C_{34} to reach equilibrium. Characterization of the accumulated hydrocarbons was not determined, however, alkanes from C_{10}–C_{34} were identified in the aquatic worms. The accumulation of higher molecular weight alkanes may be due to ingestion of organic matter to which the chemicals are sorbed. Depuration was not studied.

Overall, BCF values determined for various PAHs (Table A5.5 in Appendix 5) were highly variable, ranging from 180 to over 9000 L/kg ww. The majority of BCF studies on PAHs have found that bioconcentration can occur after short exposure times but that the majority of organisms also exhibit rapid depuration once the contaminant is removed..

Three studies on BAFs of PAHs in aquatic organisms (fish and clams) were found. Hence, experimental values of BAFs from the work of Neff et al. (1976), Zhou et al. (1997) and Burkhard and Lukasewyez (2000) were compiled for comparison with modelled data (Arnot and Gobas 2003) (Table A5.4 in Appendix 5). In general, the modelled values approximate those measured (Table A5.6 in Appendix 5) for the selected PAHs. None of the measured and modelled values were shown to be bioaccumulative according to the BAF criterion (BAF $\geq$ 5000) in the *Persistence and Bioaccumulation Regulations* (Canada 2000) with the exception of the substituted PAH, isoheptylfluorene (see Table A5.6 in Appendix 5).

Characterizing BCF/BAF

In characterizing bioaccumulation, the derivation of a BAF is preferred over a BCF since chemical exposure through the diet is not accounted for in the latter (Barron 1990). BCFs are typically derived under laboratory controlled conditions. According to Arnot and Gobas (2006), the BCF is a poor descriptor of biomagnification in food webs because it is derived from laboratory experiments and does not include dietary exposure. Thus, BCFs have been shown to underestimate bioaccumulation potential or biomagnification of chemicals in the food web, as predators consume prey containing lipophilic compounds (U.S. EPA 1995). As hydrophobicity increases, dietary uptake is likely to be more important than absorption from water (Arnot and Gobas 2003). Further, laboratory BCFs have been shown to overestimate bioaccumulation potential when a chemical is bound or strongly sorbed to sediment (i.e., less bioavailable).

Due to the scarcity of measured BAF values (Table A5.4 in Appendix 5), BCFs from various published work were compiled (Table A5.7a in Appendix 5) and used to help verify measured and modelled BAF values. In contrast to the few available experimental BAFs on PAHs, a suite of BCFs for components of gas oils were found, including alkanes, isoalkanes, two-ring cycloalkanes, one-ring aromatics, cycloalkane monoaromatics, cycloalkane diaromatics and polyaromatics (Table A5.7a in Appendix 5). Model estimates of these BCFs were also produced using a kinetic mass-balance model (Arnot and Gobas 2003) to fit the model kinetic elimination constants to agree with the observed BCF data in order to generate BAF predictions that reflect the known elimination rates.

A kinetic mass-balance model is, in principle, considered to provide the most reliable prediction method for determining bioaccumulation potential because it allows for correction of the kinetic rate constants and bioavailability parameters, when possible. BCF and BAF model predictions are considered “in domain” for this hydrocarbon assessment because it is based on first principles. As long as the mechanistic domain (passive diffusion), global parameter domain (range of empirical log K_{ow} and molecular weight), as

well as metabolism domain (corrected metabolic rate [k_M]) are satisfied, predictions are considered valid (Arnot and Gobas 2003, 2006). The kinetic mass-balance model developed by Arnot and Gobas (2003, 2004) was employed using metabolic rate constants normalized to both conditions of the study and a representative middle trophic level fish as outlined in Arnot et al. (2008a,b) when a BCF or growth corrected elimination rate constant is known. Both BCF and biomagnifications factor (BMF) empirical data were used to correct default model uptake and elimination parameters, which are summarized in Table A5.7b (Appendix 5).

In Table A5.7b (Appendix 5), some metabolic rate constants calculated from the empirical BCF data were negative, suggesting that the metabolic rate is essentially zero and that other routes of elimination are more important. Accordingly, no metabolic rate correction was used when predicting the BCF and BAF for these structures. Gut and tissue metabolism is generally not regarded as an important elimination process for chemicals with log K_{ow} less than ~4.5 (Arnot et al. 2008a,b; Arnot and Gobas 2006), but this can depend on the size and lipid content of fish used in testing.

In Table A5.7a (Appendix 5), only the C_{15} isoalkane (2,6,10-trimethyldodecane), C_8 one-ring cycloalkane (ethylcyclohexane), and C_{13} two-ring aromatic (2-isopropylnaphthalene) had measured and/or modelled BCFs or BAFs $\geq$ 5000. However, the measured diaromatic (2-isopropylnaphthalene) that was found to be highly bioaccumulative contains the isopropyl functional group that is considered atypical in petroleum and requires a more thorough appraisal of reasonableness of model predictions based on available experimental information (Lampi et al. 2010). As well, Neff et al. (1976) found that the C_{12} and C_{13} diaromatics (alkylated naphthalenes and biphenyls) were not highly bioaccumulative in clams upon exposure to an oil-in-water dispersion of Fuel Oil No. 2. Thus, the combined weight of evidence suggests that these C_{12} and C_{13} diaromatics are not likely to be highly bioaccumulative. For the C_8 cyclohexane (ethyl cyclohexane), the predicted BAF (Arnot and Gobas 2004) for the middle trophic level fish is 5495 L/kg ww, which just exceeds the criterion (BAF $\geq$ 5000), suggesting that it is bioaccumulative when all routes of uptake are considered. This prediction, however, was generated with a metabolic rate equal to zero because of the potential error associated with the estimate of metabolism rates (see Table A5.7b in Appendix 5). Factoring in metabolism, it is expected that the BAF would be lower and likely below 5000. As well, the experimental BCF suggests this C_8 cycloalkane is not highly bioaccumulative (Table A5.7a in Appendix 5). Combining these lines of reasoning suggests that this C_8 cycloalkane is also not likely to be bioaccumulative according to the Canadian criteria. For the C_{15} isoalkane (2,6,10-trimethyldodecane), two predicted BAFs are presented (575 and 47 863 L/kg ww). The latter BAF of 47 863 L/kg ww is preferred, as the depuration rate constant from the study was available to calculate the metabolic rate constant. This higher predicted BAF value is also in agreement with the slow rate of metabolism. Combining these lines of reasoning suggests that this C_{15} isoalkane is likely bioaccumulative according to the Canadian criteria.

Most components > C_{20} have an estimated log K_{ow} > 8 and were excluded from the modelling, as predictions may be highly uncertain due to limitations of the model (Arnot

and Gobas 2003). In Arnot and Gobas (2006), 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 the Canadian criterion of BCF ≥ 5000. Examination of Environment Canada's empirical BCF/BAF database for DSL and non-DSL chemicals developed by Arnot and Gobas (2003) and further by Arnot (2005, 2006) shows that these are all 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 L/kg ww (Fox et al. 1994; Gobas et al. 1989; Oliver and Niimi 1988), and all have log K_{ow} values < 8. Therefore, the predicted BCF and BAF values with log K_{ow} > 8 were considered out of the parametric domain of the Arnot-Gobas model (2003) and considered highly uncertain and not reliable.

BCF and BAF model estimates were also generated for an additional 26 C_9–C_{22} linear and cyclic representative structures using the modified Arnot-Gobas three trophic level model (2004) (Table A5.6 in Appendix 5), as no empirical bioaccumulation data were identified for these substances. Metabolism and dietary assimilation efficiency kinetics were corrected for these predictions based on analogue BCF and BMF test data. From this analysis, only the C_{14} polycycloalkane was predicted to have a BCF suggesting a high bioconcentration potential. However, one isoalkane, one one-ring cycloalkane, one two-ring cycloalkane, two polycycloalkanes, one one-ring aromatic, two cycloalkane monoaromatics, and one cycloalkane diaromatic were found to have high BAFs; the log K_{ow} for these structures suggests that dietary uptake can predominate (up to 87% of total uptake) but will not be the sole route of exposure, as some substances are expected to have 90% bioavailable fraction in the water column. BAF is, therefore, considered the most appropriate metric to assess the bioaccumulation potential of these structures and represents a comparison of whole body burdens compared with concentrations in water. The BCF and BAF predictions for these fractions are within the parametric, mechanistic and metabolic domains of the model and so are considered reliable.

Biomagnification Factors (BMF) and Trophic Magnification Factors (TMFs)

BMF values from ExxonMobil Biomedical Sciences Inc. (EMBSI), used to derive kinetic information for 15 substances, are included in Table A5.7a (Appendix 5) (Lampi et al. 2010). None of these analogues have BMFs > 1, suggesting that these hydrocarbons will not biomagnify when compared to the concentrations expected in food items. A combination of metabolism, low dietary assimilation efficiency and growth dilution appear to limit the biomagnification potential of these compounds (see Tables A5.7a and A5.7b in Appendix 5).

Lampi et al. (2010) also summarized TMFs for PAHs from three field studies. The TMFs for various PAHs are summarized in Table A5.8 (Appendix 5).

Field-based TMFs for the PAHs studied are mostly < 1, except fluorene and acenaphthene, which are approximately 1. A combination of metabolism, low dietary assimilation efficiency and growth dilution appear to limit the trophic magnification potential of these compounds as well. Therefore, it is not likely that the linear, cyclic and

aromatic components of these gas oils will undergo biomagnification or trophic magnification.

Biota-sediment Accumulation Factors (BSAFs)

Lampi et al. (2010) also summarized the available BSAF data for several PAHs from a database compiled by the U.S. EPA (2008a). Median field-based fish BSAF values for PAHs expected to be found in gas oils (acenaphthylene, acenaphthene, fluoranthene, fluorene, naphthalene and phenanthrene) ranged from 0.001–0.1. Ninetieth percentile BSAF values ranged from 10^{-4} to just less than one, with naphthalene being the only PAH with a BSAF close to but below one. None of the PAHs have fish BSAFs greater than one. This is expected, given the same rationale for low BMF and TMF values. However, data were not extracted for invertebrate BSAFs from the U.S. EPA database. In the case of invertebrates, these factors can be much greater than one, because invertebrates do not have the same metabolic competency as fish (e.g., B[*a*]P) (Muijs and Jonker 2010; Stegeman and Teal 1973; Neff et al. 1976).

As previously noted, Muijs and Jonker (2010) studied the bioaccumulation of oil in the aquatic worm, *L. variegatus.* Resulting BSAFs varied from 0.01–2.3. The wide range is likely related to the differences in oil weathering status. The BSAF values for separate hydrocarbon blocks appeared to be relatively constant up to C_{22}, indicating that *L. variegatus* proportionally accumulated these fractions from sediment. Beyond C_{22}, BSAFs decreased for all sediments studied, likely due to the reduced bioavailability of the higher boiling point fractions such as PAHs. Likewise, there may be enhanced sorption of PAHs to sediment and in some cases the nonaqueous phase liquid (NAPL). Muijs and Jonker (2010) also suggest that the studied aquatic worm may even avoid NAPLs, which may also limit the bioaccumulation of the very hydrophobic fractions.

Bioaccumulation Conclusion

Non-PAH Components

As noted previously, of the parameters that have prescribed Canadian regulatory criteria, BAF values are preferred over BCF values because they represent the potential accumulation in biota from all exposure sources and thus represent a more complete picture of the total body burden of chemicals. Biomagnification (BMF), trophic or foodweb magnification (TMF) and biota-sediment accumulation factors (BSAF) are also considered very important for understanding the pattern of bioaccumulation and are used in a weight of evidence for the overall bioaccumulation potential of a chemical.

In general, the C_{10}–C_{15} alkanes, C_{10} one-ring cycloalkanes, C_9 one-ring aromatics and C_{10} cycloalkane monoaromatics were not found to meet the bioaccumulation criterion as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000). This conclusion is based on consistencies found between available BCF and BAF experimental data, BCF and BAF kinetic mass-balance model predictions (Arnot and Gobas 2003) and modelled results using the Arnot-Gobas three trophic level model (2004).

The majority of components > C_{20} (alkanes, isoalkanes, two-ring cycloalkanes and one-ring aromatics) have estimated log K_{ow}s > 8 and were therefore excluded from modelling, as predictions may be highly uncertain due to limitations of the model (Arnot and Gobas 2003). Likewise, for these > C_{20} components, no experimental measured BCFs were found.

In terms of the polycycloalkanes, the C_{18} polycycloalkane (hydrochrysene) did not meet the criteria of BCF or BAF ≥ 5000 for its modelled BAF prediction using the modified Arnot-Gobas three trophic level model (2004) (Table A5.6 in Appendix 5), whereas the C_{14} and C_{22} polycycloalkanes were found to meet the criteria based on the same model. The metabolic rate constant (0.45/day) for hydrochrysene suggests a rapid rate of metabolism in comparison to the lower metabolic rate constants (0.01/day and 0.04/day) for the C_{14} and C_{22} polycycloalkanes. Study details from experimental evidence for a similar polycycloalkane could not be obtained to determine predicted BCFs and BAFs, thus the available evidence suggests that the C_{18} polycycloalkane (hydrochrysene) is not bioaccumulative based on modelled results alone.

The C_{14} and C_{22} polycycloalkanes, C_{15} one-ring aromatics, C_{15}–C_{20} cycloalkane monoaromatics and C_{20} cycloalkane diaromatics were found to meet the bioaccumulation criterion based on modelled results from the Arnot-Gobas three trophic level model (2004). For these particular components, the metabolic rate constants (normalized to a 184 g fish at 10°C) range from 0.01–0.13 (day^{-1}), suggesting a slow rate of metabolism. In the case of C_{14} and C_{22} polycycloalkanes, the C_{15} one-ring aromatic and the C_{20} cycloalkane monoaromatic, only experimental BMFs for comparative analogues were available. The BMFs were all < 1, suggesting that these components will not biomagnify. In the case of the C_{15} cycloalkane monoaromatic, only an experimental BCF (3418 L/kg ww) for a similar component (octahydro-phenanthrene) was found. However, considering the slow rate of metabolism of 0.197 (day^{-1}) for octahydrophenanthrene, there is the potential that predicted BCFs and BAFs for the C_{15} cycloalkane monoaromatic could exceed the Canadian criteria, although this cannot be determined due to the lack of details from the relevant study. Lastly, the only analogue similar to the C_{20} cycloalkane diaromatic (isoheptylfluorene) is fluorene, which has an experimental BCF of 1030 L/kg ww. However, the presence of an isoheptyl group may affect the bioaccumulation potential of fluorene and the low k_M value suggests a slow rate of metabolism. Overall, the available evidence suggests that these components are likely to bioaccumulate based on available modelled and experimental results.

BMF values for 19 substances comprising some isoalkanes, one- and two-ring cycloalkanes, polycycloalkanes, one-ring aromatics, cycloalkane monoaromatics, cycloalkane diaromatics, and three- and four-ring aromatics (see Table A5.7a in Appendix 5) show that no components have BMFs > 1. This suggests that these particular hydrocarbons will not biomagnify when tissue concentrations are compared to concentrations in food items. Thus, the available evidence suggests that there is limited biomagnification of petroleum hydrocarbons. It is possible that BSAFs will be > 1 for invertebrates (up to 2.3 for total petroleum hydrocarbons in *L. variegatus* (Mujis and

Jonker 2010) as they do not have the same metabolic competency as fish, but BSAFs will likely decrease beyond C_{22} due to reduced bioavailability of the higher boiling point fractions (Muijs and Jonker 2010).

Overall, there is consistent empirical and predicted evidence to suggest that nine representative structures (C_{15} isoalkane, C_{15} one-ring cycloalkane, C_{15} two-ring cycloalkane, C_{14} and C_{22} polycycloalkanes, C_{15} one-ring aromatic and C_{15}–C_{20} cycloalkane monoaromatics) meet the bioaccumulation criteria as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000). These components are associated with a slow rate of metabolism and are highly lipophilic. Exposures from water and the diet, when combined, suggest that the rate of uptake would exceed that of the total elimination rate. However, these components are not expected to biomagnify in aquatic food webs, largely because a combination of metabolism, low dietary assimilation efficiency and growth dilution allows the elimination rate to exceed the total uptake rate from the diet.

PAH Components

In general, the C_{12}–C_{15} cycloalkane diaromatics and C_{15} three-ring aromatics were not found to meet the bioaccumulation criteria as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000). This conclusion is based on consistencies found between available BCF and BAF experimental data, BCF and BAF kinetic mass-balance model predictions (Arnot and Gobas 2003) and modelled results using the Arnot-Gobas three trophic level model (2004).

Experimental BAFs and BCFs suggest that PAHs, as a whole, have low bioaccumulation potential in fish. This is due in part to the metabolism of PAHs by fish, resulting in low or nondetectable concentrations of the parent PAHs in fish tissues (Varanasi et al. 1989). Regarding BAF, none of the measured or modelled values were shown to meet the bioaccumulation criterion (BAF $\geq$ 5000) as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000) with the exception of modelled BAF values for isoheptyl fluorene (see Table A5.6 in Appendix 5). Lampi et al. (2010) found that isopropyl functional groups increased the bioaccumulation potential of naphthalene although isopropyl groups are considered atypical in petroleum. Thus highly alkylated PAHs, especially those with iso- groups, likely have a greater potential to bioaccumulate simply from increased partitioning to lipophillic tissues in biota and possibly some hindrance of biotransformation. With regards to the modelled BAF value for isoheptyl fluorene, the only similar analogue (fluorene) has an experimental BCF of 1030 L/kg ww which is slightly higher than the predicted BCF using the mass-balance kinetic model (Table A5.6 in Appendix 5). However, there is some uncertainty surrounding the kinetic rate constants used to model BCFs and BAFs for these two compounds (e.g., the metabolic rate constants were either estimated from QSARs or based on analogue data) as well as the degree of trophic magnification within the foodweb used by the model), suggesting that the BAFs may be overestimated. However, given that the log K_{ow} of this compound is 7.4, the optimal range for high bioaccumulation from the diet and water coupled with a possible slow rate of metabolism and that a TMF for fluorene is

approximately one (Table A5.8 in Appendix 5), a high bioaccumulation potential may still be likely.

None of the modelled BCF values for representative PAHs were shown to meet the bioconcentration criterion (BCF ≥ 5000) as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000) (see Table A5.6 in Appendix 5). This is largely due to the lower contribution of chemical uptake from water from highly hydrophobic substances, but also because PAHs such as naphthalene and phenanthrene are metabolized by fish resulting in very low or nondetectable concentrations of the parent PAHs in fish tissues (Varanasi et al. 1989). However, measured BCFs in fish for phenanthrene exceed the bioaccumulation criterion (Table A5.5 in Appendix 5). For fluoranthene, Weinstein and Oris (1999) reported a BCF of 9054 L/kg ww in fathead minnows, Burkhard and Lukasewycz (2000) determined a BAF of 1550 L/kg ww in trout and De Maagd (1996) determined a BCF of 3388 L/kg ww in fathead minnows. As previously mentioned, the Weinstein and Oris (1999) and De Voogt et al. (1991), as well as the Peterson and Kristensen (1998) studies reporting high BCF values contain sufficient levels of uncertainty or the early life stage results cannot easily be interpreted versus other studies or regulatory criteria for bioaccumulation. The findings of these studies were thus considered equivocal and received a lower weighting for determining bioaccumulation potential according to criteria. The high laboratory BCFs are also not consistent with field measured BAFs in fish. Consequently there is greater evidence weight and consistency from kinetic data, modelled BCF and BAF values, laboratory and field evidence for vertebrates (i.e., fish) to suggest that vertebrates possess sufficient metabolic capacities and other elimination processes to mitigate body burdens of PAHs below levels considered by criteria to be high leels of bioaccumulation.

Empirical BCF data for invertebrates, namely molluscs (fluoranthene) have been shown to be relatively high. In the case of blue mussels, a 96-hour study with fluoranthene resulted in a BCF value of 5920 L/kg ww which exceeds the bioaccumulation criterion (Table A5.5 in Appendix 5). This indicates that there is significant potential for body burdens to reach toxic levels in these lower trophic level organisms as they lack the metabolic capability to eliminate PAHs in comparison to fish. Thus, high accumulation patterns are found in both the lab and field. There is also potential for these body burdens to exceed the internal narcotic thresholds, assuming PAH exposure is constant and continuous. However, the majority of BCF studies on PAHs have found that bioconcentration by invertebrates can occur quickly but that the majority of organisms also exhibit rapid depuration once the contaminant is removed. Therefore, exposure duration is critical to bioaccumulation and toxicity.

Field-based TMFs for PAHs were mostly < 1, with the exception of fluorene and acenaphthene which are approximately one (Table A5.8 in Appendix 5). It appears that biomagnification and trophic magnification are mitigated by a combination of metabolism, low dietary assimilation efficiency and growth dilution through the food-chain. Thus, the available evidence suggests that there is limited biomagnification and trophic magnification for PAHs.

As PAHs tend to accumulate in sediments, benthic organisms may be continuously exposed to the contaminants. Because invertebrates do not have the same metabolic competency as fish (Muijs and Jonker 2010; Stegeman and Teal 1973; Neff et al. 1976), the bioaccumulation potential in invertebrates is expected to be higher than in fish. While only BSAFs for fish were found for some PAHs and were below one, it is possible that BSAFs will be > 1 for invertebrates as they have lower metabolic competencies than fish. However, BSAFs will likely decrease beyond C_{22} due to reduced bioavailability of the higher boiling point fractions (Muijs and Jonker 2010).

Overall, there is consistent empirical and predicted evidence to suggest that one PAH representative structure (C_{20} cycloalkane diaromatic) meets the bioaccumulation criteria as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Proportion of Bioaccumulative Components in Gas Oils

There is a lack of detailed compositional information for these gas oils. As such, the proportion of bioaccumulative structures in these gas oils cannot be determined with certainty. However, it can be compared to the compositional analyses of diesel fuel from Canadian sources. This analysis, based on the empirical and predicted analysis of BCF and BAFs, indicates that the total potentially bioaccumulative fraction based on diesel ranges from 20–25% by weight (Yang 2001). The majority of this fraction is composed of dicycloalkanes and alkylated monoaromatics.

Based on the combined evidence of empirical and predicated analysis of BCF and BAFs, the gas oils assessed in this report may contain components that meet the bioaccumulation criteria defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

Information relevant to the toxicity of gas oils to various organisms is provided below. As well, PAHs are components of gas oils and have been considered in a previous risk assessment. PAHs are on the List of Toxic Substances under Schedule 1 of CEPA 1999 (Environment Canada 2010).

Evidence from field and laboratory studies using field samples indicates that biota are adversely affected at various Canadian sites contaminated by PAHs of different industrial origins (Canada 1994).

There are potential hazards associated with the metabolism of PAHs such as B[*a*]P. This process may create metabolites that are potent mutagens. Under laboratory conditions, neoplastic and genotoxic effects have been associated with exposure to PAHs for both terrestrial and aquatic organisms. In field studies, preliminary stages of chemically induced carcinogenesis have been shown (Canada 1994).

Aquatic Compartment

Shell (2011) provides a numerical score for acute and chronic aquatic toxicity indicating that 64741-82-8 is very toxic to aquatic life (Hazard Statement H400 under the Globally Harmonized System of Classification and Labelling of Chemicals [UNECE 2011] and a classification value of 1), and very toxic to aquatic life with long-lasting effects (Hazard Statement H410 and a classification value of 1). Under this schema, a classification value of 1 for acute aquatic toxicity means a median lethal concentration (LC_{50}) or median effect concentration (EC_{50}) ≤ 1 mg/L in either a 96-hour $L(E)C_{50}$ test for fish, 48-hour $L(E)D_{50}$ for invertebrates or 72- to 96-hour ErC_{50} for algae. For chronic toxicity to aquatic life, a classification value of 1 means that for substances that are non-rapidly biodegradable (assumed), a no-observed-effect concentration (NOEC) ≤ 0.1 mg/L or, if absent, an $L(E)C_{50}$ ≤ 1 mg/L.

However, no experimental data were available for the aquatic toxicity of these gas oils; therefore, data from similar diesel fuels and Fuel Oil No. 2, as well as modelled data were used to estimate the potential for aquatic toxicity.

CONCAWE developed an aquatic toxicity model specific for petroleum hydrocarbon mixtures called PETROTOX (2009). This model assumes chemical action via narcosis and therefore accounts for additive effects according to the toxic unit approach. It can model petroleum hydrocarbon toxicity for C_4–C_{41} compounds dissolved in the water fraction. Substances smaller than C_4 are considered too volatile 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 (LL_{50}) rather than a LC_{50} due to the insolubility of petroleum substances in water. The LL_{50} value is the amount of petroleum substance needed to generate a water-accommodated fraction (WAF) that is toxic to 50% of the test organisms. It is not a measure of the concentration of the petroleum components in the water-accommodated fraction.

The modelled ecotoxicological data in Table A5.9 (Appendix 5) with different aromatic to aliphatic ratios were restricted to marine organisms since the only significant route of transportation of these industry-restricted gas oils is by marine tanker. The data indicate that these gas oils have a high potential to cause harm to most aquatic organisms at relatively low concentrations (majority ≤ 1 mg/L). The likelihood of harm is largely related to the aromatic content, as the 80:20 (aromatic/aliphatic content) ratio used in modelling is more toxic to marine organisms than the 61:39 ratio or the 50:50 ratio.

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 these gas oils 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–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 A5.10 and A5.11 (Appendix 5).

Aquatic LC_{50} values for Fuel Oil No.2 and diesel fuel range from 0.9–23.7 mg/L. The modelled aquatic LL_{50}s from PETROTOX (0.1–9.8 mg/L) fall within this range, although the LL_{50} is not a direct measurement of the concentration of the dissolved fraction that would cause toxicity (Table A5.9 in Appendix 5). Therefore, the modelled data from PETROTOX are within the appropriate range of measured toxicity values for similar commercial products.

The LC_{50} from Fuel Oil No. 2 is 0.9 mg/L, based on exposure of mysid shrimp to the water-soluble fraction over 48 hours (Anderson et al. 1974). The aromatic content of Fuel Oil No. 2 is usually 25%, while the gas oil 64741-59-9 has a much higher aromatic content of 61–80% by volume. The lowest modelled data for the water-accommodated fractions of gas oil 64741-59-9 are 0.06–0.08 mg/L, based on acute exposures of a marine amphipod (*Rhepoxynius abronius*). Such a difference could be explained by the high proportion (up to 80%) of aromatics in this gas oil. The modelled ecotoxicological data in Table A5.9 (Appendix 5) indicate that this industry-restricted gas oil has the potential to cause harm to many marine organisms at relatively low concentrations (≤ 1 mg/L). Unfortunately, compositional data for 64741-82-8 were insufficient to run PETROTOX; however, statements from the European manufacturer confirm a range of toxicity values, generally ≤ 1 mg/L. Thus, the average of the modelled data for WAFs for CAS RN 64741-59-9 (0.07 mg/L) was used to represent the critical toxicity value (CTV) for these industry-restricted gas oils.

Terrestrial Compartment

The acute oral median lethal dose (LD_{50}) to rats was 3200 mg/kg-bw (API 1982, 1985a). As there were no inhalation studies for industry-restricted gas oils beyond acute durations, a read-across to other gas oils, including fuels, was considered. Acute inhalation toxicity in rats was 3350–5400 mg/m^3 air (API 1986a, b). At necropsy, the main effects observed were marked inflammation both of the respiratory tract and lungs (CONCAWE 1996). It is expected that wild animals would react in a similar manner if exposed to these levels of these substances; therefore, 3350 mg/m^3 will be used for the CTV for inhalation by non-human mammals.

Ecological Exposure Assessment

Estimations of releases of these gas oils were made using information on volumes transported by each mode identified in submissions under section 71 of CEPA 1999 (Environment Canada 2009). Estimations of losses to the sea were determined based on information from Canada's east coast developed by the Risk Management Research Institute (RMRI 2007) in addition to spill data fromEnvironment Canada's Spill Line database (Environment Canada 2011).

Aquatic Compartment

Release scenarios were developed for ship to water for loading only since it is likely the predominant source based on confidential information received in response to section 71 of CEPA 1999 (Environment Canada 2009). There were no other transportation methods or releases to water examined.

To determine the predicted environmental concentration (PEC) in water, the volume of water predicted to be in contact with spilled oil was provided by a report prepared by the Risk Management Research Institute (RMRI 2007). This work estimated the risk of oil spills in Hazard Zones around the southern coast of Newfoundland and Labrador based on the nature of the water (open or partially constricted), the type of vessels travelling through the zones, and the quantities of oil transported. The estimated volume of water in contact with spilled oil was dependent on the volume of oil spilled during the event and the Hazard Zone of the spill.

For the ship loading scenarios, the volume of water in contact with oil is from Hazard Zone 1, as this region includes loading operations at Whiffen Head and Come By Chance refinery in Newfoundland and Labrador (RMRI 2007). The area of a slick created within Hazard Zones around Newfoundland was estimated for specific volume ranges of oil using ocean spill dispersion models, and then the volume of contacted water was estimated by multiplying the area by 10 to represent the top 10 meters of water. This estimate assumes that all of the water is equally contacted by the petroleum substance spilled. This work was originally developed for crude oil, but it can be applied to gas oils as they have a similar density.

In the case of the loading of gas oils onto ships, an estimated 144 L (122 kg) of gas oil could be lost in an average event. This is approximately equivalent to 1 barrel (U.S.), and is therefore expected to be in contact with 40×10^{6} m^3 of water (Table A5.12 in Appendix 5). The resulting concentration in water would be 0.003 mg/L (i.e., 1.22×10^{8} mg in 4.0×10^{10} L), which is considered the PEC for ship loading.

Terrestrial Compartment

The quantities of these gas oils transported by truck were too minor to warrant an exposure assessment.

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine available scientific information and develop conclusions based on a weight-of-evidence approach as required under CEPA 1999. For each endpoint organism, an estimate of the potential to cause adverse effects, or predicted no-effect concentration (PNEC), was determined. The PNEC is the lowest CTV for the organism of interest divided by an appropriate assessment factor. An assessment factor of 100 was used to account for the extrapolation of modelled acute toxicity data to chronic effects in the field. Also, a PEC was determined. A risk quotient (RQ = PEC/PNEC; Table 3) was calculated for each endpoint

organism and is an important line of evidence in evaluating the potential risk to the environment. In the case of the loading of gas oils onto ships, the PEC for an average spill, as calculated above, is 0.003 mg/L; the average modelled value for WAF was used as the CTV..

Table 3. Risk quotient calculated for industry-restricted gas oil (CAS RNs 64741-59-9 and 64741-82-8).

Medium	Organism	PEC	CTV	Assessment factor	PNEC	Risk quotient
Marine water (ship loading)	*Rhepoxynius abronius*	0.003 mg/L	0.07 mg/L	100	0.0007 mg/L	4.3

To yield a risk quotient of 1, a marine spill during loading would need to be greater than 33 L given the scenario presented here. Only four marine spills recorded in Canada from 2000–2009 were of that volume or greater, therefore < 1 spill per year is expected to be potentially harmful.

This critical spill volume was calculated based on models developed by RMRI (2007) relating the volume spilled and concentration of petroleum substance in the water. These models take into consideration dispersion of the petroleum substance spilled and, therefore, the calculated spill volume relating to a risk quotient of 1 is not for the acute, initial exposure to the spilled material. It is recognized that local, acute effects may occur during the inital phase of a spill before significant dispersion occurs.

The physical-chemical properties of gas oils may increase the potential risk of gas oils to the aquatic environment. Light refined products, such as diesel fuel and Fuel Oil No. 2 (and these gas oils), are narrow-cut fractions that have low viscosity and spread rapidly into thin sheens. As low-viscosity, moderately persistent oils, light distillates tend to disperse readily into the water column by gentle wave action. Thus, they have the highest potential of any oil type for vertical mixing, which in turn causes a greater potential for dissolution to occur—from both surface sheens and droplets dispersed in the water column. The water-soluble fractions are dominated by two- and three-ring PAHs, which may affect aquatic life. Thus, spills of light distillates have the greatest potential to affect water-column resources (NRC 2003). A major difference between CAS RN 64741-59-9 and both Fuel Oil No. 2 and diesel fuel is that it has a higher aromatic content ranging from 61–80%, while Fuel Oil No. 2 has an aromatic content around 25% and diesel fuel can range up to 37%. This can have a major impact on the toxicity of this gas oil compared to finished, blended fuels as toxicity increases as the aromatic fraction increases (Table A2.1 in Appendix 2).

Based on results from AOPWIN (2008), all components of gas oils will degrade readily by interactions with hydroxyl radicals in air. Based on the primary and ultimate biodegradation modelling, the C_{15}–C_{20} two-ring cycloalkanes, C_{14}–C_{22} polycycloalkanes, C_{10}–C_{20} cycloalkane monoaromatics, C_{15} two-ring aromatics and C_{12}–C_{15} cycloalkane diaromatics in these gas oils meet the persistence criteria in water, soil and sediment

(half-lives in soil and water ≥ 182 days and half-life in sediment ≥ 365 days). The cycloalkanes represent a relatively small fraction (8–10%) of gas oils. There is no detailed information on the specific aromatic content of these gas oils; however, CAS RN 64741-59-9 may include up to 80% aromatics (by volume), which would include the persistent aromatics listed here. Thus, these gas oils are expected to contain an unknown proportion of components that meet the persistence criteria in soil, water and sediment as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Based on the combined evidence of empirical and predicted analysis of BCFs, BAFs, BMFs, TMFs and BSAFs, the gas oils assessed in this report may contain components (up to approximately 25% by weight) that meet the criteria for bioaccumulation as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000), but are not likely biomagnified in food webs. Both empirical and predicted BCF and predicted BAFs are ≥ 5000 for isoalkane, cycloalkane and some aromatic substances. There is consistent steady-state and kinetic evidence to suggest that these components do not metabolize very quickly and have sufficient dietary assimilation efficiency, that when tissue levels are compared with the bioavailable fraction in water, accumulation factors are expected to be high.

In general, fish can efficiently metabolize aromatic compounds. Of the aromatic representative structures of gas oils with high bioaccumulation potential, only a C_{20} cycloalkane diaromatic was bioaccumulative (i.e., BCF or BAF > 5000). This structure contains an isoalkyl functional group which may hinder biotransformation. There is some evidence that alkylation increases bioaccumulation of naphthalene (Neff et al. 1976, Lampi et al. 2010) but it is not known if this can be generalized to larger PAHs or if any potential increase in bioaccumulation due to alkylation will be sufficient to exceed the Canadian criteria.

Bioaccumulation of aromatic compounds might be lower in natural environments than what is observed in the laboratory. PAHs may sorb to organic material suspended in the water column (dissolved humic material) which decreases their overall bioavailability primarily due to an increase in size. This has been observed with fish (Weinstein and Oris 1999) and *Daphnia* (McCarthy et al. 1985).

In general, fish can efficiently metabolize aromatic compounds. However, there is evidence that fluoranthene is highly bioconcentrated in molluscs. There is potential for such bioaccumulative components to reach toxic levels in organisms if exposure is constant, continuous and of sufficient magnitude; however, this is unlikely in the water column following a spill scenario due to relatively rapid dispersal.

As shown in Table A5.13 (Appendix 5), some components may meet both the persistence and bioaccumulation criteria in the *Persistence and Bioaccumulation Regulations*. These include the C_{15} dicycloalkanes, C_{14} and C_{22} polycycloalkanes, and C_{15}–C_{20} cycloalkane monoaromatics.

With regard to invertebrates, fluoranthene, which has high bioaccumulation potenetial in molluscs, is also persistent in sediments which could lead to exposure of longer duration. Based on the Level III fugacity modelling of this substance (Table A5.1), fluoranthene is expected to partition to sediments when released to water where it might accumulate in benthic invertebrates species with low metabolic capacities. However, the proportion of fluoranthten in these gas oils is low. In addition, given that there are on average approximately 4 spills per year of diesel, light oil, and petroleum distillate between 2000 and 2009, of which only a fraction would be the two gas oils under assessment in this report, it is expected that spills of gas oils in water during loading are likely not harmful to aquatic organisms.

Based on the information presented in this screening assessment on the frequency and magnitude of spills, there is low risk of harm to organisms or the broader integrity of the environment from these substances. It is concluded that the industry-restricted gas oils (CAS RNs 64741-59-9 and 64741-82-8) do not meet the criteria under paragraph 64(*a*) or 64*(b*) of the *Canadian Environmental Protection Act, 1999* (CEPA 1999) as they are not entering the environment in a quantity or concentration or under conditions that 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.

Uncertainties in Evaluation of Ecological Risk

This analysis addresses uncertainty associated with each component of the current assessment, including but not limited to representative structures selection and quantification, exposure estimation, effects estimation, and risk characterization.

All modelling of the substances' physical-chemical properties, and persistence, bioaccumulation and toxicity characteristics is based on chemical structures. As these gas oils are complex UVCBs, they cannot be represented by a single, discrete chemical structure. The specific chemical composition of the substances falling under CAS RNs 64741-59-9 and 64741-82-8 are variable and not well defined. Gas oil streams under the same CAS RNs can vary significantly in the number, identity and proportion of components, depending on operating conditions, feedstocks and processing units. Therefore, for the purposes of modelling, a suite of representative structures that provide estimates for the entire range of components likely present was identified. Specifically, these structures were used to assess the fate and hazard properties of gas oils. Given that more than one representative structure may be used for the same carbon range and type of component, it is recognized that structure-related uncertainties exist for this substance. The physical-chemical properties of 24 representative structures were used to estimate the overall behaviour of these gas oils, in order to represent the expected range in physical-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.

Uncertainty arises from the variability of spill data. The available data on spills generally do not report values for each specific substance by CAS RN. For marine transportation,

Environment Canada reported spills data for substances similar to these gas oils, specifically fuel oils, gasoline, diesel fuel and jet fuel. Spill data specific to these industry-restricted gas oils are not available for each mode of transportation.

This assessment involves the prediction of effects on biota using measured inputs and modelled accumulation or exposures, which typically relies on modelled exposures for organisms at higher trophic levels. However, all models are simplifications of natural systems or processes, and therefore rely on a number of assumptions. These, in turn, create uncertainties in the outcomes.

The BAF model calculations were derived from a large database of measured BAF values from the Great Lakes for chemicals that are poorly metabolized (e.g., PCBs). With metabolic biotransformation, the BAF model predictions are in general agreement with measured BAFs in fish. Many petroleum hydrocarbons are readily metabolized, somewhat by invertebrates and at much higher levels in fish (Arnot and Gobas 2003; Arnot et al. 2008a, b). There is some uncertainty when estimating the biotransformation used by the model at the first trophic level. Thus, the BAF model predictions may be an overestimate in consideration of these factors.

The significance and impact of bioaccumulation is species-specific and is dependent on a range of factors such as species, size and the environmental conditions. At present, there are no field data on the study of bioaccumulation of gas oils as a class; therefore, predicting effects is based on modelling BAFs of representative structures based on laboratory-acquired partitioning data.

Potential to Cause Harm to Human Health

Exposure Assessment

The exposure characterization for industry-restricted petroleum substances focuses on fugitive releases. This includes evaporative emissions during the various modes of transportation of petroleum substances. The unintentional release (leaks or spills) data used in the ecological assessment are, for the purposes of assessing the potential to cause harm to human health, considered to be releases that occur on a non-routine or unpredictable basis in specific geographical locations. These unintentional releases typically do not contribute to the potential for exposure of the general population in Canada.

Due to the relatively low volatility of the industry-restricted gas oils (see Table 1), as well as relevant regulations that limit potential releases during the handling of petroleum substances (see Appendix 3), non-occupational exposure of the general population as a result of loading or unloading is not expected. Despite relatively low volatility, evaporative emissions of the industry-restricted gas oils during transit (i.e., during transport by ships between facilities), as well as during loading and unloading stops in

port, will enter ambient air. As such, inhalation is the primary route of potential exposure for the general population in the vicinity of such transporation corridors.

Inhalation

As monitoring data on gas oils in the environment are not available, gas oil vapour concentrations in ambient air were estimated using SCREEN3 (1996), a screening-level Gaussian air dispersion model based on the Industrial Source Complex (ISC) model (for assessing pollutant concentrations from various sources in an industry complex). The driver for air dispersion in the SCREEN3 model is wind. The maximum calculated exposure concentration is selected based on a built-in meteorological data matrix of different combinations of meteorological conditions, including wind speed, turbulence and humidity. This model directly predicts concentrations resulting from point, area and volume source releases. SCREEN3 gives the maximum concentrations of a chemical at chosen receptor heights and at various distances from a release source for a given population in the vicinity of the release source in the direction downwind from the prevalent wind one hour after a given release event. During a 24-hour period, for point emission sources, the maximum 1-hour exposure (as assessed by the ISC Version 3) is multiplied by a factor of 0.4 to account for variable wind directions. This gives an estimate of the air concentration over a 24-hour exposure (U.S. EPA 1992). Similarly, for exposure events happening over the span of a year, it can be expected that the direction of the prevalent winds will be more variable and not correlated with the wind direction for a single event. Thus, the maximum amortized exposure concentration for one year is determined by multiplying the maximum 1-hour exposure by a factor of 0.08. Such scaling factors are not used for non-point source emissions. However, to prevent overestimation of the exposures originating from area sources, a scaling factor of 0.2 was used to obtain the yearly amortized concentration from the value of the maximum 1-hour exposure concentration determined by SCREEN3. Detailed input parameters for SCREEN3 are listed in Table A6.1 (Appendix 6). It should be noted that the estimated exposure concentrations are considered to be conservative, as SCREEN3 is, by design, a conservative screening-level tool used as a rapid approach to estimate the air dispersion of various chemicals.

As a conservative estimate, the regular evaporative emissions determined for one day of the port stop process are assumed to originate from a defined area rather than a moving source (i.e., the 1-day exposure scenario used to represent all 7 days of the typical port stop process is the worst-case scenario, whereby the ship is in port and stationary); as such, actual levels are expected to be lower, considering that the release source is moving for a portion of the 7-day port stop process (i.e., when the ship is coming into and leaving port). Estimated regular evaporative emissions of industry-restricted gas oils to air during ship transit (including time during which the ship is in port) are approximately 1100 kg/year or 3.2 kg/day (Table A6.2 in Appendix 6). The emission rate (7.4×10^{-5} g/s·m^2) is derived based on the emission of 3.2 kg/day and the estimated emission area of 50 m × 10 m. This emission rate (7.4×10^{-5} g/s·m^2) is used in SCREEN3 for determining the concentration of the gas oil vapours in ambient air (SCREEN3 1996). Exposure to the evaporated gas oils will occur over a typical port stop of one week.

The estimated maximum concentration of ambient gas oil vapours during 24 hours is presented in Table A6.3 (Appendix 6). For a conservative estimate of exposure to the general population in the vicinity of these transportation corridors, the concentration at 1000 m was used for ambient air concentrations of gas oil vapours from evaporative emissions during the 7-day port stop process. The maximum concentration in ambient air at 1000 m was estimated to be 1.0 $\mu g/m^3$.

Due to the use of an evaporative emissions value from a point source rather than a moving vessel, the placement of the receptor at 1000 m from the release source, and the conservative nature of SCREEN3 modelling, the estimated exposure concentration to the general population is considered to be conservative.

Health Effects Assessment

Health effects of the two industry-restricted gas oils (CAS RNs 64741-59-9 and 64741-82-8) were assessed primarily using data specific to these two CAS RNs. However, given the limited number of studies available that specifically evaluate the health effects of the industry-restricted gas oil substances for certain endpoints and/or routes of exposure, additional gas oils in the PSSA that are similar from both a process and a physical-chemical perspective were also considered. Because both the industry-restricted and additional gas oil substances have similar physical-chemical properties, their toxicological properties are likely similar. The health effects data were therefore pooled and used to construct a toxicological profile to represent all gas oils. Accordingly, the health effects of gas oils are represented as a group, not by individual CAS RNs.

Appendix 7 contains a summary of the available health effects information for CAS RNs 64741-59-9 and 64741-82-8 in laboratory animals. A summary of key studies is presented below. The health effects literature has referred to different stream samples of CAS RN 64741-59-9 as API 83-07, API 83-08, MD-7 light cycle oil (LCO), Mobil LCO and light catalytic cracked distillate (LCCD). Different stream samples of CAS RN 64741-82-8 have been referred to as Mobil coker light gas oil (CLGO), DGMK No. 8 and light thermal cracked distillate.

Gas oils have low acute toxicity. API 83-07 exhibited an oral LD_{50} of 3200 mg/kg-bw in female rats and an inhalation LC_{50} of 3350 mg/m^3 in male rats (API 1982, 1985a, 1986a). API 83-07 and 83-08 exhibited a dermal LD_{50} of > 2000 mg/kg-bw in rabbits (API 1982, 1985a,b). Slight to severe skin irritation was observed in all cases of acute dermal exposure. Acute studies were not identified for CAS RN 64741-82-8.

In short-term and subchronic dermal studies of CAS RNs 64741-59-9 and 64741-82-8, moderate to severe skin irritation and inflammation were observed in laboratory animals at all doses tested. In a short-term study that exposed pregnant Sprague-Dawley rats to Mobil LCO from gestation days 0–19 or 6–15, a lowest-observed-adverse-effect level (LOAEL) of 50 mg/kg-bw per day was established based on decreased maternal body weight gain and body weight (likely due to reduced feed consumption), as well as skin irritation

(Mobil 1988a). In a subchronic study that exposed male and female Sprague-Dawley rats to CAS RN 64741-82-8, 5 days/week for 13 weeks, a LOAEL of 30 mg/kg-bw per day was established based on increased lymphocytes in females and a 10% decrease in thymus weight in males (Mobil 1991). Four further short-term and subchronic dermal studies were identified for CAS RN 64741-59-9. These studies found decreased thymus weights and increased liver weights in rats, as well as varying degrees of skin irritation in rats and rabbits (API 1985c,d; Mobil 1985; Feuston et al. 1994). Two further short-term and subchronic dermal studies were reported for CAS RN 64741-82-8. Light thermal cracked distillate was applied to the skin of pregnant Sprague-Dawley rats at doses of 15, 60, 250 or 500 mg/kg-bw per day on gestation days 0–19. Maternal effects such as moderate to severe skin irritation, erythema, flaking, scabbing and thickening of the skin were observed at an unspecified dose (Mobil 1988b). In the second study, doses of 30, 125, 500 or 2000 mg/kg-bw per day were applied to male and female Sprague-Dawley rats, 5 days/week for 13 weeks. Increased relative liver weights were observed at 125 mg/kg-bw per day (Feuston et al. 1994).

Repeated-exposure studies assessing the health effects due to inhalation of the industry-restricted gas oils were not identified. Thus, critical effect levels were derived from health effects studies on related gas oil substances (as mentioned above). In a short-term (4 week) repeated-exposure study of male and female Sprague-Dawley rats exposed to CAS RN 64742-80-9 (hydrodesulfurized middle distillates), 25 mg/m^3 was identified as a lowest-observed-adverse-effect concentration (LOAEC) based on microscopic changes in nasal tissue and subacute inflammation of the respiratory mucosa (API 1986c). An increased leukocyte count (~30%) was also noted, but no corresponding macroscopic changes were observed at necropsy. In a repeated-exposure subchronic inhalation study of another gas oil (CAS RN 68334-30-5; diesel fuel), 250 mg/m^3 was identified as a LOAEC based on decreased body weight and increased response time in an acoustic startle reflex assay at all exposure levels tested in both male and female Sprague-Dawley rats exposed 2 days/week for 13 weeks; however, no corresponding histological changes in the nervous system were noted (Lock et al. 1984). Therefore, 25 and 250 mg/m^3 were considered the short-term and subchronic inhalation critical effect levels, respectively, for the industry-restricted gas oils.

CAS RNs 64741-59-9 and 64741-82-8 have been evaluated in a limited number of *in vitro* and *in vivo* genotoxicity assays. *In vivo,* API 83-07 and API 83-08 did not affect the mitotic index of rat bone marrow cells in two cytogenetic assays (API 1985e, 1986d), but API 83-07 was positive for sister chromatid exchange in mice (API 1989a). *In vivo* studies for CAS RN 64741-82-8 were not identified. *In vitro,* MD-7 LCO exhibited a mutagenicity index of 14 in a modified Ames assay and was found to contain 8.7% polycyclic aromatic compounds (Nessel et al. 1998). Positive results for both API 83-07 (with metabolic activation) and API 83-08 (with and without metabolic activation) were also observed in the mouse lymphoma assay (API 1985f,g). Equivocal results for one sister chromatid exchange assay were observed for API 83-07, both with and without metabolic activation (API 1988). CAS RN 64741-82-8 exhibited positive results in a modified Ames assay in two different studies (Blackburn et al. 1984, 1986; Conaway et al. 1984; DGMK 1991).

Thus, the industry-restricted gas oils demonstrate genotoxic potential, as evidenced by positive *in vivo* and *in vitro* results for the sister chromatid exchange, mouse lymphoma and Ames assays. However, given the limited number of experiments conducted for the two industry-restricted CAS RNs, other PSSA high priority gas oils were also considered. The potential genotoxicity of the two industry-restricted gas oils is supported by the overall genotoxicity database for additional gas oil substances, although it is recognized that the results were variable depending on the substance tested and the assay used. Overall, gas oils, including CAS RNs 64741-59-9 and 64741-82-8, demonstrate genotoxic potential.

Regarding the carcinogenic potential of the industry-restricted gas oils, CAS RNs 64741-59-9 and 64741-82-8 were classified as Category 2 carcinogens (R45: *may cause cancer*) by the European Commission (ESIS 2008). The United Nations' Globally Harmonized System of Classification and Labelling of Chemicals has classified these substances as Category 1B carcinogens (H350: *may cause cancer*) (European Commission 2008a). The International Agency for Research on Cancer (IARC) has also indicated that CAS RN 64741-59-9 exhibits *sufficient evidence in experimental animals* for carcinogenicity (consistent with a Group 2A *probably carcinogenic to humans* classification). The data supporting this conclusion were considered when they classified "occupational exposures in petroleum refining" as Group 2A (*probably carcinogenic to humans*), although CAS RN 64741-59-9 was not directly assigned to an IARC carcinogen group *per se* (IARC 1989a). Other gas oils have been classified by IARC as Group 3 carcinogens (*not classifiable as to their carcinogenicity to humans*) (IARC 1989b,c).[4]

The dermal carcinogenic potential of CAS RN 64741-59-9 has been investigated in multiple skin painting studies in mice. A statistically significant increase in the number of mice with skin tumours occurred after mice were chronically exposed to MD-7 LCO at 343 mg/kg-bw per day, the lowest test dose applied (Nessel et al. 1998). Tumour types and relative incidences were consistent across different studies, with squamous cell carcinomas exhibiting the highest incidence, followed by fibrosarcomas and papillomas (Skisak et al. 1994; Broddle et al. 1996; Nessel et al. 1998). One study investigated the tumour initiating and promoting activity of LCCD (Skisak et al. 1994). Skin tumours formed in 93% of mice when LCCD was used as a tumour growth promoter, but only 30% of mice developed tumours when it was used as a tumour initiator. Together, the results indicate that CAS RN 64741-59-9 may exhibit significant tumour promoting and carcinogenic activity when applied chronically to the skin of mice.

The dermal carcinogenic potential of CAS RN 64741-82-8 was assessed as a test substance blend with three other gas oil substances. Mice were dermally exposed to 1389 mg/kg-bw of the blended substance twice per week for 80 weeks. At 80 weeks, 98% of exposed mice had developed skin tumours (ARCO 1980a,b, 1981). It is difficult to ascribe a carcinogenic effect to CAS RN 64741-82-8 based on this study, however, given that the substance was administered in combination with three other substances.

[4] This category is used most commonly for agents, mixtures and exposure circumstances for which the evidence of carcinogenicity is inadequate in humans and inadequate or limited in experimental animals.

Regarding the tumourigenicity of gas oils, it is recognized that these substances may contain appreciable concentrations of components that are tumourigenic, such as PAHs, and the quantity of this fraction can vary depending on the nature and amount of diluent fractions and whether the residue component is cracked or uncracked. The Government of Canada has previously completed a human health risk assessment of five PAHs, including a critical review of relevant data, under the Priority Substances Program. Based primarily on the results of carcinogenicity bioassays in animal models, these PAHs were classified as *probably carcinogenic to humans*: substances for which there is believed to be some chance of adverse effects at any level of exposure (Canada 1994). Due to the lack of exposure to gas oils, evaluating the contribution of gas oil components to carcinogenic activity is beyond the scope of the current assessment.

The potential for CAS RNs 64741-59-9 and 64741-82-8 to affect reproduction and development has also been evaluated. The only reproductive or developmental LOAELs available for any gas oil substance were identified for CAS RN 64741-59-9 and were observed only at the highest dose tested. Mobil LCO exhibited a reproductive LOAEL of 1000 mg/kg-bw per day based on an increased incidence of resorptions after the substance was applied dermally to rats on gestation days 6–15 (Feuston et al. 1994). In a similar study, a LOAEL of 1000 mg/kg-bw per day was established for developmental toxicity based on statistically significant decreased fetal body weights after pregnant rats were dermally exposed to the substance on gestation days 0–6 and 6–15 (fetal body weights also trended lower in the group exposed to 500 mg/kg-bw per day on gestation days 0–19) (Mobil 1988a). Three studies assessing CAS RN 64741-82-8 found no developmental or reproductive effects when it was tested dermally in rats. Doses ranged from 15–2000 mg/kg-bw per day (Mobil 1988b, 1991; Feuston et al. 1994). All studies identified for other PSSA high priority gas oils administered dermally or via inhalation were noted to have negative results at all doses/concentrations tested. The available data indicate that, when applied dermally or via inhalation to laboratory animals during gestation, the industry-restricted gas oils do not exhibit significant reproductive or developmental toxicity.

No human epidemiological literature specific to the industry-restricted gas oils was identified. However, examination of studies that evaluated other gas oils revealed a case report involving repeated dermal exposure to diesel oil, resulting in adverse health effects, including renal failure (Crisp et al. 1979). Additionally, a case-control study of male cancer patients revealed a correlation between prostate cancer and occupational exposures to diesel fuels; however, there was no evidence for a positive dose-response relationship (Siemiatycki et al. 1987). Due to confounding variables and limited data, the evidence gathered from these studies is considered to be inadequate for a conclusion to be drawn on the effects of human exposure to gas oils.

Characterization of Risk to Human Health

Industry-restricted gas oils were identified as high priorities for action during categorization of the DSL because they were determined to present greatest potential for exposure of individuals in Canada, and were considered to present a high hazard to human health. A critical effect for the initial categorization of industry-restricted gas oil substances was carcinogenicity, based primarily on classifications by international agencies. These substances are classified as Category 2 carcinogens by the European Commission (ESIS 2008), Category 1B carcinogens using the Globally Harmonized System (European Commission 2008a) and Group 2A or 3 carcinogens by IARC (IARC 1989a,b,c). Several cancer studies conducted in laboratory animals reported the development of skin tumours following repeated dermal application of CAS RN 64741-59-9 (Skisak et al. 1994; Broddle et al. 1996; Nessel et al. 1998). Gas oils demonstrated genotoxicity in *in vivo* and *in vitro* assays. There are no carcinogenicity studies by the inhalation route to inform the carcinogenic potential of these substances in the general population following inhalation exposure.

The long-term health effects of the gas oils have primarily been examined through the dermal route of exposure; this is likely due in part to their relatively low volatility (Table 1). The rodent health effects studies from which the short-term and subchronic LOAECs were selected (as representative data for the industry-restricted gas oils) both used artificial methods (atomizer and heat) to generate aerosols and increase the concentrations of the substances in ambient air, thus underscoring the low volatility of gas oil substances in general and indicating that under normal conditions, the volatilization of the industry-restricted gas oils would be minimal (i.e., would not lead to significant vapour concentrations in ambient air).

Given that the potential for general population exposure to the industry-restricted gas oils results primarily from inhalation of ambient air containing gas oil vapours due to evaporative emissions during transportation and that the estimate of maximum air concentration (1.0 $\mu g/m^3$) is considered to be low, the risk to human health is likewise considered to be low. The ambient air concentration estimate is very conservative and highlighted by the assumption of total daily evaporative emissions occurring within a defined geographic area from a stationary point source (under normal operating conditions, evaporative emissions occur predominantly from a moving source; thus, the releases are diluted across a large geographic area).

General population exposure to industry-restricted gas oils via the dermal and oral routes is not expected; therefore, risk to human health from these routes of exposure is not expected.

No data were available that were specific to the industry-restricted gas oils with respect to non-cancer effects (identified in laboratory animals) following inhalation exposures. Therefore, the lowest concentrations causing health effects due to inhalation, identified from the pooled toxicological dataset for gas oil substances, were used as representative data for CAS RNs 64741-59-9 and 64741-82-8. The short-term LOAEC identified from

the pooled data on gas oil substances was 25 mg/m^3, based on inflammation of the respiratory mucosa in Sprague-Dawley rats following 4 weeks of repeated daily exposure to CAS RN 64742-80-9. The subchronic LOAEC identified was 250 mg/m^3, based on decreased rat body weights and increased response time in the acoustic startle reflex assay following 13 weeks of exposure to CAS RN 68334-30-5. Comparison of these non-cancer effect levels for inhalation exposure in rodents with the estimated maximum ambient air concentration of 1.0 µg/m^3 (based on the vapour concentration in air at 1000 m from a stationary release source) results in MOEs of 25 000 and 250 000 for short-term and subchronic effects, respectively. These margins are considered adequate to address uncertainties in the exposure and cancer and non-cancer health effects databases, especially in light of the highly conservative nature of the maximum air concentration estimate and the use of the lowest critical effect levels from the pooled toxicological dataset for gas oil substances.

Uncertainties in Evaluation of Human Health Risk

The PSSA screening assessments evaluate substances that are UVCBs composed of a number of substances in various proportions due to the source of the crude oil or bitumen and its subsequent processing. Monitoring information or provincial and territorial release limits from petroleum facilities target broad releases, such as oils and grease to water or total volatile organic compounds to air. These release categories are too broad to allow specific UVCB substances to be identified as the source. 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.

There is uncertainty regarding the magnitude of the conservatism built into the estimation of human exposure because, in the absence of ambient air monitoring data for gas oils, SCREEN3 modelling was used to profile gas oil vapour dispersion. Assumptions made in SCREEN3 (see Tables A6.1 and A6.2 in Appendix 6) also contribute uncertainty.

Uncertainty also exists in the equations used for estimating evaporative emissions. It is noted that transit evaporative emissions can vary with the tightness of transport vessels, valve settings, loading modes at terminals (e.g., submerge, splash or bottom) and use of a vapour balance system. The estimation of evaporative emissions does not account for these variables.

The specific chemical compositions of the streams falling under CAS RNs 64741-59-9 and 64741-82-8 are not well defined given that gas oils are UVCBs. Gas oil streams under the same CAS RN can vary significantly in the number, identity and proportions of components, depending on feedstocks and operating conditions of processing units. Consequently, the toxicological dataset reflects this variability. For this reason, there is some uncertainty in the characterization of risk to human health given that health effects data derived from studies of a particular stream may not be entirely representative of the spectrum of streams falling under the same CAS RN. More research by the scientific community and/or the petroleum sector to elucidate the exact compositions of petroleum

substances would support more robust characterization of the potential health risks associated with potential exposure to these substances.

Uncertainty in the evaluation of risk also exists due to the fact that studies assessing repeated oral and inhalation exposures to CAS RNs 64741-59-9 and 64741-82-8 were generally not available, and studies assessing other gas oil substances were occasionally used for the purpose of the health effects assessment. As such, to derive margins of exposure for inhalation exposure to these substances, representative data from other gas oils were used, which introduced additional uncertainty. However, in each case where appropriate, conservative assumptions were made regarding exposure and health effects.

A full mode of action analysis regarding tumourigenesis was not conducted for this screening assessment of gas oils. Inherent differences of sensitivity between laboratory animals and humans were also not considered.

Conclusion

Based on a comparison of levels expected to cause harm to organisms with estimated exposure levels, the gas oils identified in this report have the potential to harm aquatic life in the relatively confined waters around a loading wharf. However, given the low frequency of gas oil spills to marine water during ship loading (on average <1 per year), spills of these industry-restricted gas oile are not expected to result in harm to the environment.
Based on the information presented in this screening assessment on the frequency and magnitude of spills, there is low risk of harm to organisms or the broader integrity of the environment from these substances. It is concluded that the industry-restricted gas oils (CAS RN 64741-59-9 and 64741-82-8) do not meet the criteria under paragraph 64(a) or 64(b) of the *Canadian Environmental Protection Act, 1999* (CEPA 1999) as they are 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.

Based on adequate margins of exposure between critical effect levels and upper-bounding estimates of general population exposure, it is concluded that the industry-restricted gas oils (CAS RNs 64741-59-9 and 64741-82-8) do not meet the criteria under paragraph 64(c) of CEPA 1999 as they are not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

It is therefore concluded that the industry-restricted gas oils (CAS RNs 64741-59-9 and 64741-82-8) do not meet any of the criteria set out in section 64 of CEPA 1999.

References

[AEROWIN] Aerosols for Microsoft Windows [Estimation Model]. 2008. Version 1.92a. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Anderson JW, Neff JM, Cox BA, Tatem HE, Hightower GM. 1974. Characteristics of dispersions and water-soluble extracts of crude and refined oils and their toxicity to estuarine crustaceans and fish. Mar Biol 27:75–88.

[AOPWIN] Atmospheric Oxidation Program for Microsoft Windows [Estimation Model]. 2008. Version 1.92a. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[API] American Petroleum Institute. 1978. Mutagenicity evaluation of diesel fuel. Washington (DC): API. API Medical Research Publication No.: 26-60102. [cited in API 2003b].

[API] American Petroleum Institute. 1982. Acute oral toxicity study in rats. Acute dermal study in rabbits. Primary dermal irritation study in rabbits. Primary eye irritation study in rabbits. Dermal sensitization study in guinea pigs. API 83-07, light catalytically cracked distillate (CAS 64741-59-9). Washington (DC): API. API Report No.: 33-30162. Washington (DC): American Petroleum Institute. [cited in API 2003a].

[API] American Petroleum Institute. 1985a. Acute oral toxicity study in rats. Acute dermal toxicity study in rabbits. Primary dermal irritation study in rabbits. Primary eye irritation study in rabbits. Dermal sensitization study in guinea pigs. API 83-07, light catalytic cracked distillate, CAS No. 64741-59-9. Study conducted by Hazleton Laboratories America, Inc. Washington (DC): API. API Report No.: 33-30162. [cited in CONCAWE 1996; API 2003a].

[API] American Petroleum Institute. 1985b. Acute oral toxicity study in rats. Acute dermal toxicity study in rabbits. Primary dermal irritation study in rabbits. Primary eye irritation study in rabbits. Dermal sensitization study in guinea pigs. API 83-08, light catalytic cracked distillate, CAS No. 64741-59-9. Study conducted by Hazleton Laboratories America, Inc. Washington (DC): API. API Report No.: 32-32859. [cited in CONCAWE 1996; API 2003a].

[API] American Petroleum Institute. 1985c. 28-day dermal toxicity study in the rabbit. API 83-07 light catalytic cracked distillate (CAS 64741-59-9). Washington (DC): API. API Report No.: 32-32751. [cited in API 2003a].

[API] American Petroleum Institute. 1985d. 28-day dermal toxicity study in the rabbit. API 83-08, light catalytic cracked distillate (CAS 64741-59-9). Washington (DC): API. API Report No.: 32-32753. [cited in API 2003a].

[API] American Petroleum Institute. 1985e. Activity of API 83-08 in the acute *in vivo* cytogenetic assay in male and female rats, TEM CAS No. 51-18-3. Washington (DC): API. API Report No.: 33-30493. [cited in API 2003a].

[API] American Petroleum Institute. 1985f. Mutagenicity evaluation of API 83-07 in the mouse lymphoma forward mutation assay. Washington (DC): API. API Medicine and Biological Science Department Report No.: 32-32167. [cited in API 2003a].

[API] American Petroleum Institute. 1985g. L5158Y TK+/− mouse lymphoma mutagenesis assay of API 83-08. Washington (DC): API. API Medicine and Biological Science Department Report No.: 32-31709. [cited in API 2003a].

[API] American Petroleum Institute. 1986a. Acute inhalation toxicity evaluation in rats. API 83-07, light catalytic cracked distillate, CAS No. 64741-59-9. Study conducted by Hazleton Laboratories America, Inc. Washington (DC): API. API Report No.: 33-30549. [cited in CONCAWE 1996; API 2003a].

[API] American Petroleum Institute. 1986b. Acute inhalation toxicity evaluation in rats. API 83-08, light catalytic cracked distillate, CAS No. 64741-59-9. Study conducted by Hazleton Laboratories America, Inc., Report No. 33-30444. Washington (DC): American Petroleum Institute. [cited in CONCAWE 1996; API 2003a].

[API] American Petroleum Institute. 1986c. Four week subchronic inhalation toxicity study in rats. Final report. API 81-07 hydrodesulfurized kerosene (petroleum) (CAS 64742-81-0); API 81-09 hydrodesulfurized middle distillate (petroleum) (CAS 64742-80-9); API 81-10 hydrodesulfurized middle distillate (petroleum) (CAS 64742-80-9). Washington (DC): API. API Health and Environmental Sciences Department Report No.: 33-32724. [cited in API 2003a].

[API] American Petroleum Institute. 1986d. Mutagenic evaluation in the rat bone marrow cytogenetic assay. API 83-07 light catalytic cracked distillate (CAS 64741-59-9). Washington (DC): API. API Health and Environmental Sciences Department Report No.: 33-30929. [cited in API 2003a].

[API] American Petroleum Institute. 1987. Comprehensive analytical analysis of API generic refinery streams. Washington (DC): American Petroleum Institute. [cited in CONCAWE 1996].

[API] American Petroleum Institute. 1988. Sister chromatid exchange assay in Chinese hamster ovary (CHO) cells with API 83-07: light catalytic cracked distillate. Washington (DC): API. API Health and Environmental Sciences Department Report No.: 35-32432. [cited in API 2003a].

[API] American Petroleum Institute. 1989a. *In vivo* sister chromatid exchange assay with API 83-07 (light catalytic cracked distillate). Washington (DC): API. API Report No.: 36-31429. [cited in API 2003a].

[API] American Petroleum Institute. 1989b. Twenty-four month dermal carcinogenesis/chronic toxicity screening bioassay of refinery streams in C3H/HeJ mice (AP-190R). Study conducted by Primate Research Institute, New Mexico State University, Las Cruces, NM. Washington (DC): API. API Report No.: 36-33220.

[API] American Petroleum Institute. 2003a. High production volume (HPV) chemical challenge program. Robust summary of information on gas oils. Washington (DC): API. 65 p. Available from: www.epa.gov/hpv/pubs/summaries/gasoilct/c14835rsa.pdf

[API] American Petroleum Institute. 2003b. High production volume (HPV) chemical challenge program. Robust summary of information on distillate fuels. Washington (DC): API. Available from: www.epa.gov/hpv/pubs/summaries/gasoilct/c14835rsb.pdf

[ARCO] Atlantic Richfield Company. 1980a. Letter from Atlantic Richfield Company to US Environmental Protection Agency regarding information on Wellaid PG-100 with attachments. La Palma (CA): ARCO. NTIS New Document ID No. 88-8000327; NTIS/OTS0200616.

[ARCO] Atlantic Richfield Company. 1980b. Letter from Atlantic Richfield Company to US Environmental Protection Agency regarding information on the 37th week of the 80-week mouse painting projected study on ARCO LB-7979 and Provalent 4A. La Palma (CA): ARCO. NTIS New Document ID No. 86-8000075; NTIS/OTS0200616.

[ARCO] Atlantic Richfield Company. 1981. The carcinogenicity of two petroleum samples with cover letter dated 040181. La Palma (CA): ARCO. NTIS New Document ID No. 88-8100210; NTIS/OTS0200616.

Arnot JA. 2005. Bioconcentration factor and bioaccumulation factor assessments for organic chemicals on the Canadian domestic substances list: Task 1: Supplementation of Environment Canada's BCF database. Report to Environment Canada, New Substances Branch. March

Arnot JA. 2006. Bioconcentration factor and bioaccumulation factor assessments for organic chemicals on the Canadian domestic substances list: Database update. Report to Environment Canada, New Substances Branch. March.

Arnot JA, Gobas FA. 2003. A generic QSAR for assessing the bioaccumulation potential of organic chemicals in aquatic food webs. QSAR Comb Sci [Internet]. [restricted access]. [cited 2007 Mar 15]; 22(3):337–345. Available from: www3.interscience.wiley.com/journal/104557877/home

Arnot J, Gobas F. 2004. A food web bioaccumulation model for organic chemicals in aquatic ecosystems. Environ Toxicol Chem 23:2343–2355.

Arnot JA, Gobas FAPC. 2006. A review of bioconcentration factor (BCF) and bioaccumulation factor (BAF) assessments for organic chemicals in aquatic organisms. Environ Rev 14(4):257–298.

Arnot JA, Mackay D, Bonnell M. 2008a. Estimating metabolic biotransformation rates in fish from laboratory data. Environ Toxicol Chem 27(2):341–351.

Arnot JA, Mackay D, Parkerton TF, Bonnell M. 2008b. A database of fish biotransformation rates for organic chemicals. Environ Toxicol Chem 27(11):2263–2270.

Arthurs P, Stiver WH, Zytner RG. 1995. Passive volatilization of gasoline from soil. J Soil Contam. 4: 1-13.

[ATSDR] Agency for Toxic Substances and Disease Registry. 1995. Toxicological profile for fuel oils. Atlanta (GA): U.S. Department of Health and Human Services, Public Health Service. [cited 2009 Aug 1]. Available from: www.atsdr.cdc.gov/toxprofiles/tp75.pdf

Banerjee S. 1984. Solubility of organic mixtures in water. Environ Sci Technol 18:587–591.

Barron MG. 1990. Bioconcentration. Environ Sci Technol 24:1612–1618.

Beliles RP, Mecler FJ. 1983. Inhalation teratology of jet fuel A, fuel oil and petroleum naphtha in rats. In: MacFarland HN, editor. Proceedings of the symposium on the toxicology of petroleum hydrocarbons (May 1982). Washington (DC): American Petroleum Institute. [cited in ATSDR 1995].

[BioHCWin] Biodegradation Prediction of Petroleum Hydrocarbons, EPI Suite. 2008. Version 1.01a. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[BIOWIN]. Biodegradation Estimation Program for Windows. 2009. Version 4.10. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Blackburn GR, Deitch RA, Schreiner CA, Mehlman MA, Mackerer CR. 1984. Estimation of the dermal carcinogenic activity of petroleum fractions using a modified Ames assay. Cell Biol Toxicol 1:67–80.

Blackburn GR, Deitch RA, Schreiner CA, Mackerer CR. 1986. Predicting carcinogenicity of petroleum distillation fractions using a modified *Salmonella* mutagenicity assay. Cell Biol Toxicol 2:63–84.

Boethling RS, Howard PH, Beauman JA, Larosche ME. 1995. Factors for intermedia extrapolations in biodegradability assessment. Chemosphere 30(4):741–752.

Broddle WD, Dennis MW, Kitchen DN, Vernot EH. 1996. Chronic dermal studies of petroleum streams in mice. Fundam Appl Toxicol 30:47–54.

Brost EJ, DeVaull GE. 2000. Non-aqueous phase liquid (NAPL) mobility limits in soil. API Soil and Groundwater Research Bulletin No. 9. Washington (DC): American Petroleum Institute (API).

Bruner KA, Fisher SW, Landrum PF. 1994. The role of the zebra mussel, *Dreissena polymorpha*, in contaminant cycling: I. The effect of body size and lipid content on the bioconcentration of PCBs and PAHs. J Great Lakes Res 10(4):725–734.

Burkhard L, Lukasewycz M. 2000. Some bioaccumulation factors and biota–sediment accumulation factors for polycyclic aromatic hydrocarbons in lake trout. Environ Toxicol Chem 19(5):1427–1429.

Canada. 1994. Polycyclic aromatic hydrocarbons [Internet]. Ottawa (ON): Environment Canada; Health Canada. (Priority substances list assessment report). Available from: www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/psl1-lsp1/hydrocarb_aromat_polycycl/hydrocarbons-hydrocarbures-eng.pdf

Canada. 1999. *Canadian Environmental Protection Act, 1999*. S.C., 1999, c. 33. Canada Gazette, Part III, vol. 22, no. 3. Available from: www.gazette.gc.ca/archives/p3/1999/g3-02203.pdf

Canada. 2000. *Canadian Environmental Protection Act, 1999: Persistence and Bioaccumulation Regulations*, P.C. 2000-348, 23 March, 2000, SOR/2000-107, Canada Gazette. Part II, vol. 134, no. 7, p. 607−612. Available from: www.gazette.gc.ca/archives/p2/2000/2000-03-29/pdf/g2-13407.pdf

Canada. 2001. *Canada Shipping Act, 2001*. Canada Gazette, Part III, vol. 24, no. 4, chapter 26. Available from: www.gazette.gc.ca/archives/p3/2001/g3-02404.pdf

Canada. 2010. *Petroleum Refinery Liquid Effluent Regulations* (C.R.C., c. 828) to the *Fisheries Act*. [cited 2010 Feb 19]. Available from: http://laws.justice.gc.ca/eng/C.R.C.-c.828/index.html

[CanLII] Canadian Legal Information Institute [database on the Internet]. 2001– . Ottawa (ON): CanLII. [cited 2009]. Available from: www.canlii.org/en/index.php

Carlson RM, Oyler AR, Gerhart EH, Caple R, Welch KJ, Kopperman HL, Bodenner D, Swanson D. 1979. Implications to the aquatic environment of polynuclear aromatic hydrocarbons liberated from northern great plains coal. U.S. Environmental Protection Agency Environmental Research Laboratory (EPA 600/3-79-093).

[CATABOL] Probabilistic assessment of biodegradability and metabolic pathways [Computer Model]. c2004-2008. Version 5.10.3. Bourgas (BG): Bourgas Prof. Assen Zlatarov University, Laboratory of Mathematical Chemistry. Available from: http://oasis-lmc.org/?section= software&swid=1

[CITI] Chemicals Inspection and Testing Institute. 1992. Bioaccumulation and Biodegradation Data on Existing Chemicals Based on the CSCL Japan. Tokyo, Japan.

Coast Guard. 1985. Chemical Hazard Response Information System (CHRIS): Hazard assessment handbook. Washington (DC): U.S. Department of Transportation, U.S. Coast Guard. Commandant Instruction M.16465.12A.

Colombo J, Cappelletti N, Migoya M, Speranza E. 2007. Bioaccumulation of anthropogenic contaminants by detritivorous fish in the Río de la Plata estuary: 1—Aliphatic hydrocarbons. Chemosphere 68:2128–2135.

Conaway CC, Schreiner CA, Cragg ST. 1984. Mutagenicity evaluation of petroleum hydrocarbons. In: MacFarland HN, MacGregor JA, Call RW, Lane ML, editors. Advances in modern environmental

toxicology, vol. VI. Applied toxicology of petroleum hydrocarbons. Princeton (NJ): Princeton Scientific Publishers. p. 89–107. [cited in IARC 1989a].

[CONCAWE] CONservation of Clean Air and Water in Europe. 1996. Gas oils (diesel fuels/heating oils). Prepared by CONCAWE's Petroleum Products and Health Management Groups. Brussels (BE): CONCAWE. Product Dossier No. 95/107. 66 p.

Cravedi J, Tulliez J. 1981. Distribution and elimination routes of a naphthenic hydrocarbon (dodecylcyclohexane) in rainbow trout *(Salmo gairdneri)*. Bull Environ Contam Toxicol 26:337–344.

Cravedi J, Tulliez J. 1983. Hydrocarbon disposition, lipid content, and fatty acid composition in trout after long-term dietary exposure to *n*-alkanes. Environ Res 32(2):398–413.

Crisp AJ, Bhalla AK, Hoffbrand BI. 1979. Acute tubular necrosis after exposure to diesel oil. Br Med J 2:177.

Curry P, Kramer G, Newhook R, Sitwell J, Somers D, Tracy B, Oostdam JV. 1993. Reference values for Canadian populations. Prepared by the Environmental Health Directorate Working Group on Reference Values. Ottawa (ON): Health Canada. [update of 1988 version].

De Maagd PGJ. 1996. Polycyclic aromatic hydrocarbons: fate and effects in the aquatic environment. Ph.D. Thesis. Utrecht University. Utrecht (NL) [cited in European Commission 2008b].

De Voogt P, van Hattum B, Leonards P, Klamer JC, Govers H. 1991. Bioconcentration of polycyclic heteroaromatic hydrocarbons in the guppy (*Poecilia reticulata*). Aquat Toxicol 20:169–194.

[DGMK] German Society for Petroleum and Coal Science and Technology. 1991. Middle distillates. Analytical investigations and mutagenicity studies. Hamburg (DE): DGMK. Research Report No.: 412-1 (May). [cited in CONCAWE 1996; API 2003a].

[ECB] European Chemicals Bureau. 2000. IUCLID dataset for distillates (petroleum), light catalytic cracked (CAS RN 64741-59-9). European Commission, European Chemicals Bureau. Available from: http://esis.jrc.ec.europa.eu/doc/IUCLID/data_sheets/64741599.pdf

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2004a. Fish, dietary bioaccumulation study, study no. 0400947. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2004b. Fish, aqueous bioaccumulation study, study no. 0409544. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2005a. Fish, dietary bioaccumulation study, study no. 0409547. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2005b. Fish, aqueous bioaccumulation test, study no. 0523644. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2005c. Fish, dietary bioaccumulation study, study no. 0523747. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2005d. Fish, dietary bioaccumulation study, study no. 0531047. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2006a. Fish, dietary bioaccumulation study, study no. 0674247. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2006b. Fish, dietary bioaccumulation test, study no. 0681647. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2007a. Fish, dietary bioaccumulation study, study no. 0796347T. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2007b. Fish, dietary bioaccumulation study, study no. 0796347C. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2008a. Fish, dietary bioaccumulation study, study no. 0711047. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2008b. Fish, dietary bioaccumulation study, study no. 0821047. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2008c. Fish, dietary bioaccumulation study, study no. 0818447. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2009. Fish, dietary bioaccumulation study, study no. 0818447. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2010a. Fish, dietary bioaccumulation study, study no. 0818447. Supplement. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

[EMBSI] ExxonMobil Biomedical Sciences Inc. 2010b. Fish, dietary bioaccumulation study, study no. 0681647. Annandale (NJ): ExxonMobil Biomedical Sciences Inc.

Environment Canada. 2007. Guidance for conducting ecological assessments under CEPA 1999. Science Resource Technical Series, Draft Module on QSARs. Draft document prepared by Environment Canada, Existing Substances Division. Available from: Environment Canada, Existing Substances Division, Ottawa (ON).

Environment Canada. 2008. Data for petroleum sector stream substances collected under the *Canadian Environmental Protection Act, 1999*, section 71: Notice with respect to certain high priority petroleum substances. Data prepared by: Environment Canada, Oil, Gas, and Alternative Energy Division.

Environment Canada. 2009. Data for petroleum sector stream substances collected under the *Canadian Environmental Protection Act, 1999*, section 71: Notice with respect to potentially industry-limited high priority petroleum substances. Data prepared by: Environment Canada, Oil, Gas, and Alternative Energy Division.

Environment Canada. 2010. CEPA Environmental Registry. Toxic Substances List – Schedule 1. Available from: www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=0DA2924D-1

Environment Canada. 2011. Spill Line data report on petroleum product spills 2000–2009. Gatineau (QC): Environment Canada, Environmental Emergencies Division. Unpublished information.

[EPI Suite] Estimation Programs Interface Suite for Microsoft Windows [Estimation Model]. 2008. Version 4.0. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[EQC] Fugacity Based Equilibrium Criterion Model. 2003. Version 2.02. Peterborough (ON): Trent University, Canadian Environmental Modeling Centre. Available from: www.trentu.ca/cemc/

[ESIS] European Chemical Substances Information System [database on the Internet]. 2008. Database developed by the European Chemicals Bureau (ECB). [cited 2011 Aug 29]. Available from: http://esis.jrc.ec.europa.eu/

European Commission. 2008a. Details on substances classified in Annex VI to Regulation (EC) No 1272/2008 [database on the Internet]. Database developed by the European Commission. [cited 2011 Aug 29]. Available from: http://esis.jrc.ec.europa.eu/index.php?PGM=cla

European Commission. 2008b. European Union risk assessment report. Coal-tar pitch, high temperature. CAS No.: 65996-93-2. EINECS No.:266-028-2. Risk assessment. Environment. May 2008. Luxembourg (NL): Office for Official Publications of the European Communities. Available from: http://echa.europa.eu/documents/10162/13630/trd_rar_env_netherlands_pitch_en.pdf

Evans MS, Landrum PF. 1989. Toxicokinetics of DDE, benzo*(a)*pyrene, and 2,4,5,2', 4',5'-hexachlorobiphenyl in *Pontoporeia hoyi* and *Mysis relicta*. J Great Lakes Res 15:589–600.

Feuston MH, Low LK, Hamilton CE, Mackerer CR. 1994. Correlations of systemic and developmental toxicities with chemical component classes of refinery streams. Fundam Appl Toxicol 22:622–630.

Fingas M. 2001. Basics of oil spill cleanup. 2nd ed. Boca Raton (FL): CRC Press LLC. 233 p.

Fox K, Zauke GP, Butte W. 1994. Kinetics of bioconcentration and clearance of 28 polychlorinated biphenyl congeners in zebrafish (*Brachydanio rerio*). Ecotoxicol Environ Saf 28(1):99–109.

Gobas F, Clark K, Shiu W, Mackay D. 1989. Bioconcentration of polybrominated benzenes and biphenyls and related superhydrophobic chemicals in fish: role of bioavailability and elimination into the feces. Environ Toxicol Chem 8:231–245.

Gossiaux DC, Landrum PF, Fisher SW. 1996. Effect of temperature on the accumulation kinetics of PAHs and PCBs in the zebra mussel, *Dreissena polymorpha*. J Great Lakes Res 22(2):379–388.

Gustafson JB, Tell JG, Orem D. 1997. Selection of representative TPH fractions based on fate and transport considerations. Vol. 3. Total Petroleum Hydrocarbon Criteria Working Group Series, Association for Environmental Health and Sciences Foundation. 109 p. Available from: www.aehsfoundation.org/publications.aspx

Hardy R, Mackie P, Whittle K, McIntyre A. 1974. Discrimination in the assimilation of *n*-alkanes in fish. Nature 252:577–578.

Health Canada. 1998. Exposure factors for assessing total daily intake of priority substances by the general population of Canada. Ottawa (ON): Health Canada, Environmental Health Directorate. Unpublished report.

[HENRYWIN] Henry's Law Constant Program for Microsoft Windows [Estimation Model]. 2008. Version 3.20. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Hopkinson R. 2008. Priority substances under Environment Canada's Chemical Management Plan for the petroleum sector. Richmond (BC): Levelton Consultants Ltd.

[HYDROWIN]. Aqueous Hydrolysis Fate Program for Windows. 2008. Version 2.00. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[IARC] IARC Working Group on the Evaluation of Carcinogenic Risks to Humans. 1989a. Occupational exposures in petroleum refining. IARC Monogr Eval Carcinog Risks Hum 45:39–117.

[IARC] IARC Working Group on the Evaluation of Carcinogenic Risks to Humans. 1989b. Fuel oils. IARC Monogr Eval Carcinog Risks Hum 45:239–270.

[IARC] IARC Working Group on the Evaluation of Carcinogenic Risks in Humans. 1989c. Diesel fuels. IARC Monogr Eval Carcinog Risks Hum 45:219–238.

Jimenez BD, Cirmo CP, McCarthy JF. 1987. Effects of feeding and temperature on uptake, elimination and metabolism of benzo(a)pyrene in the bluegill sunfish (*Lepomis macrochirus*). Aquat Toxicol 10:41–57.

[JNITE] Japanese National Institute of Technology and Evaluation [database on the Internet]. 2010. Official Bulletin of Economy, Trade and Industry. [accessed 2010 September]. Available from: http://www.nite.go.jp/index-e.html

Jonsson G, Bechmann RK, Bamber SD, Baussant T. 2004. Bioconcentration, biotransformation, and elimination of polycyclic aromatic hydrocarbons in sheepshead minnows (*Cyprinodon variegates*) exposed to contaminated seawater. Environ Toxicol Chem 23:1538–1548.

Khan AA, Coppock RW, Schuler MM. 2001. Effects of multiple exposures of small doses of Pembina Cardium crude oil and diesel in rats. Arch Environ Contam Toxicol 40:418–424.

[KOCWIN] Organic Carbon Partition Coefficient Program for Windows [Estimation Model]. 2009. Version 2.00. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[KOWWIN] Octanol–Water Partition Coefficient Program for Windows [Estimation Model]. 2008. Version 1.67a. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Koyama J, Uno Seiichi, Kohno K. 2004. Polycyclic aromatic hydrocarbon contamination and recovery characteristics in some organisms after the *Nakhodka* oil spill. Mar Poll Bull 49:1054–1061.

Lampi M, Paumen ML, Parkerton T. 2010. An evaluation of the persistence, bioaccumulation and toxicity of petroleum hydrocarbons. Report Prepared for CONCAWE, Brussels (BE) by ExxonMobil Biomedical Sciences, Inc., Annandale (NJ) and ExxonMobil Petroleum and Chemical, Machelen (BE).

Lee WY, Winters K, Nicol JAC. 1978. The biological effects of the water-soluble fractions of a no. 2 fuel oil on the planktonic shrimp, *Lucifer faxoni.* Environ Pollut 15:167–183.

Lock S, Dalbey W, Schmoyer R, Griesemer R. 1984. Chemical characterization and toxicologic evaluation of airborne mixtures: inhalation toxicology of diesel fuel obscurant aerosol in Sprague-Dawley rats. Final report, phase 3: subchronic exposures. Oak Ridge (TN): Oak Ridge National Laboratory. Report No.: ORNL/TM-9403. [cited in ATSDR 1995].

Lockhart WL, Danelle RW, Murray DAJ. 1987. Acute toxicity bioassays with petroleum products: influence of exposure conditions. In: Vandermeulen JH, Hurdy SE, editors. Oil in fresh water: chemistry, biology and counter-measure technology. Oxford (UK): Pergamon Press. [cited in CONCAWE 1996].

Lyman W, Reehl W, Rosenblatt D. 1990. Handbook of chemical property estimation methods. Washington (DC): American Chemical Society.

MacLean MM, Doe KG. 1989. The comparative toxicity of crude and refined oils to *Daphnia magna* and *Artemia*. Manuscript Report EE-111. Ottawa (ON): Environment Canada. 72 p. [cited in Environment Canada 2010].

McCain BB, Hodgins HO, Gronlund WD, Hawkes JW, Brown DW, Myers MS. 1978. Bioavailability of crude oil from experimentally oiled sediment to English sole *Parophrys vetulus*. J Fish Res Board Can 35(5):657–664.

McCarthy JF, Jimenez BD, Barbee T. 1985. Effect of dissolved humic material on accumulation of polycyclic aromatic hydrocarbons: Structure-activity relationships. Aquat Toxicol 7:145–156.

McKee RH, Amoruso MA, Freeman JJ, Pryzgoda RT. 1994. Evaluation of the genetic toxicity of middle distillate fuels. Environ Mol Mutagen 23:234–238.

McLeese DW, Burridge LE. 1987. Comparative accumulation of PAHs in four marine invertebrates. In: Capuzzo IM, Kester DR, editors. Oceanic processes in marine pollution. Malabar (FL): Kirger RE. p.109-118 [cited in European Commission 2008b].

[Mobil] Mobil Oil Corporation. 1985. Thirteen week dermal administration of light cycle oil to rats. Study No. 20535. Princeton (NJ): Mobil Oil Corporation, Environmental and Health Science Laboratory. [cited in API 2003a].

[Mobil] Mobil Oil Corporation. 1988a. Light cycle oil developmental toxicity screen in rats. Study No. 50511. Princeton (NJ): Mobil Oil Corporation, Environmental and Health Science Laboratory. [cited in API 2003a].

[Mobil] Mobil Oil Corporation. 1988b. Developmental toxicity study in rats exposed dermally to coker light gas oil (CLGO). Study No. 61998. Princeton (NJ): Mobil Oil Corporation, Environmental and Health Science Laboratory. [cited in API 2003a].

[Mobil] Mobil Oil Corporation. 1991. Thirteen week dermal administration of Beaumont coker light gas oil to rats. Final report of Study No. 61996. Princeton (NJ): Mobil Oil Corporation, Environmental and Health Science Laboratory. [cited in API 2003a].

[MPBPWIN] Melting Point Boiling Point Vapour Pressure for Windows. 2008. Version 1.43. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Muijs B, Jonker MTO. 2010. A closer look at bioaccumulation of petroleum hydrocarbon mixtures in aquatic worms. Environ Toxicol Chem 29:1943–1949.

[NCI] National Chemical Inventories [database on a CD-ROM]. 2006. Issue 1. Columbus (OH): American Chemical Society, Chemical Abstracts Service. Available from: http://www.cas.org/products/other-cas-products/nci-on-cd

Neff JM, Cox BA, Anderson JW. 1976. Accumulation and release of petroleum derived aromatic hydrocarbons by four species of marine animals. Mar Biol 38(3):279–289.

Nessel CS, Priston RA, McKee RH, Cruzan G, Riley AJ, Hagermann R, Plutnick RT, Simpson BJ. 1998. A comprehensive evaluation of the mechanism of skin tumourigenesis by straight-run and cracked petroleum middle distillates. Toxicol Sci 44:22–31.

Newsted JL, Giesy JP. 1987. Predictive models for photoinduced acute toxicity of polycyclic aromatic hydrocarbons to *Daphnia magna*, Strauss (Cladocera, crustacean). Environ Toxicol Chem 6:445–461.

Nfon E, Cousins IT, Broman D. 2008. Biomagnification of organic pollutants in benthic and pelagic marine food chains from the Baltic Sea. Sci Total Environ 397:190–204. [cited in Lampi et al. 2010].

Niimi A, Palazzo V. 1986. Biological half-lives of eight polycyclic aromatic hydrocarbons (PAHs) in rainbow trout *(Salmo gairdneri).* Wat Res 20(4):503–507.

[NRC] National Research Council. 2003. Oil in the sea III: inputs, fates, and effects. Washington (DC): National Academy Press. 114 p.

[OECD] Organisation for Economic Co-operation and Development. 2009. Emission scenario document on transport and storage of chemicals. OECD series on emission scenario documents, No. 24. Available from: http://www.oecd.org/officialdocuments/displaydocumentpdf?cote=env/jm/mono(2009)26&doclanguage=en

Oliver B, Niimi A. 1988. Trophodynamic analysis of polychlorinated biphenyl congeners and other chlorinated hydrocarbons in the Lake Ontario ecosystem. Environ Sci Technol 22:388–397.

Pancirov R, Brown R. 1975. Analytical methods for polynuclear aromatic hydrocarbons in crude oils, heating oils, and marine tissues. In: Proceedings of a Conference on Prevention and Control of Oil Pollution, San Francisco, California. Washington (DC): American Petroleum Institute. p. 103–113. [cited in Potter and Simmons 1998].

Peterson GI, Kristensen P. 1998. Bioaccumulation of lipophilic substances in fish early life stages. Environ Toxicol Chem 17:1385-1395.

[PETROTOX] Spreadsheet model to calculate toxicity of petroleum hydrocarbons to aquatic organisms. 2009. Version 3.04. Brussels (BE): CONservation of Clean Air and Water in Europe (CONCAWE). [Internet]. [restricted access]. Available from: www.concawe.be/Content/Default.asp?PageID=241

Potter T, Simmons K. 1998. Composition of petroleum mixtures. Vol. 2. Total Petroleum Hydrocarbon Criteria Working Group Series, Association for Environmental Health and Sciences Foundation. 109 p. Available from: www.aehsfoundation.org/publications.aspx

[RMRI] Risk Management Research Institute. 2007. Quantitative assessment of oil spill risk for the south coast of Newfoundland and Labrador. St. John's (NL): RMRI (Canada). Draft report for Transport Canada.

Rossi SS, Anderson JW, Ward GS. 1976. Toxicity of water-soluble fractions of four test oils for the polychaetous annelids, *Neanthes arenaceodentata* and *Capitella capitata*. Environ Pollut 10:9–18.

Salazar-Coria L, Amezxua-Allieri MA, Tenorio-Torres M, Gonzales-Marcias C. 2007. Polyaromatic hydrocarbons (PAHs) and metal evaluation after a diesel spill in Oaxaca, Mexico. Bull Environ Contam Toxicol 79:462–467.

Salem H, Katz SA, editors. 2006. Inhalation toxicology. 2nd ed. Boca Raton (FL): CRC Press, Taylor & Francis Group.

[SCREEN3] Screening Tool Program for Windows [Screening Model]. 1996. Version 4.10. Research Triangle Park (NC): U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Emissions, Monitoring, and Analysis Division. Available from: www.epa.gov/scram001/dispersion_screening.htm

[SENES] SENES Consultants Limited. 2009. Review of current and proposed regulatory and non-regulatory management tools pertaining to selected petroleum substances under the Chemicals Management Plan. Report to Health Canada. Richmond Hill (ON): SENES.

[Shell] Shell Trading International Limited. 2011. Distillates (petroleum), light thermal cracked - CAS 64741-82-8 Safety Data Sheet. [accessed 2011 October 14]. Available from: http://www-static.shell.com/static/shipping_trading/downloads/trading_shipping/msds/in_country/uk_stasco/distillates_petroleum_light_thermal_cracked_64741-82-8_stl_en.pdf

Siemiatycki J, Dewar R, Nadon L, Gerin M, Richardson L, Wacholder S. 1987. Associations between several sites of cancer and twelve petroleum-derived liquids. Scand J Work Environ Health 13:493–504.

Simpson BJ. 2005. Analysis of petroleum hydrocarbon streams on the Health Canada CEPA/DSL Draft Maximal List. Report to the Canadian Petroleum Products Institute.

Skisak CM, Furedi-Machacek EM, Schmitt SS, Swanson MS, Vernot EH. 1994. Chronic and initiation/promotion skin bioassays of petroleum refinery streams. Environ Health Perspect 102:82–87.

[SPARC] Sparc Performs Automated Reasoning in Chemistry. 2007. [Internet]. US Environmental Protection Agency. Ecosystems Research Division.

Stegeman JJ, Teal JM. 1973. Accumulation, release and retention of petroleum hydrocarbons by the oyster *Crassostrea virginica*. Mar Biol 22:37–44.

Takeuchi I, Miyoshi N, Mizukawa K, Takada H, Ikemoto T, Omori K, Tsuchiya K. 2009. Biomagnification profiles of polycyclic aromatic hydrocarbons, alkylphenols and polychlorinated biphenyls in Tokyo Bay elucidated by $\delta^{13}C$ and $\delta^{15}N$ isotope ratios as guides to trophic web structure. Mar Pollut Bull 58:663–671.

Tolls J, van Dijk J. 2002. Bioconcentration of n-dodecane and its highly branched isomer 2,2,4,6,6-pentamethylheptane in fathead minnows. Chemosphere 47:1049–1057.

[TOPKAT] TOxicity Prediction by Komputer Assisted Technology [Internet]. 2004. Version 6.1. San Diego (CA): Accelrys Software Inc. Available from: http://accelrys.com/mini/toxicology/predictive-functionality.html

[UBTL] Utah Biomedical Testing Laboratory Inc. 1986. Twenty-eight day dermal toxicity study in rat on Watson Cherry point diesel fuel No. 2 (F-75-01). Study No. 60764. Salt Lake City (UT): Utah Biomedical Testing Laboratory Inc. [cited in API 2003b].

[UNECE] United Nations Economic Commission for Europe. 2011. Globally Harmonized System of Classification and Labelling of Chemicals. Revision 4. [accessed 2011 October 14]. Available from: http://www.unece.org/trans/danger/publi/ghs/ghs_rev04/04files_e.html

[U.S. EPA] United States Environmental Protection Agency. 1992. Screening procedures for estimating the air quality impact of stationary sources. Revised. Office of Air and Radiation, Office of Air Quality Planning and Standards. EPA-454/R-92-019. Available from: http://www.epa.gov/opptintr/exposure/pubs/usepa_1992b_sp_for_estim_aqi_of_ss.pdf

[U.S. EPA] United States Environmental Protection Agency. 1995. Great Lakes Water Quality Initiative technical support document for the procedure to determine bioaccumulation factors. Washington (DC): U.S. EPA. Report No.: EPA-820-B-95-005.

[U.S. EPA] United States Environmental Protection Agency. 2008. Transportation and marketing of petroleum liquids. In: AP 42, Compilation of air pollutant emission factors, vol. 1. 5th ed. Washington (DC): U.S. EPA. Available from: www.epa.gov/ttn/chief/ap42/ch05/final/c05s02.pdf

Varanasi U, Stein J, Nishimoto M. 1989. Biotransformation and disposition of PAH in fish. In: Varanasi U, editor, Metabolism of Polycyclic Aromatic Hydrocarbons in the Aquatic Environment. Boca Raton (FL): CRC Press. p. 93–150. [cited in Burkhard and Lukasewycz 2000].

Wan Y, Jin X, Hu J, Jin F. 2007. Trophic dilution of polycyclic aromatic hydrocarbons (PAHs) in a marine food web from Bohai Bay, North China. Environ Sci Technol 41:3109–3114.

Weinstein JE, Oris JT. 1999. Humic acids reduce the bioaccumulation and photoinduced toxicity of fluoranthene to fish. Environ Toxicol Chem 18(9):2087–2094.

[WSKOWWIN] Water Solubility for Organic Compounds Program for Microsoft Windows [Estimation Model]. 2008. Version 1.41a. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Yakata N, Sudo Y, Tadokoro H. 2006. Influence of dispersants on bioconcentration factors of seven organic compounds with different lipophilicities and structures. Chemosphere 64:1885–1891.

Yang H. 2001. NCUT (National Center for Upgrading and Technology) technical information.

Zhou S, Heras H, Ackman RG. 1997. Role of adipocytes in the muscle tissue of Atlantic salmon (*Salmo salar*) in the uptake, release and retention of water-soluble fraction of crude oil hydrocarbons. Mar Biol 127:545–553.

Appendix 1: Petroleum substance grouping

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

Group[a]	Description	Example
Crude oils	Complex combinations of aliphatic and aromatic hydrocarbons and small amounts of inorganic compounds, naturally occurring under the earth's surface or under the seafloor	Crude oil
Petroleum and refinery gases	Complex combinations of light hydrocarbons primarily from C_1–C_5	Propane
Low boiling point naphthas	Complex combinations of hydrocarbons primarily from C_4–C_{12}	Gasoline
Gas oils	Complex combinations of hydrocarbons primarily from C_9–C_{25}	Diesel
Heavy fuel oils	Complex combinations of heavy hydrocarbons primarily from C_{11}–C_{50}	Fuel Oil No. 6
Base oils	Complex combinations of hydrocarbons primarily from C_{15}–C_{50}	Lubricating oils
Aromatic extracts	Complex combinations of primarily aromatic hydrocarbons from C_{15}–C_{50}	Feedstock for benzene production
Waxes, slack waxes and petrolatum	Complex combinations of primarily aliphatic hydrocarbons from C_{12}–C_{85}	Petrolatum
Bitumen or vacuum residues	Complex combinations of heavy hydrocarbons having carbon numbers greater than C_{25}	Asphalt

[a] These groups were based on classifications developed by Conservation of Clean Air and Water in Europe (CONCAWE 1996) and a contractor's report presented to the Canadian Petroleum Products Institute (Simpson 2005).

Appendix 2: Physical and chemical data tables for industry-restricted gas oils

Table A2.1. Substance identity for gas oils

CAS RN	64741-59-9	64741-82-8
DSL name	Distillates (petroleum), light catalytic cracked	Light thermal cracked distillates
National Chemical Inventories[a]	Distillates (petroleum), light catalytic cracked	Distillates, petroleum, light thermal cracked (AICS, EINECS, ESIS, IUCLID)
Chemical group (DSL Stream)	UVCB – organic	UVCB – organic
Major chemical class or use	Refinery streams	Distillate fuel oils
Major chemical subclass[b]	Complex combinations of alkanes, cycloalkanes, alkenes and aromatics (predominantly aromatic)	Complex combinations of alkanes, cycloalkanes and aromatics
Carbon range[c]	C_9–C_{25}	C_{10}–C_{22}
Aromatic content[d] (%)	61–80	57
Aliphatic content[d] (%)	Alkanes 14–23 Cycloalkanes 8–10	43
Alkene content[d] (%)	0–3.7[d]	0[c]
Boiling point range (°C)	179–382[e]	160–370[c]
Aliphatic : aromatic ratio	20:80[d,f]	43:57[d,g]

Abbreviations: AICS, Australian Inventory of Chemical Substances; DSL, Domestic Substances List; EINECS, European Inventory of Existing Commercial Chemical Substances; ESIS, European Chemical Substances Information System; IUCLID, International Uniform Chemical Information Database.

[a] NCI (2006)

[b] This substance is a UVCB (Unknown or Variable Composition, Complex Reaction Products, or Biological Materials), i.e., it is not a discrete chemical and thus may be characterized by a variety of structures.

[c] CONCAWE (1996)

[d] API (2003a)

[e] ECB (2000)

[f] The aromatic to aliphatic ratio reported for CAS RN 64741-59-9 is based on the MOBIL Light Cycle Oil sample.

[g] The aromatic to aliphatic ratio reported for CAS RN 64741-82-8 is based on the MOBIL coker light gas oil sample.

Table A2.2. Physical-chemical properties of representative substances for gas oils (EPI Suite 2008)[a]

Chemical class, name and CAS RN	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]	Henry's Law constant ($Pa \cdot m^3/mol$)[c]
Alkanes				
C_{10} decane (124-18-5)	174.1 (expt.)	−29.7 (expt.)	191	5.2×10^{5} (expt.)
C_{15} pentadecane (629-62-9)	270.6 (expt.)	9.9 (expt.)	0.5 (expt.)	1.3×10^{6} (expt.)
C_{20} eicosane (112-95-8)	343.0 (expt.)	36.8 (expt.)	6.2×10^{-4} (expt.)	5.3×10^{6}
Isoalkanes				
C_{10} 4-methylnonane (17301-94-9)	165.7 (expt.)	−99 (expt.)	339	5×10^{4}
C_{15} 2-methyltetradecane (1560-95-8)	250.2	1.5	5.8	3.7×10^{5}
C_{20} 3-methyl-nonadecane (6418-45-7)	326.3	39.5	0.09	2.4×10^{6}
One-ring cycloalkanes				
C_{10} butylcyclohexane (1678-93-9)	180.9 (expt.)	−74.7 (expt.)	180 (expt.)	2×10^{4}
C_{15} nonylcyclohexane (2883-02-5)	282 (expt.)	−10 (expt.)	1.2 (expt.)	5.8×10^{4}
Two-ring cycloalkanes				
C_{9} cis-bicyclononane (4551-51-3)	167 (expt.)	−53 (expt.)	320.0	2100

C_{15} pentamethyldecalin	248	8.6	6.6	2.8×10^4
C_{20} 2,4-dimethyloctyl-2-decalin	329	78	0.03	8.2×10^4
Polycycloalkanes				
C_{14} hydrophenanthrene	255	21	4.5	8×10^3
C_{18} hydrochrysene	316	66.4	0.004	6×10^3
C_{22} hydropicene	365	117	0.003	4×10^3
One-ring aromatics				
C_9 ethylmethylbenzene (25550-14-5)	165.2 (expt.)	−80.8 (expt.)	384 (expt.)	324.2
C_{15} *n*-nonylbenzene (1081-77-2)	280.5 (expt.)	−24 (expt.)	0.76 (expt.)	4200
C_{20} 1-benzyl-4,8-dimethyl-dodecane	334.6	49.2	4	82 100
Cycloalkane monoaromatics				
C_{10} tetralin (tetrahydronaphthalene) 119-64-2	207.6 (expt.)	-35.7 (expt.)	49.1 (expt.)	138 (expt.)
C_{15} methyloctahydro-phenanthrene	284.8	50.9	0.337	939
C_{20} ethyldodecahydro-	351.3	115.7	0.00279	1710

chyrsene				
Two-ring aromatics				
C_{10} naphthalene (91-20-3)	218 (expt.)	80.2 (expt.)	11.3 (expt.)	44.6 (expt.)
C_{15} 4-isopropylbiphenyl	309	43.7	0.1	23.8
Cyclolkane diaromatics				
C_{12} acenaphthene (83-32-9)	279 (expt.)	93.4 (expt.)	0.287 (expt.)	5.95
C_{15} ethylfluorene	321	89.5	0.0202	24.8
C_{20} isoheptylfluorene	374	119	0.0011	102
Three-ring aromatics				
C_{15} 4-methylphenanthrene (2531-84-2)	340	94	0.02	5 (expt.)
Four-ring PAHs				
C_{16} fluoranthene (206-44-0)	348.0	107.8	1.2×10^{-3}	0.9

Table A2.2 cont. Physical-chemical properties of representative substances for gas oils (EPI Suite 2008)[a]

Chemical class, name and CAS RN	**Log K_{ow}**	**Log K_{oc}**	**Aqueous solubility (mg/L)[d]**
Alkanes			
C_{10} decane (124-18-5)	5.01 (expt.)	2.2×10^{4}	0.052 (expt.)
C_{15}	7.7	6.7	7.6×10^{-5}

Chemical class, name and CAS RN	**Log K_{ow}**	**Log K_{oc}**	**Aqueous solubility (mg/L)[d]**
pentadecane (629-62-9)			(expt.)
C_{20} eicosane (112-95-8)	10.2	5.9	0.002 (expt.)
Isoalkanes			
C_{10} 4-methylnonane (17301-94-9)	5.2	3×10^{4}	0.087
C_{15} 2-methyltetradecane (1560-95-8)	7.6	6.6	0.003
C_{20} 3-methylnonadecane (6418-45-7)	10*	8.8	1.1×10^{-5}
One-ring cycloalkanes			
C_{10} butylcyclohexane (1678-93-9)	5.1	4.4	1.2
C_{15} nonylcyclohexane (2883-02-5)	7.5	4.6	0.004 (expt.)
Two-ring cycloalkanes			
C_{9} cis-bicyclononane (4551-51-3)	3.7	3.0	19.3
C_{15} pentamethyldecalin	6.3	5.5	0.05
C_{20} 2,4-dimethyloctyl-2-decalin	8.9	7.7	1.1×10^{-4}
Polycycloalkanes			
C_{14}	5.2	4.4	0.5

Chemical class, name and CAS RN	**Log K_{ow}**	**Log K_{oc}**	**Aqueous solubility (mg/L)[d]**
hydrophenanthrene			
C_{18} hydrochrysene	6.2	5.3	0.03
C_{22} hydropicene	7.3	6.3	0.002
One-ring aromatics			
C_9 ethylmethylbenzene (25550-14-5)	3.6 (expt.)	2.93	74.6 (expt.)
C_{15} *n*-nonylbenzene (1081-77-2)	7.1 (expt.)	4.4	0.04
C_{20} 1-benzyl-4,8-dimethyl-dodecane	8.78	5.67	0.0005
Cycloalkane monoaromatics			
C_{10} tetralin (tetrahydronaphthalene) 119-64-2	3.49 (expt.)	3.19	47 (expt.)
C_{15} methyloctahydro-phenanthrene	5.40	4.43	0.37
C_{20} ethyldodecahydro-chyrsene	6.91	5.74	0.00274
Two-ring aromatics			
C_{10} naphthalene (91-20-3)	3.3 (expt.)	731	31 (expt.)
C_{15}	5.5	4.63	0.9

Chemical class, name and CAS RN	**Log K_{ow}**	**Log K_{oc}**	**Aqueous solubility (mg/L)[d]**
4-isopropylbiphenyl	(expt.)		
Cycloalkane diaromatics			
C_{12} acenaphthene (83-32-9)	3.92 (expt.)	3.70	2.534
C_{15} ethylfluorene	5.05	4.45	0.198
C_{20} isoheptylfluorene	7.44	5.68	0.0009
Three-ring aromatics			
C_{15} 4-methylphenanthrene (2531-84-2)	4.9	2.6×10^4	1.7
Four-ring PAHs			
C_{16} fluoranthene (206-44-0)	5.2	4.5	0.3

[a] All values are modelled unless denoted with an (expt.) 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}; WSKOWWIN (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] Henry's Law constants for C_{20} representative substances were calculated with HENRYWIN Version 3.10 from EPI Suite (2007), 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.

[d] Maximum water solubility was estimated for each representative substance based on its individual physical-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).

Appendix 3: Measures designed to prevent, reduce or manage unintentional releases

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 *Petroleum Refinery Liquid Effluent Regulations* and guidelines in the *Fisheries Act* (Canada 2010). These regulations set the discharge limits of oil and grease, phenol, sulfides, 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 specifies 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) are also in place at petroleum sector facilities to reduce unintentional releases. Such control measures include appropriate material selection during the design and setup processes; regular inspection and maintenance of storage tanks, pipelines 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 or spills (SENES 2009).

Under the *Canada Shipping Act, 2001* (Canada 2001), releases of petroleum substances from marine loading and unloading and transportation are managed by pollution prevention and response provisions (Parts 8 and 9), including the establishment of pollution prevention plans and pollution emergency plans for any discharges during loading or unloading activities.

For those substances containing highly volatile components (e.g., low boiling point naphthas, gasoline), a vapour recovery system is generally implemented or recommended at loading terminals of Canadian petroleum facilities (SENES 2009). Such a system is intended to reduce evaporative emissions during handling procedures.

Appendix 4: Unintentional release estimation of diesel fuel spills to the marine environment

Table A4.1. Diesel fuel, light oil and petroleum distillates spills information, 2000–2009, from Environment Canada Spill Line database to selected marine locations (Environment Canada 2011)[a]

Year	Average spill volume (litres)	Maximum single spill volume (litres)	Median spill volume (litres)	Number spills reported	% of spills with unknown volume	Total known volume spilled (litres)	Extrapolated total volume spilled (litres)[b]
2009	100	100	100	2	50	100	244
2008	-	-	-	1	100	-	144
2007	7	20	4	7	43	29	460
2006	1700	1700	1700	2	50	1700	1844
2005	-	-	-	3	100	-	431
2004	46	91	46	5	60	92	523
2003	8	20	4	9	56	31	748
2002	29	57	29	7	71	59	777
2001	-	-	-	0	-	-	-
2000	-	-	-	0	-	-	-
Total volume spilled				36		2010	5169

[a] Does not include releasess due to aircraft crash, collision, ice/frost, road conditions, subsidence, or vandalism.

[b] The extrapolated total volume was calculated using a proportional estimate of known spills to determine the frequency and volume of unknown spill volumes assuming that the distribution of reported volumes released was representative of all releases.

Table A4.2a. Sources of diesel fuel, light oil, and petroleum distillates releases in Canada to selected marine locations, 2000–2009 (Environment Canada 2011)[a]

Source	Total number of releases	Total volume of releases (litres)	Proportion of volume	Average release (litres)
Other motor vehicle	4	1700	0.85	1700
Other industrial plant	1	91	0.05	91
Unknown	19	125	0.06	31
Other watercraft	7	85	0.04	21
Marine terminal	1	4	0.00	4
Pipeline	1	2	0.00	2
Tank truck	1	2	0.00	2
Marine tanker	1	1	0.00	1
Other	1	0	0.00	0
Total	**36**	**2010**	**1.00**	**144**

[a] Does not include releasess due to aircraft crash, collision, ice/frost, road conditions, subsidence, or vandalism.

Table A4.2b. Causes for diesel fuel, light oil, and petroleum distillates releases in Canada to selected marine locations 2000–2009 (Environment Canada 2011)[a]

Cause	Total number of releases	Total volume of releases (litres)	Proportion of volume	Average release (litres)
Unknown	23	1734	0.86	248
Container leak	2	191	0.09	95
Discharge	6	59	0.03	29
Other	4	22	0.01	11
Valve, fitting leak	1	4	0.00	4
Total	**36**	**2010**	**1.00**	**144**

[a] Does not include releasess due to aircraft crash, collision, ice/frost, road conditions, subsidence, or vandalism.

Table A4.2c. Reasons for diesel fuel, light oil, and petroleum distillates releases in Canada to selected marine locations 2000–2009 (Environment Canada 2011)[a]

Reason	Total number of releases	Total volume of releases (litres)	Proportion of volume	Average release (litres)
Unknown	24	1803	0.90	258
Human error	2	100	0.05	100
Vandalism	1	91	0.05	91

Equipment failure	4	10	0.00	3
Material failure	1	4	0.00	4
Corrosion	1	2	0.00	2
Other	2	0	0.00	0
Subsidence	1	0	0.00	0
Total	**36**	**2010**	**1.00**	**144**

[a] Does not include releasess due to aircraft crash, collision, ice/frost, road conditions, subsidence, or vandalism.

Appendix 5: Modelling results for environmental properties of industry-restricted gas oils

Table A5.1. Results of Level III fugacity modelling of representative gas oil hydrocarbons (EQC 2003)

Compartment of release (100%)	**Percentage (%) of substance partitioning into each compartment**			
***n*-Alkanes**	**Air**	**Water**	**Soil**	**Sediment**
C_{10}				
Air	99.5	0.02	0.5	0.02
Water	1.5	48.0	0.0	50.5
Soil	0.1	0.0	99.9	0.0
C_{15}				
Air	98.4	0.01	1.5	0.1
Water	0.01	8.7	0.0	91.3
Soil	0.1	0.0	99.9	0.02
C_{20}				
Air	16.0	1.3	61.3	21.5
Water	0.0	5.5	0.0	94.5
Soil	0.0	0.0	99.9	0.03
Isoalkanes				
C_{10}				
Air	99.8	0.0	0.2	0.0
Water	3.3	85.7	0.0	11.0
Soil	6.2	0.0	93.7	0.0
C_{15}				
Air	99.0	0.0	1.0	0.01
Water	0.01	9.6	0.0	90.4
Soil	0.04	0.0	99.9	0.01
C_{20}				
Air	94.0	0.05	5.1	0.9
Water	0.0	5.0	0.0	95.0
Soil	0.0	0.0	99.9	0.03
One-ring cycloalkanes				
C_{10}				
Air	99.8	0.0	0.2	0.0
Water	2.8	93.4	0.0	3.8
Soil	3.2	0.0	96.8	0.0
C_{15}				
Air	97.3	0.03	2.3	0.4
Water	0.01	7.0	0.0	93.0
Soil	0.0	0.0	99.9	0.02
Two-ring cycloalkanes				

C_9				
Air	99.0	0.1	0.8	0.0
Water	4.7	87.0	0.0	8.3
Soil	3.4	0.1	96.5	0.0
C_{15}				
Air	96.8	0.0	3.0	0.1
Water	0.05	6.0	0.0	94
Soil	0.06	0.0	99.9	0.04
C_{20}				
Air	15.8	0.8	25.4	58.1
Water	0.0	1.3	0.0	98.7
Soil	0.0	0.0	99.8	0.2
Polycycloalkanes				
C_{14}				
Air	93.1	0.2	6.0	0.8
Water	0.2	18.1	0.02	81.6
Soil	0.03	0.0	99.9	0.03
C_{18}				
Air	7.7	0.6	60.4	31.2
Water	0.0	2.0	0.05	97.9
Soil	0.0	0.0	99.8	0.2
C_{22}				
Air	3.0	0.05	91.8	5.2
Water	0.0	1.0	0.02	99.0
Soil	0.0	0.0	99.7	0.3
One-ring aromatics				
C_9				
Air	99.4	0.3	0.3	0.0
Water	4.4	94.6	0.01	0.9
Soil	1.0	0.08	98.9	0.0
C_{15}				
Air	98.4	0.05	1.1	0.4
Water	0.03	11.5	0	88.5
Soil	0.0	0.0	100	0.01
C_{20}				
Air	92.1	0.1	0.0	1.5
Water	0.0	7.8	0.0	92.2
Soil	0.0	0.0	100	0.02
Cycloalkane monoaromatics				
C_{10}				
Air	99.8	0.2	0.05	0.0
Water	2.02	97.8	0.0	0.1
Soil	0.2	0.02	99.8	0.0
C_{15}				

Air	81.4	1.7	1.5	15.4
Water	0.2	9.7	0.0	90.0
Soil	0.0	0.0	100	0.04
C_{20}				
Air	24.7	0.9	24.3	50
Water	0.01	1.8	0.01	98.2
Soil	0.0	0.0	99.9	0.1
Two-ring aromatics				
C_{10}				
Air	97.4	2.2	0.4	0.02
Water	1.3	98.0	0.8	0
Soil	0.08	0.2	99.8	0
C_{15}				
Air	89.9	4	1.3	4.8
Water	0.1	45.6	0.0	54.3
Soil	0.0	0.0	100	0.0
Cycloalkane diaromatics				
C_{12}				
Air	91.6	6.7	1.4	0.4
Water	0.4	94.1	0.01	5.5
Soil	0.0	0.04	100	0.0
C_{15}				
Air	92.6	4.2	1.7	1.5
Water	1.5	72.6	0.03	25.9
Soil	0.0	0.0	100	0.0
C_{20}				
Air	94.1	0.6	4.6	0.7
Water	0.1	44.8	0.0	55.1
Soil	0.0	0.0	100	0.0
Three-ring aromatics				
C_{15}				
Air	68.5	9.7	11.6	10.2
Water	0.1	48.7	0.02	51.2
Soil	0.0	0.01	99.98	0.01
Four-ring aromatics				
C_{16}				
Air	13.1	4.7	58.1	24.1
Water	0.0	16.2	0.04	83.7
Soil	0.0	0.0	99.9	0.1

Table A5.2. Modelled data for primary (BioHCWin 2008; BIOWIN4 2009) and ultimate (BIOWIN3,5,6 2009; CATABOL, TOPKAT) degradation of gas oils components

	Primary Biodegradation	
	BioHCWin (2008)[a] (days)	**BIOWIN 4 (2009) Expert Survey[b]**
Alkanes		
C_{10} decane	8.6	4.18
C_{15} pentadecane	19	4.08
C_{20} eicosane	40	3.98
Isoalkanes		
C_{10} 4-methylnonane	7.7	3.91
C_{15} 2-methyltetradecane	17	3.81
C_{20} 3-methylnonadecane	36	3.71
One-ring cycloalkanes		
C_{10} butylcyclohexane	11.6	3.91
C_{15} nonylcyclohexane	25	3.81
Two-ring cycloalkanes		
C_9 cis-bicyclononane	56	3.67
C_{15} 2-isopentadecylin	88	3.55
C_{20} 2,4-dimethyloctyl-2-decalin	250	3.56
Polycycloalkanes		
C_{14} hydrophenanthrene	117	3.57
C_{18} hydrochrysene	678	3.49
C_{22} hydropicene	4416	3.41
One-ring aromatics		
C_9 ethylmethylbenzene	4.9	3.54
C_{15} 2-nonylbenzene	14	3.76

	Primary Biodegradation	
	BioHCWin (2008)[a] (days)	**BIOWIN 4 (2009) Expert Survey[b]**
C_{20} tetradecylbenzene	31	3.66
Cycloalkane monoaromatics		
C_{10} tetralin	1.5	3.52
C_{15} methyloctahydro-phenanthrene	466	3.42
C_{20} ethyldodecahydro-chyrsene	469	3.32
Two-ring aromatics		
C_{10} naphthalene	5.6	3.32
C_{15} 4-isopropylbiphenyl	72.6	3.50
Cycloalkane diaromatics		
C_{12} acenaphthene	18.8	3.49
C_{15} ethylfluorene	16.5	3.50
C_{20} isoheptylfluorene	40.9	3.33
Three-ring PAHs		
C_{15} 2-methylphenanthrene	24	3.50
Four-ring PAHs		
C_{16} fluoranthene	191	2.85

Table A5.2 cont. Modelled data for primary (BioHCWin 2008; BIOWIN4 2009) and ultimate (BIOWIN3,5,6 2009; CATABOL, TOPKAT) biodegradation of gas oil components

	Ultimate Biodegradation					
	BIOWIN 3 (2009) Expert Survey[b]	**BIOWIN 5 (2009) MITI linear probability[c]**	**BIOWIN 6 (2009) MITI non-linear probability[c]**	**CATABOL (2008) % BOD**	**TOPKAT (2004) Probability of biodegradability**	**Extrapolated half-life compared with criteria (days)**
Alkanes						

	Ultimate Biodegradation					
	BIOWIN 3 (2009) Expert Survey[b]	**BIOWIN 5 (2009) MITI linear probability[c]**	**BIOWIN 6 (2009) MITI non-linear probability[c]**	**CATABOL (2008) % BOD**	**TOPKAT (2004) Probability of biodegradability**	**Extrapolated half-life compared with criteria (days)**
C_{10} decane	3.48	0.69	0.87	100	1	< 182
C_{15} pentadecane	3.33	0.72	0.88	99.94	1	< 182
C_{20} eicosane	3.17	0.76	0.89	89	1	< 182
Isoalkanes						
C_{10} 4-methylnonane	3.18	0.54	0.72	15.6	1	< 182
C_{15} 2-methyltetra-decane	3.03	0.57	0.75	91.11	1	< 182
C_{20} 3-methyl-nonadecane	2.87	0.61	0.77	97.9	1	< 182
One-ring cycloalkanes						
C_{10} butylcyclo-hexane	3.19	0.55	0.70	9.0	1	< 182
C_{15} nonylcyclo-hexane	3.04	0.57	0.65	57.9	1	< 182
Two-ring cycloalkanes						
C_9 cis-bicyclononane	2.92	0.51	0.58	0	0.001	< 182
C_{15} 2-isopenta-decylin	2.74	0.32	0.19	4.49	0	≥ 182
C_{20} 2,4-dimethyl-octyl-2-decalin	2.67	0.45	0.26	4.5	0	≥ 182
Polycyclo-alkanes						
C_{14} hydro-phenanthrene	2.77	0.39	0.24	0	0	≥ 182
C_{18} hydro-chrysene	2.65	0.29	0.07	0	0	≥ 182
C_{22}	2.54	0.19	0.02	0	0	≥ 182

	Ultimate Biodegradation					
	BIOWIN 3 (2009) Expert Survey[b]	**BIOWIN 5 (2009) MITI linear probability[c]**	**BIOWIN 6 (2009) MITI non-linear probability[c]**	**CATABOL (2008) % BOD**	**TOPKAT (2004) Probability of biodegradability**	**Extrapolated half-life compared with criteria (days)**
hydropicene						
One-ring aromatics						
C_9 ethylmethyl-benzene	2.78	0.37	0.44	10.67*	0.086	< 182
C_{15} 2-nonylbenzene	2.99	0.44	0.53	50.9	0.11	< 182
C_{20} tetradecyl-benzene	2.84	0.47	0.56	90.6	0.001	< 182
Cycloalkane mono-aromatics						
C_{10} tetralin	2.76	0.28	0.36	0.71	0.003	< 182
C_{15} methyl-octahydro-phenanthrene	2.61	0.19	0.13	0.91*	0	≥ 182
C_{20} ethyl-dodecahydro-chyrsene	2.46	0.10	0.04	0.7	0	≥ 182
Two-ring aromatics						
C_{10} naphthalene	2.33	0.40	0.45	3.2	0.001	< 182
C_{15} 4-isopropyl-biphenyl	2.71	0.19	0.15	12.16	0	≥ 182
Cycloalkane diaromatics						
C_{12} acenaphthene	2.71	0.19	0.19	3.82	0	≥ 182
C_{15} ethylfluorene	2.70	0.15	0.10	1.03*	0	< 182
C_{20} isoheptyl-fluorene	2.47	-0.03	0.036	2.36*	0.916	< 182
Three-ring PAHs						
C_{15}	2.70	0.26	0.16	21.23*	0.004	< 182

	Ultimate Biodegradation					
	BIOWIN 3 (2009) Expert Survey[b]	**BIOWIN 5 (2009) MITI linear probability[c]**	**BIOWIN 6 (2009) MITI non-linear probability[c]**	**CATABOL (2008) % BOD**	**TOPKAT (2004) Probability of biodegradability**	**Extrapolated half-life compared with criteria (days)**
2-methyl-phenanthrene						
Four-ring PAHs						
C_{16} fluoranthene	1.95	0.19	0.11	19.67*	0	≥ 182

Abbreviations: BOD, biological oxygen demand; MITI, Ministry of International Trade & Industry, Japan
[a] Half-life estimations are for non-specific media (i.e., water, soil and sediment).
[b] Output is a numerical score from 0–5.
[c] Output is a probability score.
* Modelled results were found to be out of domain and therefore not considered for persistence. For modelled results of CATABOL that were found to be out of domain, it was assumed that results for TOPKAT, BIOWIN 5, 6 were also out of domain because these models use the same dataset. In these cases, only BIOWIN 3, 4 and BioHCWin were considered when determining the persistence of the component.

Table A5.3. Modelled atmospheric degradation of representative structures in gas oils via reaction with hydroxyl radicals (AOPWIN 2008)

	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
One-ring cycloalkanes	
C_{10}	0.7
C_{15}	0.4
Two-ring cycloalkanes	
C_9	0.8
C_{15}	0.4
C_{20}	0.3
Polycycloalkanes	
C_{14}	0.4
C_{18}	0.3
C_{22}	0.2
One-ring aromatics	
C_9	1.4
C_{15}	0.7

C_{20}	0.2
Cycloalkane monoaromatics	
C_{10}	0.3
C_{15}	0.5
C_{20}	0.3
Two-ring aromatics	
C_{10}	0.5
C_{15}	1.1
Cycloalkane diaromatics	
C_{12}	0.2
C_{15}	0.6
C_{20}	0.5
Three-ring aromatics	
C_{15}	0.3
Four-ring aromatics	
C_{16}	0.4

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

Table A5.4. Experimental BAFs for aromatic hydrocarbons

	Reference; Study	**Log K_{ow}**	**BAF Experimental (L/kg ww)**
One-ring aromatics			
C_6 benzene	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (water-soluble fraction [WSF] of crude oil)	2.13 (expt.)	4
C_7 toluene	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (WSF of crude oil)	2.73 (expt.)	11
C_8 ethylbenzene	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (WSF of crude oil)	3.15 (expt.)	26
C_8 xylenes	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (WSF of crude oil)	3.12 (expt.)	47
C_9 isopropylbenzene	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (WSF of crude oil)	3.66 (expt.)	20
C_9 propylbenzene	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (WSF of	3.69 (expt.)	36

	crude oil)		
C_9 ethylmethylbenzene	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (WSF of crude oil)	3.98 (expt.)	51
C_9 trimethylbenzene	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (WSF of crude oil)	3.66 (expt.)	74
Two-ring aromatics			
C_{10} naphthalene	Neff et al. 1976 Clam; 24-hour (oil-in-water dispersion of No. 2 fuel oil) lab study	3.30 (expt.)	2.3
C_{11} methyl naphthalenes	Zhou et al. 1997 Atlantic salmon (white muscle); 96-hour (WSF of crude oil) lab study	3.87 (expt.)	230
C_{11} 1-methylnaphthalene	Neff et al. 1976 Clam; 24-hour (oil-in-water dispersion of No. 2 fuel oil) lab study	3.87 (expt.)	8.5
C_{11} 2-methylnaphthalene	Neff et al. 1976 Clam; 24-hour (oil-in-water dispersion of No. 2 fuel oil) lab study	3.86 (expt.)	8.1
C_{12} dimethylnaphthalene	Neff et al. 1976: Clam; 24-hour (oil-in-water dispersion of No. 2 fuel oil) lab study	4.31 (expt.)	17.1
C_{13} trimethylnaphthalene	Neff et al. 1976: Clam; 24-hour (oil-in-water dispersion of No. 2 fuel oil) lab study	4.81	26.7
Three-ring aromatics			
C_{14} phenanthrene	Burkhard and Lukasewycz 2000 Lake trout; field study	4.57	87
C_{16} fluoranthene	Burkhard and Lukasewycz 2000 Lake trout; field study	5.23	1550

Abbreviation: (expt.), experimental log K_{ow} data

Table A5.5. Summary of empirical aquatic bioconcentration factors (BCFs) for various PAHs (adapted from European Commission 2008b)

Substance	**Species**	**Exposure time**	**BCF (L/kg ww)**	**Reference**
Fish				
fluoranthene	*Pimephales*	24 hours	9054	Weinstein and Oris

	promelas (fathead minnow)			1999
Molluscs				
fluoranthene	*Mytilus edulis* (blue mussel)	96 hours	5920	McLeese and Burridge 1987
	Mya arenaria (clam)		4120	
Crustaceans				
fluoranthene	*Daphnia magna* (water flea)	24 hours	1742	Newsted and Giesy 1987
	Cragon septemspinosa (sand shrimp)	96 hours	180	McLeese and Burridge 1987
Polychaetes				
fluoranthene	*Nereis virens* (sandworm)	96 hours	720	McLeese and Burridge 1987

Table A5.6. Fish BAF and BCF predictions for representative structures of gas oils using Arnot-Gobas three trophic level model (2004) with corrections for metabolism rate (k_M) and dietary assimilation efficiency (E_d)

	Log K_{ow}	**Metabolic rate constant for MTL fish (day^{-1})[a]**	**BCF[b] MTL fish (L/kg ww)**	**BAF[b] MTL fish (L/kg ww)**
Alkanes*				
C_{10} decane (124-18-5)	5.0 (expt.)	0.37[g]	479	513
C_{15} pentadecane (629-62-9)	**7.7**	0.44[c]	42	550
Isoalkanes*				
C_{10} 4-methylnonane (17301-94-9)	**5.2**	0.13	1259	1584
C_{15} 2-methyltetradecane (1560-95-8)	**7.5**	0.020[d]	1148	**181 970**[q]
One-ring cycloalkanes*				
C_{10} butylcyclohexane (1678-93-9)	**5.1**	0.13	1445	1820
C_{15} nonylcyclohexane (2883-02-5)	**7.5**	0.023[f]	2630	**22 909**
Two-ring cycloalkanes*				
C_9	3.7	0.15	300	310

cis-bicyclononane (4551-51-3)				
C_{15} pentamethyldecalin	**6.5**	0.04[h]	2884	**8511**
Polycycloalkanes*				
C_{14} hydrophenanthrene	**5.2**	0.01[i]	**5888**	**8511**
C_{18} hydrochrysene	**6.2**	0.45[j]	1023	3548
C_{22} hydropicene	**7.3**	0.04[k]	871	**31 623**
One-ring aromatics*				
C_9 ethylmethylbenzene (25550-14-5)	3.6	0.31	191	191
C_{15} *n*-nonylbenzene (1081-77-2)	**7.1**	0.01	4365	**151 356**
Cycloalkane monoaromatics*				
C_{10} tetralin (tetrahydronaphthalene) 119-64-2	3.5 (expt.)	0.00	214	562
C_{15} methyloctahydro-phenanthrene	**5.6**	0.13[m]	2630	**5445**
C_{20} ethyldodecahydro-chyrsene	**6.9**	0.08[n]	1698	**25 119**
Two-ring aromatics*				
C_{10} naphthalene (91-20-3)	3.3	0.00	138	148
C_{15} 4-isopropylbiphenyl	**5.5**	0.20[o]	871	1175
Cyclolkane diaromatics*				
C_{12} acenaphthene (83-32-9)	3.92 (expt.)	0.10	275	380
C_{15} ethylfluorene	**5.1**	0.23	730	809
C_{20} isoheptylfluorene	**7.4**	0.06[p]	501	**26 915**
Three-ring aromatics*				
C_{15} 4-methylphenanthrene (2531-84-2)	4.9	0.20	789	851
Four-ring aromatics				
C_{16}	5.2 (expt.)	0.13	516	563

fluoranthene (206-44-0)				

[a] Metabolic rate constant normalized to middle trophic level fish in Arnot-Gobas three trophic level model (2004) at weight = 184 g, temperature = 10°C, lipids = 6.8%) based on estimated QSAR vaues from BCFBAF v3.01, unless otherwise indicated.
[b] Arnot-Gobas BCF and BAF predictions for midde trophic level fish using three trophic level model (Arnot and Gobas 2004) using normalized rate constant and correcting for observed or estimated dietary assimilation efficiency reported in Tables A5.7a and A5.7b (Appendix 5).
[c] Based on rate constant for C_{15} *n*-pentadecane.
[d] Based on BCF and BMF rate constant for C_{15} 2,6,10-trimethyldodecane.
[e] Based on rate constant for C_9 1,2,3-trimethylbenzene.
[f] Based on rate constant data for octylcyclohexane.
[g] Based on rate constant for *n*-octane.
[h] Based on rate constant data for isopropyldecalin and diisopropyldecalin.
[i] Based on rate constant data for isopropyl hydrophenanthrene and 1-methyl-7-(isopropyl)-hydrophenanthrene.
[j] Based on rate constant data for octahydrochrysene, perhydrochrysene and hexahydrochrysene.
[k] Based on rate constant data for dodecahydrochrysene.
[l] Based on rate constant data for octylbenzene and decylbenzene.
[m] Based on rate constant data for octahydrophenanthrene.
[n] Based on rate constant data for dodecahydrochrysene.
[o] Based on rate constant data for ethylbiphenyl.
[p] Based on rate constant data for fluorene as worst case (more bioavailable).
[q] Bolded values refer to BAFs ≥ 5000 based on the *Persistence and Bioaccumulation Regulations* (Canada 2000a).
[*] Note: Alkanes C_{20}, isoalkanes C_{20}, two-ring cycloalkanes C_{20} and one-ring aromatics C_{20} all having values of log K_{ow} > 8 were excluded from this comparison, as model predictions may be highly uncertain for chemicals that have estimated log K_{ow} values > 8 (Arnot and Gobas 2003).
(expt.) = experimental log K_{ow} data.

Table A5.7a. Experimental BCFs for selected representative structures

	Log K_{ow}	**Study Endpoint**	**BCF or BMF Measured (L/kg ww)**	**Predicted BCF[a] (L/kg ww)**		**Predicted BAF[a] (L/kg ww)**		**Reference; species**
				Study conditions[b]	**MTL fish[c]**	**Study conditions[b]**	**MTL fish[c]**	
Alkanes								
C_8 octane[h]	5.18 (expt.)	BCF_{ss}[1]	530	537	490	560	537	JNITE 2010; carp
C_{12} *n*-dodecane[h]	6.10 (expt.)	BCF_{ss}[1]	240	240	794	251	1950	Tolls and van Dijk 2002; fathead minnow
C_{15} *n*-pentadecane	7.71	BCF_{ss}[1]	20	21	18	100	112	CITI 1992; carp
C_{15} *n*-pentadecane	7.71	BCF_{ss}[1]	26	27	23	162	182	JNITE 2010; carp
C_{16} *n*-hexadecane[h]	8.20	BCF_{ss}[1]	46	47	41	1778	1995	CITI 1992; carp
C_{16} *n*-hexadecane[h]	3.15 (expt.)	BCF_{ss}[1]	20	20	20	21	21	JNITE 2010; carp

Isoalkanes								
C_{15} 2,6,10-trimethyl-dodecane[h]	7.49	BCF_{ss}[1]	152	151 1000[d]	85 575[d]	490 16 595[d]	575 47 863[d]	EMBSI 2006a; rainbow trout
C_{15} 2,6,10-trimethyl-dodecane[h]	7.49	$BMF_{kinetic}$	0.97[f]	n/a	n/a	n/a	n/a	EMBSI 2004a, 2005b; rainbow trout
One-ring cycloalkanes								
C_6 cyclohexane[h]	3.44 (expt.)	BCF_{ss}[1]	77	77	89	77	89	CITI 1992; carp
C_7 1-methylcyclohexane[h]	3.61 (expt.)	BCF_{ss}[1]	240	190*	275*	229*	426*	CITI 1992; carp
C_8 ethylcyclohexane[h]	4.56 (expt.)	BCF_{ss}[1]	2529	1622*	2344*	4467*	5495*	CITI 1992; carp
C_{14} *n*-octylcyclohexane[h]	7.0	$BMF_{kinetic}$	0.06	n/a	n/a	n/a	n/a	EMBSI 2006a; BMF rainbow trout
Two-ring cycloalkanes								
C_{10} trans-decalin[h]	4.20	BCF_{ss}[1]	2200	724*	1072*	1288*	1660*	CITI 1992; carp
C_{10} cis-decalin[h]	4.20	BCF_{ss}[1]	2500	724*	1072*	1288*	1660*	CITI 1992; carp
C_{13} isopropyldecalin[h]	5.50	$BMF_{kinetic}$	0.02	n/a	n/a	n/a	n/a	EMBSI 2006a; BMF rainbow trout
C_{16} diisopropyldecalin[h]	6.85	$BMF_{kinetic}$	0.1	n/a	n/a	n/a	n/a	EMBSI 2008a; BMF rainbow trout
Polycycloalkanes								
C_{17} isopropylhydro-phenanthrene[h]	6.5	$BMF_{kinetic}$	0.45	n/a	n/a	n/a	n/a	EMBSI 2006b; BMF rainbow trout
C_{18} 1-methyl-7-(isopropyl)-hydro-phenanthrene[h]	7.0	$BMF_{kinetic}$	0.35	n/a	n/a	n/a	n/a	EMBSI 2008a; BMF rainbow trout
C_{18}	6.0	$BMF_{kinetic}$	0.38	n/a	n/a	n/a	n/a	EMBSI

per-hydrochrysene[h]								2008b; BMF rainbow trout
One-ring aromatics								
C_9 1,2,3-trimethyl-benzene[h]	3.66 (expt.)	BCF_{ss}[1]	133[e]	135	155	135	155	CITI 1992; carp
C_{10} 1,2-diethylbenzene[h]	3.72 (expt.)	BCF_{ss}[1]	516[e]	245*	355*	309*	427*	CITI 1992; carp
C_{11} 1-methyl-4-tertbutylbenzene[h]	3.66 (expt.)	BCF_{ss}[1]	< 1.0	214*	309*	263*	263*	JNITE 2010; carp
C_{14} *n*-octylbenzene[h]	6.3 (expt.)	$BMF_{kinetic}$	0.02[f]	n/a	n/a	n/a	n/a	EMBSI 2007a, 2007b; BMF rainbow trout and carp
C_{16} decylbenzene[h]	7.4 (expt.)	$BMF_{kinetic}$	0.18	n/a	n/a	n/a	n/a	EMBSI 2005d; BMF rainbow trout
Cycloalkane monoaromatics								
C_{10} tetralin	3.49 (expt.)	BCF_{ss}[1]	230	145*	214*	166*	562*	CITI 1992; carp
C_{14} octahydro-phenanthrene[h]	5.9	BCF_{ss}[1]	3418	n/a	n/a	n/a	n/a	EMBSI 2005d; BCF rainbow trout
C_{14} octahydro-phenanthrene[h]	5.9	$BMF_{kinetic}$[1]	0.13	n/a	n/a	n/a	n/a	EMBSI 2009; BMF rainbow trout
C_{18} dodecahydro-chyrsene[h]	6.00	BCF_{ss}[1]	4588	n/a	n/a	n/a	n/a	EMBSI 2008c; rainbow trout
C_{18} dodecahydro-chyrsene[h]	6.00	$BMF_{kinetic}$[1]	0.17	n/a	n/a	n/a	n/a	EMBSI 2010a; BMF rainbow trout
Two-ring aromatics								
C_{10} naphthalene	3.30 (expt.)	BCF_{ss}[1]	94	95*	138*	105*	148*	JNITE 2010; carp

	3.30 (expt.)	BCF_{ss}[1]	93[e]	95*	138*	105*	148*	CITI 1992; carp
C_{11} 2-methylnaphthalene[h]	3.86 (expt.)	BCF_{ss}[1] $BMF_{kinetic}$[1]	2886[e] 3930[f]	2884*	n/a	2884*	n/a	Jonsson et al. 2004; sheepshead minnow
C_{12} 1,3-dimethyl-naphthalene[h]	4.42 (expt.)	BCF_{ss}[1] $BMF_{kinetic}$[1]	4039[e] 5751[f]	4073	n/a	4073	n/a	Jonsson et al. 2004; sheepshead minnow
C_{13} 2-isopropyl-naphthalene[h]	4.63	BCF_{ss}[1] $BMF_{kinetic}$[1]	12 902[e] 33 321[f]	12 882	n/a	12 882	n/a	Jonsson et al. 2004; sheepshead minnow
C_{14} 4-ethylbiphenyl[h]	4.80	BCF_{ss}[1]	839[e]	832	759	851	813	Yakata et al. 2006; carp
Cycloalkane diaromatics								
C_{12} acenaphthene	3.92 (expt.)	BCF_{ss}[1]	991[e]	389	562	977	741	CITI 1992; carp
C_{18} hexahydroterphenyl[h]	6.44	BCF_{ss}[1]	1646	n/a	n/a	n/a	n/a	EMBSI 2008c; rainbow trout
C_{18} hexahydroterphenyl[h]	6.44	$BMF_{kinetic}$	0.06	n/a	n/a	n/a	n/a	EMBSI 2009; rainbow trout
C_{18} octahydrochrysene[h]	6.0	$BMF_{kinetic}$	0.05	n/a	n/a	n/a	n/a	EMBSI 2010a; BMF rainbow trout
C_{18} hexahydrochrysene[h]	5.8	$BMF_{kinetic}$	0.05	n/a	n/a	n/a	n/a	EMBSI 2010a; BMF rainbow trout
Three- and Four-ring aromatics								
C_{12} acenaphthylene[h]	3.94 (expt.)	BCF_{ss}[1]	275[e]	275	380	275	390	Yakata 2006; Carp
C_{13} fluorene[h]	4.18 (expt.)	BCF_{ss}[1]	1030[e]	1023	1071	1023	3311	CITI 1992 (carp); Carlson et al. 1979 (fathead minnow)
C_{14} phenanthrene[h]	4.46 (expt.)	BCF_{ss}[1]	2944[e]	2951	1905*	2884	3890*	Carlson et al. 1979; fathead minnow

C_{16} fluoranthene[h]	5.16 (expt.)	BCF_{ss}[1]	277[e]	275	646	281	724	EMBSI 2007a, 2007b (cited in Lampi et al. 2010); rainbow trout
C_{16} fluoranthene[h]	5.16 (expt.)	BCF_{ss}[1]	1700	1698	1288	1820	1621	Carlson et al. 1979 (cited in Lampi et al. 2010); fathead minnow
C_{16} fluoranthene[h]	5.16 (expt.)	BCF_{ss}[1]	0.021[f]	n/a	n/a	n/a	n/a	EMBSI, 2007a, 2007b 2008b, 2009; BMF; rainbow trout
C_{18} 1-methyl-7-(1-methylethyl)-phenanthrene[h]	6.4	$BMF_{kinetic}$	0.03	n/a	n/a	n/a	n/a	EMBSI 2008a; BMF rainbow trout

[a] BCF and BAF predictions were performed using the Arnot-Gobas mass-balance kinetic model normalizing the metabolic rate constant according to fish weight, lipid content and temperature reported in study or protocol.
[b] Fish weight, lipid content and water temperature used when specified in study. For CITI/NITE tests when conditions not known, fish weight = 30 g, lipid = 4.7%, temperature = 22°C for carp in accordance with MITI BCF test protocol. When more than one study was reported, the geomean of study values was used for model normalization inputs.
[c] Kinetic mass-balance predictions made for middle trophic level fish (weight = 184 g, temperature = 10°C, lipid = 6.8%) in Arnot-Gobas three trophic level model (Arnot and Gobas 2004).
[d] Calculated using growth-rate-corrected elimination half-life reported in BCF study.
[e] Geometric mean of reported steady-state values.
[f] Geometric mean of reported kinetic values.
[g] Corrected BAF using dietary assimilation efficiency of 3.2%.
[h] Structures that are included as analogues for the chosen representative structures.
*Predictions generated with metabolism rate equal to zero due to negative predicted metabolism rate constant. Metabolism rate constant deemed erroneous or not applicable given log K_{ow} and BCF result (see kinetic rate constants table).
n/a – not applicable; study details could not be obtained to determine predicted BCFs and BAFs.

Table A5.7b. Calculated kinetic rate constants for selected representative structures of gas oils

Substance	**Study endpoint**	**Uptake rate constants day^{-1} (k_1)**	**Total elimination rate constant day^{-1} (k_T)[b]**	**Gill elimination rate constant day^{-1}**

				(k_2)
Alkanes				
C_8 octane[e]	BCF_{ss}[1]	406	0.742	0.077
C_{12} *n*-dodecane[e]	BCF_{ss}[1]	1525	5.00	0.035
C_{15} *n*-pentadecane	BCF_{ss}[1]	407	1.69	0.000
C_{15} *n*-pentadecane	BCF_{ss}[1]	407	1.30	0.000
C_{16} *n*-hexadecane[e]	BCF_{ss}[1]	407	0.252	0.000
C_{16} *n*-hexadecane[e]	BCF_{ss}[1]	379	19.28	5.720
Isoalkanes				
C_{15} 2,6,10-trimethyldodecane[e]	BCF_{ss}[1]	1317	0.2103[b] 1.139	0.000[c] 0.005
C_{15} 2,6,10-trimethyldodecane[e]	$BMF_{kinetic}$		0.071 0.036[d]	0.000
One-ring cycloalkanes				
C_6 cyclohexane[e]	BCF_{ss}[1]	392	5.090	3.031
C_7 1-methylcyclohexane[e]	BCF_{ss}[1]	397	2.081	2.072
C_8 ethylcyclohexane[e]	BCF_{ss}[1]	405	0.247	0.238
C_{14} *n*-octylcyclohexane[e]	$BMF_{kinetic}$		0.130 0.095	0.000
Two-ring cycloalkanes				
C_{10} trans-decalin[e]	BCF_{ss}[1]	404	0.519	0.510
C_{10} cis-decalin[e]	BCF_{ss}[1]	404	0.551	0.542
C_{13} isopropyldecalin[e] and C_{16} diisopropyldecalin[e]	$BMF_{kinetic}$		0.478 0.136	0.000
Polycycloalkanes				
C_{17} isopropylhydrophenanthrene[e]	$BMF_{kinetic}$		0.078 0.043	0.000
C_{18} 1-methyl-7-(isopropyl)-hydro-phenanthrene[e]	$BMF_{kinetic}$		0.071 0.036	0.000
C_{18} perhydrochrysene[e]	$BMF_{kinetic}$		0.091 0.056	0.000
One-ring aromatics				
C_9 1,2,3-trimethylbenzene[e]	BCF_{ss}[1]	398	2.989	1.852
C_{10}	BCF_{ss}[1]	398	1.679	1.617

1,2-diethylbenzene[e]				
C_{11} 1-methyl-4-tertbutylbenzene[e]	BCF_{ss}[1]	398	398.2	1.852
C_{14} *n*-octylbenzene[e]	$BMF_{kinetic}$		0.643 0.608	0.000
C_{16} decylbenzene[e]	$BMF_{kinetic}$		0.324 0.289	0.000
Cycloalkane monoaromatics				
C_{10} tetralin	BCF_{ss}[1]	394	2.720	2.711
C_{14} octahydrophenanthrene[e]	BCF_{ss}[1]			
C_{14} octahydrophenanthrene[e]	$BMF_{kinetic}$[1]		0.239 0.204	0.000
C_{18} dodecahydrochrysene[e]	BCF_{ss}[1]	n/a	n/a	n/a
C_{18} dodecahydrochrysene[e]	$BMF_{kinetic}$[1]		0.174 0.139	0.000
Two-ring aromatics				
C_{10} naphthalene	BCF_{ss}[1]	387	4.138	4.129
C_{11} 2-methylnaphthalene[e]	BCF_{ss}[1] $BCF_{kinetic}$[1]	 1089	0.610[d] 0.610	 0.607
C_{12} 1,3-dimethylnaphthalene[e]	BCF_{ss}[1] $BCF_{kinetic}$[1]	2322[d] 1100	0.406[d] 0.406	 0.403
C_{13} 2-isopropylnaphthalene[e]	BCF_{ss}[1] $BCF_{kinetic}$[1]	3961[d]	0.120[d] 0.120	 0.551[f]
C_{14} 4-ethylbiphenyl[e]	BCF_{ss}[1]		1.140	0.480
Cycloalkane diaromatics				
C_{12} acenaphthene	BCF_{ss}[1]	401	1.037	1.028
C_{18} hexahydroterphenyl[e]	BCF_{ss}[1]	n/a	n/a	n/a
C_{18} octahydrochrysene[e]	$BMF_{kinetic}$		1.424 1.390	0.000
C_{18} hexahydrochrysene[e]	$BMF_{kinetic}$		1.424 1.390	0.000
Three- and Four-ring aromatics				
C_{12} acenaphthylene[e]	BCF_{ss}[1]	456	1.611	1.273
C_{13} fluorene[e]	BCF_{ss}[1]	622	0.901	0.892
C_{13}	$BMF_{kinetic}$[1]		0.100 (k_e)	0.000

fluorene[e]				
C_{14} phenanthrene[e]	BCF_{ss}[1]	957	0.833	0.821
C_{16} fluoranthene[e]	BCF_{ss}[1]	197	0.548	0.151
C_{18} 1-methyl-7-(1-methylethyl)-phenanthrene[e]	$BMF_{kinetic}$		1.815 1.78	0.000

Table A5.7b cont. Calculated kinetic rate constants for selected representative structures of gas oils

Substance	**Study endpoint**	**Metabolic rate constant day^{-1} (k_M)[a]**	**Growth rate constant day^{-1} (k_G)**	**Fecal egestion rate constant day^{-1} (k_E)[c]**	**Dietary assimilation efficiency (α, E_D)**	**Reference; species**
Alkanes						
C_8 octane[e]	BCF_{ss}[1]	0.657	0.001	0.007		JNITE 2010; carp
C_{12} *n*-dodecane[e]	BCF_{ss}[1]	4.95	0.002	0.013		Tolls and van Dijk 2002; fathead minnow
C_{15} *n*-pentadecane	BCF_{ss}[1]	1.69	0.001	0.003		CITI 1992; carp
C_{15} *n*-pentadecane	BCF_{ss}[1]	1.30	0.001	0.003		JNITE 2010; carp
C_{16} *n*-hexadecane[e]	BCF_{ss}[1]	0.249	0.001	0.002		CITI 1992; carp
C_{16} *n*-hexadecane[e]	BCF_{ss}[1]	13.30	0.001	0.008		JNITE 2010; carp
Isoalkanes						
C_{15} 2,6,10-trimethyl-dodecane[e]	BCF_{ss}[1]	0.158[h] 1.119	0.0425[d] 0.008	0.002 0.005		EMBSI 2004b, 2005b; rainbow trout
C_{15} 2,6,10-trimethyl-dodecane[e]	$BMF_{kinetic}$	0.032[h]	0.035	0.004	28%[e]	EMBSI 2004a, 2005a; rainbow trout
One-ring cycloalkanes						
C_6 cyclohexane[e]	BCF_{ss}[1]	2.050	0.001	0.008		CITI 1992; carp
C_7 1-methylcyclohexane[e]	BCF_{ss}[1]	-0.429	0.001	0.008		CITI 1992; carp

C_8 ethylcyclohexane[e]	BCF_{ss}[1]	-0.087	0.001	0.008		CITI 1992; carp
C_{14} *n*-octylcyclohexane[e]	$BMF_{kinetic}$	0.087[h]	0.035	0.008	5%	EMBSI 2006a; BMF rainbow trout
Two-ring cycloalkanes						
C_{10} trans-decalin[e]	BCF_{ss}[1]	-0.336	0.001	0.008		CITI 1992; carp
C_{10} cis-decalin[e]	BCF_{ss}[1]	-0.390	0.001	0.008		CITI 1992; carp
C_{13} isopropyldecalin[e] and C_{16} diisopropyldecalin[e]	$BMF_{kinetic}$	0.128[h]	0.035	0.008	6%	EMBSI 2006a
Polycycloalkanes						
C_{17} isopropyl-hydrophenanthrene[e]	$BMF_{kinetic}$	0.035[h]	0.035	0.008	13%	EMBSI 2006b; rainbow trout
C_{18} 1-methyl-7-(isopropyl)-hydrophenanthrene[e]	$BMF_{kinetic}$	0.030[h]	0.035	0.006	9%	EMBSI 2008a; rainbow trout
C_{18} perhydrochrysene[e]	$BMF_{kinetic}$	0.048[h]	0.035	0.008	15%	EMBSI 2008b; rainbow trout
One-ring aromatics						
C_9 1,2,3-trimethylbenzene[e]	BCF_{ss}[1]	1.128	0.001	0.008		CITI 1992; carp
C_{10} 1,2-diethylbenzene[e]	BCF_{ss}[1]	-0.854	0.001	0.008		CITI 1992; carp
C_{11} 1-methyl-4-tertbutyl-benzene[e]	BCF_{ss}[1]	395.6	0.001	0.008		JNITE 2010; carp
C_{14} *n*-octylbenzene[e]	$BMF_{kinetic}$	0.600[h]	0.035	0.008	10%	EMBSI 2007a, 2007b; BMF rainbow trout and carp
C_{16} decylbenzene[e]	$BMF_{kinetic}$	0.284[h]	0.035	0.005		EMBSI 2005c; BMF rainbow

						trout
Cycloalkane monoaromatics						
C_{10} tetralin	BCF_{ss}[1]	-1.009	0.001	0.008		CITI 1992; carp
C_{14} octahydro-phenanthrene[e]	BCF_{ss}[1]					EMBSI 2005d; BCF rainbow trout
C_{14} octahydro-phenanthrene[e]	$BMF_{kinetic}$[1]	0.197[h]	0.035	0.007	19%	EMBSI 2009; BMF rainbow trout
C_{18} dodecahydro-chyrsene[e]	BCF_{ss}[1]	n/a	n/a	n/a	n/a	EMBSI 2008c; rainbow trout
C_{18} dodecahydro-chyrsene[e]	$BMF_{kinetic}$[1]	0.132[h]	0.035	0.007	18%	EMBSI 2008c; rainbow trout
Two-ring aromatics						
C_{10} naphthalene	BCF_{ss}[1]	-0.020	0.001	0.008		JNITE 2010; carp
C_{11} 2-methylnaphthalene[e]	BCF_{ss}[1] $BCF_{kinetic}$[1]	0.000	0.002	0.001	3.2%[g]	Jonsson et al. 2004; sheepshead minnow
C_{12} 1,3-dimethyl-naphthalene[e]	BCF_{ss}[1] $BCF_{kinetic}$[1]	0.000	0.002	0.001	3.2%[g]	Jonsson et al. 2004 (cited in Lampi et al. 2010); sheepshead minnow
C_{13} 2-isopropyl-naphthalene[e]	BCF_{ss}[1] $BCF_{kinetic}$[1]	-0.447	0.002	0.014	3.2%[g]	Jonsson et al. 2004; sheepshead minnow
C_{14} 4-ethylbiphenyl[e]	BCF_{ss}[1]	0.645	0.002	0.013		Yakata et al. 2006; carp
Cycloalkane diaromatics						
C_{12} acenaphthene	BCF_{ss}[1]	-0.632	0.001	0.008		CITI 1992; carp
C_{18} hexahydroterphenyl[e]	BCF_{ss}[1]	n/a	n/a	n/a	n/a	EMBSI 2008c;

						rainbow trout
C_{18} octahydrochrysene[e]	$BMF_{kinetic}$	1.383[h]	0.034	0.007	55%	EMBSI 2010a; BMF rainbow trout
C_{18} hexahydrochrysene[e]	$BMF_{kinetic}$	1.383[h]	0.034	0.007	49%	EMBSI 2010a; BMF rainbow trout
Three- and Four-ring aromatics						
C_{12} acenaphthylene[e]	BCF_{ss}[1]	0.370	0.001	0.010		Yakata et al. 2006; carp
C_{13} fluorene[e]	BCF_{ss}[1]	-0.302	0.001	0.012		CITI 1992; Carlson et al. 1979; fathead minnow
C_{13} fluorene[e]	$BMF_{kinetic}$[1]	0.098	n/a	0.002	14%	Niimi and Palazzo 1986
C_{14} phenanthrene[e]	BCF_{ss}[1]	-0.512	0.002	0.012		Carlson et al. 1979; fathead minnow
C_{16} fluoranthene[e]	BCF_{ss}[1]	0.383	0.002	0.012		Carlson et al. 1979
C_{18} 1-methyl-7-(1-methylethyl)-phenanthrene[e]	$BMF_{kinetic}$	1.773[h]	0.035	0.007	4%	EMBSI 2008a; BMF rainbow trout

[a] Negative values of k_M indicate possible kinetic model error, as the estimated rate of metabolism exceeds the total of all other elimination rate constants combined. Observed BCFs may thus not be explained by kinetic modelling of metabolic rate (e.g., steric hindrance, low bioavailability) and could also point to study exposure error. Negative values of k_M are not included in the estimate of k_T.
[b] $k_T = (k_E + k_G)$.
[c] Calculated using kinetic mass-balance BCF or BAF model based on reported rate kinetics of empirical study and correcting for log K_{ow}, fish body weight, temperature and lipid content of fish from cited study.
[d] As reported in empirical study (geomean used when multiple values reported).
[e] Structures that are included as analogues for the chosen representative structures.
[f] Value adjusted so that predicted k_T agrees with observed k_2 reported in study.
[g] Based on assimilation efficiency data for 6-*n*-butyl-2,3-dimethylnaphthalene.
[h] Calculated using kinetic mass-approach when k_e is known (Arnot et al. 2008a) and correcting for log K_{ow}, fish body weight, temperature and lipid content of fish from cited study.
[1] BCF steady state (tissue conc./water conc.).
n/a – not applicable; study details could not be obtained to determine predicted BCFs and BAFs.

Table A5.8. Trophic magnification factors[a] (TMF) for PAH in the marine food webs of Bohai Bay, Baltic Sea and Tokyo Bay

Compound	TMF (Wan et al. 2007)	TMF (Nfon et al. 2008)	TMF (Takeuchi et al. 2009)
acenaphthylene	0.45*		
acenaphthene	1.02		
phenanthrene	0.43	0.82*	0.75*

[a] Antilogs of the slopes of the regression equations for the lipid-based PAH concentrations versus $\delta^{15}N$ were used to calculate the TMFs.
* Indicates a significant TMF slope.

Table A5.9. Modelled acute aquatic toxicity data for CAS RN 64741-59-9 (PETROTOX 2009)[a]

Test organism	Common name	LL_{50}[b] (mg/L) 80:20 Ar:Al	LL_{50}[b] (mg/L) 61:39 Ar:Al
Palaemonetes pugio	Grass shrimp	0.13	0.44
Rhepoxynius abronius	Marine amphipod	0.06	0.08
Neanthes arenaceodentata	Marine worm	1.13	2.55
Nitocra spinipes	Harpacticoid copepod	1.11	2.49
Oitona davisae	Marine copepod	0.65	1.36
Portunus pelagicus	Blue crab	0.12	0.19
Menidia beryllina	Inland silverside	3.78	9.83

[a] PETROTOX was run in the low resolution mode that requires only an aromatic to aliphatic ratio and a boiling point range for each hydrocarbon block.
[b] LL_{50} refers to lethal loading, the amount of substance necessary to be added in order to kill 50% of test organisms (Ar:Al, aromatic: aliphatic ratio).

Table A5.10. Aquatic toxicity of Fuel Oil No. 2

Organism	Common name	Duration	Endpoint	Test type	Value (mg/L)	Reference
Fundulus similis	Longnose killifish	48 hours (acute)	LC_{50}	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 (acute)	LC_{50}	WSF	2.2	MacLean and Doe 1989
Artemia spp.	Brine shrimp	48 hours (acute)	LC_{50}	WSF	11.2	MacLean and Doe

						1989
Lucifer faxoni	Planktonic shrimp	48 hours (acute)	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 A5.11. Aquatic toxicity of diesel fuel

Organism	**Common name**	**Duration**	**Endpoint**	**Test type**	**Value (mg/L)**	**Reference**
Oncorhynchus mykiss	Rainbow trout	48 hours (acute)	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

Table A5.12. Estimated volume of water in contact with medium persistence oil for loading and transport processes via ship for various spill sizes (RMRI 2007)

	Volume of water in contact with oil ($\times 10^6$ m^3)	
Spill size (barrels)	**Loading**	**Transport**
1–49	40	5300
50–999	60	5500
1000–9999	150	8100
10 000–99 999	500	14 000
100 000–199 999	3500	37 000
>200 000	33 000	62 000

Table A5.13. An analysis of modelled and experimental persistence and bioaccumulation data on petroleum hydrocarbons with respect to the Canadian *Persistence and Bioaccumulation Regulations* (Canada 2000)[a]

C#	**C_9**	**C_{10}**	**C_{12}**	**C_{13}**	**C_{14}**	**C_{15}**	**C_{18}**	**C_{20}**	**C_{22}**
***n*-Alkanes**	*						*	*	*
***i*-Alkanes**	*					B	*	*	*
Monocycloalkane	*		*	*	*	B	*	*	*

Dicycloalkane	*		*	*	*	**PB**	P*	P*	*
Polycycloalkane	(-)	(-)	(-)	(-)	**PB**	P	P	P	**PB**
Monoaromatic		*	*	*	*	B	*	*	*
Cycloalkane monoaromatic	*		*	*	*	**PB**	**PB**	**PB**	*
Diaromatic	(-)					P	*	*	*
Cycloalkane diaromatic	(-)	(-)	P				*	B	*
Three-ring PAH	(-)	(-)	*	*	*		*	*	*
Four-ring PAH	(-)	(-)	(-)	(-)	(-)	(-)	*	*	*

[a] Bioaccumulation potential for carbon number with no experimental data will be assumed to be the same as for carbon numbers bracketing them. For example, the C_{15} and C_{20} cycloalkane monoaromatics were found to bioaccumulative, therefore, the carbon numbers between the ranges of C_{15}–C_{20} for the cycloalkane monoaromatics will be assumed to be bioaccumulative.

P = Predicted persistence based on data from BioHCWin (2008), BIOWIN (2008), CATABOL (c2004–2008) and TOPKAT (2004).

B = Predicted fish BCFs and/or BAFs using the Arnot-Gobas three trophic level model (2003) with corrections for metabolism rate (k_M) and dietary assimilation efficiency (E_d).

PB = representative structures that are potentially persistent and bioaccumulative.

Blank cells mean the representative structures are neither persistent nor bioaccumulative.

(-) indicates that no such carbon numbers exist within the group.

* Not modelled for bioaccumulation as there was no chosen representative structure, or the representative structure was excluded due to a log K_{ow} > 8 as model predictions may be highly uncertain for chemicals that have estimated log K_{ow} values > 8 (Arnot and Gobas 2003).

Appendix 6: Modelling results for human exposure to industry-restricted gas oils

Table A6.1. Variable inputs to SCREEN3

Variables	Input
Source type	Area
Effective emission area[a]	50 m × 10 m (for ships)
Emission rate	7.4×10^{-5} g/s·m^{2} [b]
Receptor height[c]	1.74 m
Source release height[a]	3 m
Adjustment factor for highest 1 h to 24 h wind averaging[d]	0.4
Urban/rural option	Urban
Meteorology[e]	1 (full meteorology)
Minimum and maximum distance to use	50–3000 m

[a] Professional judgement.
[b] Emission rate (g/s) is available in Table A6.2.
[c] Curry et al. (1993).
[d] U.S. EPA (1992).
[e] Default value in SCREEN3 (1996).

Table A6.2. Estimated regular evaporative emissions of gas oil to air in transit in Canada, 2004–2005

Substance	Estimated regular evaporative emissions to air		
	kg/year	kg/day[a]	g/s
Industry-restricted gas oil	1100	3.2	3.7×10^{-2}

[a] The Risk Management Research Institute (RMRI 2007) summarized the industry-related shipping traffic in Placentia Bay, Newfoundland and Labrador, during 2004–2005, showing approximately 3900 transits per year from tankers, bulk cargo, tugboat or other means. For the Come By Chance refinery only, more than approximately 230 tanker transits per year are related to shipping petroleum substances. Thus, it is reasonable to assume an average transportation period of 350 days/year for marine transportation.

Table A6.3. Modelling results of industry-restricted gas oil dispersion profile in ambient air with 24-hour averaging of wind direction in Canada using SCREEN3

Substance	Maximum concentration with 24-hour wind averaging (µg/m^3)[a]			
	50 m	1000 m	2000 m	3000 m
Industry-restricted gas oil	150	1.0	0.36	0.21

[a] These estimations are conservative, as they are based on release from a stationary source. The actual concentration in ambient air in the vicinity of the moving release source, for any given location, will be considerably lower than that represented by the modelling results based on a stationary release source.

Appendix 7: Summary of health effects information for the industry-restricted gas oils

Table A7.1. Critical health effects information on gas oil substances

Endpoints	CAS RNs[a]	Effect levels[b]/results
Acute health effects	64741-59-9	**Lowest oral LD_{50}** (female rat): 3200 mg/kg-bw for sample API 83-07 (API 1982, 1985a). **Lowest inhalation LC_{50}** (male rat): 3350 mg/m^3 for sample API 83-07 (API 1986a). **Lowest dermal LD_{50}** (rabbit): > 2000 mg/kg-bw for samples API 83-07 and API 83-08 (API 1982, 1985a,b).
	64741-82-8	No studies identified.
Short-term repeated-exposure health effects	64741-59-9	**Lowest dermal LOAEL:** 50 mg/kg-bw per day was identified based on decreased maternal rat body weight gain and body weight (likely due to reduced feed consumption), as well as skin irritation. Pregnant Sprague-Dawley rats were exposed to 0, 25, 50, 125, 250 and 500 mg/kg-bw per day of Mobil LCO on GDs 0–19 and to 1000 mg/kg-bw per day on GDs 6–15. Increased cholesterol and triglycerides were observed at doses ≥ 250 mg/kg-bw per day, and severe sensory irritation was noted at doses ≥ 500 mg/kg-bw per day (Mobil 1988a). **Other dermal studies:** API 83-07 (0, 250, 500 and 1000 mg/kg-bw per day) and API 83-08 (0, 200, 1000 and 2000 mg/kg-bw per day) were applied to the clipped dorsal skin of New Zealand White rabbits (five of each sex per group) 3 times per week for 4 weeks. Dose-dependent skin irritation was observed, from no irritation in the control groups to moderate and severe irritation in the test groups. Histological examination revealed moderate to severe proliferation and inflammation in the high-dose groups. Other findings were not considered treatment related and included decreased body weight gain and body weight, reduced ovary weight, hypoplasia of the seminiferous tubules and mortality (API 1985c,d).
	64741-82-8	**Dermal study:** Doses of 15, 60, 250 or 500 mg/kg-bw per day were applied to the shaved dorsal skin of pregnant Sprague-Dawley rats (10 animals per dose) from GD 0–19. Decreased maternal body weight and feed consumption were observed at 250 and 500 mg/kg-bw per day. Moderate to severe skin irritation, erythema, flaking, scabbing and thickening of the skin were noted to occur at an unspecified dose (Mobil 1988b).
	64742-80-9 (hydrodesulfurized middle distillates)	**Lowest inhalation LOAEC:** 25 mg/m^3 was identified based on microscopic changes in nasal tissue and subacute inflammation of the respiratory mucosa in rats. Male and female Sprague-Dawley rats (20 animals of each sex) were exposed to test substances API 81-09 and API 81-10 at a

Endpoints	CAS RNs[a]	Effect levels[b]/results
		single concentration of 25 mg/m^3 for 6 hours/day, 5 days/week, for 4 weeks. An approximate 30% increase in leukocytes 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 1986c).
Subchronic repeated-exposure health effects	64741-59-9	**Dermal NOAEL:** 25 mg/kg-bw per day. Male Sprague-Dawley rats were exposed to Mobil LCO at 0, 8, 25, 125, 500 or 1250 mg/kg-bw per day, 5 times per week for 13 weeks (the highest dose was applied for only 2 weeks). Test substance was applied unoccluded to the clipped back skin of 10 animals of each sex per group. Dose-dependent, slightly reduced thymus weights (likely due to lymphocyte depletion) were observed at 125 mg/kg-bw per day. Severe erythema and edema with visibly thick, stiffened skin were observed in the 500 mg/kg-bw per day group; histological examination confirmed moderate chronic inflammatory changes in the skin and hair follicles. Systemic toxicity was noted at 500 and 1250 mg/kg-bw per day (Mobil 1985). **Other dermal study:** In a similar study, a statistically significant increase in relative liver weights occurred in male and female Sprague-Dawley rats (TAC:N(SD)fBR MPF) dermally exposed to LCO at 500 mg/kg-bw per day for 13 weeks (Feuston et al. 1994). Liver weights of animals exposed to 1250 mg/kg-bw per day were not reported.
	64741-82-8	**Lowest dermal LOAEL:** 30 mg/kg-bw per day was identified based on increased lymphocytes in female rats and a 10% decrease in thymus weight in male rats. Sprague-Dawley rats (10 animals of each sex per group) were exposed 5 days/week for 13 weeks to 30, 125, 500 or 2000 mg/kg-bw via application of the substance to shaved skin. At doses ≥ 125 mg/kg-bw, changes in megakaryocytes, increased lymphocytes and decreased body weight in male rats were observed. Additional effects were observed at doses ≥ 500 mg/kg-bw, including severe skin irritation and decreased body weight in females. Daily exposure to the highest dose, 2000 mg/kg-bw, resulted in increased leukocytes 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 study:** Sprague-Dawley rats were exposed to 30, 125, 500 or 2000 mg/kg-bw per day of test substance 5 days/week for 13 weeks. Increased relative liver weights in male and female rats were noted at

Endpoints	CAS RNs[a]	Effect levels[b]/results
		125 mg/kg-bw per day. Other possible effects, noted at unspecified doses, included decreased body and thymus weights, skin irritation and altered serum chemistry and hematology. However, the study examined several different substances, and the authors did not explicitly state whether any or all of the latter aforementioned effects were due to CAS RN 64741-82-8 (Feuston et al. 1994).
	68334-30-5 (diesel fuel)	**Lowest inhalation LOAEC:** 250 mg/m^3 was identified based on decreased body weight and increased response time in an acoustic startle reflex assay (no histological changes in the nervous system were noted, however) in rats. Male and female Sprague-Dawley rats (24 animals of each sex per concentration) were exposed to diesel fuel at 250, 750 or 1500 mg/m^3 for 4 hours/day, 2 days/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).
Carcinogenicity	64741-59-9	***Chronic dermal studies*** **Lowest dermal effect level:** 343 mg/kg-bw per day. A statistically significant ($p < 0.05$) increase in the number of mice with squamous cell carcinomas or papillomas occurred after long-term dermal exposure to 343 mg/kg-bw per day of MD-7 LCO. Groups of male mice (C3H/HeNCrlBR; 50 per group) were exposed daily for 104 weeks to 35 µL of highly refined mineral oil (negative control), 50 µL of 5% heavy clarified oil (positive control), 28.5% MD-7 LCO (7 times per week = 343 mg/kg-bw per day[c,d,e,f]), 50% MD-7 LCO (4 times per week = 601 mg/kg-bw per application[c,d,e,f]) or 100% MD-7 LCO (2 times per week = 1203 mg/kg-bw per application[c,d,e]). Of mice exposed to 28.5% (343 mg/kg-bw) MD-7 LCO, 7/50 developed skin tumours (compared with 0/50 in the negative control and 47/50 in the positive control), with the first tumour visible by day 301. Mice exposed to 50% (601 mg/kg-bw) MD-7 LCO also developed skin tumours (17/50, $p < 0.01$), and these were confirmed histologically (the first tumour was visible by day 266). In addition to the 17 mice with confirmed tumours in this group, other mice had unconfirmed tumours (1/50) or developed only fibrosarcomas (4/50) or melanomas (1/50). An insignificant increase in skin

Endpoints	CAS RNs[a]	Effect levels[b]/results
		tumours occurred in the group exposed to 100% (1203 mg/kg-bw) MD-7 LCO (1/50, tumour visible by day 651). The lack of tumours in this group was thought to be due to substantial cellular necrosis of skin cells due to the high concentration of the substance (Nessel et al. 1998). **Other chronic dermal studies:** Application twice weekly of 50 µL (1203 mg/kg-bw per application[c,d,e]) LCCD to the shaved interscapular region of the backs of 50 C3H/HeJ male mice for 104 weeks resulted in a statistically significant ($p < 0.05$) increased incidence of skin tumours, with 63% of mice developing at least one skin tumour (mean latency of onset = 79 weeks). Squamous cell carcinomas (13/50) and fibrosarcomas (12/50) were predominantly formed (compared with a zero tumour incidence in controls). An ~50% reduction in survival (relative to the control group) at 78 weeks was noted for mice exposed to LCCD, and only 6% survived to 104 weeks (compared with 52% of control mice) (Broddle et al. 1996). Application twice weekly of 50 µL (1203 mg/kg-bw per application[c,d,e]) LCCD to the shaved intrascapular region of the backs of 50 C3H/HeJ male mice for 104 weeks resulted in the formation of squamous cell carcinomas (54% of test mice) and papillomas (14% of test mice), as well as fibrosarcomas (24% of test mice) (39/50 test mice developed skin tumours, mean latency of onset = 40 weeks) (Skisak et al. 1994). ***Initiation/promotion dermal studies*** *Initiation*: 30 male CD-1 mice received five consecutive daily applications of 50 µL (1203 mg/kg-bw[c,d,e]) LCCD and then 50 µL of tumour promoter (phorbol-12-myristate-13-acetate) twice weekly for 25 weeks. Squamous cell papillomas and keratoacanthomas developed in 9/30 mice, but this was not considered statistically significant (3/30 tumours in the negative versus 30/30 in the positive control groups). *Promotion*: 30 mice were initiated with 50 µL 7,12-dimethylbenzanthracene and then received 50 µL (1203 mg/kg-bw[c,d,e]) LCCD twice weekly for 25 weeks. Mice treated with LCCD exhibited a statistically significant increased incidence of skin tumours (28/30 versus zero incidence in the negative control group), with a 90% incidence of squamous cell papillomas and a 33% incidence of keratoacanthomas. Two malignant tumours were noted in the LCCD-exposed group (Skisak et al. 1994).

Endpoints	CAS RNs[a]	Effect levels[b]/results
		Other dermal studies with similar results have been described in API (1989b). No oral or inhalation studies were identified.
	64741-82-8 (64741-54-4, 64741-83-9 and 64741-81-7 were also part of the test substance)	Test substance was a blend of the CAS RNs listed. Two different formulations (ARCO Base LB-7979 and Provalent 4A) were used. **Chronic dermal studies:** C3H/HeJ mice (50 animals per group) were exposed to 50 mg (1389 mg/kg-bw[c,g]) ARCO LB-7979 twice per week for 80 weeks. Substance was applied to shaved interscapular skin. Benign skin tumours developed in 2/50 exposed mice after 17 weeks of observation, with a mean latency period of 14 weeks (the positive control group, exposed to benzo[*a*]pyrene, developed 3/50 tumours after 10 weeks). Following 37 weeks of observation, 47/50 mice in the test group had skin tumours (and of the mice with tumours, 29 were moribund), with a mean latency period of 24.5 weeks (28/50 mice in the positive control group had tumours, and 9 of the 28 were moribund after 27.8 weeks). After 80 weeks of observation, 46/47 mice in the test group had skin tumours (39 malignant, 7 benign) (in the positive control group, 47/49 mice had tumours, with 32 malignancies) (ARCO 1980a,b, 1981). Provalent 4A was tested as above. After 17 weeks of observation, 16/50 exposed mice developed benign skin tumours, with a mean latency period of 15.8 weeks (3/50 mice of the positive control group had tumours after 10 weeks). Following 37 weeks of observation, 47/50 exposed mice had tumours, and 41 with tumours were moribund (mean latency period of 20.7 weeks) (27/50 mice in the positive control group had tumours after 27.8 weeks, and 9 with tumours were moribund). After 80 weeks of observation, 46/47 exposed mice had skin tumours (42 malignant, 4 benign) (47/49 in positive control, with 32 malignancies) (ARCO 1980a,b, 1981).
Reproductive and developmental health effects	64741-59-9	**Dermal reproductive LOAEL:** 1000 mg/kg-bw per day was identified based on a statistically significant increased incidence of resorptions after dermal application of 0, 25, 50, 125, 250 or 500 mg/kg-bw per day of Mobil LCO to 11-week-old pregnant CD rats (VAF/Plus Crl:CD(SD)BR) on GDs 0–19 and of 1000 mg/kg-bw per day on GDs 6–15 (Feuston et al. 1994). **Dermal developmental LOAEL:** 1000 mg/kg-bw per day was identified based on statistically significant decreased fetal body weights after dermal application of 0, 25, 50, 125, 250 or 500 mg/kg-bw per day of Mobil LCO to the

Endpoints	CAS RNs[a]	Effect levels[b]/results
		shorn dorsal skin of pregnant Sprague-Dawley rats on GDs 0–19 and of 1000 mg/kg-bw per day on GDs 0–6 and 6–15. Fetal body weights were decreased at 500 mg/kg-bw per day, but this was not statistically significant. No developmental malformations or reproductive effects were noted (Mobil 1988a).
	64741-82-8	**Dermal studies:** Doses of 15, 60, 250 or 500 mg/kg-bw were applied to the shaved dorsal skin of pregnant Sprague-Dawley rats (10 animals per group) from GD 0–19. No differences were observed in the number of females who aborted, dams with viable fetuses, dams with resorptions, corpora lutea, implantation sites, percent preimplantation loss, viable fetuses or resorptions. No differences were observed in litter sizes, viable male/female fetuses, dead fetuses, fetal body weight or fetal crown-to-rump length (Mobil 1988b). Pregnant Sprague-Dawley rats were exposed to 15 or 60 mg/kg-bw per day of test substance from GD 0–19 or to 250 mg/kg-bw per day from GD 0–15. No increased incidence of resorptions was observed (Feuston et al. 1994). Sprague-Dawley rats (10 animals of each sex per dose) were exposed to test substance at 30, 125, 500 or 2000 mg/kg-bw per day, 5 days/week for 13 weeks. No effects were observed on spermatid and spermatozoa counts or morphology of testes and epididymides. Effects in females were not reported (Mobil 1991).
	68334-30-5	**Inhalation NOAEC:** 3777 mg/m^3 for developmental toxicity. A concentration of 3777 mg/m^3 (401.5 ppm[h,i]) of diesel fuel was administered to pregnant rats from GD 6–15. No developmental effects were noted (Beliles and Mecler 1983).
	68476-34-6	**Highest 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[j,k]) of diesel fuel No. 2 were applied to Sprague-Dawley rats (10 animals of each sex per dose), 5 days/week for 4 weeks. No effects on testes or ovaries were observed (UBTL 1986).
Genotoxicity: *in vivo*	64741-59-9	**Cytogenetic assay** **Negative:** API 83-07 was administered by intraperitoneal injection to Sprague-Dawley rats (15 of each sex per group) at doses of 0, 0.2, 0.67 and 2 g/kg-bw. Bone marrow was obtained at 6, 24 and 48 h after exposure to the test substance. Lethargy and mortality were noted for some rats receiving the highest dose. API 83-07 was found not to affect the mitotic index of bone marrow cells.

Endpoints	CAS RNs[a]	Effect levels[b]/results
		Testing of API 83-08, using the same protocol, was also observed to be negative (API 1985e, 1986d). **Sister chromatid exchange assay** **Positive:** API 83-07 was positive for sister chromatid exchange when administered to mice via intraperitoneal injection at doses of 340, 1700 and 3400 mg/kg-bw (API 1989a).
	64741-82-8	No studies identified.
	68476-34-6	**Cytogenetic assay** **Positive:** Groups of male rats (five animals per dose) were exposed by intraperitoneal injection to 486, 1620 or 4860 mg/kg-bw (0.6, 2.0 or 6.0 ml/kg-bw[j,k]) of No. 2-DA 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).
	68476-30-2	**Cytogenetic assay** **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).
	68334-30-5	**Cytogenetic assay** **Positive:** Groups of Sprague-Dawley rats were exposed by intraperitoneal injection to diesel fuel at concentrations of 493, 1644 or 4933 mg/kg-bw (0.6, 2.0 or 6.0 ml/kg-bw[j,l]) for 1 or 5 days. Increased number of aberrant cells reported in bone marrow at the highest dose level (Conaway et al. 1984).
	68476-30-2 64742-46-7 64742-30-9	**Micronuclei induction** **Negative:** Groups of CD-1 mice (15 of each 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).
Genotoxicity: *in vitro*	64741-59-9	**Mutagenicity** **Positive:** Of 10 petroleum middle distillates, MD-7 LCO exhibited the highest mutagenicity index (14) in a modified Ames assay. The mutagenicity of the 10 distillates positively correlated with the percentage of three- to seven-ring hydrocarbons (PAHs) found in each distillate, and MD-7 LCO contained 8.7% PAHs (Nessel et al. 1998). **Mouse lymphoma assay** **Positive:** API 83-07 was tested at 5–80 nL/mL (without activation) and 2.5–30 nL/mL (with activation) in a forward mutation assay using the cell line L5178Y TK +/−. Cells were exposed for 4 h followed by a 2-day

Endpoints	CAS RNs[a]	Effect levels[b]/results
		recovery period. API 83-07 was negative for mutagenicity without activation but positive with activation. When tested with activation, API 83-07 exhibited a positive response for mutant frequency (API 1985f). In another study, API 83-08 was positive both with and without activation (API 1985g). **Sister chromatid exchange assay** **Equivocal:** API 83-07 was tested at 5–80 µg/mL in Chinese hamster ovary cells with and without activation. In the absence of activation, API 83-07 produced a statistically significant increase in sister chromatid exchanges per cell at 10 and 20 µg/mL (the highest concentrations for which data were available), but no concentration–response was observed. In a repeat study, an increase was statistically significant only at 30 µg/mL. With activation, API 83-07 exhibited statistically significant increases in the frequency of sister chromatid exchanges at 10, 40 and 80 µg/mL, but a clear concentration–response was not observed (API 1988).
	64741-82-8	**Mutagenicity** **Positive:** DGMK No. 8 was tested with S9 metabolic activation in *Salmonella typhimurium* TA98 using a modified Ames assay. A mutagenic index of 2.1 was observed, and the test substance contained 8% PAH content (Blackburn et al. 1984, 1986; DGMK 1991). **Positive:** Test substance was positive when tested at concentrations of 0.26–42 mg/plate, with and without S9 metabolic activation, in *S. typhimurium* TA98 and TA100 (Conaway et al. 1984).
Human studies	Case report: diesel oil	Diesel oil used over several weeks as an arm and hand cleaner resulted in epigastric and loin pains, nausea, anorexia, degeneration of kidney tubular epithelium and renal failure. The patient subsequently made a good recovery. There was no history of exposure to any other nephrotoxin (Crisp et al. 1979).
	Case–control study: diesel fuel	A case–control study of various cancers revealed an adjusted odds ratio of 1.9 (90% confidence interval 1.2–3.0) for prostate cancer in men exposed to diesel fuel. There was no evidence for a positive dose–response relationship (Siemiatycki et al. 1987).

Abbreviations: CLGO, coker light gas oil; GD, gestation day; LCCD, light catalytic cracked distillate; LCO, light cycle oil; PAH, polycyclic aromatic hydrocarbon.

[a] Different samples of CAS RN 64741-59-9 are referred to as API 83-07, API 83-08, LCCD, Mobil LCO and MD-7 LCO. CAS RN 64741-82-8 is referred to as Mobil CLGO, DGMK No. 8 and light thermal cracked distillate.

[b] 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.

[c] Body weight not provided; thus, laboratory standards from Salem and Katz (2006) were used.
[d] The following formula was used for conversion of provided values into mg/kg-bw: (% of dilution × *x* mL × ρ)/kg-bw.
[e] Density (ρ) not provided; thus, a density value from ECB (2000) was used.
[f] A volume/volume dilution was assumed.
[g] The following formula was used for conversion of provided value into mg/kg-bw: *x* mg/kg-bw.
[h] 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.
[i] MM of diesel fuel estimated to be 230 g/mol (www.epa.gov/athens/learn2model/part-two/onsite/es.html).
[j] The following formula was used for conversion of provided values into mg/kg-bw: *x* ml/kg-bw × ρ.
[k] Density (ρ) not provided; thus, a density from Khan et al. (2001) was used.
[l] Density (ρ) not provided; thus, a density from API (2003b) was used.