Final Screening Assessment
Petroleum Sector Stream Approach

Heavy Fuel Oils
[Industry-Restricted]

Chemical Abstracts Service Registry Numbers

64741-75-9
68783-08-4
70592-76-6
70592-77-7
70592-78-8

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 heavy fuel oils (HFOs):

CAS RN[a]	DSL[b] name
64741-75-9	Residues (petroleum), hydrocracked
68783-08-4	Gas oils (petroleum), heavy atmospheric
70592-76-6	Distillates (petroleum), intermediate vacuum
70592-77-7	Distillates (petroleum), light vacuum
70592-78-8	Distillates (petroleum), vacuum

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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 or intermediate 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 HFOs are a group of complex combinations of petroleum hydrocarbons that serve as blending stocks in final fuel products or as intermediate products of distillation or residue derived from refinery distillation or cracking units. The final fuel products usually consist of a blend of HFOs, as well as higher-quality hydrocarbons as diluents. The HFOs considered in this assessment are complex combinations composed of aromatic, aliphatic and cycloalkane hydrocarbons with carbon ranges spanning C_7–C_{50} and a typical boiling point range of 121–600°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.

The HFOs considered in this screening assessment have been identified as industry restricted (i.e., they are a subset of HFOs that may leave a petroleum sector facility and 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 HFOs are transported in large volumes from refinery or upgrader facilities to other industrial facilities by pipelines, ships, trains and trucks; therefore, exposure of the environment is expected.

Based on results of comparison of levels expected to cause harm to organisms with estimated exposure levels and the relatively low expected frequency of spills to water and soil during loading/unloading and transport operations, these five HFOs have a low risk of harm to aquatic or soil 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 HFOs (CAS RNs 64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7 and 70592-78-8) 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.

A critical effect for the initial categorization of industry-restricted HFO 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 HFO substances. HFOs demonstrated genotoxicity in *in vivo* and *in vitro* assays and may also adversely affect reproduction and 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 HFO substances in the PSSA that are similar from a processing and physical-chemical perspective was considered for characterization of human health effects.

General population exposure to industry-restricted HFOs results primarily from inhalation of ambient air containing HFO vapours due to evaporative emissions during transportation. Due to the relatively low volatility of the HFO substances, as defined by their physical-chemical properties, evaporative emissions into the air are expected to be minimal. The margins between the upper-bounding estimate of exposure, the maximum air concentration of HFOs (1.28 $\mu g/m^3$), and the critical inhalation effect levels are considered to be highly conservative and adequately protective to account for uncertainties related to health effects and exposure. The likelihood of inhalation exposure of the general population is considered to be low; thus, the risk to human health is likewise considered to be low. General population exposure to industry-restricted HFOs via the oral and dermal routes is not expected; therefore, risk to human health from the industry-restricted HFOs via these routes is not expected.

Based on the information presented in this screening assessment, it is concluded that the industry-restricted HFOs (CAS RNs 64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7 and 70592-78-8) 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 five industry-restricted HFOs listed under CAS RNs 64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7 and 70592-78-8 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].

[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.

Grouping of Petroleum Substances

The high priority petroleum substances fall into nine groups of substances (Table A1.1 in Appendix 1) based on similarities in production, toxicity and physical-chemical properties. In order to conduct the screening assessments, each high priority petroleum substance was placed into one of five categories ("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 (HFOs), gas oils, petroleum and refinery gases, low boiling point naphthas and crude oils.

This screening assessment addresses five industry-restricted HFO substances described under Chemical Abstracts Service Registry Numbers (CAS RNs) 64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7 and 70592-78-8. These substances were identified as GPE or IPE 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), these substances can be consumed on-site or transported from refineries and upgraders to other industrial facilities, but they are not sold directly to consumers. These substances were included in the PSSA because they are related to the petroleum sector and are all complex combinations of petroleum hydrocarbons.

Seven site-restricted HFOs were previously assessed under Stream 1, and an additional nine HFOs are being assessed separately, as they belong to Streams 3 and 4 (as described above). The health effects of the industry-restricted HFOs were assessed using health effects data pooled across all high priority HFOs due to insufficient data specific to the industry-restricted HFOs.

Included in this Stream 2 screening assessment is the consideration of information on chemical properties, uses, exposure and effects, including the additional information

[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.

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 March 2010 for the human exposure and environmental sections of the document and up to September 2011 for the health effects section of the document. Key studies were critically evaluated, and modelling results were used to reach conclusions.

Characterizing risk to the environment involves the 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 HFOs, 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 a negative impact on non-human organisms. As well, other lines of evidence including fate, temporal/spatial presence in the environment, and hazardous properties are taken into account. The ecological portion of the screening assessment summarizes the most pertinent data on environmental behaviour and effects and does not represent an exhaustive or critical review of all available data. Environmental models and comparisons with similar petroleum 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 HFO 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/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. Michael Dourson (TERA), Dr. Stephen Embso-Mattingly (NewFields Environmental Forensics Practice, LLC), Dr. Susan Griffin (United States Environmental Protection Agency [U.S. EPA]) and Dr. Donna Vorhees (Science Collaborative). 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 final screening assessment is based are summarized below.

Substance Identity

These HFOs are a group of complex petroleum combinations of petroleum hydrocarbons that serve as blending constituents in final fuel products or as intermediate products of distillate or residue derived from refinery distillation or cracking units with a typical carbon range of C_{20}–C_{50} (CONCAWE 1998). The final fuel product usually consists of a blend of HFOs and high-quality hydrocarbons that have been produced in the refinery or upgrader facilities. The HFOs considered in this assessment are complex mixtures composed of aromatic, aliphatic and cycloalkane hydrocarbons with carbon ranges spanning C_7–C_{50} and boiling point ranges of 121–600°C (Table A2.1 and A2.2 in Appendix 2; API 2004; CONCAWE 1998). The ratio of aliphatic to aromatic hydrocarbons is important for estimating environmental behaviour; however, very few data exist for these five CAS RNs, so a ratio of 50:50 has been assumed. This ratio will not bias results and is within the range of other types of HFOs (50–79% aromatics) (ATSDR 1999; API 2004).

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 HFOs vary depending upon the sources of crude oils or bitumen and the processing steps involved. A summary of experimental data on the physical-chemical properties of industry-restricted HFOs is presented in Table 1.

Table 1. Experimental physical-chemical properties of HFOs in general

Property	Value	Temperature (°C)	Reference
Pour point (°C)	< 30		API 2004
Boiling point (°C)	121–600		API 2004
Density (kg/m^3)	900–1100	20	API 2004; MSDS 2007
Vapour pressure (Pa)	282.6–3519.6	21	Rhodes and Risher 1995
Log K_{oc} (dimensionless)	3.0–6.7		Rhodes and Risher 1995
Log K_{ow} (dimensionless)	2.7–6.0	20	API 2004
Water solubility (mg/L)	< 100	20	API 2004

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

The theoretical vapour pressures of individual substances comprising HFOs are low to moderate due to their high molecular weights. However, the actual vapour pressures will be influenced by the substance composition of the HFO in which they occur. Water

solubilities of all HFOs are low, and octanol–water partition coefficient estimations vary considerably due to the complex nature of these substances.

To predict the environmental behaviour and fate of complex petroleum products such as these HFOs, representative structures were selected from each chemical class contained within the mixture. Forty-seven structures were selected from a database in PETROTOX (2009) based on boiling point ranges for each HFO (Table A2.3 in Appendix 2), the number of data on each structure and the middle of the boiling point range of similar structures. As the compositions of most HFOs are not well defined and are indeed variable, representative structures could not be chosen based on their proportion in the mixture. This resulted in the selection of representative structures for alkanes, isoalkanes, one-ring cycloalkanes, two-ring cycloalkanes, polycycloalkanes, cycloalkane monoaromatics, cycloalkane diaromatics and one-, two-, three-, four-, five- and six-ring aromatics ranging from C_9–C_{50} (Table A2.4 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 U.S. EPA's Estimation Programs Interface Suite (EPI Suite 2008) (Table A2.4 in Appendix 2).

Sources

Industry-restricted HFOs 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 HFOs. Information submitted under section 71 of CEPA 1999 shows that these substances can be intermediate streams consumed within a facility or be transported off-site by pipeline, truck, train and ship for use as a feedstock in other industrial facilities or for disposal (Environment Canada 2008, 2009).

CAS RN 64741-75-9 is a residual fraction from distillation of hydrocracking effluents in both refineries and upgraders.

CAS RN 68783-08-4 is a general description of distillates from atmospheric distillation of crude oil in refineries, primarily ranging from C_7–C_{35}.

CAS RNs 70592-76-6, 70592-77-7 and 70592-78-8 have slight differences in their dominant carbon range, but they all refer to distillates from vacuum fractionation of the residue produced from atmospheric distillation of crude oil.

Uses

According to the information collected through the *Notice with respect to certain high priority petroleum substances* published under section 71 of CEPA 1999 (Environment Canada 2008) and the *Notice with respect to potentially industry-limited high priority petroleum substances* (Environment Canada 2009), these industry-restricted HFO substances have been identified as being consumed at the facility or transferred to another

industrial facility for use as feedstock or for disposal. 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 these industry-restricted HFOs (i.e., the CAS RNs identified in this screening assessment) may leave a refinery or an upgrading facility and be transported to another industrial facility for use as a feedstock, or for disposal, but do not reach the public market in the form originally acquired.

Releases to the Environment

Potential releases of industry-restricted HFOs consist of releases within facilities from activities associated with processing these substances, as well as releases related to transportation of these 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 or maintenance 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 substance into ambient air and which may occur on a routine basis. Fugitive releases can be reduced but may not be

Terminology	Definition
	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 HFO 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 unplanned releases due to 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 HFOs considered in this screening assessment originate from distillation columns in a refinery or an upgrader, either as a residue (bottom product) or as a distillate. Thus, the potential locations for the controlled release of these HFOs include relief valves, venting valves and drain valves on the piping or vessels where these streams are generated.

Under typical operating conditions, controlled releases of these HFO 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 HFOs is not expected.

Unintentional Releases

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

[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.

Conclusion for Potential On-site Releases

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

Potential Releases from Transportation

As these industry-restricted HFOs can be transported between facilities, releases may also occur during transportation. In general, three operating procedures are involved during the process of transportation: loading, transit and unloading.

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

Storage of industry-restricted HFOs may be required before they are transported off-site. Releases of HFO vapours from the storage tanks into the air are expected to be small because the HFOs have low volatility. All relevant releases from storage, including leaks, spills and breathing loss (expulsion of vapour due to changes in temperature and pressure), will be similar to the aforementioned potential on-site releases and will be managed under the relevant legislation currently in place.

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 2008a; OECD 2009). As such, exposure of the general population and the environment to the HFOs considered in this screening assessment from tank cleaning is not expected. Cleaning facilities require processing of grey-water to meet local and provincial release standards.

Release Estimation

Information on the transportation quantities and relevant transportation modes was collected under section 71 of CEPA 1999 (Environment Canada 2009) with respect to each CAS RN considered in this screening assessment. Four modes of transportation—ships, pipelines, trucks and trains—were identified as being involved in moving industry-restricted HFOs to other industrial facilities. The total transport quantity of the five HFOs considered in this assessment is about 3 million tonnes (2.9×10^9 L) (year 2006). Two types of potential releases 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 tightness of transport vessels and settings of valves. Ambient air is the receiving medium for evaporative emissions.

Evaporative emissions to the environment were considered in transportation by ships, trucks and trains and were estimated based on empirical equations from the U.S. EPA (2008a), physical-chemical properties (e.g., vapour pressure, molecular weight and density of vapours) of these HFO substances, and the annual transported quantities. No evaporative emissions are considered for pipeline systems, as typical releases are generated as a result of leaks through seals, flanges and valves and are defined as unintentional releases.

Unintentional releases of the HFO substances due to spills generally enter water or soil, depending on the modes of transportation involved. Due to the relatively low volatility of the HFOs, as defined by their physical-chemical properties, evaporative emissions into the air from spills would occur in a lower proportion compared with the proportions entering water or soil.

Potential releases associated with the transport of these HFOs to marine, freshwater and soil environments were assessed through analysis of historical spill data (2000–2009) from the Environment Canada Spill Line database (Environment Canada 2011). There was no spills category for HFOs; spills of Bunker C fuel oil were therefore used. The releases labelled as Bunker C fuel oil (Fuel Oil No. 6) would also include these industry-restricted HFOs. There were also a small number of releases that were generically labelled as just "Bunker," and there was no indication as to what specific type of Bunker was released. Thus, all releases labelled as "Bunker" were considered to be Bunker C fuel oil. Bunker C is considered a heavy fuel oil but is not industry-restricted and has a wider distribution. Thus, it is expected that the actual number and volume of industry-restricted HFO spills are considerably lower than those of Bunker C fuel oil spills, but this could not be reliably determined. Of note was the large-volume spill of 734 000 L in 2005, which is known to be a Bunker C fuel oil spill into Lake Wabamun, Alberta; it was not included in the release estimate, as it was known not to be an industry-restricted HFO spill. As well, extremely large spills with no known origin were not included, as these were likely from environmental emergencies training exercises, which are not differentiated from actual events in the Environment Canada Spill Line database (Environment Canada 2011). Spills where collisions, poor road conditions and/or adverse weather-related events were listed as a source, reason or cause of spill were not included in the release estimate.
Many of the individual reports had no estimate of the volume released into the environment. In order to account for the underestimation of the volume released, the estimated total volumes were 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 HFOs to all media (soil, salt water and fresh water) was 2.4 million litres from 339 spills (Table A4.1 in Appendix 4).

The historical spill data were also separated into the specific compartment affected, so that the estimated average release quantity per spill to each compartment could be determined. Within each compartment, a similar extrapolation was conducted to account for reported spills with no associated volumes. The estimated average quantities of these

HFOs released per spill to fresh water and salt water from ship transport are shown in Table 3. These average spill volumes were based on Bunker C releases from the Spills Line database because HFOs are handled the same as Bunker C fuel oil for loading/unloading and ship transport. However, spills that were specifically known to be Bunker C were not included in the release estimate. There is no distinction in the database as to whether the spills occur during loading, transport or unloading. Thus, the average spill volume will be used for each of the scenarios.

Table 3. Average release quantities per spill of industry-restricted HFOs to various compartments (L/spill) based on historical Bunker C spill data from 2000–2009 from Environment Canada (2011)

Compartment affected	Average release quantities per spill	
	kg[a]	L[b]
Marine (salt water)	13 646	13 122
Fresh water	15 262	14 675
Soil	5105	4909

[a] Determined based on an average density of 1.04 kg/L (API 2004).

[b] Average release of industry-restricted HFOs to each compartment was determined by separating all HFO releases from 2000–2009 into specific compartments (marine, fresh water, soil), determining the extrapolated total released within each compartment (see Table A4.1 in Appendix 4) and then dividing this extrapolated total by the total number of spills affecting that compartment.

[c] Does not include the 2005 Lake Wabamun spill (734 000 L).

The largest fraction of HFO spills documented by Environment Canada from 2000–2009 affected land (130 incidents), followed by 108 releases to sea water and 53 releases to fresh water. For some reported spills, the compartment affected was not documented, whereas for others, multiple compartments were included; thus, this total does not equate to the total reported spills shown in Table A4.1 (Appendix 4). These numbers are considered to be a low estimate of actual releases, as not all provinces were reporting their spills to Environment Canada for all years, and some provinces have minimum reportable spill quantities. Releases to groundwater were not included in the analysis.

The Environment Canada (2011) Spill Line database provides three columns of data (sources, causes and reasons) for many releases of Bunker C fuel oil. The data in these columns were analyzed to determine how and why the majority of HFO releases occur (Tables A4.2a–c in Appendix 4).

The industrial areas where the majority of HFO releases occurred (Table A4.2a in Appendix 4) were other watercraft (25% of the volume), pipelines (20% of the volume) and marine tankers (20% of the volume). Releases at storage depots and facilities accounted for about 2% of the volume, refineries accounted for 2%, tank and transport trucks accounted for 3%, trains accounted for 4% and "other" sources accounted for 9%. The majority of truck releases were in New Brunswick (50%), and the rest were reported in Newfoundland and Labrador, Nova Scotia, Quebec, Prince Edward Island, Ontario and British Columbia.

The Environment Canada Spill Line data were also analyzed for causes of HFO leaks (Table A4.2b in Appendix 4). It was found that pipe leaks accounted for 38% of the

volume released, which is consistent with pipelines being a major source of Bunker C releases (see Table A4.2a). Likewise, sinking and grounding of vessels accounted for 13% and 6% of the total volume, respectively, which is also consistent with the high total spill volume by watercraft as a source. Twenty-five percent of the volume spilled was due to unknown causes, and 8% was due to "other" causes.

Analyzing reasons for releases, the data (Table A4.2c in Appendix 4) identified material failure as a major cause of releases, accounting for 16% of the volume released. Unknown reasons accounted for 43% of the volume, human error and negligence accounted for 18%, and fire and explosion accounted for 6% of the volume (from a single spill). The remaining 17% was divided over a wide variety of reasons.

For purposes of assessing the potential exposure of the environment from the transportation of industry-restricted HFOs, the ecological assessment focuses on unintentional releases to water and soil due to spills. Releases to water contributed significantly greater volumes than releases to soil. In comparison, assessment of potential exposure of the general population from transportation of industry-restricted HFOs focuses on evaporative emission, which occurs during regular operation 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, as relevant legislation and best practices are in place for on-site handling of these industry-restricted HFOs (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.

This assessment does not include illegal releases of fuel oil at sea in Canadian jurisdictions. Transport Canada has in place a National Aerial Surveillance Program to monitor and deter such releases (Transport Canada 2010).

Environmental Fate

When petroleum substances are released into the environment, four major fate processes will take place: 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, another fate process, 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 component class is as follows: alkenes ≈ alkanes > aromatics ≈ cycloalkanes. The most soluble and volatile components have the lowest molecular weight; thus, there is a general shift to higher molecular weight components 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). Degradation occurs both in the presence and absence of oxygen. Two key factors that determine degradation rates are oxygen supply and molecular structure. In general, degradation is more rapid under aerobic conditions. Decreasing trends in degradation rates according to structure are (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)).

These trends typically result in the depletion of the more readily degradable components and the accumulation of the most resistant in residues.

Level III fugacity modelling of representative hydrocarbons contained in the HFO group of substances was performed using EQC (2003) (Table A5.1 in Appendix 5) based on their physical-chemical properties as given in Table A2.4 (Appendix 2).

If released solely to air, all C_9–C_{15} representative structures will remain in air. With an increase in molecular size, the proportion remaining in air declines. Some of the C_{20} components will also remain primarily in air, except for alkanes, polycycloalkanes, cycloalkane monoaromatics, and four-, five- and six-ring PAHs. Moderate amounts of the C_{30} isoalkanes (70%) will also remain in air with the same pattern of decreasing partitioning to air with increasing molecular size (Table A5.1 in Appendix 5). Aside from the C_{30} isoalkanes, the C_{30} and C_{50} representative structures of HFOs will partition almost entirely to soil.

If released solely to water, most C_9 representative structures will remain in water, with the exception of alkanes, which will partition almost equally between sediment and

water. The C_{15} one- to three-ring aromatics will also undergo significant partitioning between sediments and water (12–49% into water), while all other representative structures will partition largely to sediment. Volatilization from water surfaces is not expected to be an important fate process despite the presence of some representative structures with moderate to very high estimated Henry's Law constants. Thus, if water is a receiving medium, all HFOs are expected to have a large proportion of the mixture partitioning to sediment (Table A5.1 in Appendix 5). It is likely, with a release situation into water where the HFO is not immediately in contact with sediments or suspended matter, that the moderate to high Henry's Law constants will drive the C_9–C_{20} representative structures out of the water. The tendencies for evaporation and sorption are competing and the exact nature of the release would dictate how the HFO behaves.

If released to soil, all representative structures of HFOs are expected to have high sorption to soil (i.e., expected to be immobile with > 99% remaining in the soil). Competing with this tendency are evaporative forces. Volatilization from moist soil surfaces may be an important fate process based upon estimated Henry's Law constant values of 5.1 to 1.3×10^6 Pa·m^3/mol. Lower molecular weight representative structures of HFOs (alkanes, isoalkanes, cycloalkanes and one-ring aromatics) may slightly to substantially volatilize from dry soil surfaces based upon their moderate vapour pressures (Table A5.1 in Appendix 5).

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).

Persistence and Bioaccumulation Potential

Environmental Persistence

In water, hydrolysis half-lives could not be predicted for hydrocarbons using 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 HFOs as complex mixtures, a QSAR-based weight-of-evidence approach (Environment Canada 2007) was applied using the BioHCWin (2008), BIOWIN 3,4,5,6 (2009), CATABOL (c2004-2008) and TOPKAT (2004) biodegradation models (Table A5.2 in Appendix 5).

Primary biodegradation (estimated with BioHCWin and BIOWIN 4) 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 to 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 in BIOWIN (2009) and BioHCWin agree that these compounds would degrade quickly and would not likely be persistent (Table A5.2 in Appendix 5). The following show persistence (half-life ≥ 182 days in water based on criteria in the *Persistence and Bioaccumulation Regulations* [Canada 2000]) in the environment: C_{30}–C_{50} isoalkanes, C_{30}–C_{50} one-ring cycloalkanes, C_{15}–C_{50} two-ring cycloalkanes, C_{14}–C_{22} polycycloalkanes, C_{30}–C_{50} one-ring aromatics, C_{15}–C_{20} cycloalkane monoaromatics, C_{15}–C_{50} two-ring aromatics, C_{12} cycloalkane diaromatics, C_{20}–C_{50} three-ring aromatics, C_{16}–C_{20} four-ring aromatics, C_{20}–C_{30} five-ring aromatics and C_{22} six-ring aromatics. Many of the C_{50} components were found to have extrapolated half-lives < 182 days; however, BioHCWin (2008) indicates that these components do not degrade easily, with half-lives ≥ 182 days. Thus, these C_{50} components are expected to be persistent based on primary degradation results from BioHCWin, as it is specific to petroleum hydrocarbons. The potential presence of these persistent components in each CAS RN is shown in Table A5.3 (Appendix 5).

Using an extrapolation ratio of 1:1:4 for a water : soil : sediment biodegradation half-life (Boethling et al. 1995), the representative structures that are persistent in water are also persistent in soil (half-life ≥ 182 days) and in sediments (half-life ≥ 365 days).

Using compositional data on Fuel Oil No. 6 and reading across to these HFOs (Tables A5.3 and A5.4 in Appendix 5), the average weight percent of components that are expected to be persistent ranges from approximately 50–60%.

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. Although the low vapour pressures of these representative structures indicate that volatilization may not be a very significant fate process, oxidation half-lives of less than 1 day (Table A5.5 in Appendix 5) indicate that this would be a relatively rapid removal process if these substances were introduced into the atmosphere (Atkinson 1990; API 2004).

Persistence Conclusion

Based on results from AOPWIN (2008), there would be a relatively rapid removal process if these HFOs were introduced into the atmosphere, based on oxidation half-lives of less than 1 day. These HFOs thus do not meet the criterion for persistence in air (half-life ≥ 2 days) as defined in the *Persistence and Bioaccumulation Regulations* (Canada

2000). With regard to the primary and ultimate biodegradation modelling, the C_{30}–C_{50} isoalkanes, C_{30}–C_{50} one-ring cycloalkanes, C_{15}–C_{50} two-ring cycloalkanes, C_{14}–C_{22} polycycloalkanes, C_{30}–C_{50} one-ring aromatics, C_{15}–C_{20} cycloalkane monoaromatics, C_{15}–C_{50} two-ring aromatics, C_{12} cycloalkane diaromatics, C_{20}–C_{50} three-ring aromatics, C_{16}–C_{20} four-ring aromatics, C_{20}–C_{30} five-ring aromatics and C_{22} six-ring aromatics in these HFOs meet the criteria for persistence (half-lives in soil and water ≥ 182 days and half-life in sediment ≥ 365 days). These HFOs are estimated to contain approximately 50–60% of components (C_{10}–C_{50}) by weight 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 HFOs or its components were found, empirical data on the bioaccumulation of components of Fuel Oil No. 6 was used in a read-across approach. A predictive approach using a bioconcentration/bioaccumulation factor (BCF/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 the 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 fish organs examined showed rapid accumulation of naphthalenes within the 2-hour exposure period, with the gallbladder 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 A5.6 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-labelled PAHs (naphthalene, phenanthrene, pyrene and benzo[*a*]pyrene B[*a*]P. 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*), water and sediment concentrations of PAHs from three separate published

works and used the data to derive BAFs. BAFs for PAHs in these fish were 87, 1550 and 3990 L/kg ww for phenanthrene, fluoranthene and chrysene/triphenylene, respectively (Table A5.6 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} 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, and *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 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. *n*-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 (only 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 fresh crude oil and settling particulates. The bioaccumulation factors (BAFs: 0.4–6.4 dw or 0.07–0.94 lipid-organic carbon) plotted 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 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, producing 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). The fish were capable of depurating pyrene completely within 160 hours of cessation of exposure. However, anthracene was only 70% and fluorene only 20% depurated within 200 hours. The BCF results for anthracene and pyrene by De Voogt et al. (1991) were not considered reliable in determining the bioconcentration potential of these substances due the lack of evidence that a steady-state had been reached within the 48-hour exposure. Likewise, there was poor recovery of pyrene at the end of the static bioconcentration experiment (62%) which had the BCF of 11 300 L/kg ww.

Jimenez et al. (1987) exposed bluegill sunfish (*Lepomis macrochirus*) to [^{14}C]B[*a*]P in a flow-through system for 48 hours to determine the effects of temperature and feeding on B[*a*]P uptake and elimination. The uptake of B[*a*]P was twice as fast for fish that were fed compared to those denied food in fish and uptake was slower at lower temperatures. A BCF of 608 L/kg ww was found for B[*a*]P for fed bluegill sunfish at 23ºC and it appears that steady-state was reached.

Jonsson et al. (2004) used a long-term (36-day) study to determine the bioconcentration of pyrene in sheepshead minnows (*Cyprinodon variegatus*). Fish reached a steady state after 4–7 days of exposure. The BCFs were 145 and 97 L/kg ww for PAH concentrations of 7.57 and 72.3 µg/L, respectively, which were likely due to biotransformation of PAHs by the fish.

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 A5.7 in Appendix 5). Unlike fish and some crustaceans, molluscs are unable to rapidly metabolize aromatic hydrocarbons. Accumulation can occur in stable tissue compartments with low hydrocarbon turnover and that are not readily exchangeable (Stegeman and Teal 1973; Neff et al. 1976).

The zebra mussel (*Dreissena polymorpha*) showed fast uptake of B[*a*]P and pyrene over a 6-hour exposure which led to high BCF values (Bruner et al. 1994; Gossiaux et al. 1996). After 3 days of depuration, body concentrations of B[*a*]P had dropped to less than 50%, and after 2 weeks, the concentrations had been reduced to 5–20% (Gossiaux et al.

1996). Pyrene elimination was highly temperature dependent, with depuration occurring more rapidly at higher temperatures and occurring very slowly at colder temperatures (Gossiaux et al. 1996). Lipid content was also important to the bioconcentration values, with higher lipid contents accumulating PAHs more readily, whereas body size did not affect the BCF values (Bruner et al. 1994).

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, pyrene, triphenylene and perylene produced high BCF values in mussels (*Mytilus edulis*) (5920, 4430, 11 390 and 10 500 L/kg ww, respectively) and clams (*Mya arenaria*) (4120, 6430, 5540 and 10 000 L/kg ww, respectively) 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 for fluoranthene, 5000 L/kg ww for pyrene and 9500 L/kg ww for perylene). All of these substances can be depurated from molluscs given time, but heavier PAHs (triphenylene and perylene) depurate more slowly than lighter PAHs (phenanthrene, fluoranthene and pyrene). Shrimps and polychaetes did not readily bioaccumulate PAHs.

Although some crustaceans can readily bioaccumulate higher-weight PAHs, they can also rapidly depurate PAHs. After 6 hours of exposure to B[*a*]P, the amphipod *Pontoporeia hoyi* and the freshwater shrimp *Mysis relicta* showed rapid uptake (Evans and Landrum 1989), but also had rapid depuration over 10–26 days (Evans and Landrum 1989). In *Daphnia magna* exposed to PAHs for 24 hours, high bioconcentration (>5000 L/kg) was observed with 11 higher-weight PAHs, ranging from 6100 L/kg ww for chrysene to 50 000 L/kg ww for dibenz[*ah*]anthracene (Newsted and Giesy 1987). Depuration was not studied.

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, though 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 possibly 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 A5.7 in Appendix 5) were highly variable, ranging from 180 to over 28 000 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. However, some components have been shown to meet the persistence criteria.

Three studies on BAFs of PAHs in aquatic organisms 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 A5.6 in Appendix 5). In general, the modelled values approximate the measured (Table A5.8 in Appendix 5) for the selected PAHs. None of the measured and modelled values were shown to be bioaccumulative according to the criteria (BAF ≥ 5000) in the *Persistence and Bioaccumulation Regulations* (Canada 2000), with the exception of the substituted PAH isoheptylfluorene and 2-isohexylphenanthrene (see Table A5.8 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 included 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 based on laboratory studies 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). Furthermore, laboratory BCFs have been shown to overestimate bioaccumulation potential when a chemical is bound or tightly sorbed to sediment (i.e., less bioavailable).

Due to the scarcity of measured BAF values (Table A5.6 in Appendix 5), BCFs from various published works were compiled (Table A5.9a 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 HFOs were found, including alkanes, isoalkanes, two-ring cycloalkanes, one-ring aromatics, cycloalkane monoaromatics, cycloalkane diaromatics and polyaromatics (Table A5.9a 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 the BCF or growth-corrected

elimination rate constant is known. Both BCF and biomagnification factor (BMF) empirical data were used to correct default model uptake and elimination parameters, which are summarized in Table A5.9b (Appendix 5).

In Table A5.9b (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 A5.9a (Appendix 5), only the C_{15} isoalkane (2,6,10-trimethyldodecane), C_8 one-ring cycloalkane (ethylcyclohexane), and C_{13} two-ring aromatics (2-isopropylnaphthalene) had measured and/or modelled BCFs or BAFs ≥ 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 ≥ 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 A5.9b 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 A5.9a in Appendix 5). Combining these lines of reasoning, this 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, this 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 octachloro naphthalene 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 < 8.0. 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 twenty-six C_9–C_{22} linear and cyclic representative structures using the modified Arnot-Gobas three trophic level model (2004) (Table A5.8 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 one C_{14} polycycloalkane was predicted to have a BCF that suggested a high bioconcentration potential. However, one isoalkane, several polycycloalkanes, one- and two-ring cycloalkanes and one-, two- and three-ring aromatics were found to have high bioaccumulation factors. 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 a 90% bioavailable fraction in the water column. BAF is therefore considered the most appropriate metric for assessing 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 reported in Table A5.9a (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 A5.9a and A5.9b 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 A5.10 (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 HFOs will undergo biomagnification or trophic magnification.

Broman et al. (1990) studied TMFs for 19 PAHs in a marine food chain (seston to mussels (*M. edulis*) to ducks (*Somateria mollissima*)), and did not find TMFs > 1.

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 HFOs (acenaphthylene, acenaphthene, benzo[*a*]anthracene, B[*a*]P, benzo[*e*]pyrene, benzo[*b*]fluoranthene, benzo[*b+k*]fluoranthene, benzo[*j+k*]fluoranthene, benzo[*k*]fluoranthene, benzo[*ghi*]perylene, chrysene, fluoranthene, fluorene, indeno[*123-cd*]pyrene, dibenz[*ah*]anthracene, perylene, naphthalene, phenanthrene and pyrene) ranged from 10^{-4} to 10^{-1}. Ninetieth percentile BSAF values ranged from 10^{-4} to just less than 1, with naphthalene being the only PAH with a BSAF close to but below 1. 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 majority of $< C_{15}$ components (alkanes, isoalkanes and cycloalkane monoaromatics) were not found to meet the *Persistence and Bioaccumulation Regulations* (Canada 2000). This conclusion is based on consistencies found between available BCF and BAF experimental data and BCF and BAF kinetic mass-balance model predictions using the Arnot-Gobas (2004) three trophic level model.

The majority of components ≥ C_{20} (alkanes, isoalkanes, one-ring cycloalkanes, 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 criterion of BCF or BAF ≥ 5000 for its modelled BAF prediction using the modified Arnot-Gobas three trophic level model (2004), whereas the C_{14} and C_{22} polycycloalkanes were found to meet this criteria based on the same model (Table A5.8 in Appendix 5) 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 criteria based on modelled results from the Arnot-Gobas (2004) three trophic level model. For these particular components, the metabolic rate constants range from 0.01–0.08 (day^{-1}), suggesting a slow rate of metabolism. In the case of C_{14} and C_{22} polycycloalkanes, C_{15} one-ring aromatic and 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 metabolic rate 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 fluorine, 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 15 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 A5.9a in Appendix 5) show that no components have BMFs > 1. This suggests that these particular hydrocarbons will not biomagnify when compared to concentrations expected 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* (Muijs and Jonker 2010)) as they do not have the same metabolic competency as 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 10 representative structures (C_{15} isoalkane, C_{15} one-ring cycloalkanes, C_{15} two-ring cycloalkane, C_{14} and C_{22} polycycloalkane, 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, suggests that the rate of uptake would exceed that of the total elimination rate. However, these components are not expected to biomagnify in aquatic foodwebs largely because a combination of metabolism, low dietary assimilation efficiency and growth dilution allows the elimination rate to exceed the total uptake rate.

PAH Components

In general, the majority of < C_{15} components (cycloalkane diaromatics and three-ring PAHs) were not found to meet the *Persistence and Bioaccumulation Regulations* (Canada 2000). The majority of components ≥ C_{20} (two-, three- and five-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).

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 ≥ 5000) as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000) with the exception of modelled BAF values for isoheptylfluorene and 2-isohexylphenanthrene (see Table A5.8 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. Lack of experimental or field data for alkyl-PAHs larger than naphthalene prevents drawing a concrete conclusion for these substances, albeit Neff et al. (1976) found that as naphthalene becomes increasingly alkylated, there is an increase in bioaccumulation potential. With regards to the modelled BAF values for isoheptylfluorene and 2-isohexylphenanthrene, the only similar analogues (fluorene and phenanthrene) have experimental BCFs of 1030 L/kg ww and 2944 L/kg ww, respectively, which are both slightly higher than the predicted BCFs using the mass-balance kinetic model (Table A5.8 in Appendix 5). However, there is some uncertainty surrounding the kinetic rate constants used to model BCF and BAF for isoheptylfluorene and 2-isohexylphenanthrene (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 these compounds is between 7.0 and 7.5, 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 1 (Table A5.10 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 A5.8 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, phenanthrene and B[*a*]P 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 some of the PAHs exceed the bioaccumulation criterion, including fluoranthene, anthracene and pyrene (Table A5.8 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) studies, as well as Peterson and Kristensen (1998), reported high BCF values and 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 for fluoranthene. Consequently there is greater evidence weight and consistency from kinetic data, modelled BCF and BAF values, and 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 levels of bioaccumulation.

Empirical BCF data for invertebrates, namely molluscs (fluoranthene and pyrene) and *Daphnia magna* (chrysene, benzo[*a*]anthracene, benzo[*k*]fluoranthene, B[*a*]P, benzo[*e*]pyrene and benzo[*ghi*]perylene) have been shown to be high. In the case of ***D. magna***, benzo[*a*]anthracene, B[*a*]P, benzo[*e*]pyrene and benzo[*ghi*]perylene have BCF values exceeding bioaccumulation criteria at approximately 10 000 L/kg ww (Table A5.7 in Appendix 5). This indicates that there is 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 A5.10 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, but BSAFs will likely decrease beyond C_{22} due to reduced bioavailability of the higher boiling point fractions (Muijs and Jonker 2010).

Overall, the evidence indicates that 4 representative polycyclic aromatic hydrocarbon structures (C_{20} three-ring PAHs, C_{18} four-ring PAHs, C_{20} five-ring PAHs and C_{22} six-ring PAHs) meet the bioaccumulation criteria as defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Proportion of Bioaccumulative Components in HFOs

Based on the boiling point ranges of each individual CAS RN (Table A2.4 in Appendix 2), the proportions of components that are expected to be bioaccumulative range from approximately 5 to 25% by weight. These proportions are based on Canadian samples of Fuel Oil No. 6, as the chemical characterization of these industry-restricted HFOs is unknown (Table A5.11 in Appendix 5). A more detailed analysis of how these bioaccumulative proportions were determined is shown in Table A5.11 (Appendix 5).

Thus, up to approximately 25% of components by weight of these industry-restricted HFOs may be bioaccumulative based on criteria in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

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

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 (Environment Canada 1994).

Aquatic Compartment

No experimental data were available for the aquatic toxicity of these industry-restricted HFOs; therefore, data from Fuel Oil No. 6 were used in a read-across approach to estimate the potential for aquatic toxicity. Other studies have shown that, with HFOs, variations in aquatic toxicity exist, in part, due to differences in boiling point ranges determining the composition of the HFOs (ECB 2000b).

Table A5.12 (Appendix 5) presents Fuel Oil No. 6 acute toxicity data. Aquatic median lethal concentration (LC_{50}) values range from 0.9–> 10 000 mg/L. Oil-in-water dispersions have been shown to be not nearly as hazardous to aquatic organisms as the water-soluble fraction. The lowest marine toxicity value of 0.9 mg/L was determined in a 48-hour acute LC_{50} test using water-soluble fractions with *Mysidopsis almyra* (a mysid shrimp) (Neff and Anderson 1981). The same value was determined in a 96-hour LC_{50} with *Capitella capitata* (a marine worm) (Rossi et al. 1976). The lowest freshwater value of 4.1 mg/L was determined by MacLean and Doe (1989) in a 48-hour EC_{50} test with*Daphnia magna*.

Avian Effects

HFOs can have a wide variety of effects on birds, especially sea birds. Heavy oils, including HFOs, can destroy the insulation provided by feathers, resulting in increased mortality due to exposure. HFOs are also directly toxic to birds through ingestion. The preening of feathers to clean them of oil, and the reduced insulation from oiled feathers increases metabolic requirements to the point where birds may starve to death while trying to keep warm.

As well, nesting birds that come into contact with fuel oils may transfer oil from their feathers and feet to their eggs during incubation. Toxicity to bird eggs via this route has been shown (Environment Canada 2010b; Michigan 2010). Fuel Oil No. 6 is similar to four of the HFOs considered here (64741-75-9, 70592-76-6, 70592-77-7 and 70592-78-8) and can be used in a read-across approach for toxicity. Szaro (1979) found that 5 µL of Fuel Oil No. 6 applied to eggs significantly reduced hatching success to 36% and 6-day survival to 52% in mallard ducks (*Anas platyrhyncos*).

Fuel Oil No. 2 is similar to the light HFO (CAS RN 68783-08-4) and can be used as a toxicity surrogate. In tests on mallard duck eggs, lowest-observed-effect concentrations (LOECs) were found at 1 µL/egg (20% reduction in hatchability with a 28% reduction in duckling survival post-hatch) (Albers and Szaro 1978; Szaro et al. 1978). Coon et al. (1979) determined that a 5 µL/egg treatment reduced hatchability by 28% compared with

controls with eggs of great black-backed gull (*Larus marinus*). Common eider duck (*Somateria mollissima*), Louisiana heron (*Hydranassa tricolour*), laughing gull (*Larus atricilla*) and sandwich tern (*Sterna sandvicensis*) eggs experienced from 20–81% mortality at 20 µL/egg (Albers and Szaro 1978; White et al. 1979).

Terrestrial Compartment

The Canada-Wide Standards for Petroleum Hydrocarbons in Soil (CCME 2008) were used as a data source for effects of HFOs on terrestrial ecosystems. These standards were developed based on consideration of four fractions of total petroleum hydrocarbons (TPHs): F1 (C_6–C_{10}), F2 (> C_{10}–C_{16}), F3 (> C_{16}–C_{34}) and F4 (> C_{34}). Fraction 3 (F3) is most like HFOs. Standards were developed for four land-use classes (agricultural, residential, commercial, industrial) and two soil types (coarse grained and fine grained). The land-use and soil type with the lowest standard is typically agricultural coarse-grained soils. The F3 standard for soil contact by non-human organisms for agricultural coarse-grained soils is 300 mg/kg dw (CCME 2008).

Ecological Exposure Assessment

Estimations of releases of these HFOs were made using data included in responses to a notice published under section 71 of CEPA 1999 (Environment Canada 2009), along with estimations of losses to the sea on Canada's east coast by Risk Management Research Institute (RMRI 2007) and Environment Canada's Spill Line database (Environment Canada 2011).

Aquatic Compartment

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 and unloading 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). For the ship transport scenarios, the estimated volume of water in contact with oil is the average volume of water from Hazard Zone 2 (outer Placentia Bay), as this area is a major ship transportation corridor. 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 product spilled. This work was originally developed for crude oil, but it can be applied to HFOs as they have a similar density.

In the case of marine loading and unloading of HFOs by ship, an estimated 13 646 kg of fuel oil on average could be lost in one event to salt water (Table 3). At an average density of 1.04 kg/L (API 2004) this is equivalent to 83 barrels of fuel oil and is therefore expected to be in contact with 150×10^9 litres of water (Table A5.13 in Appendix 5). This volume is estimated from the enclosed waters found at wharves and loading terminals. The resulting concentration in water would be 0.09 mg/L (1.38×10^{10} mg/150×10^9 litres), which is considered the marine PEC for ship loading and unloading.

The situation is similar for marine transportation of HFOs by ship. In this case, 83 barrels of fuel oil is expected to be in contact with 6250×10^9 litres of water (Table A5.13 in Appendix 5). This volume is estimated from the open ocean of Placentia Bay. The resulting concentration in water would be 0.002 mg/L (1.38×10^{10} mg/6250×10^9 litres), which is considered the marine PEC for ship transport.

In the case of the freshwater loading and unloading of HFOs by ship, an estimated 15 262 kg of fuel oil could be lost in one event to fresh water (Table 3). At an average density of 1.04 kg/L (API 2004) this is equivalent to 92 barrels of fuel oil and is therefore expected to be in contact with 150×10^9 litres of water (Table A5.13 in Appendix 5). This volume is estimated from the enclosed waters found at wharves and loading terminals. The resulting concentration in water would be 0.1 mg/L (1.53×10^{10} mg/150×10^9 litres), which is considered the freshwater PEC for ship loading and unloading.

In the case of the freshwater transportation of HFOs by ship, an estimated 15 262 kg of fuel oil could be lost in one event to fresh water (Table 3). At an average density of 1.04 kg/L (API 2004) this is equivalent to 92 barrels of fuel oil and is therefore expected to be in contact with 6250×10^9 litres of water (Table A5.13 in Appendix 5). This volume is estimated from the open ocean of Placentia Bay. The resulting concentration in water would be 0.002 mg/L (1.53×10^{10} mg/6250×10^9 litres), which is considered the freshwater PEC for ship transport.

Terrestrial Compartment

Less than one release event per year for pipeline transport of HFOs is predicted based on the short distance of transport determined from information submitted under section 71 of CEPA 1999 (Environment Canada 2009) and the average spill rate per length of pipeline (1 spill per 11 100 km of pipeline, as found in NEB 2008). Likewise, only two of the five industry-restricted HFOs are transported by pipeline. From the historical Canadian data from the Spill Line database for Bunker C (Environment Canada 2011), only 13 spills of HFOs from pipelines were reported over 10 years (2000–2009). Thus, less than 1 release event per year is expected for pipeline loading, transport and unloading for industry-restricted HFOs.

It is estimated that there will be ≤ 1 release event per year each for train and truck loading, unloading and transport based on historical release information from the Spill Line database (Environment Canada 2011). Spill events are expected to generally occur at industrial facilities for industry-restricted HFOs. It was additionally considered that these infrequent releases would likely occur on a hard surface and not on soil; therefore releases from truck and train are not considered to be of high importance under these circumstances. It is expected that the actual release frequency for these industry-restricted HFOs is lower, as the Spill Line database release information was for Bunker C.

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 and predicted no-effect concentration (PNEC) was determined. Also, a PEC was determined from the aquatic exposure scenario. The PNEC is the lowest critical toxicity value (CTV) for the organism of interest divided by an appropriate assessment factor. A risk quotient (RQ = PEC/PNEC) was calculated for each endpoint organism and is an important line of evidence in evaluating the potential risk to the environment.

Since a read-across approach can be used with Fuel Oil No. 6, the CTVs for this assessment are selected from empirical data available for Fuel Oil No. 6 (Table A5.12 in Appendix 5). For the marine scenarios, a CTV of 0.9 mg/L is selected based on the 48-hour acute LC_{50} value for *Mysidopsis almyra*. For the freshwater exposure scenarios for ship loading/unloading and transport, the selected CTV is the 96-hour acute EC_{50} (immobilization) of 4.1 mg/L for *Daphnia magna* (Table A5.12). An assessment factor of 10 is used to account for the extrapolation of modelled data to field effects.

Table 4 is the summary of the risk quotients for the industry-restricted HFOs. Only spills to marine water during the loading/unloading of ships were determined to be potentially harmful to fish, as the RQ ≥ 1.

Table 4. Risk quotients calculated for industry-restricted HFOs

Compartment affected	Organism	PEC	CTV	Assessment factor	PNEC	Risk quotient
Fresh water (loading/ unloading)	*Daphnia magna*	0.1 mg/L	4.1 mg/L	10	0.4 mg/L	0.25
Freshwater (transport)	*Daphnia magna*	0.002 mg/L	4.1 mg/L	10	0.4 mg/L	0.005
Marine (loading/ unloading)	*Mysidopsis almyra*	0.09 mg/L	0.9 mg/L	10	0.09 mg/L	1
Marine (transport)	*Mysidopsis almyra*	0.002 mg/L	0.9 mg/L	10	0.09 mg/L	0.02

For all aquatic spill scenarios, the critical spill volume for HFOs required to obtain an RQ = 1 and the frequency of spills above that threshold was determined from the Environment Canada Spill Line database (Environment Canada 2011) (see Table 5).

Table 5. Spill volumes required to create harmful conditions to aquatic organisms and the proportion of reported spills of HFOs above this threshold volume[a]

Compartment affected	Critical spill volume required to obtain risk quotient = 1 (threshold volume) (L)	Proportion of *reported* spills above the threshold volume	Number of spills per year expected to be above the threshold volume
Fresh water (loading/unloading)	58 000	8%	< 1
Fresh water (transport)	6 700 000	0%	0
Marine (loading/unloading)	13 000	15%	1.6
Marine (transport)	835 000	0%	0

[a] HFO spills were assumed to be equal to Bunker C spills due to the inability of the dataset to distinguish between these two substances. Actual number and volume of industry-restricted HFO spills are expected to be less than reported here.

For the marine and freshwater scenarios during ship transport, critical spill volumes of 835 000 L and 6 700 000 L of fuel oil, respectively, are needed to obtain an RQ of 1 for aquatic organisms (Table 5) based on toxicity estimations and spill dispersion models of the volume of water affected. None of the reported spills from 2000–2009 were greater than these threshold volumes during ship transport and therefore, the expected number of spills per year above this volume is zero. As well, the whole dataset from the Environment Canada Spill Line database for Bunker C was used as a surrogate for these HFOs. The amount of HFOs released is unknown, but is certainly less than the total volume of Bunker C. Thus, spills to fresh water and salt water during transport are not considered harmful to aquatic organisms.

For the scenarios for ship loading/unloading, spill volumes of 13 000 L and 58 000 L of fuel oil are needed to obtain an RQ of 1 for aquatic organisms in marine and fresh waters, respectively (Table 5). There are some reported spills above these threshold volumes during the loading/unloading of ships in marine (15% of spills) and fresh water (8% of spills). However, these frequencies equate to an expected less than 2 spills per year above the threshold volume in marine waters and less than one spill per year in fresh water. These frequencies are based on the entire dataset from the Environment Canada Spill Line database for spills of Bunker C, which are expected to be more frequent than spills of industry-restricted HFOs. The RQ for marine loading was 1, and for fresh water loading the risk quotient was below 1, based on average spill volumes. Thus, based on the RQs and relatively low expected number of spills per year, spills of these HFOs to water

during loading and unloading are considered to be infrequent and pose a low risk of harm to aquatic organisms.

These spill volumes were 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.

Both field reports and experiments have shown that commercial blends of HFOs can be toxic to aquatic birds through ingestion (CONCAWE 1998; Environment Canada 2010b; Michigan 2010), contact with feathers (Environment Canada 2010b) and contact with eggs (Albers and Szaro 1978; Coon et al. 1979; CONCAWE 1998). The negative effects of oil on feathers, however, are not specific to HFOs and are primarily based on Bunker C fuel oil. Indeed, average spills to marine water for these industry-restricted HFOs are based on the Environment Canada Spill Line data for Bunker C fuel oil (Environment Canada 2011). Use of this data overestimates the number of spills of the industry-restricted HFOs considered in this assessment. Thus, there is a low frequency of releases of these industry-restricted HFOs to marine waters, and thus low risk to sea birds through direct toxicity and indirect effects.
Based on the estimated < 1 HFO release event per year for pipeline transport, HFOs pose a low risk of harm to terrestrial non-human organisms.

With regard to truck and train releases, a risk quotient was not determined. Release frequency and volumes from trains are less certain due to a lack of definitive data. The Spill Line database reports small numbers of Bunker C spills via train (11 spills) and truck (32 spills) from 2000–2009. Considering the cause and reason of spill, it was determined that for each scenario of loading, transport and unloading of trains, less than 1 spill per year is expected. By the same analysis, ≤ 1 spill per year each for loading, transport and unloading by truck is expected. Thus, terrestrial impacts from train and truck transport of HFOs are unlikely to cause harm due to their low frequency (less than 1 spill per year for loading/unloading and transport). Likewise, the estimated spills from truck loading and unloading were not considered to be of high importance, as they would likely occur on a hard surface and not on soil.

Based on results from AOPWIN (2008), there would be a relatively rapid removal process if these HFOs are introduced into the atmosphere, based on oxidation half-lives of less than 1 day. With regard to the primary and ultimate biodegradation modelling, the C_{30}–C_{50} isoalkanes, C_{30}–C_{50} one-ring cycloalkanes, C_{15}–C_{50} two-ring cycloalkanes, C_{14}–C_{22} polycycloalkanes, C_{30}–C_{50} one-ring aromatics, C_{10}–C_{20} cycloalkane monoaromatics, C_{15}–C_{50} two-ring aromatics, C_{12}–C_{20} cycloalkane diaromatics, C_{20}–C_{50} three-ring aromatics, C_{16}–C_{20} four-ring aromatics, C_{20}–C_{30} five-ring aromatics and C_{22} six-ring aromatics in these HFOs meet or exceed the criteria for persistence (half-lives in soil and water ≥ 182 days and half-life in sediment ≥ 365 days) defined in the *Persistence and*

Bioaccumulation Regulations (Canada 2000). Based on the available predicted information, these HFOs contain approximately 50–60% by weight of components that may persist sufficiently in soil, water and sediment to meet the regulatory criteria.

Based on the combined evidence of empirical data and predicted analysis of BCFs, BAFs, BMFs, TMFs and BSAFs, the HFOs assessed in this report may contain approximately 25 % by weight of components 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 BCFs and predicted BAFs are ≥ 5000 for isoalkanes, cycloalkanes 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 HFOs with high bioaccumulation potential, only two (a C_{20} cycloalkane diaromatic and a C_{20} three-ring PAH) were bioaccumulative (i.e., BCF or BAF > 5000). Both structures contain isoalkyl functional groups 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.

Some lower trophic level organisms (i.e., invertebrates) appear to lack the capacity to efficiently metabolize aromatic compounds, resulting in bioaccumulation that can be above Canadian criteria for some aromatic components of HFOs. This is the case for the C_{18} four-ring PAHs, C_{20} five-ring PAHs, and C_{22} six-ring PAHs, which were bioconcentrated to high levels (BCF > 5000) by invertebrates (e.g., *Daphnia*, molluscs) but not by fish. 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.

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).

As shown in Table A5.14 (Appendix 5), some components may meet both the persistence and bioaccumulation criteria in the *Persistence and Bioaccumulation Regulations.* The HFOs assessed in this report may contain approximately 15% of these components by weight. These include the C_{15} dicycloalkanes, C_{14} and C_{22} polycycloalkanes, C_{15}–C_{20} cycloalkane monoaromatics, C_{20} three-ring aromatics, C_{18} four-ring aromatics, C_{20} five-ring aromatics and C_{22} six-ring aromatics.

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 these industry-restricted HFOs (CAS RNs 64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7 and 70592-78-8) 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.

Uncertainties in Evaluation of Ecological Risk

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

All modelling of the substance's physical-chemical properties, as well as persistence, bioaccumulation and toxicity characteristics, is based on chemical structures. As these industry-restricted HFO are UVCBs, they cannot be represented by a single, discrete chemical structure. The specific chemical compositions of these HFOs are variable and not well defined. HFO 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 average estimates for the entire range of components likely present was identified. Specifically, these structures were used to assess the fate and hazard properties of HFOs. 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 these substances. The physical-chemical properties of 48 representative structures were used to estimate the overall behaviour of these HFOs, 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 HFOs, there is uncertainty in the results associated with modelling.

Uncertainty arises from the non-uniformity of spill data. The available data on spills generally do not report values for each specific transported substance by CAS RN. For marine transportation, Environment Canada reported spills data for substances similar to these heavy fuel oils, specifically Bunker C fuel oil. Spill data specific to these industry-restricted HFOs are not available for each mode of transportation. The use of a generic loss fraction factor, derived from the available data, introduces uncertainty in the estimation of transportation releases.

Similarly, historical spills data classified as Bunker C fuel oil from the Emergencies Spill Line database (Environment Canada 2011) were used in the ship, truck and train transport release scenarios for these industry-restricted HFOs. The amount of HFOs released is

unknown, but is certainly less than the total volume of Bunker C. There is uncertainty in the estimation of the actual HFO loading, transport and unloading releases.

The fate, food chain interactions and toxicity of a number of petroleum hydrocarbons depend to a large extent upon their chemical form. As such, conservative assumptions about chemical form, bioavailability, and absorption through the digestive tract were generally carried forward in the risk assessment. HFO representative structures were assessd with the conservative assumption that all of them were bioavailable.

This assessment involves the prediction of effects on biota using measured inputs and modelled accumulation or exposures. The process 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. There is some uncertainty when estimating the biotransformation used by the model at the first trophic level. Many petroleum hydrocarbons are readily metabolized, somewhat by invertebrates and at much higher levels in fish.

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 industry-restricted HFOs as a class; therefore, predicting effects is based on modelling their BAFs based on laboratory-acquired partitioning data.

Potential to Cause Harm to Human Health

Exposure Assessment

HFO substances are a group of heavy petroleum streams produced in oil refinery and upgrader facilities. Due to the physical-chemical properties of HFOs, the dermal route is an important route of occupational exposure. In a recent study to quantify such workplace exposures, Yvette et al. (2011) found that dermal exposures were generally low. However, the authors indicated that the presence of HFO components with some degree of carcinogenic potential identified in all of the HFO blends they investigated requires that control measures to maintain low dermal exposure levels should be strictly adhered to, and additional means of reducing HFO exposure even further should continue to be sought.

Due to the relatively low volatility of the industry-restricted HFOs (see Table 1) and relevant regulations in place to limit potential releases during handling of petroleum substances, general population exposure to these substances by ingestion and inhalation

during loading and unloading is expected to be negligible and will not be considered further.

Significant concentrations of hydrogen sulfide are known to accumulate in the headspaces of storage tanks that contain HFOs. Heating of such tanks may cause the decomposition of some of the sulfur-containing compounds, which release hydrogen sulfide. There is also evidence that vapours of light hydrocarbons accumulate in the headspaces of HFO tanks (CONCAWE 1998).

The human health assessment of industry-restricted petroleum substances focuses on the fugitive releases that occur when petroleum substances escape into ambient air. These include evaporative emissions from tanks 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 refer to releases that occur on a non-routine or unpredictable basis in specific geographical locations. These unintentional releases (leaks or spills) typically do not contribute to the potential for exposure of the general population in Canada.

Evaporative emissions of the industry-restricted HFO substances during transit will enter ambient air. As such, inhalation is the primary potential route of bystander exposure, which may occur as the substances are being transported between facilities, and is therefore the focus of the current human health exposure assessment.

Inhalation from Ambient Air

As monitoring data on HFOs in the environment are not available, the HFO vapour level in ambient air was 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 estimates the maximum concentrations of a chemical at chosen receptor heights and at various distances for a given population in the vicinity of the release source in the direction downwind from the prevalent wind 1 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 maximum concentration within 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 even more variable and uncorrelated to the wind direction for a single event; thus, the maximum 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 required for non-point source emissions. However, to prevent overestimation of the exposures, we use a scaling factor

of 0.2 to obtain the yearly exposure concentration from the value of the maximum 1-hour exposure determined from SCREEN3 calculations. Detailed input parameters for SCREEN3 are listed in Table A6.1 (Appendix 6). As a conservative estimate, the regular evaporative emission during 1 day of transit is assumed to originate from a defined area rather than a moving line source; as such, actual levels are expected to be lower, considering that the release source is typically moving.

Estimated regular evaporative emission to air during transit of industry-restricted HFOs is presented in Table A6.2 (Appendix 6) as a range to cover the losses from the various transportation modes involved. Formulas for evaporative emissions of HFOs from truck and train transit of HFOs are not available in the AP 42 guidelines (U.S. EPA 2008a). A conservative estimate for these transit losses may be calculated by using stationary storage tank formulas adapted to typical dimensions of truck and train tanks. Even at this level of conservatism, due to the low volatility of the HFOs, the evaporative emissions from truck and train transit are small. The upper value in the range is related to evaporative emission from ship transit. Emission rates in grams per second per square metre ($g/s \cdot m^2$) are derived based on the loss quantity of kilograms per day (Table A6.2 in Appendix 6) and the estimated emission areas for different transportation modes (Table A6.1 in Appendix 6). This emission rate ($g/s \cdot m^2$) was used for determining the concentration of the HFO vapours in ambient air by SCREEN3 (1996).

As evaporative emission quantities are different for various transportation modes, for those industry-restricted HFOs with more than one mode of transportation, the maximum concentrations of ambient HFO vapours during 24 hours are presented as a range in Table A6.3 (Appendix 6). A conservative estimate of exposure was chosen by using the maximum concentrations at 50 m (for transportation by trains), as these were the highest exposure values obtained, compared with those at distances farther from the release sources. The upper-bounding estimate of the maximum concentration in ambient air at 50 m was 1.28 $\mu g/m^3$.

It should be noted that the estimated air concentrations of HFOs 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. Another consideration is that the releases of the industry-restricted HFO vapours that occur during the transit process occur continuously from a moving source (a line source) rather than from a stationary point source. As such, the actual concentration of the HFO vapours around a moving line source, for any given location, will be considerably lower than that represented by the total daily release quantity from a point release source, as was used in this assessment. Thus, the assumption of total daily evaporative emission within one defined area is considered to be a conservative estimate of the actual substance concentration in ambient air. Placing the receptor at 50 m from the release source is also conservative, as most Canadians do not reside within 50 m of HFO transport.

Health Effects Assessment

Given the limited number of studies available that specifically evaluate the health effects of the industry-restricted HFO substances, an adequately representative toxicological dataset unique to these substances could not be obtained. Therefore, to characterize the health effects of these HFOs, additional HFOs in the PSSA that are similar from both a process and a physical-chemical perspective were also considered. Because both the industry-restricted and the additional HFO 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 HFOs. Accordingly, the health effects of HFOs are represented as a group, not by individual CAS RNs.

Appendix 7 contains a summary of available health effects information on HFOs in laboratory animals. A summary of key studies is presented below. The HFO category of petroleum mixtures represented in Table A7.1 (Appendix 7) includes both residual fuels from distillation or cracking units and blended products. It consists of aromatic, aliphatic and cycloalkane hydrocarbons. Heavy fuels may also contain hydrogen sulfide, as well as a broad range of chemicals that are tumourigenic (e.g., PAHs), and the quantities present in HFOs can vary (CONCAWE 1998; Yvette et al. 2011).

HFOs have low acute toxicity. Inhalation exposure resulted in an LC_{50} of > 3700 mg/m^3 in rats. Oral exposure resulted in a median lethal dose (LD_{50}) of > 2000–> 25 000 mg/kg-bw in rats. Dermal exposure resulted in an LD_{50} of > 2000–> 5350 mg/kg-bw in rabbits and > 2000 mg/kg-bw in rats (CONCAWE 1998; ECB 2000a; API 2004; U.S. EPA 2005). Minimal to moderate skin irritation was observed for acute dermal exposure. Available data indicate that HFOs and HFO components are not eye irritants (CONCAWE 1998).

In an acute oral study conducted for CAS RN 64741-62-4, a single dose of 2000 mg/kg-bw or a single dose of 125, 500 or 2000 mg/kg-bw was administered to pregnant Sprague-Dawley rats on one of gestation days 11–15 or on gestation day 12, respectively. Decreased maternal body weight gain and thymus weights were reported, regardless of treatment day, for the gestation day segment of the study. Dose-related decreased maternal body weight gain and thymus weights were reported for the dose-response segment of the study (Feuston et al. 1989; Feuston and Mackerer 1996).

One short-term inhalation study was conducted for CAS RN 64742-90-1. A lowest-observed-adverse-effect concentration (LOAEC) of 540 mg/m^3 was observed for decreased body weight (concentration-related) and increased liver weight in Fischer 344 rats following administration of 540 or 2000 mg/m^3, 6 hours/day for 9 days (Gordon 1983).

Short-term and subchronic dermal studies conducted over periods of 3 days to 13 weeks are available for HFO substances, including one industry-restricted substance (CAS RN 68783-08-4). Slight to severe skin irritation was observed in several studies; the lowest

dose reported for skin irritation was 8 mg/kg-bw per day (Mobil 1994a, b). Selected systemic effects observed in these studies included decreased body weight gain and body weight, decreased thymus weights, increased liver weights and changes in hematological parameters (e.g., platelets, hemoglobin, red blood cells) and serum chemistry (i.e., liver enzymes and other indicators of liver toxicity) (API 1983; Mobil 1988, 1990, 1992, 1994a, b; UBTL 1990, 1994; Feuston et al. 1994, 1997). A lowest-observed-adverse-effect level (LOAEL) of 1 mg/kg-bw per day was reported for maternal toxicity following dermal exposure of pregnant CD rats to CAS RN 64741-62-4 at doses of 0.05, 1, 10, 50 or 250 mg/kg-bw per day from gestation days 0–19. Effects observed at the LOAEL included significantly decreased body weight gain, body weight and feed consumption, as well as decreased gravid uterine weight and the occurrence of red vaginal exudates (Hoberman et al. 1995). For subchronic exposure, a LOAEL of 8 mg/kg-bw per day was established following dermal exposure of male and female rats to CAS RN 64741-62-4 or 64741-81-7 at doses of 8, 30, 125, 500 or 2000 mg/kg-bw per day for 13 weeks. Effects noted at the LOAEL included decreased platelet counts and increased liver weights, as well as dose-related skin irritation (Mobil 1988, 1992, 1994b; Feuston et al. 1994, 1997). Lack of testing at doses lower than 8 mg/kg-bw per day lowers confidence in the LOAEL.

The genotoxicity of HFOs has been evaluated in *in vivo* and *in vitro* assays. Results from *in vivo* genotoxicity testing of three HFO substances were mixed (i.e., both positive and negative results were obtained for the same assay and endpoint). Positive results were observed in mice and rats for micronuclei induction, sister chromatid exchange and unscheduled deoxyribonucleic acid (DNA) synthesis when HFOs were administered orally or by intraperitoneal injection (Khan and Goode 1984; API 1985a, b). Negative results were also observed for micronuclei induction, as well as for chromosomal aberrations (API 1985c; Mobil 1987a).

In vitro assays evaluating the genotoxicity of HFOs also exhibited mixed results. Positive results were obtained in the Ames test battery and mouse lymphoma assays, as well as for cell transformation and unscheduled DNA synthesis (Brecher and Goode 1983, 1984; Blackburn et al. 1984, 1986; API 1985c,d, 1986a; Mobil 1985; Feuston et al. 1994). Regarding CAS RN 68553-00-4, negative results were obtained in the Ames and mouse lymphoma assays, as well as for forward mutations and sister chromatid exchange (Farrow et al. 1983; Vandermeulen et al. 1985; Vandermeulen and Lee 1986). Additional negative results were observed only for one cytogenetic assay and one forward mutation assay for CAS RNs 64741-57-7 and 64741-62-4, respectively (API 1985e; Mobil 1987b). Equivocal results were observed in one forward mutation assay and one sister chromatid exchange assay and for cell transformation (Papciak and Goode 1984; API 1985f, 1986b).

The overall genotoxicity database indicates that although the results varied depending on the substance tested and the assay used, HFOs do exhibit genotoxic potential.

The European Commission has classified industry-restricted HFOs as Category 2 carcinogens (R45: *may cause cancer*) (European Commission 1994; 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 classified residual (heavy) fuel oils as Group 2B carcinogens (*possibly carcinogenic to humans*) (IARC 1989a).

A number of skin-painting studies were conducted in laboratory animals to investigate the dermal carcinogenicity of HFOs using both chronic and initiation/promotion methodologies. Skin tumours, including both malignant carcinomas and benign papillomas, were frequently observed in mice, rabbits and monkeys (Smith et al. 1951; Shubik and Saffiotti 1955; Shapiro and Getmanets 1962; Saffiotti and Shubik 1963; Getmanets 1967; Weil and Condra 1977; Bingham and Barkley 1979; Sun Petroleum Products Co. 1979; Bingham et al. 1980; Lewis 1983; Blackburn et al. 1984, 1986; API 1989a, b; McKee et al. 1990). Exposure durations for the chronic studies ranged from 25 weeks to lifetime, with reported tumour latency periods ranging from 8 to 113 weeks. In several studies, however, the durations of exposures and latencies were not specified. In a chronic study, male mice were dermally treated with CAS RN 64741-62-4 at doses of 8.4, 16.8, 42.0, 83.8 or 167.6 mg/kg-bw, 3 times per week for a lifetime. Significant skin tumour formation was observed at all doses in a dose-response fashion (McKee et al. 1990). In the one initiation study that was identified, male mice were dermally treated with CAS RN 64741-62-4 at a dose of 16.8 mg/kg-bw once per day for 5 consecutive days. Significant skin tumour formation was observed at this dose. In the corresponding promotion study, no increase in histologically confirmed tumour incidence was observed. A statistically significant increase in the number of mice with gross masses (and shortened latency periods) was observed, however, indicating possible weak promoting activity (API 1989a).

Regarding the tumourigenicity of HFOs, 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 HFOs, evaluating the contribution of HFO components to carcinogenic activity is beyond the scope of the current assessment.

HFOs have also been investigated for their reproductive and developmental effects. A LOAEL of 1 mg/kg-bw per day was identified for reproductive toxicity after dermal exposure of pregnant rat dams to CAS RN 64741-62-4 during gestation days 0–19 (the no-observed-adverse-effect level [NOAEL] was 0.05 mg/kg-bw per day). Reproductive effects included decreased number of live fetuses, increased incidences of resorptions and early resorptions and increased percentage of dead or resorbed conceptuses per litter. Fetal developmental variations were also observed in this study but were determined by

the authors not to be treatment related (Hoberman et al. 1995). A LOAEL of 8 mg/kg-bw per day for treatment-related developmental toxicity was determined in another study, based on an increased incidence of fetal external abnormalities, including cleft palate, micrognathia (shortened lower jaw) and kinked tail, when catalytically cracked clarified oil was applied dermally to pregnant rats (Mobil 1987c; Feuston et al. 1989). These effects were noted to occur at low incidences. Reproductive toxicity and further developmental effects were observed at 30 mg/kg-bw per day. Reproductive effects included an increased incidence of resorptions and a decreased number of viable fetuses at and above 30 mg/kg-bw per day. At 250 mg/kg-bw per day, no viable offspring were produced (Mobil 1987c; Feuston et al. 1989). In another study, various HFO substances were applied dermally to rats. Substance-dependent LOAELs ranged from 30 to 500 mg/kg-bw per day based on fetal resorption rates ranging from 35.1–78.0% (Feuston et al. 1994).

Only one oral reproductive and developmental study was identified for any HFO substance. A LOAEL of ≥ 125 mg/kg-bw was established based on a dose-related increase in resorptions (concomitant decrease in litter size), decreased fetal body weight and increased incidences of skeletal malformations in this acute study that exposed pregnant Sprague-Dawley rats to CAS RN 64741-62-4 during gestation (Feuston and Mackerer 1996). No reproductive or developmental studies were identified for any HFO substance via the inhalation route of exposure.

Although results varied depending on the substance tested, the overall weight of evidence suggests that HFOs exhibit reproductive and developmental toxicity in laboratory animals. The most sensitive LOAEL is 1 mg/kg-bw per day for reproductive and developmental effects.

Epidemiological data were not available for consideration in the human health effects evaluation of HFO substances.

Characterization of Risk to Human Health

Industry-restricted HFOs were identified as high priorities for action during categorization of the DSL because they were determined to present greatest potential or intermediate 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 HFO substances was carcinogenicity, based primarily on classifications by international agencies. These substances are classified as Category 2 carcinogens by the European Commission (European Commission 1994; ESIS 2008), Category 1B carcinogens using the Globally Harmonized System (European Commission 2008a) and Group 2B carcinogens by IARC (1989a). Several cancer studies conducted in laboratory animals resulted in the development of skin tumours following repeated dermal application of HFO substances (API 1989a; McKee et al. 1990). Skin carcinomas and papillomas developed in 100% of mice tested after 36 weeks of dermal exposure to an HFO substance at 167.6 mg/kg-bw per day, whereas tumours developed in 18% of the mice exposed to the lowest dose of 8.4 mg/kg-bw per day (McKee et al. 1990). HFOs

demonstrated genotoxicity in *in vivo* and *in vitro* assays when applied dermally, and a mode of action for the induction of tumours involving direct interaction with genetic material cannot be precluded. There are no carcinogenicity studies by the inhalation route to inform the carcinogenic potential of these substances in the general population following inhalation exposure.

Given that the potential for general population exposure to the industry-restricted HFOs results primarily from inhalation of ambient air containing HFO vapours due to evaporative emissions during transportation and that the estimated maximum air concentration (1.28 $\mu g/m^3$) is considered to be low, the risk to human health is likewise considered to be low. The conservative nature of the ambient air concentration estimated is highlighted by a bystander being placed at 50 m and 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 HFOs via the dermal and oral routes is not expected; therefore, risk to human health from these routes of exposure is not expected.

With respect to non-cancer effects, decreased body weights and increased liver weights in rats were the primary adverse effects observed following a short-term repeated inhalation exposure of 6 hours/day for 9 days. A critical LOAEC of 540 mg/m^3 was reported in the single available inhalation study. Comparison of this critical effect level for inhalation exposure in rats with the estimated maximum daily exposure concentration of 1.28 $\mu g/m^3$ in ambient air results in an MOE of approximately 420 000. The margin is considered more than adequately protective to account for the uncertainties in the data set for the human health risk assessment for both cancer and non-cancer effects, especially in light of the highly conservative nature of the estimated exposures.

Uncertainties in Evaluation of Human Health Risk

The PSSA screening assessments evaluate substances that are complex combinations of hydrocarbons (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 release limits from petroleum facilities target broad releases, such as releases of oils and grease, to water or air. These widely encompassing release categories do not allow for the detection of individual complex mixtures or production streams. As such, the monitoring of broad releases cannot provide sufficient data to associate a detected release with a specific substance identified by a CAS RN, nor can the proportion of releases attributed to individual CAS RNs be defined.

Uncertainty exists by using empirical equations for the estimation of evaporative emissions. It is noted that the transit evaporative emissions also vary with physical conditions, such as the tightness of transport vessels or the valve settings. The screening estimation of evaporative emissions does not account for these.

There is uncertainty regarding the conservative estimation of human exposure because of the lack of monitoring data of HFOs in the ambient air and the use of modelling. SCREEN3 modelling of the dispersion profile of HFO vapours requires limited input parameters and non-site-specific meteorological data. These assumptions will introduce more uncertainty compared with other complex dispersion models (Tables A6.1 and A6.2 in Appendix 6).

Because the relative differences in absorption of HFOs through the inhalation, dermal and oral routes of exposure are not well documented, a conservative assumption of 100% absorption was made. Thus, the internal (systemic) doses were considered to be equivalent to the external doses that were used for treatment of the laboratory animals.

As the industry-restricted HFOs are UVCBs, their specific compositions are not well defined. HFO streams under the same CAS RN can vary significantly in the number, identity and proportion of components. Consequently, it is difficult to obtain a representative toxicological dataset for these specific HFO CAS RNs. For this reason, all available health effects data on HFO substances were pooled across CAS RNs to develop a comprehensive toxicological profile. More research by the scientific community or the petroleum sector to elucidate the compositions of petroleum substances would allow for better characterization of the potential health risks associated with possible exposure to these substances.

Uncertainty also exists due to the paucity of data available regarding the physical-chemical properties of certain HFOs. The densities of the specific CAS RNs were not provided in the health effects studies; thus, these properties were often obtained from alternative sources. However, because each sample of a particular CAS RN can be slightly different in its composition (as stated previously), these properties may not be entirely representative of a specific sample tested in any one study.

Uncertainty also exists because certain details of the laboratory animals (i.e., sex, strain, body weight and minute volume) were often not stated in the health effects studies and were obtained from laboratory standard data. Thus, these data may not be entirely representative of the physical features of the actual test animals used in the studies.

Conclusion

Based on comparison of levels expected to cause harm to organisms with estimated exposure levels, these HFOs have low risk to cause harm to aquatic life in the confined marine waters around loading wharfs due to the low estimated frequency of — and, hence, exposure to the environment from — unintentional spills of these HFOs during ship loading.

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 five industry-restricted HFOs (CAS RNs 64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7 and 70592-78-8) do not meet the criteria under paragraphs 64(a) or 64(b) of 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 the information presented in this screening assessment, the critical effect for the initial categorization of risk to human health was carcinogenicity. However, because the estimates of exposure indicate that the potential exposure of the general population to industry-restricted HFOs from ambient air is expected to be very low, resulting in an extraordinarily large MOE (approximately 420 000), the likelihood of inhalation exposure of Canadians is considered to be very low. Exposure of the general population to industry-restricted HFOs via the dermal and oral routes is not expected. Therefore, based on the adequacy of the margins between estimated exposure to industry-restricted HFO substances and critical effect levels, it is concluded that the five industry-restricted HFOs (CAS RNs 64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7 and 70592-78-8) 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 these five industry-restricted HFOs listed under CAS RNs 64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7 and 70592-78-8 do not meet any of the criteria set out in section 64 of CEPA 1999.

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Appendix 1. Petroleum substance groupings

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 combination of hydrocarbons primarily from C_4–C_{12}	Gasoline
Gas oils	Complex combination of hydrocarbons primarily from C_9–C_{25}	Diesel
Heavy fuel oils	Complex combination of heavy hydrocarbons primarily from C_{11}–C_{50}	Fuel Oil No. 6
Base oils	Complex combination of hydrocarbons primarily from C_{15}–C_{50}	Lubricating oils
Aromatic extracts	Complex combination of primarily aromatic hydrocarbons from C_{15}–C_{50}	Feedstock for benzene production
Waxes, slack waxes and petrolatum	Complex combination of primarily aliphatic hydrocarbons from C_{12}–C_{85}	Petrolatum
Bitumen or vacuum residues	Complex combination 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) and a contractor's report presented to the Canadian Petroleum Products Institute (Simpson 2005).

Appendix 2. Physical and chemical data tables for industry-restricted HFOs

Table A2.1. Substance identity of industry-restricted HFOs

CAS RN and DSL Name	64741-75-9 Residues (petroleum), hydrocracked	NCI 2006	
	68783-08-4 Gas oils (petroleum), heavy atmospheric	NCI 2006	
	70592-76-6 Distillates (petroleum), intermediate vacuum	NCI 2006	
	70592-77-7 Distillates (petroleum), light vacuum	NCI 2006	
	70592-78-8 Distillates (petroleum), vacuum	NCI 2006	
Chemical group	Petroleum – HFOs		
Major components	Aromatic and aliphatic hydrocarbons		CONCAWE 1998
Carbon range	CAS RN 64741-75-9	> C_{20}	CONCAWE 1998
	CAS RN 68783-08-4	C_7–C_{35}	CONCAWE 1998
	CAS RN 70592-76-6	C_{14}–C_{42}	CONCAWE 1998
	CAS RN 70592-77-7	C_{11}–C_{35}	CONCAWE 1998
	CAS RN 70592-78-8	C_{15}–C_{50}	CONCAWE 1998
Approximate ratio of aromatics to non-aromatics	50:50		API 2004
Three- to Seven-ring polynuclear aromatic hydrocarbons (PAHs) (weight %)	6–20%		CONCAWE 1998

Table A2.2. Boiling point ranges for HFOs (CONCAWE 1998)

CAS RN	Boiling point range (°C)	Carbon range	Reference
64741-75-9	> 350	> C_{20}	CONCAWE 1998; API 2004
68783-08-4	121–510	C_7–C_{35}	CONCAWE 1998; API 2004
70592-76-6	250–545	C_{14}–C_{42}	CONCAWE 1998; API 2004
70592-77-7	250–545	C_{11}–C_{35}	CONCAWE 1998; API 2004
70592-78-8	270–600	C_{15}–C_{50}	CONCAWE 1998; API 2004

Table A2.3. Representative structures attributed to each CAS RN

	Boiling point (°C)	**CAS RN**				
		64741-75-9	**68783-08-4**	**70592-76-6**	**70592-77-7**	**70592-78-8**
Alkanes						
C_9	151		Yes			
C_{15}	271		Yes	Yes	Yes	Yes
C_{20}	343		Yes	Yes	Yes	Yes
C_{30}	450	Yes	Yes	Yes	Yes	Yes
C_{50}	548	Yes				Yes
Isoalkanes						
C_9	141		Yes			
C_{15}	250		Yes	Yes	Yes	
C_{20}	326		Yes	Yes	Yes	Yes
C_{30}	350	Yes	Yes	Yes	Yes	Yes
C_{50}	548	Yes				Yes
One-ring cycloalkanes						
C_9	144		Yes			
C_{15}	282		Yes	Yes	Yes	
C_{20}	360	Yes	Yes	Yes	Yes	Yes
C_{30}	421	Yes	Yes	Yes	Yes	Yes
C_{50}	699	Yes				
Two-ring cycloalkanes						
C_9	167		Yes			
C_{15}	244		Yes			
C_{20}	339		Yes	Yes	Yes	Yes
C_{30}	420	Yes	Yes	Yes	Yes	Yes
C_{50}	687	Yes				
Polycycloalkanes						
C_{14}	255		Yes	Yes	Yes	
C_{18}	316		Yes	Yes	Yes	Yes
C_{22}	365	Yes	Yes	Yes	Yes	Yes
One-ring aromatics						
C_9	165		Yes			
C_{15}	281		Yes	Yes	Yes	Yes
C_{20}	359	Yes	Yes	Yes	Yes	Yes
C_{30}	437	Yes	Yes	Yes	Yes	Yes
C_{50}	697	Yes				
Cycloalkane monoaromatics						

	Boiling point (°C)	CAS RN				
		64741-75-9	**68783-08-4**	**70592-76-6**	**70592-77-7**	**70592-78-8**
C_{10}	208		Yes			
C_{15}	285		Yes	Yes	Yes	Yes
C_{20}	351	Yes	Yes	Yes	Yes	Yes
Two-ring aromatics						
C_{15}	308		Yes	Yes	Yes	Yes
C_{20}	373	Yes	Yes	Yes	Yes	Yes
C_{30}	469	Yes	Yes	Yes	Yes	Yes
C_{50}	722	Yes				
Cycloalkane diaromatics						
C_{12}	279		Yes	Yes	Yes	Yes
C_{15}	321		Yes	Yes	Yes	Yes
C_{20}	374	Yes	Yes	Yes	Yes	Yes
Three-ring aromatics						
C_{15}	350		Yes	Yes	Yes	Yes
C_{20}	398	Yes	Yes	Yes	Yes	Yes
C_{30}	493	Yes	Yes	Yes	Yes	Yes
C_{50}	746	Yes				
Four-ring aromatics						
C_{16}	384	Yes	Yes	Yes	Yes	Yes
C_{20}	480	Yes	Yes	Yes	Yes	Yes
Five-ring aromatics						
C_{20}	495	Yes	Yes	Yes	Yes	Yes
C_{30}	545	Yes		Yes	Yes	Yes
Six-ring aromatics						
C_{22}	> 500	Yes	Yes	Yes	Yes	Yes

Table A2.4. Physical-chemical properties for representative structures of HFOs[a]

Chemical class, name (CAS RN)	HFO represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]	Sub-cooled liquid vapour pressure (Pa)[c]

Alkanes					
C_9 *n*-nonane (111-84-2)	68783-08-4	151 (expt.)	−54 (expt.)	593 (expt.)	
C_{15} pentadecane (629-62-9)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	271 (expt.)	12	0.03	
C_{20} eicosane (112-95-8)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	343 (expt.)	37 (expt.)	6×10^{-4}	8×10^{-4}
C_{30} triacontane	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	450 (expt.)	65.8 (expt.)	4×10^{-9}	9×10^{-9}
C_{50}	64741-75-9, 68333-22-2, 68478-17-1, 70592-78-8	548 (expt.)	88 (expt.)	2×10^{-7}	8×10^{-7}
Isoalkanes					
C_9 2,3-dimethylheptane (3074-71-3)	68783-08-4	141 (expt.)	−116 (expt.)	1×10^{3}	
C_{15} 2-methyltetra-decane (1560-95-8)	68783-08-4, 70592-76-6, 70592-77-7	250	1.5	5.8	
C_{20} 3-methyl-nonadecane (6418-45-7)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	326	40	0.1	0.1
C_{30} hexamethyl-tetracosane (111-01-3)	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	350 (expt.)	−38 (expt.)	0.04	
C_{50}	64741-75-9, 70592-78-8	548	289	1×10^{-13}	1×10^{-9}

One-ring cycloalkanes					
C_9 1,2,3-trimethyl-cyclohexane (1678-97-3)	68783-08-4	144 (expt.)	−66.9 (expt.)	649	
C_{15} nonylcyclo-hexane (2883-02-5)	68783-08-4, 70592-76-6, 70592-77-7	282 (expt.)	−10 (expt.)	1.2 (expt.)	
C_{20} tetradecyl-cyclohexane (1795-18-2)	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	360 (expt.)	24 (expt.)	0.02	0.02
C_{30} 1,5-dimethyl-1-(3,7,11,15-tetramethyl-octadecyl)-cyclohexane	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	421	103	2×10^{-4}	9×10^{-4}
C_{50}	64741-75-9, 68333-22-2, 68478-17-1	699	300	1×10^{-13}	3×10^{-10}
Two-ring cycloalkanes					
C_9 cis-bicyclo-nonane (4551-51-3)	68783-08-4	167 (expt.)	−53 (expt.)	320.0	
C_{15} 2-isopenta-decylin	68783-08-4	244	23	2.4	
C_{20} 2,4-dimethyl-octyl-2-decalin	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	339	41	0.02	0.1
C_{30} 2,4,6,10,14-pentamethyl-dodecyl-2-decalin	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	420	106	0.0001	0.0009

C_{50}	64741-75-9	687	300	1×10^{-13}	3×10^{-10}
Polycycloalkanes					
C_{14} hydrophenanthrene	68783-08-4 70592-76-6 70592-77-7	255	21	4.5	
C_{18} hydrochrysene	68783-08-4 70592-76-6 70592-77-7 70592-78-8	316	66.4	0.004	0.03
C_{22} hydropicene	64741-75-9 68783-08-4 70592-76-6 70592-77-7 70592-78-8	365	117	0.003	0.002
One-ring aromatics					
C_9 ethylmethyl-benzene (25550-14-5)	68783-08-4	165.2 (expt.)	−80.8 (expt.)	384.0 (expt.)	
C_{15} 2-nonyl-benzene (1081-77-2)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	281 (expt.)	−24 (expt.)	0.7 (expt.)	
C_{20} tetradecyl-benzene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	359 (expt.)	16 (expt.)	0.008 (expt.)	0.003
C_{30} 1-benzyl-4,8,12,16-tetramethyl-eicosane	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	437	131	1×10^{-5}	1×10^{-4}
C_{50}	64741-75-9	697	304	1×10^{-13}	3×10^{-11}
Cycloalkane monoaromatics					
C_{10} tetralin (tetrahydro-naphthalene) (119-64-2)	68783-08-4	207.6 (expt.)	-35.7 (expt.)	49.1 (expt.)	49.1 (expt.)

C_{15}	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	284.8	50.9	0.34	0.58
C_{20} ethyldodecahydro-chrysene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	351.3	115.7	0.00279	0.016
Two-ring aromatics					
C_{15} 4-isopropyl-biphenyl	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	308	44	0.06	
C_{20} 2-isodecyl-naphthalene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	373	99	0.0007	0.007
C_{30} 2-(4,8,14,18-tetramethyl-hexadecyl)-naphthalene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	469	171	7×10^{-7}	2×10^{-5}
C_{50}	64741-75-9	722	316	1×10^{-13}	6×10^{-12}
Cycloalkane diaromatics					
C_{12} acenaphthene (83-32-9)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	279 (expt.)	93.4 (expt.)	0.287 (expt.)	1.36
C_{15} ethylfluorene	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	321	89.5	0.02	0.085
C_{20} isoheptylfluorene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	374	119	0.001	0.005
Three-ring aromatics					
C_{15}	68783-08-4,	350	65	0.009	

2-methyl-phen-anthrene (2531-84-2)	70592-76-6, 70592-77-7, 70592-78-8	(expt.)	(expt.)		
C_{20} 2-isohexyl-phenanthrene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	398	129	0.0001	0.002
C_{30} 2-(2,4,10-trimethyl-tridecyl)-phenanthrene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	493	191.6	10×10^{-8}	6×10^{-6}
C_{50}	64741-75-9	746	349	1×10^{-13}	1×10^{-12}
Four-ring PAHs					
C_{16} fluoranthene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	384 (expt.)	107.8 (expt.)	1×10^{-3} (expt.)	8×10^{-3}
C_{20} benzo[*k*]-fluoranthene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	480 (expt.)	217 (expt.)	1×10^{-7} (expt.)	1×10^{-5}
Five-ring PAHs					
C_{20} benzo[*a*]-pyrene (50-32-8)	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	495 (expt.)	177 (expt.)	7×10^{-7}	2×10^{-5}
C_{30} dimethyl-octylbenzo[*a*]-pyrene	64741-75-9 70592-76-6, 70592-77-7, 70592-78-8	545	231	2×10^{-9}	3×10^{-7}
Six-ring PAHs					
C_{22} benzo[*ghi*]-perylene (191-24-2)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	> 500 (expt.)	278 (expt.)	1×10^{-8} (expt.)	4×10^{-6} (expt.)

Table A2.4 cont. Physical-chemical properties for representative structures of HFOs[a]

Chemical class, name (CAS RN)	**HFO represented**	**Henry's Law constant ($Pa \cdot m^3/mol$)[d]**	**Log K_{ow}**	**Log K_{oc}**	**Aqueous solubility (mg/L)[e]**	**Sub-cooled liquid solubility (mg/L)[f]**
Alkanes						
C_9 *n*-nonane (111-84-2)	68783-08-4	3×10^5 (expt.)	5.7 (expt.)	3.0	0.2 (expt.)	
C_{15} pentadecane (629-62-9)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	1×10^6 (expt.)	7.7	4.6	8×10^{-5} (expt.)	
C_{20} eicosane (112-95-8)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	113	10	5.9	0.002 (expt.)	0.002 (expt.)
C_{30} triacontane	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	3×10^4	15	13	5×10^{-11}	2×10^{-10}
C_{50}	64741-75-9, 68333-22-2, 68478-17-1, 70592-78-8		25	14	5×10^{-21}	
Isoalkanes						
C_9 2,3-dimethyl-heptane (3074-71-3)	68783-08-4	4.3×10^4	4.6	2.8	3.1	
C_{15} 2-methyltetra-decane (1560-95-8)	68783-08-4, 70592-76-6, 70592-77-7	4×10^5	7.6	4.5	0.003	
C_{20} 3-methyl-nonadecane (6418-45-7)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	276	10	5.8	1×10^{-5}	0.13

C_{30} hexamethyl-tetracosane (111-01-3)	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	2×10^{9}	15	13	2×10^{-10}	5×10^{-11}
C_{50}	64741-75-9, 70592-78-8			13.8	6×10^{-21}	3×10^{-18}
One-ring cycloalkanes						
C_9 1,2,3-trimethyl-cyclohexane (1678-97-3)	68783-08-4	2×10^{4}	4.4	2.9	4.6	
C_{15} nonylcyclo-hexane (2883-02-5)	68783-08-4, 70592-76-6, 70592-77-7	6×10^{4}	7.5	4.6	0.004 (expt.)	
C_{20} tetradecyl-cyclohexane (1795-18-2)	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	63	9.9	5.9	1×10^{-5}	0.1
C_{30} 1,5-dimethyl-1-(3,7,11,15-tetramethyl-octadecyl)-cyclohexane	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	2×10^{8}	14.5	13	3×10^{-10}	2×10^{-9}
C_{50}	64741-75-9, 68333-22-2, 68478-17-1		25	14	2×10^{-21}	
Two-ring cycloalkanes						
C_9 cis-bicyclo-nonane (4551-51-3)	68783-08-4	2×10^{3}	3.7	3.0	19.3	
C_{15} 2-isopenta-decylin	68783-08-4	2×10^{4}	6.6	4.6	0.03	
C_{20}	68783-08-4,	1935	9.0	5.9	9×10^{-15}	0.02

2,4-dimethyl-octyl-2-decalin	70592-76-6, 70592-77-7, 70592-78-8					
C_{30} 2,4,6,10,14-pentamethyl-dodecyl-2-decalin	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	4×10^{7}	13.6	12	2×10^{-9}	1×10^{-8}
C_{50}	64741-75-9		24	14	5×10^{-20}	
Polycycloalkanes						
C_{14} hydro-phenanthrene	68783-08-4 70592-76-6 70592-77-7	8×10^{3}	5.2	4.4	0.5	
C_{18} hydrochrysene	68783-08-4 70592-76-6 70592-77-7 70592-78-8	6×10^{3}	6.2	5.3	0.03	
C_{22} hydropicene	64741-75-9 68783-08-4 70592-76-6 70592-77-7 70592-78-8	4×10^{3}	7.3	6.3	0.002	
One-ring aromatics						
C_9 ethylmethyl-benzene (25550-14-5)	68783-08-4	324	3.6 (expt.)	3	74.6 (expt.)	
C_{15} 2-nonyl-benzene (1081-77-2)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	4225	7.1 (expt.)	4.6	0.04	
C_{20} tetradecyl-benzene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	49	8.9	5.9	4×10^{-4}	0.02
C_{30} 1-benzyl-4,8,12,16-tetramethyl-eicosane	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	7.0×10^{5}	13.5	12	7×10^{-9}	8×10^{-8}

C_{50}	64741-75-9		24	14	2×10^{-19}	
Cycloalkane monoaromatics						
C_{10} tetralin (tetrahydro-naphthalene) (119-64-2)	68783-08-4	138 (expt.)	3.5 (expt.)	3.2	47 (expt.)	6.6×10^{-6}
C_{15} methyl-octahydro-phenanthrene	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	939	5.4	4.4	0.37	1.8×10^{-9}
C_{20} ethyl-dodecahydro-chyrsene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	1710	6.9	5.7	0.00274	4×10^{-10}
Two-ring aromatics						
C_{15} 4-isopropyl-biphenyl	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	24	5.5	4.6	0.7	
C_{20} 2-isodecyl-naphthalene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	420	8.1	5.9	0.002	0.005
C_{30} 2-(4,8,14,18-tetramethyl-hexadecyl)-naphthalene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	10×10^{3}	12.8	11	3×10^{-8}	8×10^{-7}
C_{50}	64741-75-9		23	13.9	1×10^{-18}	
Cycloalkane diaromatics						
C_{12} acenaphthene (83-32-9)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	5.95	3.92 (expt.)	3.70	2.534	1.30×10^{-6}
C_{15} ethylfluorene	68783-08-4, 70592-76-6,	24.8	5.05	4.45	0.198	9.7×10^{-9}

	70592-77-7, 70592-78-8					
C_{20} isoheptyl-fluorene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	102	7.44	5.68	0.0009	1.47×10^{-9}
Three-ring aromatics						
C_{15} 2-methyl-phen-anthrene (2531-84-2)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	6.5	4.9 (expt.)	4.5	0.3 (expt.)	
C_{20} 2-isohexyl-phenanthrene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	10	7.4	5.9	8×10^{-4}	0.05
C_{30} 2-(2,4,10-trimethyl-tridecyl)-phenanthrene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	3×10^{3}	12	10	1×10^{-8}	5×10^{-7}
C_{50}	64741-75-9		22	14	5×10^{-19}	8×10^{-16}
Four-ring PAHs						
C_{16} fluoranthene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	0.9 (expt.)	5.2	4.5	0.26 (expt.)	
C_{20} benzo[*k*]-fluoranthene	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	2.1×10^{-2}	6.1 (expt.)	5.3	0.0008 (expt.)	
Five-ring PAHs						
C_{20} benzo[*a*]-pyrene (50-32-8)	64741-75-9, 68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	5×10^{-5}	6 (expt.)	6.7	0.002	0.1

C_{30} dimethyl-octylbenzo[*a*]-pyrene	64741-75-9 70592-76-6, 70592-77-7, 70592-78-8	5.1	10.9	9.5	1×10^{-7}	1×10^{-5}
Six-ring PAHs						
C_{22} benzo[*ghi*]-perylene (191-24-2)	68783-08-4, 70592-76-6, 70592-77-7, 70592-78-8	3×10^{-3}	6.6	5.8	0.00026 (expt.)	

[a] All values are modelled unless denoted with an (expt.) for experimental data.

[b] This is the maximum vapour pressure of the surrogate; 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_9 and heaviest C_{50} representative structures were chosen to estimate a range of vapour pressures from the minimum to maximum values.

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

[d] Henry's Law constants for C_{20}–C_{30} representative structures were calculated with HENRYWIN Version 3.10 from EPI Suite (2008), using both sub-cooled liquid solubility and sub-cooled liquid vapour pressure. Henry's Law constants for C_{50} representative structures were not calculated, as sub-cooled liquid solubility data were not available. Solubility data gave anomalously high values for substances that have negligible solubility and volatility.

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

[f] Estimated sub-cooled liquid solubilities were obtained from the CONCAWE1462 database within PETROTOX (2009). The estimates contained within the database were calculated using the SPARC Performs Automated Reasoning in Chemistry (SPARC 2009). Sub-cooled liquid solubility values were only estimated for components determined to be solid at 25°C (i.e., $\geq C_{20}$). Sub-cooled liquid solubility data were not available for the C_{50} components.

Appendix 3. Measures designed to prevent, minimize 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, and lay out 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.

Intentional releases of petroleum products to Canadian marine waters have been regulated under the *Canada Shipping Act, 2001* and the *Migratory Birds Convention Act, 1994* to reduce the exposure of and hazard to seabirds through direct and indirect effects. The National Aerial Surveillance Program of Transport Canada was designed to monitor and deter such releases (Transport Canada 2010).

Appendix 4. Release estimation of industry-restricted HFOs during transportation

Table A4.1. Reported and extrapolated release volumes and spill numbers of HFO spilled in Canada based on historical Bunker C spill data from the Environment Canada Spill Line database (2000–2009) (Environment Canada 2011)

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)[1]
2009	12 592	98 000	636	16	43.8	113 330	162 834
2008	21 101	196 000	75	15	26.7	232 115	260 404
2007	27 000	222 460	200	27	22.2	566 995	609 428
2006	1197	15 000	261	32	25.0	28 726	85 303
2005	6351	127 184	227	52	36.5	209 599	343 969
2004	7523	98 000	182	39	30.8	203 131	287 997
2003	4230	79 490	132	43	34.9	118 438	224 520
2002	2325	60 000	227	58	27.6	97 662	210 815
2001	3182	65 000	216	32	18.8	82 744	125 177
2000	2083	27 822	95	25	28.0	37 491	86 995
Total volume spilled						1 690 231	2 397 441

[1] 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 HFO releases based on Bunker C spill data in Canada, 2000–2009 (Environment Canada 2011)

Source	Total spills	Volume spilled (L)	Proportion of total volume	Average volume spilled (L)
Other watercraft	43	416 759	0.247	14 371
Pipeline	13	333 431	0.197	33 343
Marine tanker	9	323 523	0.191	40 440
Other	46	156 374	0.093	4739
Other industrial plant	44	133 540	0.079	3257
Marine terminal	16	132 093	0.078	12 008
Train	11	61 304	0.036	10 217
Tank truck	21	37 431	0.022	2202
Refinery	23	31 904	0.019	1679
Other storage facilities	22	28 945	0.017	1809
Unknown	36	9294	0.005	774
Storage depot	7	6550	0.004	936
Transport truck	5	5150	0.003	1030

Barge	8	5018	0.003	1004
Bulk carrier	12	3805	0.002	951
Chemical plant	2	2270	0.001	2270
Electrical equipment	7	1274	0.001	182
Other motor vehicle	6	1129	0.001	282
Production field	4	418	0.000	139
Migration	2	20	0.000	20
Municipal sewer	1	NA[a]	NA	NA
Service station	1	NA	NA	NA
Total	**339**	**1 690 232**	**1**	**6583**

[a] NA: Data not available.

Table A4.2b. Causes of HFO releases based on Bunker C spill data in Canada, 2000–2009 (Environment Canada 2011)

Cause	Total spills	Volume spilled (L)	Proportion of volume	Average volume spilled (L)
Pipe leak	74	644 515	0.381	10 742
Unknown	72	414 993	0.246	11 216
Sinking	5	222 860	0.132	111 430
Other	47	141 964	0.084	4302
Grounding	7	98 980	0.059	32 993
Overflow	35	61 692	0.036	2056
Above-ground tank leak	19	51 597	0.031	3440
Valve, fitting leak	23	16 600	0.010	755
Container leak	21	11 267	0.007	751
Discharge	18	10 174	0.006	1130
Overturn	6	6637	0.004	1659
Process upset	3	4928	0.003	1643
Underground tank leak	2	2880	0.002	2880
Well blowout	2	500	0.000	250
Cooling system leak	2	443	0.000	221
Derailment	3	200	0.000	200
Total	**339**	**1 690 232**	**1**	**11 604**

Table A4.2c. Reasons for HFO releases based on Bunker C spill data in Canada, 2000–2009 (Environment Canada 2011)

Reason	Total spills	Volume spilled (L)	Proportion of volume	Average volume spilled (L)
Unknown	119	721 969	0.427	10 617
Material failure	42	270 403	0.160	7726
Human error	56	263 605	0.156	5380

Other	29	196 316	0.116	10 332
Fire, explosion	1	98 000	0.058	98 000
Equipment failure	65	77 178	0.046	1642
Negligence	3	35 000	0.021	35 000
Gasket, joint	11	19 011	0.011	1728
Damage by equipment	4	5520	0.003	1840
Power failure	2	2270	0.001	2270
Migration	2	20	0.000	20
Intent	2	182	0.000	182
Corrosion	2	569	0.000	569
Weld, seam failure	1	190	0.000	190
Total	**339**	**1 690 232**	**1**	**12 535**

Appendix 5. Modelling results for environmental properties of industry-restricted HFOs

Table A5.1. Results of the Level III fugacity modelling (EQC 2003)

Compartment of release (100%)	Percentage of substance partitioning into each compartment			
	Air	**Water**	**Soil**	**Sediment**
***n*-Alkanes**				
C_9				
Air	99.5	0.03	0.5	0.02
Water	1.5	48	0	50.5
Soil	0.1	0	99.9	0
C_{15}				
Air	98.4	0.01	1.5	0.1
Water	0.01	8.7	0	91.3
Soil	0.1	0.002	99.9	0.02
C_{20}				
Air	13.7	0.9	66.5	18.8
Water	0	4.6	0	95.4
Soil	0	0.002	99.9	0.04
C_{30}				
Air	0.6	0.4	79.9	19.2
Water	0	1.9	0	98.1
Soil	0	0.002	99.9	0.1
C_{50}				
Air	0.03	0.02	97.3	2.7
Water	0	0.9	0	99.1
Soil	0	0.003	99.7	0.3
Isoalkanes				
C_9				
Air	99.8	0	0.2	0
Water	3.3	85.7	7.0E-3	11
Soil	6.2	9.0E-3	93.7	1.0E-3
C_{15}				
Air	99	0.001	1.0	0.01
Water	0.01	9.6	0.0	90.4
Soil	0.04	0.001	99.9	0.01
C_{20}				
Air	94	0.05	5.1	0.9
Water	0	5	0	95
Soil	0	0.002	99.9	0.03
C_{30}				
Air	69.7	0.2	18.1	12.1
Water	0	1.3	0	98.7
Soil	0.1	0.003	99.7	0.2

Compartment of release (100%)	Percentage of substance partitioning into each compartment			
	Air	**Water**	**Soil**	**Sediment**
C_{50}				
Air	0.03	0.03	96.7	3.3
Water	0	0.9	0	99.1
Soil	0	0.003	99.7	0.3
One-ring cycloalkanes				
C_9				
Air	99.8	0	0.2	0
Water	2.8	93.4	3.8	0
Soil	3.2	9.0E-3	96.8	0
C_{15}				
Air	97.3	0.03	2.3	0.4
Water	0.006	7	0	93
Soil	0.002	0.002	99.9	0.02
C_{20}				
Air	46.5	1.4	15.7	36.4
Water	0	3.7	0	96.3
Soil	0	0.002	99.9	0.05
C_{30}				
Air	4.5	0.3	77.1	18.1
Water	0	1.9	0	98.2
Soil	0	0.002	99.9	0.1
C_{50}				
Air	0.03	0.03	96.7	3.3
Water	0	0.9	0	99.1
Soil	0	0.003	99.7	0.3
Two-ring cycloalkanes				
C_9				
Air	99.0	0.2	0.8	0.01
Water	2.7	88.8	0.02	8.5
Soil	2	0.1	97.9	0.01
C_{15}				
Air	96.8	0.008	3	0.1
Water	0.05	6	0	94
Soil	0.06	0.002	99.9	0.04
C_{20}				
Air	70.5	0.1	20.7	8.7
Water	0	1.3	0	98.7
Soil	0	0.002	99.8	0.2
C_{30}				
Air	2.7	0.05	92.1	5.2

Compartment of release (100%)	Percentage of substance partitioning into each compartment			
	Air	**Water**	**Soil**	**Sediment**
Water	0	0.9	0	99.1
Soil	0	0.003	99.7	0.3
C_{50}				
Air	0.2	0.15	87.4	12.3
Water	0	1.2	0	98.8
Soil	0	0.003	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	99.9	0.03
C_{18}				
Air	7.7	0.6	60.4	31.2
Water	0	2.0	0.05	97.9
Soil	0	0.004	99.8	0.2
C_{22}				
Air	3.0	0.05	91.8	5.2
Water	0	1.0	0.02	99.0
Soil	0	0	99.7	0.3
One-ring aromatics				
C_9				
Air	99.4	0.3	0.3	0
Water	4.4	94.6	0.01	0.9
Soil	1.0	0.1	98.9	0
C_{15}				
Air	98.4	0.05	1.1	0.4
Water	0.03	11.5	0	88.5
Soil	0.001	0.001	99.9	0.01
C_{20}				
Air	63.2	0.5	28.3	8
Water	0	5.6	0	94.4
Soil	0	0.002	99.9	0.03
C_{30}				
Air	4.7	0.2	79.5	15.5
Water	0	1.5	0	98.5
Soil	0	0.002	99.8	0.2
C_{50}				
Air	0.1	0.08	91.9	7.9
Water	0	1	0	99
Soil	0	0.003	99.7	0.27
Cycloalkane				

Compartment of release (100%)	Percentage of substance partitioning into each compartment			
	Air	**Water**	**Soil**	**Sediment**
monoaromatics				
C_{10}				
Air	99.8	0.2	0.05	0.0002
Water	2.0	97.8	0.001	0.1
Soil	0.2	0.02	99.8	0.00002
C_{15}				
Air	81.4	1.7	1.5	15.4
Water	0.2	9.7	0.004	90.0
Soil	0.002	0.004	100	0.04
C_{20}				
Air	24.7	0.9	24.3	50
Water	0.005	1.78	0.005	98.2
Soil	0.0	0.002	99.9	0.1
Two-ring aromatics				
C_{15}				
Air	65.3	6	9.6	19
Water	0.4	23.9	0.06	75.6
Soil	0.001	0.009	99.9	0.03
C_{20}				
Air	47	1.4	33	18.6
Water	0	7	0	93
Soil	0	0.002	99.9	0.02
C_{30}				
Air	3.6	0.4	77.6	18.5
Water	0	1.9	0	98.1
Soil	0	0.002	99.9	0.1
C_{50}				
Air	0.2	0.2	86.7	12.9
Water	0	1.2	0	98.8
Soil	0	0.003	99.8	0.2
Cycloalkane diaromatics				
C_{12}				
Air	91.6	6.7	1.4	0.4
Water	0.4	94.1	0.006	5.5
Soil	0.002	0.04	100	0.002
C_{15}				
Air	92.6	4.2	1.7	1.5
Water	1.5	72.6	0.028	25.9
Soil	0.001	0.005	100	0.002
C_{20}				

Compartment of release (100%)	Percentage of substance partitioning into each compartment			
	Air	**Water**	**Soil**	**Sediment**
Air	94.1	0.6	4.6	0.7
Water	0.07	44.8	0.003	55.1
Soil	< 0.001	< 0.001	100	< 0.001
Three-ring aromatics				
C_{15}				
Air	68.5	9.73	11.6	10.2
Water	0.1	48.7	0.02	51.2
Soil	0	0.01	99.98	0.01
C_{20}				
Air	41.7	2.6	9.6	46.0
Water	0.001	5.4	0	94.6
Soil	0	0.002	99.99	0.03
C_{30}				
Air	1.2	0.3	81.3	17.2
Water	0	1.6	0	98.4
Soil	0	0.002	99.9	0.1
C_{50}				
Air	0.009	0.01	98.8	1.2
Water	0	0.9	0	99.1
Soil	0	0.003	99.7	0.3
Four-ring PAHs				
C_{16}				
Air	13.1	4.7	58.1	24.1
Water	0	16.2	0.04	83.7
Soil	0	0	99.9	0.1
C_{20}				
Air	0.3	0.4	86.6	12.6
Water	0.0	3.0	0.0	97.0
Soil	0	0	99.8	0.2
Five-ring PAHs				
C_{20}				
Air	0.65	0.36	85.1	13.9
Water	0	2.6	0.002	97.4
Soil	0	0.005	99.8	0.2
C_{30}				
Air	0.06	0.05	95	4.9
Water	0	0.9	0	99.1
Soil	0	0.003	99.7	0.3
Six-ring PAHs				
C_{22}				
Air	0.3	0.3	83.7	15.6

Compartment of release (100%)	Percentage of substance partitioning into each compartment			
	Air	**Water**	**Soil**	**Sediment**
Water	0	2.1	0	97.9
Soil	0	0	99.9	0.1

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

	Primary Degradation	
	BioHCWin (2008)[a] (days)	**BIOWIN 4 (2009) Expert Survey[b]**
Alkanes		
C_9 *n*-nonane	7	4.20
C_{15} pentadecane	19	4.08
C_{20} eicosane	40	3.98
C_{30} triacontane	143	3.78
C_{50}	4581	3.37
Isoalkanes		
C_9 2,3-dimethylheptane	8	3.93
C_{15} 2-methyltetradecane	17	3.81
C_{20} 3-methylnonadecane	36	3.71
C_{30} hexamethyltetracosane	333	3.24
C_{50}	3504	3.37
One-ring cycloalkanes		
C_9 1,2,3-trimethylcyclohexane	4	3.67
C_{15} nonylcyclohexane	25	3.81
C_{20} tetradecylcyclohexane	53	3.71
C_{30} 1,5-dimethyl-1-(3,7,11,15-tetramethyl-octadecyl)cyclohexane	154	3.24
C_{50}	660	4.18

	Primary Degradation	
	BioHCWin (2008)[a] (days)	**BIOWIN 4 (2009) Expert Survey[b]**
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
C_{30} 2,4,6,10,14-pentamethyldodecyl-2-decalin	1761	3.51
C_{50}	494	4.99
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	5	3.54
C_{15} 2-nonylbenzene	14	3.76
C_{20} tetradecylbenzene	31	3.66
C_{30} 1-benzyl-4,8,12,16-tetramethyleicosane	252	3.45
C_{50}	1594	3.65
Cycloalkane monoaromatics		
C_{10} tetralin	1.46	3.52
C_{15} methyloctahydro-phenanthrene	466	3.42
C_{20} ethyldodecahydro-chyrsene	469	3.32
Two-ring aromatics		

	Primary Degradation	
	BioHCWin (2008)[a] (days)	**BIOWIN 4 (2009) Expert Survey[b]**
C_{15} 4-isopropylbiphenyl	8	3.50
C_{20} 2-isodecylnaphthalene	24	3.66
C_{30} 2-(4,8,14,18-tetramethyl-hexadecyl)naphthalene	145	3.46
C_{50}	444	4.46
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
C_{20} 2-isohexylphenanthrene	35	3.40
C_{30} 2-(2,4,10-trimethyl-tridecyl)phenanthrene	212	3.20
C_{50} alkylated anthracene	12 690	3.66
Four-ring PAHs		
C_{16} fluoranthene	191	2.85
C_{20} benzo[*k*]fluoranthene	285	2.78
Five-ring PAHs		
C_{20} benzo[*a*]pyrene	422	2.78
C_{30} dimethyloctyl-benzo[*a*]pyrene	2076	2.51
Six-ring PAHs		
C_{22} benzo[*ghi*]perylene	517	2.75

Table A5.2 cont. Modelled data for primary (BioHCWin 2008; BIOWIN4 2009) and ultimate (BIOWIN3, 5 and 6 2009; CATABOL; TOPKAT) degradation of HFO components[a]

	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 biodegrad-ability**	**Extrapolated half-life compared with criteria (days)**
Alkanes						
C_9 *n*-nonane	3.51	0.68	0.87	99.95	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
C_{30} triacontane	2.86	0.84	0.92	100	1	< 182
C_{50}	2.24	0.99	0.95	100	1	< 182
Isoalkanes						
C_9 2,3-dimethylheptane	3.21	0.38	0.50	9.45	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	91	1	< 182
C_{30} hexamethyl-tetracosane	2.26	-0.06	0.04	5.1	0*	≥ 182
C_{50}	2.24	0.84	0.87	89.9	1	≥ 182[d]
One-ring cycloalkanes						
C_9 1,2,3-trimethyl-cyclohexane	2.92	0.43	0.32	2.64	0.011*	< 182
C_{15} nonyl-cyclohexane	3.04	0.57	0.65	57.9	1	< 182
C_{20} tetradecyl-cyclohexane	2.88	0.63	0.75	64.1	1	< 182
C_{30} 1,5-dimethyl-1-(3,7,11,15-tetramethyl-octadecyl)-	2.27	-0.0007	0.02	3.5	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 biodegrad-ability**	**Extrapolated half-life compared with criteria (days)**
cyclohexane						
C_{50}	3.14	0.64	0.22	69.2	0*	≥ 182 [d]
Two-ring cycloalkanes						
C_9 cis-bicyclononane	2.92	0.51	0.58	0	0.001	< 182
C_{15} 2-isopentadecylin	2.74	0.32	0.19	1.8	0	≥ 182
C_{20} 2,4-dimethyl-octyl-2-decalin	2.67	0.45	0.26	4.5	0	≥ 182
C_{30} 2,4,6,10,14-pentamethyl-dodecyl- 2-decalin	2.57	-0.16	0.01	4.6	0*	≥ 182
C_{50}	4.04	0.34	0.01	6.4	0*	≥ 182
Polycycloalkanes						
C_{14} hydro-phenanthrene	2.77	0.39	0.24	0	0*	≥ 182
C_{18} hydrochrysene	2.65	0.29	0.07	0	0*	≥ 182
C_{22} hydropicene	2.54	0.19	0.02	0	0*	≥ 182
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
C_{30} 1-benzyl-4,8,12,16-tetramethyl-eicosane	2.53	-0.05	0.04	5.1	0*	≥ 182
C_{50}	2.56	0.22	0.09	70	0.2*	≥ 182 [d]
Cycloalkane monoaromatics						

	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 biodegrad-ability**	**Extrapolated half-life compared with criteria (days)**
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	2.91	0*	≥ 182
Two-ring aromatics						
C_{15} 4-isopropyl-biphenyl	2.71	0.19	0.15	12.16	0*	≥ 182
C_{20} 2-isodecyl-naphthalene	2.83	0.16	0.12	3.8	0*	≥ 182
C_{30} 2-(4,8,14,18-tetramethyl-hexadecyl)-naphthalene	2.52	-0.06	0.03	4.6	0*	≥ 182
C_{50}	3.46	-0.59	0.0004	3.4	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-methyl-phenanthrene	2.70	0.26	0.16	21.2*	0.004	< 182
C_{20} 2-isohexyl-phenanthrene	2.54	-0.0012	0.036	3.99*	0.302	≥ 182
C_{30} 2-(2,4,10-	2.23	-0.22	0.01	5.6	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 biodegrad-ability**	**Extrapolated half-life compared with criteria (days)**
trimethyl-tridecyl)-phenanthrene						
C_{50} alkylated anthracene	2.58	-0.11	0.01	56.6	0*	≥ 182 [d]
Four-ring PAHs						
C_{16} fluoranthene	1.95	0.19	0.11	19.67*	0	≥ 182
C_{20} benzo[*k*]-fluoranthene	1.84	0.06	0.035	9.3	0	≥ 182
Five-ring PAHs						
C_{20} benzo[*a*]pyrene	1.84	0.06	0.035	9.29*	0*	≥ 182
C_{30} dimethyloctyl-benzo[*a*]pyrene	1.46	-0.32	0.002	6.6	0*	≥182
Six-ring PAHs						
C_{22} benzo[*ghi*]-perylene	1.79	-0.011	0.018	2.9	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.
[d] Extrapolated half-life compared with criteria (days) based on BioHCWin results (2008).
* 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. Potential presence of persistent representative structures

	CAS RN				
	64741-75-9	68789-08-4	70592-76-6	70592-77-7	70592-78-8
Isoalkanes					
C_{30}	Yes	Yes	Yes	Yes	Yes
C_{50}	Yes				Yes
One-ring cycloalkanes					
C_{30}	Yes	Yes	Yes	Yes	Yes

	CAS RN				
	64741-75-9	68789-08-4	70592-76-6	70592-77-7	70592-78-8
C_{50}	Yes				
Two-ring cycloalkanes					
C_{15}		Yes			
C_{20}		Yes	Yes	Yes	Yes
C_{30}	Yes	Yes	Yes	Yes	Yes
C_{50}	Yes				
Polycycloalkanes					
C_{14}		Yes	Yes	Yes	
C_{18}		Yes	Yes	Yes	Yes
C_{22}	Yes	Yes	Yes	Yes	Yes
One-ring aromatics					
C_{30}	Yes	Yes	Yes	Yes	Yes
C_{50}	Yes				
Cycloalkane monoaromatics					
C_{15}		Yes	Yes	Yes	Yes
C_{20}	Yes	Yes	Yes	Yes	Yes
Two-ring aromatics					
C_{15}		Yes	Yes	Yes	Yes
C_{20}	Yes	Yes	Yes	Yes	Yes
C_{30}	Yes	Yes	Yes	Yes	Yes
C_{50}	Yes				
Cycloalkane diaromatics					
C_{12}		Yes	Yes	Yes	Yes
Three-ring aromatics					
C_{20}	Yes	Yes	Yes	Yes	Yes
C_{30}	Yes	Yes	Yes	Yes	Yes
C_{50}	Yes				
Four-ring aromatics					
C_{16}	Yes	Yes	Yes	Yes	Yes
C_{20}	Yes	Yes	Yes	Yes	Yes
Five-ring aromatics					
C_{20}	Yes	Yes	Yes	Yes	Yes
C_{30}	Yes		Yes	Yes	Yes
Six-ring aromatics					

	CAS RN				
	64741-75-9	68789-08-4	70592-76-6	70592-77-7	70592-78-8
C_{22}	Yes	Yes	Yes	Yes	Yes

Table A5.4. Proportion (weight %) of persistent representative structures in three samples of Fuel Oil No. 6 (Fuhr 2008)

Persistent* representative structures with boiling points > 500°C	**Boiling point (°C)**	**Weight %**			
		Sample A	**Sample B**	**Sample C**	**Average**
Isoalkane C_{50}	548	6.8	4	10.1	**7.0**
One-ring cycloalkane C_{50}	699				
Two-ring cycloalkane C_{50}	687				
One-ring aromatic C_{50}	697	22.1	21.3	24.3	**22.6**
Two-ring aromatic C_{50}	722				
Three-ring aromatic C_{50}	746				
Five-ring aromatic C_{30}	545				
Six-ring aromatic C_{22}	> 500				
Persistent* representative structures with boiling boints from 200–500°C	**Boiling Point (°C)**	**Weight %**			
		Sample A	**Sample B**	**Sample C**	**Average**
Isoalkanes C_{30}	350	8.3	2.8	3.5	**4.9**
One-ring cycloalkanes C_{30}	421	3.4	2.0	1.9	**2.4**
Two-ring cycloalkanes C_{15}	244	2.9	1.8	1.8	**2.2**
Two-ring cycloalkanes C_{20}	339				
Two-ring cycloalkanes C_{30}	420				
Polycycloalkanes C_{14}	225	2.8	2.2	3.2	**2.7**
Polycycloalkanes C_{18}	316				
Polycycloalkanes C_{22}	365				
One-ring aromatics C_{30}	437	1.7	4.2	2.2	**2.7**
Cycloalkane monoaromatics C_{15}	285	2.2	4.3	2.6	**3.0**
Cycloalkane monoaromatics C_{20}	351				
Two-ring aromatics C_{15}	308	1.1	6.0	4.5	**3.9**
Two-ring aromatics C_{20}	373				
Two-ring aromatics C_{30}	469				
Cycloalkane diaromatics C_{12}	279	0.8	1.7	2.4	**1.6**
Three-ring aromatics C_{20}	398	0.9	2.3	3.9	**2.4**
Three-ring aromatics C_{30}	493				
Four-ring aromatics C_{16}	384	1.2	1.4	2.7	**1.8**
Four-ring aromatics C_{20}	480	0.6	0.5	0.6	**0.6**
Five-ring aromatics C_{20}	495	0.4	0.4	0.2	**0.3**
Totals		55.2	54.9	63.9	**58.1**

*Based on results from Table A5.2 (Appendix 5) and as set out by the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Table A5.5. Modelled atmospheric degradation of representative structures for HFOs via reaction with hydroxyl radicals (AOPWIN 2008)

	Half-life (days) [a]
	OH•
Alkanes	
C_9	1.1
C_{15}	1
C_{20}	0.4
C_{30}	0.3
C_{50}	0.2
Isoalkanes	
C_9	1.1
C_{15}	0.6
C_{20}	0.4
C_{30}	0.3
C_{50}	0.2
One-ring cycloalkanes	
C_9	0.8
C_{15}	0.5
C_{20}	0.4
C_{30}	0.2
C_{50}	0.2
Two-ring cycloalkanes	
C_9	0.8
C_{15}	0.4
C_{20}	0.3
C_{30}	0.2
C_{50}	0.1
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}	0.5
C_{30}	0.3
C_{50}	0.2
Cycloalkane monoaromatics	
C_{10}	0.3
C_{15}	0.5

	Half-life (days) [a]
	OH•
C_{20}	0.3
Two-ring aromatics	
C_{15}	0.2
C_{20}	0.2
C_{30}	0.1
C_{50}	0.1
Cycloalkane diaromatics	
C_{12}	0.2
C_{15}	0.6
C_{20}	0.5
Three-ring PAHs	
C_{15}	0.3
C_{20}	0.3
C_{30}	0.2
C_{50}	0.1
Four-ring PAHs	
C_{16}	0.4
C_{20}	0.2
Five-ring PAHs	
C_{20}	0.2
C_{30}	0.1
Six-ring PAHs	
C_{22}	0.1

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

Table A5.6. 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 (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 crude oil)	3.69 (expt.)	36
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}	Burkhard and Lukasewycz	5.23	1550

fluoranthene	2000 Lake trout; field study		
C_{18} chrysene	Burkhard and Lukasewycz 2000 Lake trout; field study	5.81	3990

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

Table A5.7. 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 promelas* (fathead minnow)	24 hours	9054	Weinstein and Oris 1999
pyrene	*Poecilia reticulate* (guppy)	48 hours	11 300	De Voogt et al. 1991
	Cyprinodon variegatus (sheepshead minnow)	36 days	145[a], 97[b]	Jonsson et al. 2004
benzo[*a*]pyrene	*Lepomis macrochirus* (bluegill sunfish)	48 hours	608	Jimenez et al. 1987
Molluscs				
fluoranthene	*Mytilus edulis* (blue mussel)	96 hours	5920	McLeese and Burridge 1987
	Mya arenaria (clam)		4120	
pyrene	*M. edulis*	96 hours	4430	McLeese and Burridge 1987
	M. arenaria	96 hours	6430	
Crustaceans				
fluoranthene	*Daphnia magna* (water flea)	24 hours	1742	Newsted and Giesy 1987
	Cragon septemspinosa (sand shrimp)	96 hours	180	McLeese and Burridge 1987
pyrene	*D. magna*	24 hours	2702	Newsted and Giesy 1987
	C. septemspinosa	96 hours	225	McLeese and Burridge 1987
chrysene	*D. magna*	24 hours	6088	Newsted and Giesy 1987
benzo[*a*]anthracene	*D. magna*	24 hours	2920	McCarthy et al. 1985
		24 hours	10 226	Newsted and Giesy 1987

benzo[*k*]fluoranthene	*D. magna*	24 hours	13 225	Newsted and Giesy 1987
benzo[*a*]pyrene	*D. magna*	24 hours	12 761	Newsted and Giesy 1987
benzo[*e*]pyrene	*D. magna*	24 hours	25 200	Newsted and Giesy 1987
benzo[*ghi*]perylene	*D. magna*	24 hours	28 288	Newsted and Giesy 1987
Polychaetes				
fluoranthene	*Nereis virens* (sandworm)	96 hours	720	McLeese and Burridge 1987
pyrene	*N. virens*	96 hours	700	

[a] Low exposure level (7.57 µg/L).
[b] High exposure level (72.31 µg/L).

Table A5.8. Fish BAF and BCF predictions for representative structures of HFOs using the modified 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_9 *n*-nonane (111-84-2)	5.7	0.09	1905	4074
C_{15} pentadecane (629-62-9)	7.7	0.44[c]	42	550
Isoalkanes*				
C_9 2,3-dimethylheptane (3074-71-3)	4.6	0.184	2140	3000
C_{15} 2-methyltetradecane (1560-95-8)	7.5	0.020[d]	1148	**181 970**[q]
One-ring cycloalkanes*				
C_9 1,2,3-trimethyl-cyclohexane (1678-97-3)	4.4	0.09	966	1000
C_{15} nonylcyclohexane (2883-02-5)	7.5	0.023[f]	2630	**22 909**
Two-ring cycloalkanes*				
C_9 cis-bicyclononane	3.7	0.08	272	280

(4551-51-3)				
C_{15} 2-isopentadecalin	6.3	0.04[h]	3236	**7244**
Polycycloalkanes*				
C_{14} hydrophenanthrene	5.1	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} 2-nonylbenzene (1081-77-2)	7.1 (expt.)	0.01[l]	4365	**151 356**
Cycloalkane monoaromatics				
C_{10} tetralin (tetrahydro-naphthalene) (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_{15} 4-isopropylbiphenyl	5.5 (expt.)	0.65[o]	871	1175
Cyclolkane diaromatics				
C_{12} acenaphthene (83-32-9)	3.92 (expt.)	0.10	275	380
C_{15} ethylfluorene	**5.05**	0.23	730	809
C_{20} isoheptylfluorene	**7.4**	0.06[p]	501	**26 915**
Three-ring aromatics*				
C_{15} 2-methylphenanthrene	4.9	0.20	789	851

(2531-84-2)				
C_{20} 2-isohexylphenanthrene	7.2	0.04	1100	**60 256**
Four-ring aromatics				
C_{16} fluoranthene (206-44-0)	5.2 (expt.)	0.13	516	563
C_{20} benzo[*k*]fluoranthene (207-08-9)	6.1 (expt.)	0.11	393	676
Five-ring aromatics*				
C_{20} benzo[*a*]pyrene (50-32-8)	6.1 (expt.)	0.38	500	984
Six-ring aromatics				
C_{22} benzo[*ghi*]perylene (191-24-2)	6.6 (expt.)	1.13	91.2	161

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

[a] Metabolic rate constant normalized to middle trophic level (MTL) fish in Arnot-Gobas three trophic level model (2004) at W = 184 g, T = 10°C, L = 6.8%) based on estimated QSAR vaues from BCFBAF v3.01 unless otherwise indicated

[b] Arnot-Gobas BCF and BAF predictions for middle 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 A5.9a and A5.9b (Appendix 5).

[c] Based on rate constant data for C_{15} *n*-pentadecane.

[d] Based 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.

[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)

* Alkanes C_{20}–C_{50}, Isoalkanes C_{20}–C_{50}, One-ring cycloalkanes C_{20}–C_{50}, Two-ring cycloalkanes C_{20}–C_{50}, One-ring aromatic C_{20}–C_{50}, Two-ring aromatic C_{20}–C_{50}, Three-ring aromatic C_{30}–C_{50} and Five-ring aromatic C_{30} 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).

Table A5.9a. Experimental BCFs and predicted BCFs and BAFs normalized to BCF study conditions and a middle trophic level fish for selected representative structures using a modified version of the Arnot-Gobas BCFBAF model (2003)

	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, 2005a; 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-methyl-cyclohexane[h]	3.61 (expt.)	BCF_{ss}[1]	240	190*	275*	229*	426*	CITI 1992; carp
C_8 ethyl-cyclohexane[h]	4.56 (expt.)	BCF_{ss}[1]	2529	1622*	2344*	4467*	5495*	CITI 1992; carp

C_{14} *n*-octyl-cyclohexane	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} isopropyl-decalin[h]	5.50	$BMF_{kinetic}$	0.02	n/a	n/a	n/a	n/a	EMBSI 2006a; BMF rainbow trout
C_{16} diisopropyl-decalin[h]	6.85	$BMF_{kinetic}$	0.1	n/a	n/a	n/a	n/a	EMBSI 2008a; BMF rainbow trout
Polycyclo-alkanes								
C_{17} isopropyl-hydro-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} perhydro-chrysene	6.0	$BMF_{kinetic}$	0.38	n/a	n/a	n/a	n/a	EMBSI 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-diethyl-benzene[h]	3.72 (expt.)	BCF_{ss}[1]	516[e]	245*	355*	309*	427*	CITI 1992; carp
C_{11}	3.66	BCF_{ss}[1]	< 1.0	214*	309*	263*	263*	JNITE

1-methyl-4-tertbutyl-benzene[h]	(expt.)							2010; carp
C_{14} *n*-octyl-benzene[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} decyl-benzene[h]	7.4 (expt.)	$BMF_{kinetic}$	0.18	n/a	n/a	n/a	n/a	EMBSI 2005c; 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[h]	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-methyl-naphthalene[h]	3.86 (expt.)	BCF_{ss}[1] $BCF_{kinetic}$[1]	2886[e] 3930[f]	2 884*	n/a	2884*	n/a	Jonsson et al. 2004; sheepshead minnow
C_{12} 1,3-dimethyl-	4.42 (expt.)	BCF_{ss}[1] $BCF_{kinetic}$[1]	4039[e] 5751[f]	4073	n/a	4073	n/a	Jonsson et al. 2004;

naphthalene[h]								sheepshead minnow
C_{13} 2-isopropyl-naphthalene	4.63	BCF_{ss}[1] $BCF_{kinetic}$[1]	12 902[e] 33 321[f]	12 882	n/a	12 882	n/a	Jonsson et al. 2004; sheepshead minnow
C_{14} 4-ethyl-biphenyl[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} hexahydro-terphenyl[h]	6.44	BCF_{ss}[1]	1646	n/a	n/a	n/a	n/a	EMBSI 2008c; rainbow trout
C_{18} hexahydro-terphenyl[h]	6.44	$BMF_{kinetic}$	0.06	n/a	n/a	n/a	n/a	EMBSI 2009; rainbow trout
C_{18} octahydro-chrysene[h]	6.0	$BMF_{kinetic}$	0.05	n/a	n/a	n/a	n/a	EMBSI 2010a; BMF rainbow trout
C_{18} hexahydro-chrysene[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} acenaph-thylene[h]	3.94 (expt.)	BCF_{ss}[1]	275[e]	275	380	275	380	Yakata et al. 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	5.16 (expt.)	BCF_{ss}[1]	277[e]	275	646	281	724	EMBSI 2007a, 2007b;

								rainbow trout
C_{16} fluoranthene	5.16 (expt.)	BCF_{ss}[1]	1700	1698	1288	1820	1621	Carlson et al. 1979; fathead minnow
C_{16} fluoranthene	5.16 (expt.)	$BMF_{kinetic}$	0.021[f]	n/a	n/a	n/a	n/a	EMBSI, 2007b, 2007a, 2008b, 2009 BMF; rainbow trout
C_{18} chrysene[h]	5.81 (expt.)	BCF_{ss}[1]	153	n/a	n/a	n/a	n/a	EMBSI 2006b; rainbow trout BCF
C_{18} chrysene[h]	5.81 (expt.)	$BMF_{kinetic}$	0.023[f]	1546	1047	1950	1995	EMBSI 2010a, 2010b; rainbow trout BMF
C_{18} triphenylene[h]	5.49 (expt.)	BCF_{ss}[1]	61	62	54	63	55	JNITE 2010; carp
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

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

[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 (W = 184 g, T = 10°C, L = 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.

[1] BCF steady state (tissue conc./water conc.).

*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 A5.9b. Calculated kinetic rate constants for selected representative structures

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-trimethyl-dodecane[e]	BCF_{ss}[1]	1317	0.2103[b] 1.139	0.000[c] 0.005
C_{15} 2,6,10-trimethyl-dodecane[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} isopropylhydro-phenanthrene[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[m]	$BMF_{kinetic}$		0.091 0.056	0.000
One-ring aromatics				
C_9 1,2,3-trimethyl-benzene[e]	BCF_{ss}[1]	398	2.989	1.852
C_{10} 1,2-diethylbenzene[e]	BCF_{ss}[1]	398	1.679	1.617
C_{11} 1-methyl-4-tertbutyl-benzene[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} octahydro-phenanthrene[e]	BCF_{ss}[1]	n/a	n/a	n/a
C_{14} octahydro-phenanthrene[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[e]	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	n/a 0.403
C_{13} 2-isopropyl-naphthalene[e]	BCF_{ss}[1] $BCF_{kinetic}$[1]	3961[d]	0.120[d] 0.120	n/a 0.551[f]
C_{14} 4-ethylbiphenyl[e]	BCF_{ss}[1]		1.140	0.480
Cycloalkane diaromatics				
C_{12}	BCF_{ss}[1]	401	1.037	1.028

acenaphthene				
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} fluorene[e]	$BMF_{kinetic}$[1]		0.100 (k_e)	0.000
C_{14} phenanthrene[e]	BCF_{ss}[1]	957	0.833	0.821
C_{16} fluoranthene	BCF_{ss}[1]	197	0.548	0.151
C_{18} chrysene[e]	BCF_{ss}[1]	n/a	n/a	n/a
C_{18} chrysene[e]	$BMF_{kinetic}$		0.508[f]	0.000
C_{18} triphenylene[e]	BCF_{ss}[1]	406	3.512	0.009
C_{18} 1-methyl-7-(1-methylethyl)-phenanthrene[e]	$BMF_{kinetic}$		1.815 1.78	0.000

Table A5.9b cont. Calculated kinetic rate constants for selected representative structures

Substance	**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]	0.657	0.001	0.007		JNITE 2010; carp
C_{12} *n*-dodecane[e]	4.95	0.002	0.013		Tolls and van Dijk 2002; fathead minnow
C_{15} *n*-pentadecane	1.69	0.001	0.003		CITI 1992; carp
C_{15} *n*-pentadecane	1.30	0.001	0.003		JNITE 2010; carp
C_{16} *n*-hexadecane[e]	0.249	0.001	0.002		CITI 1992; carp
C_{16}	13.30	0.001	0.008		JNITE 2010;

n-hexadecane[e]					carp
Isoalkanes					
C_{15} 2,6,10-trimethyl-dodecane[e]	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]	0.032[h]	0.035	0.004	28%	EMBSI 2004a, 2005a; rainbow trout
One-ring cycloalkanes					
C_6 cyclohexane[e]	2.050	0.001	0.008		CITI 1992; carp
C_7 1-methyl-cyclohexane[e]	-0.429	0.001	0.008		CITI 1992; carp
C_8 ethylcyclohexane[e]	-0.087	0.001	0.008		CITI 1992; carp
C_{14} *n*-octyl-cyclohexane[e]	0.087[h]	0.035	0.008	5%	EMBSI 2006a; BMF rainbow trout
Two-ring cycloalkanes					
C_{10} trans-decalin[e]	-0.336	0.001	0.008		CITI 1992; carp
C_{10} cis-decalin[e]	-0.390	0.001	0.008		CITI 1992; carp
C_{13} isopropyldecalin[e] and C_{16} diisopropyldecalin[e]	0.128[h]	0.035	0.008	6%	EMBSI 2006a; rainbow trout
Polycycloalkanes					
C_{17} isopropylhydro-phenanthrene[e]	0.035[h]	0.035	0.008	13%	EMBSI 2006b; rainbow trout
C_{18} 1-methyl-7-(isopropyl)-hydro-phenanthrene[e]	0.030[h]	0.035	0.006	9%	EMBSI 2008a; rainbow trout
C_{18} perhydrochrysene[e]	0.048[h]	0.035	0.008	15%	EMBSI 2008b; rainbow trout
One-ring aromatics					
C_9 1,2,3-trimethyl-benzene[e]	1.128	0.001	0.008		CITI 1992; carp
C_{10} 1,2-diethyl-benzene[e]	-0.854	0.001	0.008		CITI 1992; carp

C_{11} 1-methyl-4-tertbutylbenzene[e]	395.6	0.001	0.008		JNITE 2010; carp
C_{14} *n*-octylbenzene[e]	0.600[h]	0.035	0.008	10%	EMBSI 2007a, b; BMF rainbow trout and carp
C_{16} decylbenzene[e]	0.284[h]	0.035	0.005		EMBSI 2005c; BMF rainbow trout
Cycloalkane monoaromatics					
C_{10} tetralin	-1.009	0.001	0.008		CITI 1992; carp
C_{14} octahydro-phenanthrene[e]	n/a	n/a	n/a	n/a	EMBSI 2005d; BCF rainbow trout
C_{14} octahydro-phenanthrene[e]	0.197[h]	0.035	0.007	19%	EMBSI 2009; BMF rainbow trout
C_{18} dodecahydro-chyrsene[e]	n/a	n/a	n/a	n/a	EMBSI 2008c; rainbow trout
C_{18} dodecahydro-chyrsene[e]	0.132[h]	0.035	0.007	18%	EMBSI 2008c; rainbow trout
Two-ring aromatics					
C_{10} naphthalene[e]	-0.020	0.001	0.008		JNITE 2010; carp
C_{11} 2-methyl-naphthalene[e]	0.000	0.002	0.001	3.2%[g]	Jonsson et al. 2004; sheepshead minnow
C_{12} 1,3-dimethyl-naphthalene[e]	n/a 0.000	n/a 0.002	n/a 0.001	n/a 3.2%[g]	Jonsson et al. 2004 (cited in Lampi et al. 2010); sheepshead minnow
C_{13} 2-isopropyl-naphthalene[e]	n/a -0.447	n/a 0.002	n/a 0.014	n/a 3.2%[g]	Jonsson et al. 2004; sheepshead minnow
C_{14} 4-ethylbiphenyl[e]	0.645	0.002	0.013		Yakata et al. 2006; carp
Cycloalkane diaromatics					
C_{12} acenaphthene	-0.632	0.001	0.008		CITI 1992; carp

C_{18} hexahydro-terphenyl[e]	n/a	n/a	n/a		EMBSI 2008c; rainbow trout
C_{18} octahydro-chrysene[e]	1.383[h]	0.034	0.007	55%	EMBSI 2010a; BMF rainbow trout
C_{18} hexahydro-chrysene[e]	1.383[h]	0.034	0.007	49%	EMBSI 2010a; BMF rainbow trout
Three- and Four-ring aromatics					
C_{12} acenaphthylene[e]	0.370	0.001	0.010		Yakata et al. 2006; carp
C_{13} fluorene[e]	-0.302	0.001	0.012		CITI 1992; Carlson et al. 1979
C_{13} fluorene[e]	0.098	n/a	0.002	14%	Niimi and Palazzo 1986
C_{14} phenanthrene[e]	-0.512	0.002	0.012		Carlson et al. 1979; fathead minnow
C_{16} fluoranthene	0.383	0.002	0.012		Carlson et al. 1979; fathead minnow
C_{18} chrysene[e]	n/a	n/a	n/a	n/a	EMBSI 2006b, 2009; rainbow trout
C_{18} chrysene[e]	0.471	0.035[f]	0.002[c]	8%[f]	EMBSI 2010a, 2010b; BMF rainbow trout
C_{18} triphenylene[e]	3.500	0.0007	0.003		JNITE 2010; carp
C_{18} 1-methyl-7-(1-methylethyl)-phenanthrene[e]	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.).
*Calculated using mass-balance approach as outlined in Arnot et al. (2008a) when BCF is known and correcting for log K_{ow}, fish body weight, temperature and lipid content of fish from cited study.

** $k_T = (k_2 + k_M + k_E + k_G)$ or when depuration rate constant is known $k_T = (k_2 + k_G)$
n/a – not applicable; study details could not be obtained to determine predicted BCFs and BAFs.

Table A5.10. Trophic magnification factors (TMFs)[1] for PAHs 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		
benz[*a*]anthracene	0.2*	0.75*	0.83
benzo[*a*]pyrene	0.24*	0.75	0.80
benzo[*e*]pyrene	0.25*	0.86	0.57
benzo[*b*]fluoranthene			0.60*
benzo[*b+k*]fluoranthene	0.27*		
benzo[*j+k*]fluoranthene			0.69*
benzo[*k*]fluoranthene		0.84	
benzo[*ghi*]perylene	0.66	0.75	0.72
chrysene	0.26*	0.66*	0.65*
fluoranthene	0.11*	0.72*	0.60*
fluorene	1.15		
Indeno[*123-cd*]pyrene	0.81	0.75	0.80
dibenz[*ah*]anthracene	0.85		
perylene	0.24*	0.67	0.77
phenanthrene	0.43	0.82*	0.75*
pyrene	0.17*	0.74*	0.62*

[1] 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 A5.11. Proportion (weight %) of bioaccumulative representative structures in three samples of Fuel Oil No. 6 (Fuhr 2008)

Bioaccumulative* representative structures	Boiling point (°C)	Weight %			
		Sample A	Sample B	Sample C	Average
Isoalkane C_{15}	250	8.3	2.8	3.5	4.9
Monocycloalkane C_{15}	282	3.4	2	1.9	2.4
Dicycloalkane C_{15}	244	2.9	1.8	1.8	2.2
Polycycloalkane C_{14}	255	2.8	2.2	3.2	2.7
Polycycloalkane C_{22}	365				
One-ring aromatic C_{15}	281	1.7	4.2	2.2	2.7
Cycloalkane monoaromatic C_{15}	285	1.3	2.8	1.6	1.9
Cycloalkane monoaromatic C_{20}	351				
Cycloalkane diaromatic C_{20}	374	1.1	1.6	2.1	1.6
Three-ring aromatic C_{20}	398	0.9	2.3	3.9	2.4

Four-ring aromatic C_{16}[a]	384–398	1.8	1.9	3.4	2.4
Four-ring aromatic C_{18}[a]	466				
Five-ring aromatic C_{20}[a]	480–509	0.4	0.4	0.2	0.3
Six-ring aromatic C_{22}[a]	>500	0.7[b]	0.4[b]	0.4[b]	0.5[b]
Totals		25.3	22.4	24.2	**24.0**

* Determined by results in the modified Arnot-Gobas Three Trophic Level Model (2003) in Table A5.8 as set out by the *Persistence and Bioaccumulation Regulations* (Canada 2000) with consideration of experimental data.

[a] Structures with empirical BCFs indicating bioconcentration in invertebrates as set out by the *Persistence and Bioacccumulation Regulations* (Canada 2000).

[b] Assumed to be unidentified aromatics in the samples of Fuel Oil No. 6 (Fuhr 2008).

Test organism	Common name	Type of test	Endpoint	Comment	Value (mg/L)	Reference
Fish						
Oncorhynchus kisutch	Coho salmon	96-hour acute	LC_{50}	OWD	4800	Hebert and Kussat 1972
		96-hour acute	LC_{50}	OWD	>10 000	Hebert and Kussat 1972
		96-hour acute	LC_{50}	OWD	7500	Hebert and Kussat 1972
Alosa sapidissma	American shad	48-hour acute	LC_{50}	Not reported	2417	Tagatz 1961
Leptocottus armatus	Staghorn sculpin	96-hour acute	LC_{50}	OWD	780	Hebert and Kussat 1972
		96-hour acute	LC_{50}	OWD	5600	Hebert and Kussat 1972
		96-hour acute	LC_{50}	OWD	3400	Hebert and Kussat 1972
Salmo salar	Atlantic salmon	96-hour acute	LC_{50}	OWD	>10 000	Sprague and Carson 1970
Pseudopleuronectes americanus	Winter flounder	96-hour acute	LC_{50}	OWD	>10 000	Sprague and Carson 1970
Fundulus similus	Longnose killifish	24-hour acute	LC_{50}	WSF*	3.8	Anderson et al. 1974
		48-hour acute	LC_{50}	WSF*	2.27	Anderson et al. 1974
		96-hour acute	LC_{50}	WSF*	1.69	Anderson et al. 1974
Menidia menidia	Atlantic silverside	96-hour acute	LC_{50}	Not reported	130	Hollister et al. 1980
Cyprinodon variegatus	Sheepshead minnow	96-hour acute	LC_{50}	WSF*	4.7	Anderson et al. 1974

		96-hour acute	LC_{50}	WSF*	4.4	Anderson et al. 1974
		96-hour acute	LC_{50}	WSF*	3.1	Anderson et al. 1974
Menidia beryllina	Inland silverside	24-hour acute	LC_{50}	WSF*	3.6	Anderson et al. 1974
		48-hour acute	LC_{50}	WSF*	2.7	Anderson et al. 1974
		96-hour acute	LC_{50}	WSF*	1.9	Anderson et al. 1974
Lepomis macrochirus	Bluegill	96-hour acute	LL_{50}	OWD	>10 000	Mobil 1987d
Invertebrates						
Daphnia magna	Water flea	48-hour acute	EC_{50} (immobilization)	WSF	4.14	MacLean and Doe 1989
		48-hour acute	LC_{50}	WSF	> 4.45	MacLean and Doe 1989
		48-hour acute	EL_{50}	OWD	>10 000	Mobil 1987e
Artemia salina	Brine shrimp	48-hour acute	EC_{50} (immobilization)	WSF	> 2.29	MacLean and Doe 1989
		48-hour acute	LC_{50}	WSF	> 2.29	MacLean and Doe 1989
Acartia tonsa	Copepod	96-hour acute	LC_{50}	Not reported	5.1	Hollister et al. 1980
Paleomonetes pugio	Grass shrimp	24-hour acute	LD_{50}	WSF*	3.2	Anderson et al. 1974
		48-hour acute	LD_{50}	WSF*	2.8	Anderson et al. 1974
		96-hour acute	LD_{50}	WSF*	2.6	Anderson et al. 1974
	Grass shrimp	96-hour acute	LC_{50}	WSF-1:9, 20-hour mix, serial dilutions, ppm dissolved total HC by IR	2.6 3.1 2.2	Tatem et al. 1978
Penaeus aztecus (postlarvae)	Brown shrimp	24-hour acute	LC_{50}	WSF*	3.8	Anderson et al. 1974
		48-hour acute	LC_{50}	WSF*	3.5	Anderson et al. 1974
		96-hour	LC_{50}	WSF*	1.9	Anderson et al.

		acute				1974
Limulus polyphemus	Horseshoe crabs (juvenile)	7 day	Increased mortality and delayed moult		2.25	Strobel and Brenowitz 1981
Mercenaria mercenaria	Quahog clam – embryo	48-hour acute	LC_{50}	WSF concentration = 25.2 ± 1.7 ppm	1.0 (0.7–1.6) ppm	Byrne and Calder 1977
	Quahog clam – larvae	48-hour acute	LC_{50}	WSF concentration = 25.2 ± 1.7 ppm	3.2 (2.3–4.5) ppm	Byrne and Calder 1977
		6 day	LC_{50}	WSF concentration = 25.2 ± 1.7 ppm	1.8 (1.0–2.6) ppm	Byrne and Calder 1977
		10 day	LC_{50}	WSF concentration = 25.2 ± 1.7 ppm	1.6 (1.1–2.2) ppm	Byrne and Calder 1977
		6 day growth test	EC_{50}	WSF concentration = 25.2 ± 1.7 ppm	1.9 (1.6–2.1) ppm	Byrne and Calder 1977
		10 day growth test	EC_{50}	WSF concentration = 25.2 ± 1.7 ppm	1.0 (0.49–2.04) ppm	Byrne and Calder 1977
Neanthes arenaceodentata	Polychaete marine worm	96-hour acute	LC_{50}	Not given	3.6	Neff and Anderson 1981
		24-hour acute	LC_{50}	WSF	> 6.3	Rossi et al. 1976
		48-hour acute	LC_{50}	WSF	4.6	Rossi et al. 1976
		96-hour acute	LC_{50}	WSF	3.6	Rossi et al. 1976
Capitella capitata	Marine worm	24-hour acute	LC_{50}	WSF	> 6.3	Rossi et al. 1976
		48-hour acute	LC_{50}	WSF	1.1	Rossi et al. 1976
		96-hour acute	LC_{50}	WSF	0.9	Rossi et al. 1976
		96-hour acute	LC_{50}	Not Reported	0.9	Neff and Anderson 1981

Mysidopsis almyra	Mysid shrimp	24-hour acute	LC_{50}	WSF	6.3	Anderson et al. 1974
		48-hour acute	LC_{50}	WSF	0.9	Anderson et al. 1974
Algae						
Skeletonema costatum	Diatom	96-hour acute	EC_{50}	Not given	160	Hollister et al. 1980
Pseudokirchneriella subcapitata (Selenastrum capricornutum)	Green alga			WSF-1:8, 16-hour mix, serial dilutions	No inhibition – 100% WSF Stimulation – 0.1% WSF	Giddings et al. 1980
	Green alga	96-hour acute	EC_{50}	Material heated, spread in container, water overlay	> 5000	Mobil 1987f
Microsystus aeruginosa	Blue-green alga			WSF-1:8, 16-hour mix, serial dilutions	No inhibition – 100% WSF Stimulation – 0.1% WSF	Giddings et al. 1980

Table A5.12. Aquatic toxicity of Fuel Oil No. 6

Definitions: LC_{50}: the concentration of a substance that is estimated to be lethal to 50% of the test organisms; EC_{50}: the concentration of a substance that is estimated to cause a defined effect on 50% of the test organisms; WSF: water-soluble fraction; OWD: oil-in-water dispersion

* WSF-1:9, 20-hour mix, serial dilutions, LC_{50} based on ppm dissolved total hydrocarbons by Infrared Spectrophometry.

Table A5.13. Estimated volume of water in contact with oil for loading/unloading and transport processes of oil via ship for various spill sizes (RMRI 2007)

	Volume of water in contact with oil ($m^3 \times 10^6$)	
Spill size (barrels)	**Loading/unloading**	**Transport**
1–49	60	5750
50–999	150	6250
1000–9999	300	9600
10 000–99 999	2200	17 350
100 000–199 999	32 500	49 500
> 200 000	35 000	74 100

Table A5.14. An analysis of modelled persistence and experimental and modelled bioaccumulation data (BCF/BAFs) of petroleum hydrocarbons with respect to the Canadian *Persistence and Bioaccumulation Regulations* (Canada 2000)[a,b]

C#	**C_9**	**C_{10}**	**C_{12}**	**C_{14}**	**C_{15}**	**C_{18}**	**C_{20}**	**C_{22}**	**C_{25}**	**C_{30}**	**C_{50}**
***n*-alkane**						*	*	*	*	*	*
***i*-alkane**		*	*	*	B	*	*	*	*	P*	P*

monocycloalkane		*	*	*	B	*	*	*	*	P*	P*
dicycloalkane		*	*	*	**PB**	P*	P	P*	P*	P*	P*
polycycloalkane	(-)	(-)	(-)	**PB**	P*	P	P*	**PB**	*	*	*
monoaromatic		*	*	*	B	*		*	*	P*	P*
cycloalkane monoaromatic	*		*	*	**PB**	**PB**	**PB**	P*	P*	*	*
diaromatic	(-)	*	*	*	P	P*	P*	P*	P*	P*	*
cycloalkane diaromatic	(-)	(-)	P			*	**B**	*	*	*	*
Three-ring PAH	(-)	(-)	*	*			**PB**	P	P	P	P
Four-ring PAH	(-)	(-)	(-)	(-)	(-)	PB[c]	P	*	*	*	*
Five-ring PAH	(-)	(-)	(-)	(-)	(-)	(-)	PB[c]	P*	P*	P*	*
Six-ring PAH	(-)	(-)	(-)	(-)	(-)	(-)	(-)	PB[c]	*	*	*

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

[b] Persistence potential for carbon numbers that were not modelled for persistence are assumed to be the same as carbon numbers bracketing them. For example, the C_{14} and C_{18} polycycloalkanes were found to be persistent; therefore, the carbon numbers between C_{14} and C_{18} for the polycycloalkanes will also be assumed to be persistent.

[c] Empirical BCFs indicate bioconcentration in invertebrates.

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

B – Predicted fish BCFs and/or BAFs using the modified 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 HFOs

Table A6.1. Variable inputs to SCREEN3

Variables	Input
Source type	Area
Effective emission area[a]	50 m × 10 m (for ships), 10 m × 2 m (for trucks), 50 m × 5 m (for trains)
Emission rate (kg/day)	Available in Table A6.2
Receptor height[b]	1.74 m
Source release height[a]	3 m
Adjustment factor for highest 1–24 h[c]	0.4
Urban–rural option	Urban
Meteorology[d]	1 (full meteorology)
Minimum and maximum distance to use	50–3000 m

[a] Professional judgement.
[b] Curry et al. (1993)
[c] U.S. EPA (1992)
[d] Default value in SCREEN3 (1996).

Table A6.2. Estimated regular evaporative emissions to air during transit[a]

Substance	Estimated regular evaporative emissions to air	
	kg/year	kg/day[b]
Industry-restricted HFOs	0.0011–8.4	3.14×10^{-6} – 0.024

[a] Numbers are presented as a range to cover losses from the various transportation modes involved.
[b] 350 days/year is used in the estimation. 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 and other means. For the Come By Chance refinery only, over 230 tanker transits per year are related to shipping petroleum substances. A personal communication with the Energy Resources Conservation Board in Alberta suggested that the utilization rate of main pipelines is normally 24 hours/day, 365 days/year. Thus, it is reasonable to assume an average of 350 days/year for the transportation period. Information on transport frequency by trucks and trains is not available.

Table A6.3. Modelling results of industry-restricted HFO dispersion profile in ambient air within 24 hours in Canada[a]

Substance	Maximum concentration within 24 hours (µg/m^3)[a]			
	50 m	1000 m	2000 m	3000 m
Industry-restricted HFOs	1.6×10^{-4} – 1.28	9.8×10^{-7} – 0.0075	3.5×10^{-7} – 0.0027	2.0×10^{-7} – 0.0016

[a] These estimates are conservative, as they are based on release from a point 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 point release source.

Appendix 7. Summary of health effects information from pooled health effects data for HFO substances

Table A7.1. Critical health effects information on HFO substances

Endpoints	CAS RN[a]	Effect levels[b]/results
Acute health effects	64742-90-1	**Inhalation LC_{50}** (rat): > 3700 mg/m^3 (both sexes) (U.S. EPA 2005).
	64741-62-4 68553-00-4	**Lowest oral LD_{50}s** (rat): 4320 mg/kg-bw (females) for sample API 81-15 and 5130 mg/kg-bw (both sexes) for sample API 79-2 (CONCAWE 1998; ECB 2000a; API 2004). **Other oral LD_{50}s** (rat): > 2000–> 25 000 mg/kg-bw (both sexes) for six CAS RN substances tested (CONCAWE 1998; ECB 2000a; API 2004; U.S. EPA 2005). **Dermal LD_{50}s** (rabbit): > 2000–> 5350 mg/kg-bw (both sexes) for six CAS RN substances tested (CONCAWE 1998; ECB 2000a; API 2004; U.S. EPA 2005).
	64741-62-4	**Other dermal LD_{50}** (rat): > 2000 mg/kg-bw (both sexes) (ECB 2000a).
Acute (non-lethal) health effects	64741-62-4	**Oral LOAEL:** ≥ 125 mg/kg-bw for maternal toxicity. A single dose of 2000 mg/kg-bw or single doses of 125, 500 or 2000 mg/kg-bw were administered to pregnant Sprague-Dawley rats (presumably via gavage) on one of gestation days 11–15 (profile of teratogenic effects as a function of gestation day) or gestation day 12 (profile of teratogenic effects as a function of dose), respectively. Two separate studies used two different samples for each study. (1) General observations (≥ 500 mg/kg-bw): Red vaginal discharge, perineal staining and decreased stool. (2) Teratogenic effects versus gestation day (2000 mg/kg-bw): Decreased maternal body weight gain and thymus weight (regardless of exposure day). (3) Teratogenic effects versus dose (125, 500, 2000 mg/kg-bw): Dose-related decrease in maternal body weight gain and thymus weight (Feuston and Mackerer 1996).
Short-term repeated-exposure health effects	64742-90-1	**Inhalation LOAEC:** 540 mg/m^3 for a concentration-related decrease in body weight (more severe in males) and an increase in liver weight (females). Concentrations of 540 or 2000 mg/m^3 were administered to male and female Fischer 344 rats (5 of each sex per concentration), 6 hours/day for 9 days. A concentration-related increase in hair loss, nasal discharge, discharge from the eyes, closed eyes and perianal soiling were observed. Yellow discoloration of the lungs and hyperplasia of the pulmonary alveolar macrophages were also observed at all concentrations. Increased liver (male and female) and lung weights (female) and decreased spleen (male and female) and heart weights (male) were observed at 2000 mg/m^3 (Gordon 1983).
	64741-62-4	**Dermal LOAEL:** 1 mg/kg-bw per day for dose-related

		decreases in gravid uterine weight, maternal body weight, body weight gain and feed consumption, as well as the occurrence of red vaginal exudates. Doses of 0.05, 1, 10, 50 or 250 mg/kg-bw per day were applied to the clipped skin of pregnant CD rats from gestation days 0 to 19 (Hoberman et al. 1995). **Other dermal study:** Doses of 4, 8, 30, 125 or 500 mg/kg-bw per day were applied to the shaved backs of pregnant Sprague-Dawley rats (15 per dose) from gestation days 0–19 (4 mg/kg-bw per day dose given as 8 mg/kg-bw every other day). Aberrant serum chemistry and decreased body weight gain, as well as vaginal discharge, were observed at 8 mg/kg-bw per day (Mobil 1990; Feuston et al. 1997). **Other dermal study:** Doses of 200, 1000 or 2000 mg/kg-bw per day were applied to the skin of male and female Fischer 344 rats (5 of each sex per dose), 3 times per week for 28 days. Moderate skin irritation was observed at 200 mg/kg-bw per day, as was liver enlargement in females. Decreased body weight gain and severe skin irritation with skin ulceration were observed at 1000 mg/kg-bw per day. One and two treatment-related deaths were observed at 1000 and 2000 mg/kg-bw per day, respectively. Liver pathological changes and enlargement in males, changes in the lymphoid organs and slight to severe hypocellularity in the bone marrow were also observed at the highest dose (API 1983).
	64741-81-7	**Other dermal study:** Doses of 8, 30, 125 or 250 mg/kg-bw per day were applied to the shaved backs of pregnant Sprague-Dawley rats (15 per dose) from gestation days 0–19. At 8 mg/kg-bw per day, decreased thymus weights (relative and absolute), increased liver weights (relative) and skin irritation (dose-related) were observed. Altered hematological parameters and aberrant serum chemistry occurred at an unspecified dose. Red vaginal discharge, paleness and emaciation were observed at 30 mg/kg-bw per day. Moribundity was observed at 250 mg/kg-bw per day (Mobil 1994a).
	68783-08-4	**Other dermal study:** Doses of 8, 30, 125 or 500 mg/kg-bw per day were applied to the shorn dorsal skin of pregnant Sprague-Dawley rats from gestation days 0–19. Maternal red vaginal discharge was observed in two rats at 125 mg/kg-bw per day (unsure if treatment-related) and in seven rats at 500 mg/kg-bw per day. Maternal body weight, body weight gain, feed consumption, thymus weight (absolute and relative), liver weight (relative), clinical chemistry and hematology parameters were also affected at unspecified doses (Mobil 1991).
Subchronic repeated-exposure health	64741-62-4	**Dermal LOAEL:** 8 mg/kg-bw per day for increased relative liver weight (male and female) and increased absolute liver weight (female). Doses of 8, 30, 125, 500 or 2000 mg/kg-bw

effects		per day were applied to the shorn backs of male and female Sprague-Dawley rats, 5 times per week for 13 weeks. Increased mortality, decreased body weights, decreased thymus weight and aberrant serum chemistry and hematology were also observed at unspecified doses (Feuston et al. 1994). Lack of testing at doses lower than 8 mg/kg-bw per day lowers confidence in the LOAEL. **Dermal LOAEL:** 8 mg/kg-bw per day for a significant reduction in platelet count. Doses of 8, 30, 125 or 500 mg/kg-bw per day were applied to the shaved backs of male and female Sprague-Dawley rats (10 of each sex per dose), 5 times per week for 13 weeks. Increased liver weight was observed for males and females at 30 mg/kg-bw per day and 125 mg/kg-bw per day, respectively. At 30 mg/kg-bw per day (male) and 125 mg/kg-bw per day (female), dose-related reductions in red blood cell, hemoglobin, hematocrit and platelet counts and a dose-related decrease in thymus weight, as well as increased mortality (20% males and 80% females), were also observed. Also at 125 mg/kg-bw per day, both sexes exhibited decreased body weight gain. All male and female rats died at 125 and 500 mg/kg-bw per day, respectively (Mobil 1988; Feuston et al. 1997).
	64741-81-7	**Dermal LOAEL:** 8 mg/kg-bw per day for moderate skin irritation (dose-related). Doses of 8, 30 or 125 mg/kg-bw per day were applied to the shaved backs of male and female Sprague-Dawley rats (10 of each sex per dose), 5 times per week for 13 weeks. Altered hematology parameters and decreased thymus weights (relative and absolute), as well as altered serum chemistry, were observed at 30 mg/kg-bw per day. Decreased body weight gain (males), as well as increased liver weight (relative and absolute) and decreased number of lymphoid cells in the thymus were observed at 125 mg/kg-bw per day (Mobil 1994b).
	68783-08-4	**Other dermal study:** Doses of 30, 125 or 500 mg/kg-bw per day were applied to male and female Sprague-Dawley rats (10 per group), 5 times per week for 13 weeks. Slight skin irritation was observed at all doses. Changes in a number of serum chemistry and hematological parameters, as well as increased liver and decreased thymus sizes were observed at 125 mg/kg-bw per day. Enlarged and reddened lymph nodes and thickening of the limiting ridge between the non-glandular and glandular sections of the stomach were also observed at this dose. Decreased body weight gain was observed at 500 mg/kg-bw per day (in males). Also at the highest dose, a reduction in hematopoiesis in the bone marrow and in the number of lymphocytes in the thymus glands, liver hypertrophy and connective tissue formation, and increased areas of hematopoiesis, focal necrosis and individual cell death in the liver were observed (Mobil 1992).
Carcinogenicity	64741-62-4	**Lowest dermal effect level:** 25 µL of catalytically cracked

		clarified oil at 1% (8.4 mg/kg-bw)[c,d,e,f] resulted in skin tumours in mice. Groups of male C3H mice (50 per dose) were treated with 25 µL of catalytically cracked clarified oil at 1%, 2%, 5%, 10% and 20% (8.4, 16.8, 42.0, 83.8 and 167.6 mg/kg-bw) in mineral oil, 3 times per week for life. At 1%, 9/50 exposed mice developed tumours (four carcinomas, five papillomas). At 2%, 34/50 exposed mice developed tumours (30 carcinomas, 4 papillomas with a latency period of 92 weeks). At 5%, 46/50 exposed mice developed tumours (46 carcinomas with a latency period of 61 weeks). At 10%, 48/50 exposed mice developed tumours (47 carcinomas, 1 papilloma with a latency period of 45 weeks). At 20%, all (50/50) exposed mice developed tumours (50 carcinomas with a latency period of 36 weeks). Of the 610 mice tested with the negative control (highly refined mineral oil) from this study and two other similar studies conducted by the same author, only two mice developed benign papillomas, and none developed carcinomas (McKee et al. 1990).
	64741-62-4	**Initiation/promotion dermal study:** ***Initiation*:** Groups of male CD mice (30 per group) were treated with 50 µL of catalytically cracked clarified oil at 1% (16.8 mg/kg-bw)[c,d,f] in toluene, once per day for 5 consecutive days. After a 2-week rest period, the promoter phorbol-12-myristate-13-acetate was applied 2 times per week for 25 weeks. A significant increase in skin tumour incidence was observed (26/30 exposed mice developed tumours after 16 days). ***Promotion*:** Details of study design not provided. No increase in histologically confirmed tumour incidence observed. However, statistically significant increase in the number of mice with grossly observed masses and shortened latency time were observed. Suggests possible weak promoting activity (API 1989a).
Developmental and reproductive health effects	64741-62-4	**Dermal reproductive LOAEL (female):** 1 mg/kg-bw per day based on a decrease in the number of live fetuses, increased incidences of resorptions and early resorptions and increased percentage of dead or resorbed conceptuses per litter (these effects were all dose-related and were observed at doses that were maternally toxic). At 1 mg/kg-bw per day, an increased incidence of fetal variations associated with a decrease in fetal body weight was observed, including slight dilatation of the lateral ventricles of the brain, moderate dilatation of the renal pelvis, bifid thoracic vertebral centrum and decreased average number of ossified caudal vertebrae, metacarpals and hindpaw phalanges (these effects were noted to be reversible delays in development). Doses of 0.05, 1, 10, 50 or 250 mg/kg-bw per day were applied to the clipped skin of pregnant CD rats from gestation days 0–19 (Hoberman et al. 1995). **Dermal developmental LOAEL:** 8 mg/kg-bw based on fetal

		external abnormalities. Doses of 4, 8, 30, 125 or 250 mg/kg-bw per day were applied to the shaved backs of pregnant Sprague-Dawley rats (10 per dose) for gestation days 0–19 (4 mg/kg-bw dose given as 8 mg/kg-bw every other day). At 8 mg/kg-bw per day, external abnormalities in living and dead fetuses, including cleft palate, micrognathia (shortened lower jaw) and kinked tail, were observed (these effects were noted to occur at low incidences). An increased incidence of resorptions, decreased number of viable offspring, reduced fetal size, visceral anomalies and skeletal variations were observed at 30 mg/kg-bw per day. There were no viable fetuses at 250 mg/kg-bw per day (Mobil 1987c; Feuston et al. 1989). **Other dermal study:** Doses of 4, 8, 30, 125 or 500 mg/kg-bw per day were applied to the shaved backs of pregnant Sprague-Dawley rats (15 per dose) from gestation days 0–19 (4 mg/kg-bw per day dose was administered as 8 mg/kg-bw every other day). At 8 mg/kg-bw per day, an increased incidence of resorptions and a decreased number of viable fetuses were observed (biologically significant). At 30 mg/kg-bw per day, a statistically significant increased incidence of resorptions was observed, as well as decreased fetal body weight. An increased incidence of fetal external, skeletal and visceral anomalies (primarily rib malformations and cleft palate) was observed at 500 mg/kg-bw per day (Mobil 1990; Feuston et al. 1997). **Other dermal study:** Doses of 8, 30, 125 or 500 mg/kg-bw per day were applied to the shaved backs of male Sprague-Dawley rats (10 per dose), 5 times per week for 13 weeks. Decreased sperm count after 9 weeks of exposure was observed at 500 mg/kg-bw per day (Mobil 1988; Feuston et al. 1997). **Oral reproductive and developmental study:** Pregnant Sprague-Dawley rats were administered 2000 mg/kg-bw on one of gestation days 11–15 (profile of teratogenic effects as a function of gestation day). Additionally, 125, 500 or 2000 mg/kg-bw was administered to pregnant Sprague-Dawley rats on gestation day 12 (profile of teratogenic effects as a function of dose). Two separate studies used two different samples (clarified slurry oil and syntower bottoms) for each study. (1) Teratogenic effects versus gestation day (2000 mg/kg-bw): The greatest incidence of resorptions/decreased litter size occurred on gestation days 11–12. Fetal body weights were reduced on all gestation days. The greatest incidence of fetal external anomalies and visceral malformations occurred on gestation days 12–14 and 12–13, respectively. Various fetal skeletal malformations occurred on all gestation days. (2) Teratogenic effects versus dose (125, 500, 2000 mg/kg-bw): dose-related response for increased resorptions, decreased

		litter size, decreased fetal body weight and increased incidence of fetal skeletal malformations. A variety of fetal external anomalies were also observed at 2000 mg/kg-bw (Feuston and Mackerer 1996).
	68783-08-4	**Other dermal studies:** Doses of 8, 30, 125 or 500 mg/kg-bw per day were applied to the shorn dorsal skin of pregnant Sprague-Dawley rats from gestation days 0–19. Pre-implantation losses (not statistically significant), as well as decreased mean fetal body weight (male pups) and increased incidence of incomplete ossification of skeletal structures (male and female pups), were observed at 125 mg/kg-bw per day. Increased mean number and percent resorptions and decreased mean fetal body weight for all viable fetuses were observed at 500 mg/kg-bw per day (Mobil 1991). A dose of 500 mg/kg-bw per day was applied to the skin of male Sprague-Dawley rats (10 rats), 5 times per week for 13 weeks. No effects on epididymal sperm or testicular sperm parameters were observed (Mobil 1992).
Genotoxicity: *in vivo*	64741-90-1	**Positive for micronuclei induction:** Groups of male and female CD Swiss mice (10 of each sex per dose) were administered 1250, 2500 or 5000 mg/kg-bw of aromatic pyrolysis oil, via oral gavage, for 2 days. One group of mice (15 of each sex per dose) was administered 5000 mg/kg-bw, via oral gavage, as a single dose. A significant increase in micronucleated polychromatic erythrocytes was observed at 1250 mg/kg-bw (in males) and at 5000 mg/kg-bw (in females) (Khan and Goode 1984).
	64741-57-7	**Negative for micronuclei induction:** Groups of male and female rats (10 of each sex per dose) were exposed dermally to 30, 125, 500 or 2000 mg/kg-bw per day, 5 days/week for 13 weeks. No increase in the frequency of micronuclei induction in bone marrow cells was observed (Mobil 1987a).
	64741-62-4	**Positive for sister chromatid exchange:** Groups of male and female B6C3F1 mice (5 of each sex per dose) were administered a single dose of 400, 2000 or 4000 mg/kg-bw of API 81-15, via intraperitoneal injection. A small but significant increase in sister chromatid exchanges/metaphase was observed in bone marrow cells at 2000 mg/kg-bw (in males) and at 4000 mg/kg-bw (in females). The response was also dose-related (API 1985a). **Positive for unscheduled DNA synthesis:** Groups of male Fischer 344 rats (3 per dose) were administered 50, 200 or 1000 mg/kg-bw of API 81-15, via oral gavage, at 2 and 12 hours. A significant increase in unscheduled DNA synthesis was observed in primary hepatocyte cultures at 200 mg/kg-bw after 12 hours and at 1000 mg/kg-bw after 2 hours (API 1985b).

		Negative for chromosomal aberrations: Groups of male and female Sprague-Dawley rats (11 of each sex per dose) were administered 100, 300 or 1000 mg/kg-bw per day of API 81-15, via intraperitoneal injection, for 5 days. No increase in the frequency of aberrations in bone marrow cells and no increase in the mitotic index were observed (API 1985c).
Genotoxicity: *in vitro*	64741-90-1	**Positive for unscheduled DNA synthesis:** Primary rat hepatocyte cultures derived from F-344 male rat liver were exposed to ethanol dilutions of aromatic pyrolysis oil at concentrations of 0.5, 2, 10 or 60 µg/mL for 18–20 hours (without S9 metabolic activation). Concentration-response observed for unscheduled DNA synthesis at ≥ 2 µg/mL (Brecher and Goode 1984). **Ambiguous for mutagenicity (forward mutations):** Chinese hamster ovary cells exposed to ethanol dilutions of aromatic pyrolysis oil at concentrations of 32, 64, 96, 128, 175 or 256 µg/mL without S9 metabolic activation and 128, 175, 256, 375, 512 or 750 µg/mL with S9 metabolic activation. A repeat experiment was conducted at concentrations of 500, 600 or 750 µg/mL with S9 metabolic activation. S9 was prepared from Aroclor 1254-induced rat liver. Reduced cell count was observed at all concentrations (with and without S9), and significant toxicity was observed at all concentrations (with S9). An increase in mutant frequency was observed at 750 µg/mL with S9 metabolic activation accompanied by a relatively linear concentration-related response from the lower concentrations. No mutagenic effects were observed without S9 metabolic activation. In the repeat experiment, an increase in mutant frequency was observed at 500 µg/mL (higher concentrations were toxic) (Papciak and Goode 1984).
	64741-62-4 64741-61-3	**Positive for mutagenicity (reverse mutations):** *Salmonella typhimurium* TA98 was exposed to dimethyl sulfoxide extracts at concentrations of 0.5, 1, 2.5, 5 or 10 µL/plate with S9 metabolic activation (Aroclor 1254-induced rat liver). A concentration-related increase in mutagenic potency was observed, and a mutagenicity index of 130 was determined (Blackburn et al. 1984). Additionally, *S. typhimurium* TA98 was exposed to dimethyl sulfoxide extracts (dissolved in cyclohexane) at concentrations of 0.5, 1, 1.5, 2 or 5 µL/plate with S9 metabolic activation (Aroclor 1254-induced Syrian golden hamster liver). A concentration-related increase in mutagenic potency was observed, and a mutagenic index of ~58 was determined (Blackburn et al. 1986).
	64741-62-4	**Positive for mutagenicity (mouse lymphoma assay):** L5178Y cells exposed to API 81-15 at concentrations ranging from 1.95–31.3 nL/mL for 4 hours with and without S9 metabolic activation (rat liver). Toxicity was noted at all levels, and survival was < 10% at concentrations above 3.9 nL/mL.

		Without activation, the test substance was weakly positive at the highest concentration only. With activation, the test substance induced a concentration-related increase in mutant frequency at concentrations > 0.977 nL/mL (API 1985c). **Ambiguous for sister chromatid exchange:** Chinese hamster ovary cells were exposed to the test substance at concentrations of 5–100 µg/mL without S9 metabolic activation and 100–5000 µg/mL with S9 metabolic activation. An increase in sister chromatid exchanges was observed with activation. No increase in sister chromatid exchanges observed without activation (API 1985f). **Ambiguous for cell transformation:** BALB/3T3 mouse embryo cells exposed to the test substance at concentrations of 1, 3, 6 and 9 µg/mL without S9 metabolic activation (for 3 days) and 10, 30, 100 and 300 µg/mL with S9 metabolic activation (for 4 days). S9 was prepared from Aroclor-induced male rat liver. An increase in cellular transformation frequency was observed at 100 µg/mL after 4 hours with S9 activation. Low survival rates were observed at concentrations > 100 µg/mL with activation. No increase in morphological transformation without activation (API 1986b).
	64741-57-7	**Negative for cellular aberrations (cytogenetic assay):** Chinese hamster ovary cells exposed to the test substance at concentrations of 5, 8, 10, 12 or 15 µL/mL with and without S9 metabolic activation (Mobil 1987b).
Human studies		No studies were identified.

[a] Industry-restricted HFO substances are indicated in bold.
[b] LC_{50}, median lethal concentration; LD_{50}, median lethal dose; LOAEC, lowest-observed-adverse-effect concentration; LOAEL, lowest-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) / bw.
[e] Density not provided; thus, a density from CONCAWE (1998) was used.
[f] A volume/volume dilution was assumed.