Government of Canada Gouvernement du Canada

Screening Assessment
Petroleum Sector Stream Approach

Distillate Aromatic Extracts

Chemical Abstracts Service Registry Numbers
64742-04-7
64742-05-8
64742-11-6

Environment and Climate Change Canada
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Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA), the Minister of the Environment and the Minister of Health have conducted a screening assessment of the following distillate aromatic extract (DAE) substances:

Table 1-1. Distillate aromatic ethers (DAEs)

CAS RN[a]	**Name on the *Domestic Substances List* (DSL)**
64742-04-7	Extracts (petroleum), heavy paraffinic distillate solvent
64742-05-8	Extracts (petroleum), light paraffinic distillate solvent
64742-11-6	Extracts (petroleum), heavy naphthenic distillate solvent

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The three DAEs identified by CAS RNs 64742-04-7 (extracts [petroleum], heavy paraffinic distillate solvent), 64742-05-8 (extracts [petroleum], light paraffinic distillate solvent) and 64742-11-6 [extracts (petroleum], heavy naphthenic distillate solvent) were identified as priorities for assessment, as they met the categorization criteria under subsection 73(1) of the CEPA. 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).

Aromatic extracts are a class of substances derived from solvent extraction of crude oil vacuum distillation distillate and residual streams. CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6 are part of the broad class of aromatic extracts and can be referred to as distillate aromatic extracts because they originate from the vacuum distillation stream. Because of their untreated nature, they have high levels of aromatic compounds, including polycyclic aromatic hydrocarbons (PAHs). These substances are consumed on-site at refineries and are also transported in Canada via trains and trucks for use at industrial and commercial facilities. They were included in the Petroleum Sector Stream Approach (PSSA) because they are related to the petroleum sector and are complex combinations of hydrocarbons.

Estimation of mixture behaviours was accomplished through the use of a suite of representative structures that are expected to be present in these DAEs. In general, the components of DAEs are poorly soluble in water, very hydrophobic, and moderately to poorly volatile, although some will evaporate readily from water. DAEs are expected to predominantly reside in sediment and soil, with some lighter components partitioning to air.

Petroleum-derived oils that include DAEs can be used as extender oils in the formulation of plastic and rubber products to achieve elasticity and make brittle materials soft and flexible. Extender oils are also a major ingredient in the production of vehicle tires and are therefore found in crumb rubber (i.e., bits of recycled tires that can be used in the production of rubberized playground and athletic surfaces). Historically, automobile tires were formulated with high PAH extender oils, although recent changes in domestic manufacturing have seen these replaced with low PAH oils. As such, there may be residual general population exposure to these DAEs if previously used as extender oils in tire production, where old tires have been recycled into crumb rubber and incorporated in rubber playground and athletic surfaces. There is the potential that these crumb rubber surfaces may release component substances, including PAHs, by off-gassing, through natural surface degradation, and during mechanical abrasion and direct contact with skin. Two of the DAEs, i.e., CAS RNs 64742-11-6 and 64742-04-7, are reported as being in industrial and professional use products such as rubbers, adhesives, sealants, solvents and roofing materials.

For the ecological assessment, environmental concentrations were estimated for major ecological exposure scenarios, including manufacturing of rubber products, manufacturing of other products and runoff from tire wear and road care products that are not mixed with asphalt. Levels of exposure in the aquatic environment are well below those expected to cause harm to aquatic organisms.

Considering all available lines of evidence presented in this screening assessment, there is low risk of harm to organisms and the broader integrity of the environment from these substances. It is concluded that the three DAEs (CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6) do not meet the criteria under paragraphs 64(*a*) or (*b*) of CEPA 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 health effect for the initial categorization of these DAEs was carcinogenicity as determined on the basis of classifications by international agencies. Skin painting studies conducted in laboratory animals show skin tumour formation following chronic dermal exposure to these substances. They have also produced positive results in in vitro genotoxicity assays and exhibit reproductive toxicity in dermally-exposed laboratory animals. These effects are attributed to the high PAH content of DAEs.

Exposure and risk to human health was characterized for DAEs CAS RN 64742-04-7, 64742-05-8 and 64742-11-6, considering that exposures may occur during their production and storage at refineries, during bulk transportation between industrial facilities, and from their potential presence in crumb rubber derived from old tire stocks. Additionally, compositional testing of Canadian marketplace plastic and rubber products was used to assess whether these substances are found in products available for purchase by the general population.

The vapour pressure of aromatic extracts is low, which means that inhalation exposure to these substances during transportation and production and storage at refineries is also low. Crumb rubber extracted with biological fluids did not release PAHs, and therefore any oral or dermal exposure to crumb rubber is not expected to give rise to a significant exposure to aromatic extracts. Air monitoring studies that quantified the benzo[a]pyrene (B[a]P) concentration in air from the off-gassing of rubberized surfaces under ideal weather conditions showed both no increase and only an incremental increase above background B[a]P levels typically found in ambient air. As exposures are either not expected or, if exposure does occur, is expected to be transient and to incremental levels, risk to human health is likewise considered to be low.

High PAH oils, including these DAEs, have the potential to be used as extender oils in the production of rubber and plastic consumer products. Results from the compositional analysis of commonly available soft rubber and plastic marketplace products in Canada indicate that these DAEs are not being used in these product formulations.

On the basis of the information presented in this screening assessment, it is concluded that the three DAEs (CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6) do not meet the criteria under paragraph 64(c) of CEPA 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.
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It is concluded that the three DAEs (CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6) do not meet any of the criteria set out in section 64 of CEPA.

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Tables

1. Introduction

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA) (Canada 1999), the Minister of the Environment and the Minister of Health conduct screening assessments of substances to determine whether these substances present or may present a risk to the environment or to human health.

A key element of the Government of Canada's Chemicals Management Plan (CMP) is the Petroleum Sector Stream Approach (PSSA), which involves the assessment of approximately 160 petroleum substances that are considered 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).

These petroleum substances fall into nine groups of substances according to similarities in production, toxicity and physical-chemical properties (Table A.1 in Appendix A). In order to conduct the screening assessments, each petroleum substance was placed into one of the following 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;[1]
> Stream 2: industry-restricted substances, which are substances that may leave a petroleum-sector facility and may be transported to other industrial facilities (for example, for use as a feedstock, fuel or blending component), but that do not reach the public market in the form originally acquired;
> Stream 3: substances that are primarily used by industries and consumers as fuels; or
> Stream 4: substances that may be present in products available to the consumer.

An analysis of the available data resulted in the determination that 67 of these petroleum substances may be present in consumer products in Stream 4, as described above. These 67 substances were further sub-grouped on the basis of their physical and chemical properties and potential uses as follows: aromatic extracts, gas oils, heavy fuel oils, low boiling point naphthas, natural gas condensates, solvents, petroleum and refinery gases, base oils, petrolatum and waxes, and asphalt.

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[1] 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.

This screening assessment addresses a subset of the "aromatic extracts" group, namely three distillate aromatic extracts (DAEs) described under Chemical Abstracts Service Registry Numbers[2] (CAS RNs) 64742-04-7, 64742-05-8 and 68742-11-6. These substances were identified as priorities for assessment as they met the categorization criteria under section 73 of CEPA (ECCC, HC [modified 2007]). These substances were included in the PSSA because they are related to the petroleum sector and are all complex combinations of hydrocarbons.

This screening assessment includes consideration of information on chemical properties, environmental fate, hazards, uses, and exposure, including additional information submitted by stakeholders. Relevant data were identified up to June 2015. Empirical data from key studies, as well as some results from models, were used to reach conclusions. When available and relevant, information presented in assessments from other jurisdictions was considered.

This screening assessment was prepared by staff in the CEPA Risk Assessment Programs at Health Canada and Environment and Climate Change Canada and incorporates input from other programs within these departments. The ecological portions of this assessment have undergone external written review and consultation. Comments on the technical portions relevant to ecological health were received from Dr. Lawrence Kapustka, Dr. Gladys Stephenson and Mr. Geoff Granville. Additionally, the draft of this screening assessment was subject to a 60-day public comment period. While comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Health Canada and Environment and Climate Change Canada.

This screening assessment focuses on information critical to determining whether a substance meets the criteria as set out in section 64 of CEPA, by examining scientific information and incorporating a weight-of-evidence approach and precaution.[3] The screening assessment presents the critical information and considerations on which the conclusion is based.

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[3] A determination of whether one or more of the criteria of section 64 of CEPA are met is based upon an assessment of potential risks to the environment and/or 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 products used by consumers. A conclusion under CEPA is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the *Hazardous 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 does not preclude actions being taken under other sections of CEPA or other Acts.

2. Substance Identity

DAEs are complex combinations of hydrocarbons produced as by-products from the extraction of condensed ring polycyclic aromatic constituents during the production of lubricating oil basestocks and waxes (API 2012a; US EPA 2012). Given their complex and variable compositions, they cannot practicably be formed by simply combining individual constituents. In these refining processes, the hydrocarbon feedstocks are treated with solvents such as furfural, n-methylpyrrolidone, sulphur dioxide or phenol, which selectively extract the aromatic and heterocyclic materials into solution (API 2003). After recovery of the solvents for re-use, the resultant products are called aromatic extracts. If, as is the case with the three substances considered in this screening assessment, the feedstock is a distillate stream from a vacuum distillation process, the resultant extract is known as a distillate aromatic extract. Such materials are commonly produced as a by-product of the production of high-quality lubricating oil basestocks (CONCAWE 1992). The other subcategories of aromatic extracts include residual aromatic extracts (RAE) and are not addressed in this assessment. RAEs are obtained from the solvent extraction of the residue that remains after vacuum distillation of crude oil.

A total of three untreated DAEs with different CAS RNs and with carbon ranges from C_{15} to C_{50} have been identified for assessment. A general description of these substances is presented in Table B.1, Appendix B. The DAEs identified by CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6 may be described as untreated DAEs because they can be further processed in a refinery via, for example, a solvent dewaxing process. After this point, the substances (and the CAS RNs) cease to exist as discrete entities, having been converted into petroleum products with other CAS RNs (e.g., those assigned to streams described as treated DAEs). Alternatively, they can be marketed as such or incorporated into other end products, such as heavy fuels.

The main difference between these three DAEs is the number of carbon atoms in individual components of the substances. The substances identified by CAS RN 64742-04-7 and 64742-11-6 are heavy DAEs, consisting of components ranging from C_{20} to C_{50}, while the substance identified by CAS RN 64742-05-8 is a light DAE, consisting of components ranging from C_{15} to C_{30} (see Table B.1, Appendix B). In addition, the three DAEs can be described as being either naphthenic or paraffinic. CAS RN 64742-05-8 is a light paraffinic DAE, CAS RN 64742-04-7 is considered a heavy paraffinic DAE, and CAS RN 64742-11-6 is a heavy naphthenic DAE. These DAEs are complex combinations of hydrocarbons obtained as the extract from a solvent extraction process, potentially with 5% by weight (wt%) or more of condensed four- to six-ring aromatic hydrocarbons (Hopkinson 2008; CONCAWE 1992).

In general, untreated DAEs are composed of approximately 60 to 90 wt% aromatics (consisting of approximately 28 to 35 wt% one- or two-ring aromatics and 17 to 23 wt% three- to five-ring aromatics) with some degree of alkylation, with the remainder consisting of polar compounds (i.e., hydrocarbon structures that also contain a hetero-atom, such as oxygen sulphur and/or nitrogen), cycloalkanes, and isoalkanes (API

2008). Table 2-1 presents a compositional analysis of different types of DAEs broken down according to light and heavy paraffinic and naphthenic categories.

Table 2-1. Compositional analysis of DAEs (API 2008)

Substance	Carbon number range (10–90 percentile)	Saturates (wt%)	Polar compounds (wt%)	Aromatics (wt%)
Light paraffinic[a]	C_{19}–C_{38}	11–25	0.6–5.2	70–88
Light naphthenic[b]	C_{22}–C_{34}	18	23	60
Heavy paraffinic[c]	C_{25}–C_{44}	6–25	4.6–13	67–85
Heavy naphthenic[b]	C_{22}–C_{38}	7.7	17	74

[a] Based on four samples, including one sample that was determined to be CAS 64742-05-8 on the basis of analytical testing.
[b] Based on one sample.
[c] Based on five samples.

Table 2-2. Polycyclic aromatic hydrocarbon (PAH) profiles of representative aromatic extracts (API 2008)

Aromatic extract type	Total % 3-7 ring
Light paraffinic DAE	8.7–12
Heavy paraffinic DAE	8.1–21
Heavy naphthenic DAE	19

The total weight percent of three- to seven-ring PAHs in these samples ranges from 8.1 to 21 wt%. There appears to be no clear relationship between the type of aromatic extract and the amount of three- to seven-ring PAHs. Aromatic concentrations in DAEs are largely dependent on the source and type of the blended crude oil from which the extract is processed (Feuston et al. 1994) as well as the degree of the refining process undergone by their parent mixtures (API 2012b). Alkylated PAHs predominate in petroleum substances (Cermak 2010).

3. Physical and Chemical Properties

As aromatic extracts are UVCBs, their compositions can only be broadly defined. The composition and physical-chemical properties of aromatic extracts vary depending on the sources of crude oils or bitumen and the processing steps involved. A summary of data on the physical-chemical properties of DAEs is presented in Table 3-1.

Table 3-1. General experimental physical-chemical properties of DAEs

Property	Value	Temperature (°C)	Reference
Boiling range (°C) (DAEs in general)	250–640	-	CONCAWE 2010
Boiling range (°C) CAS RN 64742-05-8	288–534	-	API 2012b
Boiling range (°C) CAS RN 64742-04-7	289–579	-	API 2012b
Boiling range (°C) CAS RN 64742-11-6	326–584	-	API 2012b
Pour point (°C)	-6 to 50	-	API 2012b
Bulk density (kg/m^3)	950–1030	15	API 2012b
Water solubility (mg/L)[a]	1.4–5.8	20	CONCAWE 1992
Vapour pressure (kPa)	< 0.1	20	API 2012b
log K_{ow} (dimensionless)	4.4–7.2[b]	25	API 2012a
log K_{ow} (dimensionless)	4.9 to >25[c]	-	Table C.2, Appendix C
log K_{oc} (dimensionless)	5.6–13[d] 4.4–8.1[e]	-	US EPA 2012
Aromatic components	65–85 wt%	-	API 2012b
DMSO[f] extractables (wt%)	6–30	-	API 2012b

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

[a] The exact DAE tested was not specified and the original reference was not provided.

[b] Determined for the light naphthenic DAE (CAS RN 64742-03-6; carbon range of C_{15}-C_{30}) and used for read-across to the light paraffinic DAE (CAS RN 64742-05-8) considered within this assessment.

[c] Based on representative structures in the carbon range C_{15}-$C_{50.}$

[d] Determined for CAS RN 64742-04-7 and 64742-11-6; it is unknown whether they are experimental or calculated.

[e] Determined for CAS RN 64742-05-8; it is unknown whether it is experimental or calculated.

[f] Dimethyl sulfoxide (DMSO) is used in certain analytical tests to extract polycyclic aromatic compounds (PAC) and other components from mixtures of petroleum products; the percentage of PAC extracted from the product correlates with carcinogenic potency as measured in animal tests.

Refined petroleum products are primarily made by distillation processes that separate fractions from crude oil on the basis of boiling range. Distillation does not produce sharp distinctions in boiling point cut-offs, and so there is overlap between distillate fractions. The base oil and wax distillates from which aromatic extracts are removed do not have sharp boiling point cut-offs, nor do the resulting aromatic extracts.

To predict the environmental behaviour and fate of complex substances such as these DAEs, representative structures were selected from each chemical class within these substances. Thirty-three structures were selected (see Table C.1 in Appendix C) from the database in PetroTox (2012) on the basis of the boiling point range for each DAE, the number of data on each structure, and the middle of the boiling point range of similar structures. As the compositions of these DAEs are not well defined and are indeed variable, representative structures are not considered to be proportional with respect to the actual fractions in the mixtures. The selection process resulted in representative structures for alkanes, isoalkanes, one- and two-ring cycloalkanes, polycycloalkanes, cycloalkane monoaromatics, cycloalkane diaromatics, and one- to six-ring aromatics, ranging from C_{15} to C_{50} (see Table C.1 in Appendix C). Physical-chemical data for each representative structure were assembled from the scientific literature and from the EPI Suite (c2000-2010) group of environmental models (Table C.2 in Appendix C).

The experimental water solubility for the DAEs ranged from 1.4 to 5.8 mg/L, as cited by CONCAWE (1992), but is not referenced and cannot be validated. Model predictions of individual C_{15} to C_{50} representative structures resulted in much lower water solubilities, ranging from 2.6×10^{-20} to 1.1 mg/L (Table C.2. in Appendix C). Likewise, the log K^{ow} range of 4.7 to 24 predicted for the components is much higher than that measured for the DAE identified by CAS RN 64742-03-6 (4.4 to 7.2). Nevertheless, all results suggest that these DAEs have negligible water solubility and high partitioning to octanol.

It should be noted that the physical and chemical behaviour of the representative structures will differ if these representative structures are present in a complex substance, such as aromatic extracts. The vapour pressures of components of a mixture will be lower than their individual vapour pressures based on Raoult's law (i.e., 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). Similar to Raoult's law, the water solubilities of components in a mixture are lower than when they are present individually (Banerjee 1984). Concurrently, however, when part of a mixture (or a UVCB such as in this instance), components that are normally solid under environmental conditions may have lower melting points (and therefore be in a liquid state), as well as increased vapour pressure and water solubility (Banerjee 1984).

4. Sources

DAEs are produced (i.e., manufactured) in refineries in Canada, in addition to being imported into Canada (Table 4-1). Within refineries these substances are part of intermediate streams or they are blended to make other products under a new CAS RN and so have been identified as being consumed at the facility as indicated from information collected through the *Notice with respect to certain high priority petroleum substances* (Environment Canada 2008) (see Table 4-1).

There were no manufacturing quantities reported for "extracts (petroleum), heavy naphthenic distillate solvent" (CAS RN 64742-11-6). None of the three DAEs were reported as being acquired for use as a feedstock in the petroleum sector (Environment Canada 2008).

Table 4-1. Quantities of the three DAEs in Canada (Environment Canada 2008 2012)

CAS RN	Manufacture quantity (kg) in 2006	Import, export, use and transportation quantities (kg) in 2010
64742-04-7	> 10 000 000	1 000 000 to 10 000 000
64742-05-8	> 10 000 000	0
64742-11-6	0	1 000 000 to 10 000 000

Information collected through the *Notice with respect to certain high priority petroleum substances on the* Domestic Substances List (Environment Canada 2012), published under section 71 of CEPA, indicates that two of the DAEs are imported, exported and used in industrial or commercial settings and are either imported by truck or rail car (see Table 4-1). Multiple reporters confirmed import, use and export of CAS RN 64742-04-7 and 64742-11-6.

Outside of Canada, all of these DAEs have been identified by the Organisation for Economic Co-operation and Development (OECD) as high production volume (HPV) chemicals, with 1000 tonnes or more produced per year (OECD 2004).

HPV chemicals in the United States are those produced or imported in quantities of 1 million pounds or more per year (HPVIS 2014). Information on quantities in the United States was obtained from the US EPA Chemical Data Access Tool (CDAT), which documents the annual production volume for CAS RN 64742-04-7 as between 5×10^8 and 10×10^8 lb/year (equivalent of 2.3×10^8 to 4.5×10^8 kg/year), while the volume for CAS RN 64742-05-8 was withheld under the confidential business information provisions of the US *Toxic Substances Control Act* but appeared to be at least 190 million lb/year (8.6×10^7 kg/year) from one reporter. CAS RN 64742-11-6 was reported as 231 million lb/year (1.0×10^8 kg/year) in the United States in 2012 (CDAT 2014).

The EU has also identified these DAEs as HPV chemicals (ECHA c2007-2014). In the EU, chemicals produced or imported in volumes of over 1000 tonnes per year are considered HPV substances. The European Chemicals Agency (ECHA) reported between 1 million and 10 million tonnes for CAS RN 64742-04-7 and between 100,000 and 1 million tonnes for CAS RN 64742-05-8. No volumes were identified for CAS RN 64742-11-6 (ECHA c2007-2014).

5. Uses

The *Domestic Substances List* nomination information (from 1984-1986) indicates that DAEs were used as lubricating agents, lubricant additives, and mould release agents as well as in the petroleum and natural gas sector.

According to information collected through a section 71 notice under CEPA (Environment Canada 2008), DAEs were identified as being site-restricted at refineries, as being part of an intermediate stream, as being blended to make other products under a new CAS RN or as being consumed at the facility. However, updated information collected through a later section 71 notice (Environment Canada 2012) showed DAEs were imported, exported and used for industrial products by Canadian companies outside of the petroleum sector.

Non-confidential industrial product categories collected under Environment Canada (2012) are summarized in Table 5-1. None of the refineries in Canada identified these substances as being sold or used for the purposes listed in Table 5-1.

Table 5-1. Industrial products containing the three DAEs (Environment Canada 2012)

CAS RN	Industrial and Professional Use Products
64742-04-7	Solvents Vehicle parts production Adhesives and sealant substances Corrosion inhibitors Demulsifier Viscosity adjusters
64742-05-8	No products/uses identified
64742-11-6	Adhesives and sealants Solvents Viscosity adjusters Printing inks Lubricants Rubber and plastics Paints and coatings Electrical insulating Asphalt recycling Roofing materials Process oils Fuels Road paving

Additional information on potential uses of DAEs was found through searches of the available scientific and technical literature. In general, aromatic extracts can be used as blending components in heavy fuels, as feed stock for the production of carbon black, petroleum pitches or resins, and in the manufacture of rubber and plastics (API 2012b).

The US Department of Health and Human Services' Household Products Database contains information on petroleum substances found in consumer products in the United States (Household Products Database 1993-). Some of these products may also be available in Canada. The database showed that CAS RN 64742-11-6 is found in the United States in two consumer product adhesives (Household Products

Database 1993-). Also, aromatic extracts were historically used in specialty applications such as printing inks, wood preservatives and seal coatings (API 2012b). Further data on products identified through internet and material safety data sheet (MSDS) searches and updated information from industry showed these products were discontinued, reformulated, not available in Canada, or limited to industrial use. Therefore, these DAEs were not found to be used as ingredients in Canadian marketplace products. MSDS searches also revealed that one of the DAEs (CAS RN 64742-11-6) is used in a dust suppressant product at a concentration of 100% w/w (MSDS 2005). However, use of this product from the United States in Canada is not confirmed.

Aromatic extracts in general can be used as extender oils in the manufacture of rubber and plastics. Extender oils help to achieve elasticity and are added to make brittle materials soft and flexible (API 2012b; UBA 2016). However, use of DAEs as extender oils in tires and consumer products has declined because of increased attention to their composition, including PAH content, and their potential effects on the environment and human health. Recycled tires are processed to form crumb rubber products, such rubberized playground surfaces and athletic surfaces. To this end, regulations have been introduced in the European Union. The European Commission has legislation in the form of Directive 2005/69/EC that bans the use of extender oils that are rich in PAHs for the production of tires as of January 1, 2010 (EC 2005). Tires are not to contain more than 1 mg/kg B[a]P or more than 10 mg/kg of the sum of the eight “EU-PAHs.”[4] Additionally, the use of these extender oils that contain greater than 1 mg/kg of PAH species is banned in plastic or rubber consumer products that are intended to come into direct and prolonged contact with human skin or the oral cavity (European Commission 2013). Children were also identified as a population of concern, and therefore the use of PAHs above 0.5 mg/kg (ppm) in accessible parts of toys and children’s articles is banned. These product regulations came into force in Europe on December 27, 2015.

All three DAEs are classified as carcinogens. For example, in Europe they are considered category 1B, which may cause cancer. In order to improve human health protection, substances and preparations containing these DAEs should not be placed on the market for use by the general public (ECHA c2007–2014; EU 2005). Market use of the three DAEs has therefore been restricted in the EU because of their inherent hazard (ECHA c2007-2014; EU 2005). They are included in Regulation 1272/2008 on classification, labelling and packaging of substances and mixtures (EU 2008) and in the ECHA list of CMR substances (ECHA 2012). Two of these DAEs are found on the Danish List of Undesirable Substances (2004).

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[4] Benzo[a]pyrene, benzo[e]pyrene, benzo[a]anthracene, chrysene, benzo[b]fluoranthene, benzo[j]fluoranthene, benzo[k]fluoranthene and dibenzo[a,h]anthracene, hereinafter referred to as the European Union polycyclic aromatic hydrocarbons (EU-PAHs), are classified in accordance with Annex VI to Regulation (EC) No 1272/2008 of the European Parliament and the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (2).

6. Releases to the Environment

Potential release of DAEs to the environment can be from petroleum facilities, transportation and spills, uses of consumer products, and manufacture of products containing DAEs.

6.1 Potential Release from Petroleum Facilities

The DAEs considered in this report originate from refineries. At refineries, aromatic extracts are generally obtained by solvent extraction of aromatics during the production of base oil and waxes. Thus, the potential locations for the controlled release of DAEs include relief, venting, or drain valves on piping or equipment (e.g., vessels) in the vicinity of this equipment. Under typical operating conditions, releases of DAEs would be captured in a closed system, according to defined procedures, and returned to the processing facility or to the wastewater treatment plant. In both cases, exposure of the general population or the environment is not expected.

Unintentional releases of DAEs may occur at production facilities. In Canada, legislation governing releases of DAEs is in place and includes requirements at the provincial/territorial level to prevent or manage unintentional releases of petroleum substances and streams within a facility through the use of operating permits (SENES 2009). 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).

At the federal level, unintentional releases of some petroleum substances to water from facilities are addressed under the *Petroleum Refinery Liquid Effluent Regulations* and guidelines (Environment Canada 1974) in the *Fisheries Act* (Canada 2012). 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. Non-regulatory measures (e.g., guidelines and best practices) are also in place at petroleum sector facilities to help reduce unintentional releases.

6.2 Potential Release from Transportation and Spills

The DAEs considered in this assessment can be transported between facilities by rail or truck. In general, three operating procedures are involved in the process of transportation: loading, transit, and unloading. With the transport of these substances by rail and truck (Environment Canada 2011, 2012), unintentional releases of DAEs will generally enter the air, water, or soil.

The handling of DAEs at petroleum facilities for the purpose of transportation is regulated at both the federal and provincial levels, with measures covering loading and unloading (SENES 2009). Collectively, these measures establish requirements for safe handling of petroleum substances and are intended to minimize or prevent potential releases during loading, transportation and unloading operations (SENES 2009). Given the low vapour pressure of DAEs, exposure of the general population to fugitive emissions is expected to be low (see Section 9.1).

Tanks or containers for transferring petroleum substances are typically dedicated vessels and therefore washing or cleaning is not required on a routine basis (API 2012b).

Releases associated with the transport of petroleum substances can generally be assessed through an analysis of historical spill data. There are no applicable spill data specifically for DAEs, but spills are not expected to be an important release source compared to releases from tires and road care products. The potential release of DAEs from spills is therefore not considered further in this assessment.

6.3 Potential Release of DAEs from Tires and Road Care Products

Although the use of DAEs in tires has declined (see Section 5), the release of DAEs to the aquatic environment from tires is evaluated in this assessment. Potential releases of DAEs from tire wear are conservatively estimated on the basis of estimates of tire loss, the estimated quantity of tires containing DAEs, and their concentration in the tires (see Section 8.2.3).

DAEs might be released from road care products. The release of DAEs (as a subcategory of aromatic extracts) from road-care asphalt emulsions that are mixed with asphalt has been evaluated in the screening assessment report of asphalt and oxidized asphalt (ECCC/HC 2017) and is therefore not considered in this assessment. However, release from the use of DAEs in road care products that are not mixed with asphalt is expected and evaluated in the exposure assessment (see Section 8.2.3).

6.4 Potential Releases from Manufacturing of Products Containing DAEs

Considering the reported use patterns of these DAEs, there is potential for release to the aquatic environment through wastewater effluents from industrial sources. Releases from the rubber manufacturing sector are related to rubber compounding, manufacture of rubber products, and tire retreading. Releases from manufacturing of products other than rubber are related to the formulation of corrosion inhibitors, and the manufacture of asphalt road care products and building materials. Releases to the environment are estimated on the basis of use quantity, number of operation days involved with DAEs, wastewater emission factors, and removal by wastewater treatment systems (Appendix F, Table F.1).

7. Environmental Fate and Behaviour

7.1 Environmental Distribution

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, photodegradation—another fate process—can also be significant.

As noted previously, the solubility and vapour pressure of components within a mixture will differ from those of the component alone. The interactions between the components of complex UVCBs such as petroleum hydrocarbons are complex.

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 (Potter and Simmons 1998). Thus, when a petroleum mixture is released into the environment, the principal water contaminants are likely to be aromatics, whereas the principal air contaminants will be aliphatics (Potter and Simmons 1998). Alkenes and alkanes have similar volatilities and are more volatile than aromatics and cycloalkanes, which in turn have similar volatilities. 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. Following an initial loss due to volatilization and solubilization, the remaining degradative pathway is biodegradation, usually by bacteria.

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 as follows (Potter and Simons 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 microorganisms);
(5) monoaromatics;

(6) polynuclear (polycyclic) aromatic hydrocarbons (PAHs); and
(7) higher-molecular-weight cycloalkanes (which may degrade very slowly (Pancirov and Brown 1975)).

Three weathering processes—dissolution in water, volatilization, and biodegradation—typically result in the depletion of the more readily soluble, volatile, and degradable compounds and the accumulation of those most resistant to these processes in residues. Because of the complex interaction of components within a mixture that impacts their physical-chemical properties and behaviour, it is difficult to predict the fate of a complex mixture. Therefore, as a general indication of the fate of DAEs, the physical-chemical properties of representative structures of DAEs (Tables C.1 and C.2 in Appendix C) were examined.

If released to air, the components of DAEs with carbon number less than C_{20} are likely to remain in air because of their moderate vapour pressure (1.2×10^{-3} to 5.8 Pa), whereas the heavier components will partition out of air because of their generally low vapour pressure (5.1×10^{-10} to 2.5×10^{-3} Pa) (Appendix C).

If released to water, the components will typically settle into the sediment as a result of low aqueous solubilities and high K_{ow} and K_{oc} values (Table B-3 of Appendix B). 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 (0.06 to 3.6×10^{10} $Pa \cdot m^3/mol$). The relatively low proportions of aliphatic components in these DAEs will not amount to large quantities evaporating from water. The tendencies for evaporation and sorption are competing, and the exact nature of the release would dictate how the DAEs behave.

If released to soil, most representative structures of DAEs are expected to sorb to soil because of their high log K_{oc} value (4.4 to 22). Competing with this tendency are evaporative forces. Some of the smaller structures, such as 2-methyl tetradecane (a C_{15} isoalkane), might volatize into the air because of their moderate vapour pressures. Volatilization from moist soil surfaces may be an important fate process considering the estimated Henry's law constant values. When released to the environment, these DAEs will tend to clump together rather than disperse because they are highly viscous (US EPA 2008). When large quantities of a hydrocarbon mixture enter the soil compartment, soil organic matter and other sorption sites in soil become saturated and 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, the NAPL will be immobile (Arthurs et al. 1995); 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).

7.2 Persistence and Bioaccumulation

Given the complex nature of petroleum substances such as DAEs, the persistence and bioaccumulation potential of components of these substances is characterized using empirical and/or modelled data for a suite of petroleum hydrocarbon structures. These representative petroleum hydrocarbon structures do not represent all possible structures in petroleum substances, nor do they necessarily represent the full range of persistence or bioaccumulation potential present in any given chemical class of structures (e.g., alkanes, monoaromatics) or carbon number (e.g., C_{20}). Thus, the modelling results do not indicate the persistence and bioaccumulation potential of all substances in a specific class and carbon range but instead give a more general indication of these properties. When available and applicable, empirical persistence data on whole DAEs are also considered.

7.2.1 Potential for environmental persistence

An experimental biodegradation study for a light DAE (CAS RN 64742-03-6) found that it is not biodegradable in water. No biodegradation or mineralization was observed over 28 days in a closed bottle test and modified Sturm test, respectively (Shell Research Ltd. 1994; API 2012a). Similar low biodegradation potential is expected with the light DAE considered in this assessment (CAS RN 64742-05-8). Additionally, the two heavy DAEs considered in this assessment are expected to have similar low biodegradation potential as the higher carbon number components are expected to be even less biodegradable than the lighter components found within the light DAE.

Persistence of a suite of petroleum hydrocarbons expected to occur in DAEs was characterized using empirical and/or modelled data.

Model results and the weighing of information are reported in the technical document on petroleum substance persistence and bioaccumulation (Environment Canada 2014) and are summarized in Table D.1 (Appendix D).

Empirical and modelled half-lives in the atmosphere for the components of these DAEs are less than 2 days (Environment Canada 2014). However, a number of three- to six-ring PAHs can undergo long-range transport to remote regions as a result of sorption to particulate matter (Environment Canada 2014).

Considering biodegradation in water, soil, and sediment, the following components have half-lives greater than 6 months in water and soils and greater than 1 year in sediments: C_{30} isoalkane, C_{15}–C_{50} dicycloalkanes, C_{18}–C_{22} polycycloalkanes, C_{15}–C_{20} cycloalkane monoaromatics, C_{15}–C_{50} two-ring aromatics, and C_{18}-–C_{50} three- to six-ring PAHs. The C_{30} one-ring cycloalkane, C_{15} and C_{30}–C_{50} one-ring aromatics have half-lives greater than 1 year in sediments only (Table D.1 in Appendix D).

7.2.2 Potential for bioaccumulation

Bioaccumulation potential for a suite of petroleum hydrocarbons expected to occur in DAEs was characterized using empirical and/or modelled data. Bioaccumulation factors (BAFs) are the preferred metric for assessing the bioaccumulation potential of substances, as the bioconcentration factor (BCF) may not adequately account for the bioaccumulation potential of substances via the diet, which predominates for substances with log K_{ow} values greater than approximately 4.5 (Arnot and Gobas 2003).

In addition to fish BCF and BAF data, bioaccumulation data for aquatic invertebrate species, biota-sediment/soil accumulation factors (BSAFs), trophic magnification factors and biomagnification factors were also considered in characterizing bioaccumulation potential.

Empirical and modelled bioaccumulation data for petroleum hydrocarbons, as well as the weighing of information, can be found in an Environment Canada technical report (Environment Canada 2014). A summary of the results for bioaccumulation potential is presented below and in Table D.2 (Appendix D).

Overall, there is consistent empirical and predicted evidence to suggest that the following components have the potential for high bioaccumulation with BAF/BCF values greater than 5000: C_{15} isoalkanes, C_{15} one-ring cycloalkanes, C_{15} two-ring cycloalkanes, C_{22} polycycloalkanes, C_{15} one-ring aromatics, C_{15}–C_{20} cycloalkane monoaromatics, C_{20} cycloalkane diaromatics, C_{20} three-ring aromatics, C_{16}–C_{20} four-ring PAHs, C_{20}–C_{22} five-ring PAHs, and C_{22} six-ring PAHs (Table D.2, Appendix D). These components are highly lipophilic and are associated with a slow rate of metabolism in certain organisms such that the rate of uptake greatly exceeds the total elimination rate. However, most of these components are not expected to biomagnify (relative to their concentration in the diet) in aquatic or terrestrial food webs, largely because the combination of metabolism (albeit slow), low dietary assimilation efficiency, and growth dilution allows the elimination rate to exceed the uptake rate when exposure occurs from the diet only (Environment Canada 2014). In addition, fish and other vertebrates have a higher capacity to metabolize aromatic components than invertebrates, which decreases the potential for trophic transfer of these components. However, one study (Harris et al. 2011) suggests that some alkyl-PAHs may biomagnify. While only BSAFs were found for some PAHs, it is possible that BSAFs will be greater than 1 for invertebrates, given that they do not have the same metabolic competency as fish. BSAFs will likely decrease beyond C_{22} because of reduced bioavailability of the higher boiling point fractions (Muijs and Jonker 2010).

8. Potential to Cause Ecological Harm

8.1 Ecological Effects Assessment

Information relevant to the toxicity of the DAEs to various organisms is provided below. Because of the high log K_{ow} values of components of these DAEs (4.4 to greater than 25 (Table 3-1)) and their high viscosity (semi-solid to solid at ambient temperature), the potential for these DAEs to partition to water and contribute to chronic effects in aquatic organisms is considered to be limited (API 2012b).

8.1.1 Water

Experimental data for the aquatic toxicity of two of the DAEs are presented in Table E.1 (Appendix E). Toxicity data for the heavy DAE identified by CAS RN 64742-04-7 and the light (C_{15}–C_{30}) DAE (CAS RN 64742-05-8) are presented below. Toxicity data for the heavy (C_{20}–C_{50}) DAE identified by CAS RN 64742-11-6 were not available.

All tests with the heavy DAE CAS RN 64742-04-7 were conducted using water-accommodated fractions (WAFs) at high nominal loading rates (>100 mg/L), and effects were not observed. The no-observed-effect-level (NOEL) for *Oncorhynchus mykiss* (96-hour acute test) was greater than the WAF of 1000 mg/L (BP Oil Europe 1994a). For *Daphnia magna*, a 21-day test resulted in a median effective loading rate (EL_{50}) greater than 1000 mg/L for reproduction and survival (BP Oil Europe 1994b) (see Table E.1). In a later study, the 48-hour acute EL_{50} for *D. magna* and *Selenastrum capricornutum* (now known as *Pseudokirchnerella subcapitata*) were both greater than 100 mg/L as a WAF (EMBSI 2012a and 2012b).

Experimental studies were conducted by ExxonMobil Biomedical Sciences, Inc. (EMBSI) for CONCAWE in 2012 on WAFs of prepared solutions of the light DAE CAS RN 64742-05-8 (Table E.1 in Appendix E). For *D. magna*, a 48-hour acute toxicity test had a no-observed-effect-loading-rate (NOELR) of 1 mg/L and an EL_{50} of 35.9 mg/L for mobility; the lowest-observed-effect-loading-rate (LOELR) was identified as 10 mg/L with observed lack of energy and immobilization (EMBSI 2012c). The algae *P. subcapitata* (formerly *S. capricornutum)* was more sensitive, with an EL_{50} of 18.8 mg/L, determined on the basis of growth rate inhibition, and a NOELR of 0.1 mg/L. The 72-hour growth inhibition test consisted of nine replicates per test concentration, with an algae concentration of 1.0 x 10^4 cells/mL in each replicate chamber. The study was generally conducted following the OECD 201 Guideline, with the exception of the preparation of a WAF. It was noted that for 8 hours of the 72-hour test, the temperature fell below the recommended 21ºC; however, cell densities were observed to increase by an appropriate factor in the control and the study is still considered reliable. The LOELR was identified as 1 mg/L on the basis of statistically significant growth reduction (EMBSI 2012d).

A number of samples of DAEs were characterized by EMBSI for aromatic and aliphatic content as part of a CONCAWE-sponsored project. The methodology used could only determine the aromatic and aliphatic content up to C30. The results indicate that the heavy DAE CAS RN 64742-04-7 had only 1.4 to 23 wt% total aromatic content up to C30 (EMBSI 2009), whereas DAEs generally have 65 to 85% wt% aromatic content as indicated by several sources (API 2008; US EPA 2008; CONCAWE 2010; API 2012b). Therefore, it is assumed that the majority of aromatic components from the samples of CAS RN 64742-04-7 analyzed by EMBSI have carbon numbers between C_{30} and C_{50} (CONCAWE 2013). One sample of the light DAE CAS RN 64742-05-8 was also analyzed by EMBSI; it had 87 wt% aromatic content (EMBSI 2009), which is consistent with the range reported by API (2008) (70 to 88 wt%). This is expected, as light DAEs fall entirely within the carbon range that the methodology can measure. There were no data available on the characterization of DAE CAS RN 64742-04-7 tested by BP Oil Europe in 1994 (CONCAWE 2013).

The proportions of three- to seven-ring PAHs are similar for CAS RNs 64742-05-8 and 64742-04-7 in the samples reported in US EPA (2008b), indicating their toxicity is likely similar because toxicity is found mainly in the three- to seven-ring PAHs (API 2012b). In contrast, CONCAWE reported 2077 ppm of the 16 US EPA priority PAHs[5] in a sample of CAS RN 64742-05-8 (light DAE), and only 1.2 to 302 ppm of the 16 priority PAHs in four samples of CAS RN 64742-04-7 (heavy DAE) (CONCAWE 2013). There are obvious differences in the chemical compositions between the samples reported in CONCAWE (2013) and US EPA (2008b) for the same substance. Even among the CONCAWE samples, the total aromatic proportion of CAS RN 64742-04-7 varied widely (1.4 to 23 wt%). Thus, the results of low toxicity observed by CONCAWE (2013) may not be applicable to other samples of CAS RN 64742-04-7. Differences in composition of a given sample could also explain the discrepancies observed between the aquatic toxicity results for CAS RN 64742-04-7, which showed no effects at high loading concentrations, and CAS RN 64742-05-8, which did cause effects.

CONCAWE developed an aquatic toxicity model, PetroTox, specifically for petroleum hydrocarbon mixtures. This model is based on chemical action via narcosis and therefore accounts for additive effects according to the toxic unit approach. It can model petroleum hydrocarbon toxicity for C_4–C_{41} compounds dissolved in the water fraction.[6] Substances smaller than C_4 are considered too volatile to impart any significant toxicity, and compounds larger than C_{41} are considered too hydrophobic and immobile to impart any significant aquatic toxicity. PetroTox (2012) generates estimates of toxicity with a median lethal loading (LL_{50}) rather than a median lethal concentration (LC_{50}), i.e., it takes into account the poor solubility of petroleum substances in water. The LL_{50} value is the amount of petroleum substance needed to

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[5] The 16 US EPA priority pollutant PAHs are naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benz[*a*]anthracene, chrysene, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[a]pyrene, dibenz[a,h]anthracene, benzo[ghi]perylene, and indeno[1,2,3-cd]pyrene.

[6] PETROTOX uses its own library of petroleum hydrocarbons and their associated physical chemical properties. These properties may differ from those given for the same representative structures in Tables C.1 and C.2 in Appendix C.

generate a WAF that is toxic to 50% of the test organisms. It is not a direct measure of the concentration of the petroleum components in the WAF.

PetroTox was used to estimate the aquatic toxicity of DAEs as a whole, as well as light and heavy DAEs separately (Tables E.2 to E.4, Appendix E), using available information on the boiling point ranges and aromatic-to-aliphatic ratios (see section 2). The results indicate that the toxicity of DAEs increases with the proportion of aromatics. The results also indicate that the toxicities of DAEs are generally similar, though the aquatic toxicities of heavy DAEs are slightly less than that of light DAEs. In addition, lethal loading rates were generally below 1 mg/L, except for *M. beryllina*, which appears to be quite tolerant of DAEs with estimated LL_{50} values greater than 1000 mg/L.

The Petroleum HPV Testing Group of the American Petroleum Institute used PetroTox to estimate the toxicity of the light DAE CAS RN 64742-05-8 using high resolution mode and compositional data from two-dimensional gas chromatographic analysis. Acute lethal loadings to fish (*O. mykiss*), invertebrates (*D. magna*) and algae (*P. subcapitata,* formerly *S. capricornutum*) were all greater than 1000 mg/L (API 2013). This differs from the results obtained for this DAE in Table E.3, Appendix E.

Modelled low resolution results for the three DAEs considered in this report (Appendix E) are lower than those found in the experimental studies presented above. However, because of the lack of compositional data and model uncertainties (including low toxicity observed for the light DAE when estimated using high-resolution and detailed compositional data), empirical data were given more weight when considering the overall evidence.

Some studies are available that examined the aquatic toxicity of tire debris and road wear particles. None of the studies identified DAEs as the toxic components causing adverse effects to aquatic organisms (Brophy and Graney 2004; Stephensen et al. 2005; Marwood et al. 2011).

Overall, the empirical and modelled ecotoxicological data summarized in Tables E.1, E.2, E.3 and E.4 (Appendix E) indicate that the three DAEs might have moderate to high acute toxicity to aquatic organisms. It appears that algae are most sensitive to DAEs. For the aquatic toxicity, the critical toxicity value (CTV) was chosen to be 19 mg/L on the basis of the EL_{50} (growth inhibition) resulting from exposure of algae to CAS RN 64742-05-8. This CTV is considered applicable for the three DAEs in this report, given their similar aromatic content (ranging from 67 to 88 wt%, Table 2-1) and their similar total PAHs (ranging from 8.7 to 20 wt%, Table 2-2). Whereas experimental data were not available for all three DAEs, their model predictions suggest that CAS RN 64742-05-8 would be the most hazardous of the three to aquatic organisms. In addition, as higher proportions of soluble aromatics decrease the loading rate required to cause toxicity, larger proportions of aromatics in the less than C_{30} carbon range result in greater toxicity (Swigert et al. 2014). Experimental toxicity data for sediment-dwelling organisms are not available; however, it is expected that they would have a similar sensitivity to DAEs as aquatic organisms.

8.1.2 Terrestrial

DAEs have low acute systemic toxicity in mammals. Oral LD_{50}s for both light and heavy DAEs were greater than 5000 mg/kg in rats, and a LOAEL of 125 mg/kg/day was identified in rats after a 13-week oral exposure (API 2012a; API 1986; Feuston et al. 1994; FDRL 1974).

No data on the toxicity of DAEs to soil organisms was found. However, the Canada-Wide Standard for Petroleum Hydrocarbons in Soil (CCME 2008) provides soil standards for petroleum products based on toxicity to a variety of terrestrial organisms (e.g., invertebrates and plants). These standards are based on four fractions of total petroleum hydrocarbons (fraction 1 (F1; C_6–C_{10}), fraction 2 (F2; $>C_{10}$–C_{16}), fraction 3 (F3; $>C_{16}$–C_{34}) and fraction 4 (F4; $>C_{34}$)) and assume a 20:80 ratio of aromatics to aliphatics. The standards are also divided into four land-use classes (agricultural, residential, commercial and industrial) and two soil types (coarse-grained and fine-grained) for the determination of remedial standards. The most sensitive land-use and soil type is typically agricultural coarse-grained soils.

DAEs are predominantly found in the F3 and F4 fractions, but may also partly encompass the F2 fraction for light DAEs that have a carbon range starting at C_{15}. Given that the proportion of F2 in even light DAEs would be small, the values for F3 and F4 are most relevant. The standards for soil contact by non-human organisms for F3 and F4 are 300 and 2800 mg/kg dry weight (dw) soil, respectively (CCME 2008a, 2008b). However, the Canada-wide standards were developed assuming a 20:80 ratio of aromatics to aliphatics, which is a much smaller proportion of aromatics than that present in DAEs. Considering that aromatic hydrocarbons are the main contributors to toxicity of petroleum substances, the standards may not be protective for these substances.

The major sources of environmental release of these substances are to aquatic systems (see section 8.2); thus, the risk of these substances to soil organisms was not considered further within this assessment.

8.2 Ecological Exposure Assessment

8.2.1 Exposure scenarios and predicted environmental concentrations

Exposure scenarios were developed for manufacturing of rubber and other products and for runoff from tire wear. These scenarios represent the major potential for environmental exposure to these DAEs. For each scenario, a predicted environmental concentration (PEC) is estimated in order to assess exposure to the DAEs by ecological receptors. These PECs were determined on the basis of a tiered approach (i.e., using conservative assumptions for the initial calculations and then refining these assumptions as needed to increase the level of realism of the scenario).

No data on measured environmental concentrations (e.g., water, soils, and sediments) of DAEs are available as it would be difficult to attribute the measured analytes to these complex UVCBs. Therefore, environmental concentrations have been estimated from available information including substance quantities, estimated release rates, and characteristics of the receiving environment.

8.2.2 Exposure from manufacturing of rubber and other products

An estimate of environmental exposure was derived for aquatic exposure to these DAEs resulting from their use and release from the manufacturing of rubber and other products. The CEPA section 71 notice survey results identified three types of activities involved in rubber manufacture: rubber compounding, manufacture of rubber products, and tire retreading (Environment Canada 2011, 2012). Tire manufacture was initially included in this sector on the basis of the survey data, but was removed after it was confirmed that DAEs are no longer used in tire manufacture in Canada [personal communication, Environment Canada with Canadian tire manufacturers, dated 2014; unreferenced]. The section 71 survey results identified three types of activities related to the manufacturing of products other than rubber: formulation of corrosion inhibitors, manufacture of asphalt road care products, and manufacture of building materials (Environment Canada 2011, 2012). These have been assessed as one scenario.

The PEC is estimated using available information on the quantities of these DAEs used in Canada, the number of annual operation days of manufacturing facilities for rubber and other products, estimates of losses to wastewater and removal by wastewater treatment systems, and estimates of dilution in receiving waters. The equation and values used in the calculation are provided in Appendix F (Table F.1).

As DAEs are expected to be released to water from wastewater treatment systems, and then partition to sediments, PECs were estimated for both water and sediments. The sediment PECs were estimated under the assumption that the compositions of these UVCBs do not change before and after wastewater treatment. However, the wastewater treatment system (WWTS) will remove different components preferentially, such that the composition in effluent is not the same as in influent. Concentrations for the two scenarios in water near the point of discharge vary between 5.4×10^{-5} and 0.055 mg/L, while concentrations in sediment vary between 0.013 and 213 mg/kg, as shown in (Table 8-1).

Table 8-1: Water and sediment PECs for DAEs resulting from manufacturing of rubber and other products

Scenario	Water PEC (mg/L)	Sediment PEC (mg/kg)
Manufacturing of rubber	5.4×10^{-5} to 0.054	0.013 to 170
Manufacturing of other products	1.7×10^{-4} to 0.055	0.049 to 210

8.2.3 Exposure from runoff of tire wear and from road care products

Conservative PEC estimates for water are derived for the runoff releases of these DAEs from tire wear particles and road care products. The fraction of tires used in Canada that contains DAEs is unknown; however, communication with Canadian tire manufacturers confirmed that DAEs are no longer used in the manufacture of new tires [personal communication, Environment Canada with Canadian tire manufacturers, dated 2014; unreferenced]. An upper limit for DAE-in tires was estimated on the basis of the confirmed proportion of DAE-free tires in Canada (see Table F.2 in Appendix F). This upper limit value therefore allows the derivation of conservative PEC estimates. For the same purpose, an upper limit for the DAEs present in road care products is determined from survey data (Environment Canada 2011, 2012). The two upper limits are then combined in the derivation of conservative aquatic PEC estimates.

It should be noted that road care products are divided into products mixed with asphalt and those not mixed with asphalt. As the products mixed with asphalt are covered by the screening assessment report of asphalt and oxidized asphalt (ECCC, HC 2017), they are excluded from the PEC calculations here. The PECs derived for water, presented as a distribution across 300 Canadian urban areas, are in the range of 0.0017 to 0.072 mg/L for 95% of urban areas. This further yields a range of PECs in sediment from 0.49 to 280 mg/kg derived using an equilibrium partitioning approach. The calculations and values used to derive the water and sediment PECs can be found in Appendix F (Table F.2).

8.3 Characterization of Ecological Risk

8.3.1 Risk analysis

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. For each endpoint organism, an estimate of the potential to cause adverse effects and predicted no-effect concentration (PNEC) was determined. The PNEC is the CTV selected for the organism of interest divided by an appropriate assessment factor. Also, a PEC was determined for each exposure scenario. 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.

For the exposure scenarios for the manufacture of rubber and other products and for runoff from tire and road care products, the selected critical toxicity value of 19 mg/L was based on the EL_{50} (e.g., growth inhibition) resulting from exposure of algae to CAS RN 64742-05-8. An assessment factor of 100 was applied to the CTV to account for acute to chronic extrapolations, as well as inter- and intra-species variability, resulting in a freshwater PNEC of 0.19 mg/L.

The resultant RQs for each exposure scenario are presented below (Table 8-2). These conservative RQs, calculated for each of the exposure scenarios on the basis of the available information, are below 1, which indicate low risk of harm to aquatic organisms.

Table 8-2: Summary of risk quotients (RQs) for water obtained for different conservative exposure scenarios for DAEs.

Scenario	Critical toxicity value (CTV)	Assessment factor	PNEC	PEC	RQ
Rubber manufacturing	19 mg/L	100	0.19 mg/L	0.054 mg/L	0.28
Manufacturing of other products	19 mg/L	100	0.19 mg/L	0.055 mg/L	0.29
Runoff from tire wear and road washout	19 mg/L	100	0.19 mg/L	0.072 mg/L	0.38

Once released to water, these DAEs are expected to partition to sediment. A risk quotient based on exposure in sediment may be calculated on the basis of the above PEC and PNEC values for water and used for sediment risk characterization. In the calculation, the bottom sediment, the suspended sediment, and the aqueous phase are assumed to be in equilibrium. The benthic and pelagic organisms are assumed to have similar sensitivities to DAEs. Therefore, this equilibrium approach would result in risk quotients (PEC/PNEC) for sediment that are the same as for water. The conservative RQs for water, and thus sediments, are all below 1, indicating a low risk of harm to sediment-dwelling organisms from DAEs in Canada. The equilibrium approach does not take into account the exposure of DAEs via ingestion of contaminated sediment, whereas partition to sediment is the most important fate of these DAEs, and they contain components that might persist in sediment (Table D.1 in Appendix D). However, the combination of metabolism, low dietary assimilation efficiency, and growth dilution reduces the bioaccumulation of the components (Environment Canada 2014). Some invertebrates would be more sensitive to DAEs given that they do not have the same metabolic competency as fish, but bioaccumulation will likely decrease beyond C_{22} as a result of reduced bioavailability of the higher boiling point fractions (Muijs and Jonker 2010). The release of DAEs will contribute to the loading of PAHs in the sediment that has been previously assessed (Environment Canada, Health Canada 1994).

Considering the key exposure sources identified in Section 8.2, releases to soil are not expected to be a source of concern.

8.3.2 Uncertainties in evaluation of ecological risk

All modelling of a substance’s physical and chemical properties and persistence, bioaccumulation and toxicity characteristics is based on chemical structures. As these DAEs are considered to be UVCBs, they cannot be represented by a single, discrete chemical structure. The specific chemical composition of these DAEs is not well defined; DAE streams under the same CAS RNs can vary significantly in the number, identity, and proportion of constituent components, depending on operating conditions, feedstocks, and processing units. Therefore, for the purposes of modelling, a suite of representative structures that would provide estimates for the entire range of components likely present was identified. Specifically, these structures were used to assess the fate of these DAEs. Given that more than one representative structure may be used for the same carbon range and type of component, structure-related uncertainties exist for this substance. There is also uncertainty in the results associated with modelling using representative structures, given the large number of potential permutations of the type and percentages of the structures in DAEs.

There is uncertainty in the PNEC, because limited experiments on ecological toxicity are available. In the present evaluation, the lowest experimental EL_{50} was used as a critical toxicity value, to which an assessment factor of 100 was applied to derive the PNEC. In addition, no ecological toxicity data for sediment-dwelling organisms are available. An equilibrium approach is used to evaluate the risk of sediment exposure, which assumes that the bottom sediment, the suspended sediment, and the aqueous phase are in equilibrium and that the benthic and pelagic organisms have similar sensitivities to DAEs. These assumptions tend to underestimate the risk, as it does not take into consideration the ingestion of DAEs in sediment. However, factors such as low assimilation efficiency, growth dilution, and metabolism (in some organisms) are expected to lower the accumulation potential of DAEs. Some invertebrates have decreased capacity to metabolize aromatics compared to fish, but bioavailability will likely decrease for the higher boiling point fractions (carbon range greater than C_{22}).

The lack of compositional data for the DAEs before and after wastewater treatment results in uncertainty in the estimated sediment PECs. It was assumed that the compositions of DAEs do not change during wastewater treatment. However, wastewater treatment will remove different components preferentially, such that the composition in effluent is not the same as in influent. It is speculated that the components of the lower carbon range are more easily biodegraded than those of the higher range; hence the low-molecular-weight components will be more easily removed during treatment. The lower-molecular-weight components are generally believed to be more bioavailable than the higher ones. Therefore, the risk is expected to be lower following wastewater treatment.

There are two uncertainties in estimating the PECs for the use of DAEs in road care products that are not mixed with asphalts. The breakdown in quantity between the two types of road care products (mixed or not mixed with asphalt) was not available. As a conservative estimate, the higher end value (1 000 000 kg) of the total quantity of the two products was used in the PEC estimates. This results in an overestimation the PECs. The second uncertainty is the proportion of urban runoff treated by wastewater treatment systems. This proportion can vary from one urban centre to another, depending on local stormwater collection systems. A higher proportion of runoff treated by wastewater treatment systems means lower amounts of DAEs are released to receiving waters because a portion of the DAEs will likely be removed by wastewater treatment systems. However, there was not sufficient information available to determine how runoff was collected and treated at each urban centre. In the absence of this information, all runoff was conservatively assumed to be released to receiving water without being treated. This further overestimates the PECs. Both cases lead to the conservative estimate of the PECs.

9. Potential to Cause Harm to Human Health

9.1 Exposure Assessment

The focus of the exposure assessment is to examine the potential for general population exposure to DAEs and to estimate exposure levels. Exposure is characterized for the production, storage and transportation of these DAEs. Potential exposure to DAEs from rubber surfaces is also considered, where these substances may be present as a component of crumb rubber (i.e., bits of recycled tires that can be used to create athletic tracks and playground surfaces). Product testing was also used to provide an indication of whether DAEs are being used as extender oils in soft rubber and plastic consumer products, including toys and products used by children

9.1.1 Production and storage at refineries and transportation

DAEs are reported by the Canadian petroleum industry to be used only in processing operations in refineries, including hydrotreating and solvent extraction for solvent dewaxing processes (Hopkinson 2008, Environment Canada 2008). With these uses, the substances are contained within the refineries, where they are expected to be destroyed or further refined. The potential for fugitive emissions is low given that the vapour pressure of these substances is less than 0.075 mm Hg at 25ºC (US EPA 2012); therefore, inhalation exposures to fugitive emissions of DAEs in the vicinity of petroleum facilities are expected to be low. The same considerations and conclusion apply in the vicinity of petroleum facilities exposures for other low volatility petroleum substances that have been previously assessed (Environment Canada, Health Canada 2011, 2013, 2014).

Similarly, while it is possible that fugitive emissions of DAEs may occur during transit, because volatility is low, exposure of bystanders is expected to be negligible. While no DAEs were reported to be entering the marketplace from Canadian refiners, information obtained under section 71 of CEPA (Environment Canada 2012) revealed import and use of these substances by industry in Canada. The main reported modes of transport were by truck and rail car. Analysis of these modes of transport for potential air emissions and resulting bystander exposures in the vicinity of transit ways and unloading sites was conducted for aromatic extracts using AP-42 emissions methodology (US EPA 2008). It was confirmed that releases during transit are minimal because of the low volatility of the substances. Assuming 50% of the total aromatic extracts in use were transported via tank truck and the remaining 50% transported by rail car, total losses to air based on yearly reporting volumes during both modes of transport combined were estimated to be less than 3 kg of volatiles.

9.1.2 Rubber surfaces containing crumb rubber

Tires contain up to 30% by weight extender oils and can be recycled into crumb rubber. Crumb rubber can be combined with other materials to create outdoor playground surfaces, rubberized tracks and artificial fields (crumb rubber acts to provide cushioning and extend the life of the field) (Cheng and Reinhard 2014, Schiliro 2013). Therefore, crumb rubber-containing surfaces may contain PAHs that derive from the extender oil ingredient used in the original tire formulation.

Information provided by Canadian tire manufacturers has indicated that they have recently switched to manufacturing tires that do not contain DAEs [personal communication, Environment Canada with Canadian tire manufacturers, dated 2014; unreferenced], and therefore domestic tire production incorporates low PAH oils, aligning with the European regulations for limiting PAH content (European Commission 2005). It is anticipated this is a global trend, and it is expected that future rubber surfaces containing crumb rubber will likely have a reduced PAH content. However, the general population may be exposed to DAEs from the existing stock of tires if recycled into crumb rubber and used to create rubber surfaces. The potential for dermal and inhalation exposure to PAHs derived from crumb rubber-containing surfaces has been the subject of recent studies (OEHA 2007 Cheng and Reinhard 2014, Schiliro 2013, Birkholz 2003). These data show that there is a low potential for exposure, as considered and summarized below.

The potential for PAH exposure from the ingestion of crumb rubber from degraded rubber surfaces has been considered by several groups (OEHHA 2007; Pavilonis et al. 2014; Kim et al. 2012). Bioavailability of 16 PAH species from ingested crumb rubber was estimated by mixing biological volumes of simulated digestive fluid with crumb rubber to extract PAHs, followed by quantification of PAHs in the extract (Pavilonis et al . 2014; Zhang et al . 2008). For a suite of 16 PAHs analyzed, the concentrations were found to be below the detection limits ranging from less than 0.12 mg/kg to less than 10 mg/kg (Pavilonis et al. 2014).

The potential for dermal exposure to 16 PAH species while playing on a rubber surface was investigated by extracting PAHs from crumb rubber using an artificial sweat fluid that included agitation in solution. For the suite of 16 PAHs analyzed, the concentrations were all found to be below the detection limit, which ranged from less than 0.015 mg/kg to less than 1 mg/kg (Pavilonis et al . 2014).

PAH concentrations in ambient air were measured at rubber playing fields using stationary monitors, as well as personal air samplers in the breathing zones of athletes. Benzo[a]pyrene (B[a]P) is commonly used as a marker for the presence of PAHs in ambient air (Menichini et al. 2011). Over 2 days of sampling breathing zones, with measurements taken during regular use of the rubberized floor facilities, levels of B[a]P were determined to be 0.3 and 0.5 ng/m^3 compared to background levels in ambient air of 0.2 and 0.1 ng/m^3, respectively (Menichini et al. 2011). Given the results of air monitoring studies, and the fraction of time spent on a rubber surface, exposure to PAHs is considered to be low.

9.1.3 Consumer products potentially containing the three DAEs

Information gathered under a section 71 survey (*Notice with respect to certain high priority petroleum substances on the* Domestic Substances List) on the three DAEs considered in this assessment did not reveal their use in consumer products available to the general population (Environment Canada 2012). Products that contain these substances in Canada are limited to industrial and professional uses and are not available to the general population.

Contributions to general population exposures are not expected to be significant from professional grade products because the relative volumes found in these products are limited. For more information on product searches and the information considered, see the Uses section.

9.1.4 Consumer products potentially containing DAE-based extender oil

Historically, high PAH oils, including DAEs, have been used as extender oils in some product formulations. However, this use has declined as a result of increased attention to the PAH content of such oils and their potential effects on the environment and human health.

The European Union conducted compositional testing on approximately 5300 consumer products (e.g., electrical devices, grips/handles, toys, tyres and rolls) prior to developing regulations setting upper limits for PAH content. Test methodology included processing the products to increase surface area and then extracting PAHs in an ultrasonic toluene bath at 60°C with agitation. These conditions enhance PAH extraction and provide an upper-bound estimate of the concentration to which a person might be exposed (ZEK 2010). The PAH content was predominantly low across the products, indicating the use of low PAH oils in most product formulations (BfR 2010). B[a]P was not detected in 92% of all samples analyzed and was below 1 mg/kg in another 3% of samples. The products with the highest PAH levels were from the product category ‘tyres and rolls’, indicating the use of a high PAH formulant in their production. Other tests have found higher PAH levels in products such as bicycle tires, tool handles, shoes and sports items (UBA 2016), although a smaller study conducted on 20 toys and childcare products in Denmark detected only a low level of PAHs in the products (Danish EPA 2011). Subsequent to the Danish product testing, the European Union adopted regulations (European Union 2013) to limit PAH content in consumer products (see ‘Uses’ section for more details).

Health Canada undertook a similar compositional study of readily available soft rubber and plastic consumer products in Canada in order to determine PAH levels as an indication of the presence of these DAEs in products. The levels of PAH species, including the EU-PAHs,[7] were determined for 67 product samples obtained from the Canadian marketplace (Health Canada 2014). During product selection, emphasis was given to soft rubber and plastic products that are designed for use by children. The sample preparation method was identical to that of BfR (2010), allowing a comparison of the magnitude of results (albeit from different product samples with results coming from different laboratories) (ZEK 2010). The majority of products (66 of 67) contained low or no PAHs, with 65 products below the limits of detection (LoD) of 0.04 mg/kg to 0.36 mg/kg (LoD ranged because of the PAH species being analyzed and the sample matrix). A youth sandal, found to be low in PAHs, contained chrysene at 0.79 mg/kg, slightly above the European limit of 0.5 mg/kg and lower than the adult product limit of 1 mg/kg. A single steering wheel cover was found to contain six EU-PAHs at a concentration of higher than 1 mg/kg. However, retesting of seven additional steering wheel covers found them all to be low in PAHs and below the European limit of 1 mg/kg, indicating the first sample was not representative of the product line (Health Canada 2014).

The product testing results support the contention that soft rubber and plastic consumer products as available in the Canadian marketplace are not likely to be formulated with these DAEs, and therefore exposure is not expected.

9.2 Health Effects Assessment

9.2.1 Basis for categorization

DAEs were identified as high priorities for action during categorization of the DSL because they were determined to present a high hazard to human health. A critical effect for their initial categorization was carcinogenicity, as determined primarily on the basis of classifications by international agencies. The International Agency for Research on Cancer (IARC) reviewed the available data on a broad group of ‘mineral oils’ and concluded there was sufficient evidence that aromatic oils including extracts

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[7] Health Canada analysed benzo[j]fluoranthene that is known to co-elute with benzo[b]fluoranthene.

from solvent treatment of distillates and the high-boiling fraction of catalytically cracked oils are carcinogenic to animals (IARC 1984).

The European Commission under the United Nations' Globally Harmonized System of Classification and Labelling of Chemicals classifies all three substances as Category 1B carcinogens ('may cause cancer') (EU 2008, 2009; UN 2013).

9.2.2 Health effects summary

The DAEs identified by CAS RNs 64742-05-8 and 64742-04-7 have low acute toxicity in laboratory animals via the oral (LD_{50} > 5000 mg/kg-bw) and dermal (LD_{50} > 3000 mg/kg-bw and > 2000 mg/kg-bw respectively) routes of exposure. No reliable skin sensitization studies were found but both CAS RN 64742-05-8 and 64742-04-7 can produce eye and skin irritation (slight and slight-to-severe, respectively) (API 1986a; FDRL 1974a-d).

Minimal dermal irritation, slight edema, flaky, cracked and leathery skin and lower mean serum glutamic oxaloacetic transaminase levels (~16% reduction) were seen in rabbits dermally exposed to CAS RN 64742-05-8 at 250 mg/kg-bw, three times per week for 28 days (API 1986b). In rats, dermal exposure to 50 mg/kg-bw per day, 5 days per week for 90 days affected hematology (lower red blood cell counts, hemoglobin, hematocrit, activated partial thromboplastin time, white blood cell counts, lymphocytes, eosinophils, platelet counts and higher red cell distribution widths and hemoglobin distribution widths), clinical chemistry (higher cholesterol, sorbitol dehydrogenase, blood urea nitrogen, alanine aminotransferase and triglycerides levels), and organ weight tests (weight changes in spleen, liver, thymus, pituitary, heart, and thyroid/parathyroid) (WIL Research 2012a).

Dermal exposure to 30 mg/kg-bw of CAS RN 64742-04-7 in SD rats for 5 days per week for 13 weeks showed dose-dependency for both an increase in liver weights and a decrease in thymus weights. Altered serum chemistry parameters and adverse effects on the skin were noted. Other changes included histopathologic changes in adrenals, bone marrow, kidneys, liver, lymph nodes, skin, stomach, and thymus.

A LOAEL of 150 mg/kg bw per day was identified for developmental toxicity in rats on the basis of lower mean fetal weights, increased post-implantation loss (primarily early resorptions) and a corresponding lower mean number of viable fetuses. Other effects included unossified sternebra, reduced ossification of the skull, reduced ossification of the vertebral arches, and lower incidence of ossified cervical centrum no. 1 (WIL Research 2012c).

In another developmental study, CAS RN 64742-04-7 was dermally administered to SD rats once a day on gestation days 0-19. A LOAEL of 8 mg/kg bw/day was identified for both maternal and developmental toxicity. Dams exhibited red vaginal discharge and dose-dependent reduced body weight gain. There was also a dose-dependent increase in the number of resorptions (greater than double the control group) at 30 mg/kg-bw. Other reproductive/developmental effects included increased number of dams with resorptions (at 125 and 500 mg/kg bw) and decreased viable foetuses (≥125 mg/kg bw). Foetal toxicity included decreased mean body weights (at ≥125 mg/kg). At 125 mg/kg-bw, there was a significant increase in the incidence of incompletely ossified skull bones. All treated groups showed isolated incidences of visceral malformations (Feuston et al. 1996).

These aromatic extracts also exhibit dermal carcinogenicity. Skin painting studies have used doses ranging from approximately 500 to 1600 mg/kg-bw, typically applied unoccluded two or three times per week to mice and result in approximately 10 to 100% of the animals developing skin tumours (API 1989; CITGO 1992; Doak et al. 1985; Gradiski et al. 1983; Kane et al. 1984; Sun 1978). Time to first tumour is typically 3 to 4 months. Genotoxicity results have been positive *in vivo* for chromosome aberration, but negative for epidermal DNA adduct formation and in the micronucleus assay (Booth et al. 1998; Mobil 1987; WIL Research 2012b). *In vitro* assays including cell transformation, mouse lymphoma and the Ames assay typically show positive results for genotoxicity (API 1986a; US EPA 1981; McKee and Przygoda 1987)(see Health Effects Supplement for more details, unpublished).

9.2.3 Polycyclic aromatic hydrocarbons

PAH species have a wide carcinogenic potency range. IARC (2010) recently reviewed the carcinogenicity data in experimental animals for 60 PAHs: 13 have sufficient evidence, 16 have limited evidence and 31 have inadequate evidence. Some PAHs, including B[a]P are classified as Category 1B carcinogens (‘may cause cancer’) by the European Commission (EU 2008, 2009; UN 2013). PAH species that have sufficient toxicological information can be ranked according to toxicological potency relative to B[*a*]P.

The Government of Canada previously completed a human health risk assessment of certain PAHs, including B[a]P, under the Priority Substances List Program. Based primarily on the results of carcinogenicity bioassays in animal models, five PAHs were considered “probably carcinogenic to humans”, i.e., substances for which there is believed to be some chance of adverse effects at any level of exposure (Environment Canada, Health Canada 1994). PAHs were added to the List of Toxic Substances in Schedule 1 of CEPA.

9.3 Characterization of Risk to Human Health

DAEss were identified as priorities for action during categorization of the Domestic Substances List, as they were determined to present the greatest potential or intermediate potential for exposure of individuals in Canada and were considered to present a high hazard to human health. A critical health effect for the initial categorization of DAEs was carcinogenicity, as determined on the basis of classifications by international agencies (IARC 1984).

Exposure to PAHs is generally recognized to be associated with risk to human health for repeated exposures that occur over the long-term (i.e., a carcinogenic risk). Short-term exposures to PAHs are typically required to be higher than carcinogenic doses to elicit non-carcinogenic adverse effects (Environment Canada, Health Canada 1994). High exposures to PAHs from these DAEs are not expected over the short-term or long-term.

9.3.1 Production and storage of aromatic extracts at refineries and transportation

The industry-restricted use pattern of aromatic extracts at Canadian refineries limits the potential for widespread exposure of the general population. However, exposure may occur for those living in the vicinity of such facilities. Given that aromatic extracts have low vapour pressure, general population exposure in the vicinity of these facilities is expected to be low. This is supported by the low exposures that were identified by modelling dispersions of fugitive emissions in the vicinity of refineries for other low volatility petroleum streams, including heavy fuel oils (Environment Canada, Health Canada 2011, 2013, 2014).

Fugitive emissions associated with transportation of aromatic extracts are likewise limited because of their low vapour pressure. Approximately 3 kg of combined yearly losses to air was estimated on the basis of yearly reporting volumes for the total masses in commerce for both modes of transportation. These fugitive emissions occur continuously during transportation and from a moving source (a line source) and, therefore, would be released over many kilometres, thus further diluting the concentration in air. Transient bystander exposure at any given location is therefore expected to be low.

The production, storage and transportation of aromatic extracts is not considered to constitute a risk to human health.

9.3.2 Marketplace products containing DAEs identified by CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6

Neither an MSDS search nor reporting by industry under section 71 indicated the use of the DAEs identified by CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6 in marketplace product formulations in Canada. These substances may be found in industrial or professional grade products, but such products are not available to the general population. Therefore, exposure of the general population is not expected.

9.3.3 Marketplace products containing DAE-based extender oils

Given the wide use of extender oils in producing rubber and plastic consumer products, there is the potential that high PAH oils, including these DAEs, could be used in product formulations. Test results from consumer products in Canada mirror those of the much larger subset of products tested in Europe. The results indicate that DAEs are not likely to be formulated in commonly available soft rubber and plastic consumer products found in the Canadian marketplace (Health Canada 2014). Therefore, marketplace products in Canada are not expected to contain DAEs, and exposure of the general population is not expected.

9.3.4 Rubber playground and athletic surfaces

Multiple studies have shown no or low detection of PAHs derived from crumb rubber or rubber surfaces. Extraction studies designed to assess potential exposure via the oral and dermal routes of exposure did not detect PAHs. Air monitoring studies have shown volatilized PAHs in the range of, or slightly above, ambient air background levels. There is thus expected to be limited, if any, exposure of the general population to these DAEs from crumb rubber-containing rubber surfaces. Therefore, risk to human health is considered to be low.

The European Commission has legislated in the form of directive (2005/69/EC) limits for PAHs in the production of tires effective January 2010, thus banning the use of highly aromatic oils in tire formulation (European Union 2005). Information provided by Canadian tire manufacturers confirmed that domestic companies have switched to producing tires with low PAH oils in accordance with the European PAH regulatory limits. This appears to follow a global trend moving away from the use of higher PAH oils in tire production, and results of these changes should include lower PAH levels in tires, in crumb rubber and in crumb rubber-containing rubber surfaces. Any limited exposure to these DAEs that may be currently encountered by the general population of Canada from rubber surfaces is therefore expected to be reduced in the future.

9.4 Uncertainties in Evaluation of Human Health Risk

A primary assumption is made in this assessment that PAHs that volatilize from rubber surfaces originate from these DAEs. It is acknowledged that other ingredients in tires, such as carbon black, may be a contributing source of PAHs.

10. Conclusion

Considering all available evidence presented in this screening assessment, there is low risk of harm to organisms and the broader integrity of the environment from these substances. It is concluded that the three DAEs (CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6 do not meet the criteria under paragraphs 64(*a*) or (*b*) of CEPA, 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.

Exposure of the general population to DAEs is not expected from consumer products in Canada, and exposure from crumb rubber-containing surfaces is expected to be low. Inhalation exposures to fugitive emissions of DAEs are expected to be low in the vicinity of refineries and during the transportation of these substances. Therefore, risk to human health from general population exposure to DAEs is considered to be low.

On the basis of the information presented in this screening assessment, it is concluded that the DAEs (CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6) do not meet the criteria under paragraph 64(*c*) of CEPA 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 concluded that the DAEs identified by CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6 do not meet any of the criteria set out in section 64 of CEPA.

References

[API] American Petroleum Institute. 1986a. Acute oral toxicity study in rats. Acute dermal toxicity study in rabbits, Primary dermal irritation study in rabbits. Primary eye irritation study in rabbits. Dermal sensitization study in guinea pigs. API 83-16, light paraffinic distillate solvent extract, CAS No. 64742-05-8. Washington (DC): American Petroleum Institute [API] American Petroleum Institute. 1986b. 28-day dermal toxicity study in the rabbit. API 83-16, light paraffinic distillate solvent extract, CAS No 64742-05-8. Report No.: 33-31695. Washington (DC): American Petroleum Institute.

[API] American Petroleum Institute. 1989. Twenty-four month dermal carcinogenesis/chronic toxicity screening bioassay of refinery streams in C3H/HeJ mice. Report No.: 36-33220, AP-190R, Final Report-OTS00004269, Washington (DC): American Petroleum Institute.

[API] American Petroleum Institute. 2003. High production volume chemical challenge program test plan: aromatic extracts category. Washington (DC): American Petroleum Institute. 24 p. Submitted to the US EPA by the Petroleum HPV Testing Group. http://www.petroleumhpv.org/.

[API] American Petroleum Institute. 2008. High production volume chemical challenge program revised test plan: aromatic extracts category. Washington (DC): American Petroleum Institute. Submitted to the US EPA by the Petroleum HPV Testing Group.

[API] American Petroleum Institute. 2012a. Robust summary of information on aromatic extracts. Washington (DC): American Petroleum Institute. 118 p. http://www.petroleumhpv.org/.

[API] American Petroleum Institute. 2012b. High production volume chemical challenge program: aromatic extracts category analysis and hazard characterization. Washington (DC): American Petroleum Institute. 73 p. Submitted to the US EPA by the Petroleum HPV Testing Group. http://www.petroleumhpv.org/.

[API] American Petroleum Institute. 2013. Response to EPA's hazard characterization of the aromatic extracts category. Washington (DC): American Petroleum Institute. 10 p. Submitted to the US EPA by the Petroleum HPV Testing Group. http://www.petroleumhpv.org/petroleum-substances-and-categories/aromatic-extracts.

Arnot JA, Gobas FA. 2003. A generic QSAR for assessing the bioaccumulation potential of organic chemicals in aquatic food webs. QSAR Comb Sci. 22(3):337-345.

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

[BfR] Federal Institute for Risk Assessment. 2010. Carcinogenic polycyclic aromatic hydrocarbons (PAHs_ in consumer products to be regulated by the EU – risk assessment by BfR in the context of a restriction proposal under REACH. BfR Opinion Nr. 032/2010. Berlin (DE): BfR.

Birkholz DA, Belton KL, Guidotti TL. 2003. Toxicological evaluation for the hazard assessment of tire crumb for use in public playgrounds. J Air Waste Manag Assoc. 53(7):903-907.

Blok J. 2005. Environmental exposure of road borders to zinc. Sci Total Environ. 348(1-3):173-190.

Booth ED, Brandt HC, Loose RW, Watson WP. 1998. Correlation of 32P-postlabelling-detection of DNA adducts in mouse skin in vivo with the polycyclic aromatic compound content and mutagenicity in *Salmonella typhimurium* of a range of oil products. Arch Toxicol. 72(8):505-513.

BP Oil Europe. 1994a. The acute toxicity of PSG 1860 to rainbow trout (*Oncorhynchus mykiss*). Derby (UK): Safepharm Laboratories Limited. Project No.: 692/11. [cited in CONCAWE 2013].

BP Oil Europe. 1994b. The acute toxicity of PSG 1860 to *Daphnia magna*. Derby (UK): Safepharm Laboratories Limited. Project No.: 692/10. [cited in CONCAWE 2013].

BP Oil Europe. 1995. Assessment of the effect of PSG 1860 on the reproduction of *Daphnia magna*. Derby (UK): Safepharm Laboratories Limited. Project No.: 692/12. [cited in CONCAWE 2013].

Canada. 1999. *Canadian Environmental Protection Act, 1999*. S.C., 1999, c. 33. Act current to 2012-10-02 and last amended on 2012-09-20. http://laws-lois.justice.gc.ca/eng/acts/C-15.31/index.html.

Canada. 2008. *Canadian Environmental Protection Act, 1999: Notice with respect to certain high priority petroleum substances*.

Canada Gazette, Part 1, vol. 142, no. 10. http://gazette.gc.ca/rp-pr/p1/2008/2008-03-08/pdf/g1-14210.pdf.

Canada. 2012. *Fisheries Act: Petroleum Refinery Liquid Effluent Regulations*. C.R.C., c. 828. [accessed 2015 Jul 15]. http://laws-lois.justice.gc.ca/eng/regulations/C.R.C.%2C_c._828/.

[CCME]. Canadian Council of Ministers of Environment. 2008. Canada-wide standard for petroleum hydrocarbons (PHC) in soil: user guidance. Winnipeg (MB): Canadian Council of Ministers of Environment. Report number PN-1398. [accessed 2010]. http://www.ccme.ca/en/resources/contaminated_site_management/phc_cws_in_soil.html.

[CDAT] Chemical Data Access Tool [database]. 2012. Chemical data reporting for CAS RNs 64742-04-7, 64742-05-8 and 64742-11-6 records. Washington (DC): US Environmental Protection Agency. [updated 2013 Jul 18; accessed 2014 Jun 14]. http://www.epa.gov/oppt/cdr/.

Cermak JH, Stephenson GL, Birkholz D, Wang Z, Dixon DG. 2010. Toxicity of petroleum hydrocarbon distillates to soil organisms. Environ Toxicol Chem. 29(12):2685-2694.

[Cheminfo] Cheminfo Services Inc. 2012. Tire manufacturing and tire retreading sector study: sector overview and profile along with responses to questionnaire. Confidential unpublished report. Gatineau (QC): Environment Canada, Chemical Production Division, Chemical Sectors Directorate, Environmental Stewardship Branch. March 2012.

Cheng H, Hu Y, Reinhard M. 2014. Environmental and health impacts of artificial turf: a review. Environ Sci Technol. 48:2114-2129.

[CITGO] Citgo Petroleum Corporation. 1992. Initial Submission: Letter from CITGO Petro Corp to US EPA regarding studies with petroleum products with attachments and cover letter dated 042792. Citgo Petroleum Corporation (TX): US EPA EPA/OTS; Doc #88-92008775. NTIS/OTS0546325.

[CONCAWE] CONservation of Clean Air and Water in Europe. 1992. Aromatic Extracts. Brussels (BE): CONCAWE Petroleum Products and Health Management Group. 28 p. Report No.: 92/01.

[CONCAWE] Conservation of Clean Air and Water in Europe. 2010. CONCAWE compilation of selected physical-chemical properties of petroleum substances and sulfur. Brussels (BE): CONCAWE Report No.: 6/10.

[CONCAWE] Conservation of Clean Air and Water in Europe.2013. Acute and chronic toxicity of DAEs: Summary of relevant test data. Brussels (BE): CONCAWE Ecology Group. 111 p. Report No.: 6/13.

[CWWA] Canadian Water and Wastewater Association. 2001. National survey of wastewater treatment plants. Gatineau (QC): Environment Canada, National Pollutant Release Inventory.

[Danish EPA] Danish Ministry of the Environment. 2011. PAHs in toys and childcare products. Copenhagen (DE): Danish EPA.

Danish List of Undesirable Substances 2004. Appendix G - Substances on the LOUS 2004. Danish Ministry of Environment. Copenhagen (DE): Danish Ministry of the Environment. http://www2.mst.dk/common/Udgivramme/Frame.asp?http://www2.mst.dk/udgiv/publications/2004/87-7614-477-1/html/bil07_eng.htm.

Doak SM, Hend RW, van der Wiel A, Hunt PF. 1985. Carcinogenic potential of hydrotreated petroleum aromatic extracts. Br J Ind Med. 42(6):380-388.

[ECB] European Chemicals Bureau. 2003. Technical guidance document on risk assessment, Part II, in support of Commission Directive 93/67/EEC on risk assessment for new notified substances and Commission Regulation (EC) Ispra (IT): European Chemicals Bureau. Report No. 1488/94 on risk assessment for existing substances.

[ECHA] European Chemicals Agency. 2012. CMR substances from Annex VI of the CPL Regulation registered under REACH and/or notified under CLP. Helsinki (Fl): ECHA.

[ECHA] European Chemicals Agency. c2007- 2014. Registered Substances database. Search results for CAS RNs [64742-04-7, 64742-05-8, 64742-11-6]. Helsinki (FI): ECHA. [updated on 2014 April 17; accessed 2014 Jun 4]. http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances.

[EMBSI] Exxon Mobill Biomedical Sciences Inc (Annadale, New Jersey). 2009. CONCAWE product compositional characterization – distillate aromatic extracts and treated distillate aromatic extracts. MRD-09-470, MRD-08-346, MRD-08-347, MRD-09-420, MRD-08-390, MRD-08-375. Brussels (BE): Conservation of Clean Air and Water in Europe (CONCAWE). Report No.: 09TP 19. CONCAWE sponsored project. [restricted access].

[EMBSI] Exxon Mobill Biomedical Sciences Inc (Annadale, New Jersey). 2012a. *Daphnia sp.*, acute immobilization test. Test substances: MRD-08-346, MRD-08-347, MRD-08-375. Brussels (BE): Conservation of Clean Air and Water in Europe (CONCAWE). Report No.: 12TP11. Study No.: 0834642. CONCAWE sponsored project. [restricted access].

[EMBSI] Exxon Mobill Biomedical Sciences Inc (Annadale, New Jersey). 2012b. Alga, growth inhibition test. Test substances: MRD-08-346, MRD-08-347, MRD-08-375. Brussels (BE): Conservation of Clean Air and Water in Europe (CONCAWE). Report No.: 2010TP 17. Study No.: 0834667. CONCAWE sponsored project. [restricted access].

[EMBSI] Exxon Mobill Biomedical Sciences Inc (Annadale, New Jersey). 2012c. *Daphnia sp.*, acute immobilization test. Test substance: MRD-08-346. Report No.: 10TP5. Final Report. Brussels (BE): Conservation of Clean Air and Water in Europe (CONCAWE). Study No.: 0834642A. CONCAWE sponsored project. [restricted access].

[EMBSI] Exxon Mobill Biomedical Sciences Inc (Annadale, New Jersey. 2012d. Alga, growth inhibition test. Test substance MRD-08-346. Brussels (BE): Conservation of Clean Air and Water in Europe (CONCAWE). Report No.: 10TP4. Study No.: 0834667A. CONCAWE sponsored project. [restricted access].

Environment Canada, Health Canada. 1994. *Canadian Environmental Protection Act*: Priority Substances List assessment report: polycyclic aromatic hydrocarbons. Ottawa (ON): Environment Canada; Health Canada. Report No.: C94-980182-8.

[ECCC, HC] Environment and Climate Change Canada, Health Canada. [modified 2007 Apr 20]. Categorization. Ottawa (ON): Government of Canada. [accessed 2015 Jul 02]. http://www.chemicalsubstanceschimiques.gc.ca/approach-approche/categor-eng.php.

Environment Canada, Health Canada. 2011. Screening assessment: Petroleum Sector Stream Approach: Heavy Fuel Oils [Site-Restricted]. Ottawa (ON): Environment Canada, Health Canada. http://www.chemicalsubstanceschimiques.gc.ca/petrole/group-1/index-eng.php.

Environment Canada, Health Canada. 2013. Screening assessment: Petroleum Sector Stream Approach: Heavy Fuel Oils [Industry-Restricted]. Ottawa (ON): Environment Canada, Health Canada. http://www.chemicalsubstanceschimiques.gc.ca/petrole/group-2/index-eng.php.

Environment Canada, Health Canada. 2014. Screening assessment: Petroleum Sector Stream Approach: Fuel Oil No. 4, Fuel Oil No. 6 and Residual Fuel Oil [Fuels]. Ottawa (ON): Environment Canada, Health Canada.

Environment Canada. 1974. Petroleum refinery effluent regulations and guidelines. Gatineau (QC): Environment Canada, Water Pollution Control Directorate. 29 pages. Report EPS 1-WP-74-1.

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

Environment Canada. 2011. *Canadian Environmental Protection Act, 1999,* section 71: *Notice with respect to certain high priority petroleum substances on the Domestic Substances List.* Canada Gazette, Part I, Vol. 145, no. 51, pp. 3740-3762. http://gazette.gc.ca/rp-pr/p1/2011/2011-12-17/html/notice-avis-eng.html#d101.

Environment Canada. 2012. Data collected under the *Canadian Environmental Protection Act, 1999,* section 71: *Notice with respect to certain high priority petroleum substances on the Domestic Substances List*. Data prepared by: Environment Canada and Health Canada, Existing Substances Program.

Environment Canada. 2014. Technical document on the persistence and bioaccumulation potential of petroleum hydrocarbons. Gatineau (QC): Environment Canada, Ecological Assessment Division.

Environment Canada. 2015. Supporting documentation: ecological exposure analysis of aromatic extracts. Gatineau (QC): Environment Canada. Information in support of the Screening Assessment of Petroleum Sector Stream Approach: Aromatic Extracts (Stream 4).

[EPI Suite] Estimation Program Interface Suite for Microsoft Windows [estimation model]. c2000-2010. Version 4.10. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

[EU] European Union. 2003. Opinion of the scientific committee on toxicity, ecotoxicity and the environment (CSTEE) on questions to the CSTEE relating to scientific evidence of risk to health and the environment from polycyclic aromatic hydrocarbons in extender oils and tyres. Adopted by the CSTEE during the 40th plenary meeting, November 12-13, 2003. . Brussels (BE): European Commission.

[EU] European Union. 2005. Commission Directive 2005/69/EC of the European Parliament and of the Council of 18 January 2006 amending, for the 29th time, Council Directive 76/769/EEC on the approximation of the laws, regulations and administrative provisions of the Member States relating to restrictions on the marketing and use of certain dangerous substances and preparations (substances classified as carcinogenic, mutagenic or toxic to reproduction. Official Journal of the European Union. Brussels (BE): European Commission. L323/51. http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2005:323:0051:0054:EN:PDF.

[EU] European Union. 2008. Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006. Official Journal of the European Union. Brussels (BE). December 12, 2008. http://eur-lex.europa.eu/legal-content/en/TXT/?uri=CELEX%3A32008R1272.

[EU] European Union. 2009. Commission Regulation (EU) No. 790/2009. Official Journal of the European Union. Brussels (BE). L 235, Vol. 52, September 5, 2009. http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2009:235:FULL:EN:PDF

[EU] European Union. 2013. Commission Regulation (EU) No. 1272/2013. Official Journal of the European Union. Brussels (BE). L328, Vol. 69, December 6, 2013. http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:328:0069:0071:EN:PDF

[FDRL] Food and Drug Research Laboratories Inc. 1974a. Acute oral toxicity study in rats. Waverly (NY): Food and Drug Research Laboratories. Study 11514-74. [cited in API 2003].

[FDRL] Food and Drug Research Laboratories. 1974b. Acute dermal toxicity study in rabbits. Waverly (NY): Food and Drug Research Laboratories. Report No.: 11513-74.

[FDRL] Food and Drug Research Laboratories. 1974c. Primary skin irritation study. Waverly (NY): Food and Drug Research Laboratories. Report No.: 11512-74. [FDRL] Food and Drug Research Laboratories. 1974d. Eye irritation test in rabbits. Waverly (NY): Food and Drug Research Laboratories. Report No.: 11511-74.

Feuston MH, Low LK, Mackerer CR. 1994. Correlation of system and developmental toxicities with chemical component classes of refinery streams. Fundam Appl Toxicol. 22:622-630.

Feuston MH, Hamilton CE, Mackerer CR. 1996. Systemic and developmental toxicity of dermally applied distillate aromatic extract in rats. Fundam Appl Toxicol. 30(2):276-284.

Gradiski D, Vinot J, Zissu D, Limasset JC, Lafontaine M. 1983. The carcinogenic effect of a series of petroleum-derived oils on the skin of mice. Environ Res. 32(2):258-268.

Health Canada. 2014. Determination of Polycyclic Aromatic Hydrocarbons (PAH): CMP Survey 2014-2015. Ottawa (ON): Consumer Product Safety Directorate, Product Safety Lab. Project No.: 2014-2052. Confidential Internal Report.

Hopkinson R. 2008. Priority substances under Environment Canada’s Chemical Management Plan for the petroleum sector. Final report. Victoria (BC): Levelton Consultants Ltd. File: 408-0115.

Household Products Database [database]. 1993- . Bethesda (MD): US National Library of Medicine. [updated 2013 Dec; accessed 2014 June]. http://householdproducts.nlm.nih.gov/.
[HPVIS] High Production Volume Information System [database]. 2014. Washington (DC): US Environmental Protection Agency. [updated 2013 Oct 1; accessed 2014 Jul 8] https://iaspub.epa.gov/oppthpv/public_search.html_page.

[IARC] International Agency for Research on Cancer. 1984. Mineral Oils (lubricant base oils and derived products). IARC Monogr Eval Carcinog Risks Hum. 33:87-171.

[IARC] International Agency for Research on Cancer. 2010. Some non-heterocyclic polycyclic aromatic hydrocarbons and some related exposures. IARC Monogr Eval Carcinog Risks Hum. 92:1-819.

[IUCLID] International Uniform Chemical Information Database. 2000a. IUCLID Dataset for Substance ID: 64742-04-7 (Extracts (petroleum), heavy paraffinic distillate solvent). European Commission, European Chemicals Bureau.

[IUCLID] International Uniform Chemical Information Database. 2000b. IUCLID Dataset for Substance ID: 64742-05-8 (Extracts (petroleum), light paraffinic distillate solvent). European Commission, European Chemicals Bureau.

[IUCLID] International Uniform Chemical Information Database. 2000c. IUCLID Dataset for Substance ID: 64742-11-6 (Extracts (petroleum), heavy naphthenic distillate solvent). European Commission, European Chemicals Bureau.

Kane ML, Ladov EN, Holdsworth CE, Weaver NK. 1984. Toxicological characteristics of refinery streams used to manufacture lubricating oils. Am J Ind Med. 5:183-200.

Kim HH, Lim YW, Kim SD, Yeo IY, Shin DC, Yang JY. 2012. Health risk assessment for artificial turf playgrounds in school athletic facilities: multi-route exposure estimation for use patterns. Asian J Atmos Environ. 6(3):206-221.

McKee RH, Przygoda RT. 1987. The genotoxic and carcinogenic potential of engine oils and refined lubricating oils. Environ Mutagen. 9(Suppl. 8):72. [cited in IUCLID 2000a].

Menichini E, Abate V, DeLuca S, di Domenico A, Fochi I, Forte G, Iacovella N, Iamiceli AL, Izzo P. 2011. Artificial-turf playing fields: contents of metals, PAHS, PCBs, PCDDs and PCDFs, inhalation exposure to PAHs and related preliminary risk assessment. Sci Total Environ. 409:4950-4957.

[Mobil] Mobil Corporation. 1987. Micronucleus assay of bone marrow red blood cells from rats treated for thirteen weeks 318 isthmus furfural extract. Irving (TX): Mobil Environmental Health and Safety Department. Mobil Study 67138. pg. 47-48/73.

[MSDS] Material Safety Data Sheet. 2005. Coherex. Bakersfield (CA): Tricor Refining, LLC. File number: 1900. [accessed 2015 Jul 15].

Muijs B and Jonker MTO. 2010. A closer look at bioaccumulation of petroleum hydrocarbon mixtures in aquatic worms. Environ Toxicol Chem. 29(9):1943-1949.

[OECD] Organisation for Economic Co-operation and Development. 2004. The 2004 OECD List of high production volume chemicals. Paris (FR): OECD- Environment Directorate. http://www.oecd.org/chemicalsafety/risk-assessment/33883530.pdf.

[OEHHA] Office of Environmental Health Hazard Assessment. 2007. Evaluation of health effects of recycled tires in playground and track products. Sacramento (CA): State of California.

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

Pavilonis BT, Weisel CP, Buckley B, Lioy PJ. 2014. Bioaccessibility and risk of exposure to metals and SVOCs in artificial turf field fill materials and fibers. Risk Anal. 34(1):44-55.

PetroTox [estimation model]. 2012. Version 3.06. Brussels (BE): Conservation of Clean Air and Water in Europe (CONCAWE).
https://www.concawe.eu/reach/petrotox/.

Potter T, Simmons K. 1998. TPH Working Group Series. Vol. 2., Composition of petroleum mixtures. Association for Environmental Health and Sciences Foundation. Amherst (MA): Amherst Scientific Publishers. 109 p. www.aehsfoundation.org/publications.aspx.

Safepharm Laboratories Ltd. 1994a. PSG 1854. Algal inhibition test. Project Number 599/30. [cited in IUCLID 2000b].

Safepharm Laboratories Ltd. 1994b. PSG 1854. Algal inhibition test. Project Number 599/29. [cited in IUCLID 2000b].

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

Shell Research Limited. 1994. An assessment of "Ready biodegradability". The Hague (NL): Shell Research Limited. Report No.: SBER.93.012, SBGR.85.052 [cited in API 2012a].

Schiliro T, Traversi D, Degan R, Pignata C, Alessandria L, Scozia D, Bono R, Gilli, G. 2013. Artificial turf football fields: Environmental and mutagenicity assessment. Arch Environ Contam Toxicol. 64:1-11.

Simpson B J. 2005. Analysis of petroleum hydrocarbon streams on the Health Canada CEPA/DSL Draft Maximal List. Report to the Canadian Petroleum Products Institute. Calgary (AB): Canadian Petroleum Products Institute.

Statistics Canada 2011. Population, urban and rural, by province and territory (Canada). 2011 Census. Ottawa (ON): Statistics Canada. http://www.statcan.gc.ca/tables-tableaux/sum-som/l01/cst01/demo62a-eng.htm.

[Sun] Sun Petroleum Products Co. 1978. Letter from Sun Petroleum Products Company to USEPA submitting enclosed information on the mouse skin painting testing results with attachments. Atlanta (GA): Sun Petroleum Products Co. Report Number: OTS0200438 or 8EHQ-0578-0140.

[UBA] Umwelt Bundes Amt. (German Federal Environment Agency). 2016. Polycyclic aromatic hydrocarbons: harmful to the Environment! Toxic! Inevitable? Dessau (GR): UBA.
https://www.umweltbundesamt.de/sites/default/files/medien/376/publikationen/polycyclic_aromatic_hydrocarbons_web.pdf.

[UK] United Kingdom. 1996. Statutory Instrument 1996 No. 2635. The Dangerous Substances and Preparations (Safety) (Consolidation) (Amendment) Regulations 1996 - Regulation 2(g) SCHEDULE 2 Regulations 6A, 6B and 6C. http://www.opsi.gov.uk/si/si1996/Uksi_19962635_en_2.htm.

[UN] United Nations. 2013. Globally harmonized system of classification and labelling of chemicals. ST/SG/AC.10/30/Rev.5 New York (US): United Nations.

[US EPA] Environmental Protection Agency. 1981. Letter from Gulf Oil to USEPA regarding information on the mutation assay and in vitro cell transformation testing conducted at EG&G Mason Laboratories. EPA/OTS; Doc #88-8100177. NTIS/OTS0204916. Framingham (MA): Gulf Oil.

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

[US EPA] United States Environmental Protection Agency. 2012. Screening-level hazard characterization of high production volume chemicals. Aromatic extracts. Washington (DC): US EPA. 38pp. http://www.petroleumhpv.org/petroleum-substances-and-categories/~/media/PetroleumHPV/Documents/2012_mar_Aromatic_Extracts_epa_screeninglevel_hazard_characterization.ashx.

WIL Research. 2012a. A 90-day repeat-dose dermal toxicity study in conjunction with a micronucleus assay utilizing extract, light paraffinic distillate solvent in Sprague Dawley rats. Ashland (OH): WIL Research. Consortium Registration #1100997, pp 56-59/118. #WIL-402022.

WIL Research. 2012b. A 90-day repeat-dose dermal toxicity study in conjunction with a micronucleus assay utilizing extract, light paraffinic distillate solvent in Sprague Dawley rats. Ashland (OH): WIL Research. Consortium Registration #1100997, pp 56-59/118. #WIL-402022.

WIL Research. 2012c. A dermal prenatal developmental toxicity study of extract, light paraffinic distillate solvent in rats. Ashland (OH): WIL Research, Consortium Registration #1100997, pp 109-113/118. #WIL-402015.

ZEK. 2010. Testing and validation of polycyclic aromatic hydrocarbons (PAH) in the course of GS-Mark certification. ZEK01.4-08. Munich (DE): ZEK. http://www.zls-muenchen.de/de/left/aktuell/pdf/zek_01_4_08_pak_verbindlich_engl_30112011.pdf.

Zhang J, Han IK, Zhang L, Crain W. 2008. Hazardous chemicals in synthetic turf materials and their bioaccessibility in digestive fluids. J Expo Sci Environ Epidemiol. 18(6):600-607.

Appendices

Appendix A. Petroleum substance groupings

Table A.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 to C_5	Propane
Low boiling point naphthas	Complex combinations of hydrocarbons primarily from C_4 to C_{12}	Gasoline
Gas oils	Complex combinations of hydrocarbons primarily from C_9 to C_{25}	Diesel fuel
Heavy fuel oils	Complex combinations of heavy hydrocarbons primarily from C_{11} to C_{50}	Fuel Oil No. 6
Base oils	Complex combinations of hydrocarbons primarily from C_{15} to C_{50}	Lubricating oils
Aromatic extracts	Complex combinations of primarily aromatic hydrocarbons from C_{15} to C_{50}	Feedstock for benzene production
Waxes, slack waxes and petrolatum	Complex combinations of primarily aliphatic hydrocarbons from C_{12} to C_{85}	Petrolatum
Bitumen or vacuum residues	Complex combinations of heavy hydrocarbons having carbon numbers greater than C_{25}	Asphalt

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

Appendix B. Substance identity

Table B.1. Substance identity of DAEs

CAS RN	64742-05-8	64742-04-7	64742-11-6
National Chemical Inventories[a]	Extracts (petroleum), light paraffinic distillate solvent (TSCA, DSL, EINECS, PICCS, ASIA-PAC)	Extracts (petroleum), heavy paraffinic distillate solvent (TSCA, DSL, EINECS, ECL, PICCS, ASIA-PAC, NZIoC)	Extracts (petroleum), heavy naphthenic distillate solvent (TSCA, DSL, EINECS, ECL, PICCS, ASIA-PAC, NZIoC)
Chemical group (DSL Stream)	Distillate aromatic extracts	Distillate aromatic extracts	Distillate aromatic extracts
Major chemical class or use	Organic solvents	Organic solvents	Organic solvents
Major chemical sub-class [b]	Mixtures of alkanes, cycloalkanes, and aromatic compounds	Mixtures of alkanes, cycloalkanes, and aromatic compounds	Mixtures of alkanes, cycloalkanes, and aromatic compounds
Carbon number range	$C_{15} – C_{30}$	$C_{20} – C_{50}$	$C_{20} – C_{50}$
Approximate ratio of aromatics to non-aromatics[c]	65:35 to 85:15	65:35 to 85:15	65:35 to 85:15

[a] DSL (Canada Domestic Substances List); EINECS (European Inventory of Existing Commercial Chemical Substances); TSCA (*Toxic Substances Control Act*); PICCS (Philippine Inventory of Chemicals and Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); ECL (Korean Existing Chemicals List); ASIA-PAC (Collection of inventories/lists from countries in the Asia Pacific region).

[b] These substances are UVCBs (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products, or **B**iological Materials); i.e., they are not discrete chemicals and thus may be characterized by a variety of structures.

[c] CONCAWE 1992.

n.d.: No data.

Appendix C. Physical-chemical properties

Table C.1. Representative structures that would be included for all CAS RNs

n-Alkanes

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{15}	271	Yes		
C_{20}	343	Yes	Yes	Yes
C_{30}	450	Yes	Yes	Yes
C_{50}	548		Yes	Yes

Isoalkanes

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{15}	250	Yes		
C_{20}	326	Yes	Yes	Yes
C_{30}	350	Yes	Yes	Yes
C_{50}	676		Yes	Yes

One-ring cycloalkanes

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{15}	282	Yes		
C_{20}	360	Yes	Yes	Yes
C_{30}	421	Yes	Yes	Yes

Two-ring cycloalkanes

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{20}	339	Yes	Yes	Yes
C_{30}	420	Yes	Yes	Yes

Polycycloalkanes

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{14}	255	Yes		
C_{18}	316	Yes	Yes	Yes
C_{22}	365	Yes	Yes	Yes

One-ring aromatics

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{15}	281	Yes		
C_{20}	359	Yes	Yes	Yes
C_{30}	437	Yes	Yes	Yes

Cycloalkane monoaromatics

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{15}	285	Yes		
C_{20}	351	Yes	Yes	Yes

Two-ring aromatics

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{15}	308	Yes		
C_{20}	373	Yes	Yes	Yes
C_{30}	469	Yes	Yes	Yes

Cycloalkane diaromatics

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{15}	321	Yes		
C_{20}	374	Yes	Yes	Yes

Three-ring aromatics

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{15}	350	Yes		
C_{20}	398	Yes	Yes	Yes
C_{30}	493	Yes	Yes	Yes

Four-ring aromatics

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{16}	384	Yes		
C_{20}	480	Yes	Yes	Yes

Five-ring aromatics

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{20}	495	Yes	Yes	Yes
C_{30}	545		Yes	Yes

Six-ring aromatics

Carbon number	Boiling point (°C)	64742-05-8	64742-04-7	64742-11-6
C_{22}	>500	Yes	Yes	Yes

Table C.2. Physical and chemical properties for representative structures of aromatic extracts (experimental and modelled values, c 2000-2010)[a]

Alkanes

Chemical class, name and CAS RN	**Aromatic extract represented**	**Boiling point (°C)**	**Melting point (°C)**	**Vapour pressure (Pa)[b]**
C_{15} pentadecane (629-62-9)	64742-05-8	270.6 (expt.)	9.9 (expt.)	0.5 (expt.)
C_{20} eicosane (112-95-8)	64742-05-8 64742-04-7 64742-11-6	343.0 (expt.)	36.8 (expt.)	6.2×10^{-4} (expt.)
C_{30} triacontane	64742-05-8 64742-04-7 64742-11-6	449.7 (expt.)	65.8 (expt.)	3.6×10^{-9} (expt.)
C_{50}	64742-04-7 64742-11-6	548.0 (expt.)	87.0 (expt.)	2.0×10^{-7}

Isoalkanes

Chemical class, name and CAS RN	**Aromatic extract represented**	**Boiling point (°C)**	**Melting point (°C)**	**Vapour pressure (Pa)[b]**
C_{15} 2-methyl tetradecane (1560-95-8)	64742-05-8	250.2	1.5	5.8
C_{20} 3-methyl nonadecane (6418-45-7)	64742-05-8 64742-04-7 64742-11-6	326.3	39.5	0.09
C_{30} hexamethyl tetracosane (111-01-3)	64742-05-8 64742-04-7 64742-11-6	408.5	74.7	0.04
C_{50}	64742-04-7 64742-11-6	675.5	294.6	5.1×10^{-10}

One-ring cycloalkanes

Chemical class, name and CAS RN	**Aromatic extract represented**	**Boiling point (°C)**	**Melting point (°C)**	**Vapour pressure (Pa)[b]**

C_{15} nonylcyclohexane (2883-02-5)	64742-05-8	282 (expt.)	−10 (expt.)	0.3 (expt.)
C_{20} tetradecyl cyclohexane (1795-18-2)	64742-05-8 64742-04-7 64742-11-6	360.0 (expt.)	24.0 (expt.)	0.02
C_{30} 1,5-dimethyl-1-(3,7,11,15-tetramethyloctadecyl)	64742-05-8 64742-04-7 64742-11-6	420.9	103.2	1.5×10^{-4}

Two-ring cycloalkanes

Chemical class, name and CAS RN	**Aromatic extract represented**	**Boiling point (°C)**	**Melting point (°C)**	**Vapour pressure (Pa)[b]**
C_{15} 2-isopentadecylin	64742-05-8	257.4	12.4	4.0
C_{20} 2,4-dimethyl octyl-2-decalin	64742-05-8 64742-04-7 64742-11-6	323.9	41.0	0.1
C_{30} 2,4,6,10,14 pentamethyldodecyl-2-decalin	64742-05-8 64742-04-7 64742-11-6	420.3	105.9	1.4×10^{-4}

Polycycloalkanes

Chemical class, name and CAS RN	**Aromatic extract represented**	**Boiling point (°C)**	**Melting point (°C)**	**Vapour pressure (Pa)[b]**
C_{18} hydro-chrysene	64742-05-8	353 (expt.)		4.0×10^{-3}
C_{22} hydro-picene	64742-05-8 64742-04-7 64742-11-6	364.9	108.1	2.5×10^{-3}

One-ring aromatics

Chemical class, name and CAS RN	Aromatic extract represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]
C_{15} 2-nonyl benzene (1081-77-2)	64742-05-8	281.0 (expt.)	-24.0 (expt.)	0.7 (expt.)
C_{20} tetradecyl benzene	64742-05-8 64742-04-7 64742-11-6	359 (expt.)	16 (expt.)	3.7×10^{-3} (expt.)
C_{30} 1-benzyl 4,8,12,16 tetramethyl eicosane	64742-05-8 64742-04-7 64742-11-6	437.0	131.3	1.2×10^{-5}

Cycloalkane monoaromatics

Chemical class, name and CAS RN	Aromatic extract represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]
C_{15} methyl-octahydro-phenanthrene	64742-05-8	267.1	27.9	2.34
C_{20} ethyl-dodecahydro-chyrsene	64742-05-8 64742-04-7 64742-11-6	338.4	82	0.02

Two-ring aromatics

Chemical class, name and CAS RN	Aromatic extract represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]
C_{15} 4-isopropyl biphenyl	64742-05-8	309.0	43.7	0.1
C_{20} 2-iso-decyl naphthalene	64742-05-8 64742-04-7 64742-11-6	366.4	99.5	1.4×10^{-3}
C_{30} 2-(4,8,14,18-tetramethylhexadecyl) naphthalene	64742-05-8 64742-04-7 64742-11-6	468.5	170.6	7.1×10^{-7}

Cycloalkane diaromatics

Chemical class, name and CAS RN	Aromatic extract represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]
C_{15} ethylfluorene	64742-05-8	337.6	94.6	7.3×10^{-3}
C_{20} iso-heptylfluorene	64742-05-8 64742-04-7 64742-11-6	380.8	126.3	3.2×10^{-4}

Three-ring aromatics

Chemical class, name and CAS RN	Aromatic extract represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]
C_{15} 2-methyl phenanthrene (2531-84-2)	64742-05-8	155.0-160.0 (expt.)	57.0-59.0 (expt.)	8.9×10^{-3}
C_{20} 2-isohexyl phenanthrene	64742-05-8 64742-04-7 64742-11-6	331.3	67.26	0.04
C_{30} 2-(2,4,10-trimethyltridecyl) phenanthrene	64742-05-8 64742-04-7 64742-11-6	493.0	191.6	9.8×10^{-8}

Four-ring aromatics

Chemical class, name and CAS RN	Aromatic extract represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]
C_{16} fluoranthene	64742-05-8	348.0 (expt.)	107.8 (expt.)	1.2×10^{-3} (expt.)
C_{20} benzo[k]fluoranthene	64742-04-7 64742-11-6	480.0 (expt.)	217.0 (expt.)	1.3×10^{-7} (expt.)

Five-ring aromatics

Chemical class, name and CAS RN	Aromatic extract represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]
C_{20} benzo[a]pyrene (50-32-8)	64742-05-8 64742-04-7 64742-11-6	495.0 (expt.)	177.0 (expt.)	7.3×10^{-7}

Six-ring aromatics

Chemical class, name and CAS RN	Aromatic extract represented	Boiling point (°C)	Melting point (°C)	Vapour pressure (Pa)[b]
C_{22} benzo[ghi]perylene (191-24-2)	64742-05-8 64742-04-7 64742-11-6	>500 (expt.)	278 (expt.)	1.3×10^{-8} (expt.)

Table C.2. (cont'd) Physical and chemical properties for representative structures of aromatic extracts (experimental and modelled values, EpiSuite c2000-2010)[a]

Alkanes

Chemical class, name and CAS RN	Aromatic extract represented	Henry's law constant ($Pa*m^3$/mol)	log K_{ow}	log K_{oc}	Aqueous solubility (mg/L)[c]
C_{15} pentadecane (629-62-9)	64742-05-8	1.3×10^6 (expt.)	7.7	6.7	7.6×10^{-5} (expt.)
C_{20} eicosane (112-95-8)	64742-05-8 64742-04-7 64742-11-6	2.2×10^7	10	8.8	0.02 (expt.)
C_{30} triacontane	64742-05-8 64742-04-7 64742-11-6	6.8×10^8	15.1	13.1	$5.1\ x10^{-11}$ 8.6×10^{-11}
C_{50}	64742-04-7 64742-11-6	3.6×10^{10}	25.0	21.6	2.6×10^{-21}

Isoalkanes

Chemical class, name and CAS RN	Aromatic extract represented	Henry's law constant ($Pa*m^3$/mol)	log K_{ow}	log K_{oc}	Aqueous solubility (mg/L)[c]
C_{15} 2-methyl tetradecane (1560-95-8)	64742-05-8	4.6×10^6	7.6	6.6	3.3×10^{-3}

C_{20} 3-methyl nonadecane (6418-45-7)	64742-05-8 64742-04-7 64742-11-6	2.6×10^{7}	10.0	8.8	1.1 x10^{-5}
C_{30} hexamethyl tetracosane (111-01-3)	64742-05-8 64742-04-7 64742-11-6	2.0×10^{9}	14.6	12.7	2.0×10^{-10}
C_{50}	64742-04-7 64742-11-6	1.5×10^{10}	25	21.5	6.0×10^{-21}

One-ring cycloalkanes

Chemical class, name and CAS RN	**Aromatic extract represented**	**Henry's law constant (Pa*m^3/mol)**	**log K_{ow}**	**log K_{oc}**	**Aqueous solubility (mg/L)^c**
C_{15} nonylcyclohexane (2883-02-5)	64742-05-8	5.3×10^{5}	7.5	6.5	4.9×10^{-3}
C_{20} tetradecyl cyclohexane (1795-18-2)	64742-05-8 64742-04-7 64742-11-6	2.9×10^{6}	10.0	8.6	1.7×10^{-6}
C_{30} 1,5-dimethyl-1-(3,7,11,15-tetramethyloctadecyl)	64742-05-8 64742-04-7 64742-11-6	2.9×10^{8}	14.5	12.5	4.2×10^{-7}

Two-ring cycloalkanes

Chemical class, name and CAS RN	**Aromatic extract represented**	**Henry's law constant (Pa*m^3/mol)**	**log K_{ow}**	**log K_{oc}**	**Aqueous solubility (mg/L)^c**
C_{15} 2-isopentadecylin	64742-05-8	3.0×10^{4}	6.5	5.6	0.03
C_{20} 2,4-dimethyl octyl-2-decalin	64742-05-8 64742-04-7 64742-11-6	7.15×10^{5}	8.9	7.7	1.2×10^{-4}

C_{30} 2,4,6,10,14 pentamethyldodecyl -2-decalin	64742-05-8 64742-04-7 64742-11-6	3.9×10^{7}	13.6	11.8	1.7×10^{-9}

Polycycloalkanes

Chemical class, name and CAS RN	Aromatic extract represented	Henry's law constant (Pa*m^{3}/ mol)	log K_{ow}	log K_{oc}	Aqueous solubility (mg/L)^{c}
C_{18} hydro-chrysene	64742-05-8	$5.7\ \text{x}10^{3}$	6.2	5.4	0.01
C_{22} hydro-picene	64742-05-8 64742-04-7 64742-11-6	3.8×10^{3}	7.3	6.3	2.2×10^{-3}

One-ring aromatics

Chemical class, name and CAS RN	Aromatic extract represented	Henry's law constant (Pa*m^{3}/ mol)	log K_{ow}	log K_{oc}	Aqueous solubility (mg/L)^{c}
C_{15} 2-nonyl benzene (1081-77-2)	64742-05-8	1.0×10^{4}	7.1 (expt.)	6.2	0.03
C_{20} tetradecyl benzene	64742-05-8 64742-04-7 64742-11-6	5.7×10^{4}	9.9	8.6	5.2×10^{-5}
C_{30} 1-benzyl 4,8,12,16 tetramethyl eicosane	64742-05-8 64742-04-7 64742-11-6	3.8×10^{6}	13.5	11.8	6.8×10^{-9}

Cycloalkane monoaromatics

Chemical class, name and CAS RN	Aromatic extract represented	Henry's law constant (Pa*m^{3}/ mol)	log K_{ow}	log K_{oc}	Aqueous solubility (mg/L)^{c}
C_{15} methyl-octahydro-phenanthrene	64742-05-8	1.5×10^{4}	5.6	4.9	0.2

C_{20} ethyl-dodecahydro-chyrsene	64742-05-8 64742-04-7 64742-11-6	1.4×10^{4}	7.2	6.2	3.9×10^{-3}

Two-ring aromatics

Chemical class, name and CAS RN	**Aromatic extract represented**	**Henry's law constant (Pa*m^3/ mol)**	**log K_{ow}**	**log K_{oc}**	**Aqueous solubility (mg/L)[c]**
C_{15} 4-isopropyl biphenyl	64742-05-8	98.7	5.5 (expt.)	4.8	0.9
C_{20} 2-iso-decyl naphthalene	64742-05-8 64742-04-7 64742-11-6	1.2×10^{3}	8.1	7.0	2.4×10^{-3}
C_{30} 2-(4,8,14,18-tetramethylhexadecyl) naphthalene	64742-05-8 64742-04-7 64742-11-6	5.4×10^{4}	12.8	11.1	3.0×10^{-8}

Cycloalkane diaromatics

Chemical class, name and CAS RN	**Aromatic extract represented**	**Henry's law constant (Pa*m^3/ mol)**	**log K_{ow}**	**log K_{oc}**	**Aqueous solubility (mg/L)[c]**
C_{15} ethylfluorene	64742-05-8	5.6	5.1	4.4	0.2
C_{20} iso-heptylfluorene	64742-05-8 64742-04-7 64742-11-6	32.7	7.5	6.5	5.9×10^{-4}

Three-ring aromatics

Chemical class, name and CAS RN	**Aromatic extract represented**	**Henry's law constant (Pa*m^3/ mol)**	**log K_{ow}**	**log K_{oc}**	**Aqueous solubility (mg/L)[c]**

C_{15} 2-methyl phenanthrene (2531-84-2)	64742-05-8	2.78	5.2 (expt.) and 4.9 (expt.)	4.2	0.3 (expt.)
C_{20} 2-isohexyl phenanthrene	64742-05-8 64742-04-7 64742-11-6	9.9×10^{4}	8.0	6.9	6.9×10^{-4}
C_{30} 2-(2,4,10-trimethyltridecyl) phenanthrene	64742-05-8 64742-04-7 64742-11-6	942	12.0	10.4	1.2×10^{-8}

Four-ring aromatics

Chemical class, name and CAS RN	**Aromatic extract represented**	**Henry's law constant (Pa*m^3/mol)**	**log K_{ow}**	**log K_{oc}**	**Aqueous solubility (mg/L)[c]**
C_{16} fluoranthene	64742-05-8	0.9 (expt.)	5.2 (expt.)	4.8 (expt.)	0.3 (expt.)
C_{20} benzo[k]fluoranthene	64742-04-7 64742-11-6	0.06 (expt.)	6.1 (expt.)	5.6 (expt.)	0.0008 (expt.)

Five-ring aromatics

Chemical class, name and CAS RN	**Aromatic extract represented**	**Henry's law constant (Pa*m^3/mol)**	**log K_{ow}**	**log K_{oc}**	**Aqueous solubility (mg/L)[c]**
C_{20} benzo[a] pyrene (50-32-8)	64742-05-8 64742-04-7 64742-11-6	0.05 (expt.)	6.1 (expt.)	5.9 (expt.)	1.6×10^{-3} (expt.)

Six-ring aromatics

Chemical class, name and CAS RN	**Aromatic extract represented**	**Henry's law constant (Pa*m^3/mol)**	**log K_{ow}**	**log K_{oc}**	**Aqueous solubility (mg/L)[c]**
C_{22} benzo[ghi]perylene 191-24-2	64742-05-8 64742-04-7 64742-11-6	0.03 (expt.)	6.6 (expt.)	5.8	2.6×10^{-4} (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 because of 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] Maximum water solubility was estimated for each representative structure 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).

Appendix D. Persistence and bioaccumulation

Table D.1. An analysis of persistence data for petroleum hydrocarbons representative of DAEs based on Environment Canada (2014)

C#	**C_{15}**	**C_{16}**	**C_{17}**	**C_{18}**	**C_{20}**	**C_{22}**	**C_{25}**	**C_{30}**	**C_{50}**
n-alkane	-	n/a	-	-	-	n/a	n/a	-	-
***i*-alkane**	-	n/a	n/a	n/a	-	n/a	n/a	S,W,Sd	-
***n*-alkene**	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Diene	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Monocycloalkane	-	n/a	n/a	n/a	-	n/a	n/a	Sd	S,W,Sd
Dicycloalkane	S,W,Sd	n/a	n/a	n/a	S,W,Sd	n/a	S,W,Sd	S,W,Sd	S,W,Sd
Polycycloalkane	n/a	n/a	n/a	S,W,Sd	n/a	S,W,Sd	n/a	n/a	n/a
Monoaromatic	Sd	n/a	n/a	n/a	-	n/a	n/a	Sd	Sd
Cycloalkane monoaromatic	S,W,Sd	n/a	n/a	n/a	S,W,Sd	n/a	n/a	n/a	n/a
Diaromatic	S,W,Sd	n/a	n/a	n/a	S,W,Sd	n/a	n/a	S,W,Sd	S,W,Sd
Cycloalkane diaromatic	-	n/a	n/a	n/a	-	n/a	n/a	n/a	n/a
Three-ring PAH	-	n/a	n/a	n/a	-	n/a	n/a	S,W,Sd	S,W,Sd
Four-ring PAH	n/a	A, S,W,Sd	n/a	A, S,W,Sd	S,W,Sd	n/a	n/a	n/a	n/a
Five-ring PAH	n/a	n/a	n/a	n/a	A, S,W,Sd	n/a	n/a	S,W,Sd	n/a
Six-ring PAH	n/a	n/a	n/a	n/a	n/a	A, S,W,Sd	n/a	n/a	n/a

Abbreviations: A – Predicted half-life in air of 2 days or greater, S – Predicted half-life in soil of six months or greater, W – Predicted half-life in water of six months or greater, Sd – Predicted half-life in sediment of one year or greater, - Indicates that these structures are not considered to persist for long periods of time in air, soil, water, or sediment**,** and n/a – not-applicable; indicates that no such carbon number exists within the group or it was not modelled.

Table D.2. An analysis of experimental and modelled bioaccumulation data for petroleum hydrocarbons representative of DAEs (Environment Canada 2014)

C#	**C_{15}**	**C_{16}**	**C_{17}**	**C_{18}**	**C_{19}**	**C_{20}**	**C_{22}**	**C_{25}**
***n*-alkane**	-	-	-	-	n/a	-	n/a	n/a
***i*-alkane**	B	n/a	n/a	n/a	n/a	n/a	n/a	n/a
***n*-alkene**	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Diene	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Mono-cycloalkane	B	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Dicycloalkane	B	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Polycycloalkane	n/a	n/a	n/a	-	n/a	n/a	B	n/a
Monoaromatic	B	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Cycloalkane Monoaromatic	B	n/a	n/a	n/a	n/a	B	n/a	n/a
Diaromatic	-	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Cycloalkane Diaromatic	b	-	-	n/a	n/a	B	n/a	n/a
Three-ring PAH	-	-	-	n/a	n/a	B	n/a	n/a
Four-ring PAH	n/a	B	B	B	-	B	n/a	n/a
Five-ring PAH	n/a	n/a	n/a	n/a	n/a	B	B	n/a
Six-ring PAH	n/a	n/a	n/a	n/a	n/a	n/a	B	n/a

Abbreviations: B – Predicted highly bioaccumulative with a BCF/BAF greater than 5000, and n/a – not-applicable; indicates that no such carbon number exists within the group or it was not modelled
- Indicates that these structures are not considered highly bioaccumulative.

Appendix E. Ecotoxicological information

Table E.1. Empirical aquatic toxicity data for DAEs CAN RN 64742-04-7 and 64742-05-8

Organism	Chemical (CAS RN)	Test duration	Endpoint	Value (mg/L)	Reference
Oncorhynchus mykiss	64742-04-7	96-hour acute	NOEL	1000	BP Oil Europe 1994a
Daphnia magna	64742-04-7	48-hour acute	EL_{50} NOEL	> 1000 1000	BP Oil Europe 1994b
D. magna	64742-04-7	21-day chronic	EL_{50} (survival) EL_{50} (reproduction)	> 1000 > 1000	BP Oil Europe 1995
D. magna	64742-04-7	48-hour acute	EL_{50}	> 100	EMBSI 2012a
D. magna	64742-05-8	48-hour acute	EL_{50} (mobility)	< 100	EMBSI 2012a
D. magna	64742-05-8	48-hour acute	NOELR LOELR EL_{50} (mobility)	1.0 10.0 35.9	EMBSI 2012c
Scenedesmus subspicatus (Algae)	64742-04-7	72 hours	EL_{50} NOEC	>1000 >1000	Safepharm Laboratories 1994a; API 2012
S. capricornutum (algae)	64742-04-7	48-hour acute	EL_{50}	> 100	EMBSI 2012b
Pseudokirchnerella subcapitata (microalgae)	64742-05-8	72-hour acute	NOELR EL_{50} (growth rate inhibition)	< 100 < 100	EMBSI 2012b
P. subcapitata (microalgae)	64742-05-8	72-hour acute	NOELR LOELR EL_{50} (growth rate inhibition)	0.1 1.0 18.8	EMBSI 2012d
Pseudomonas putida (Bacteria)	64742-04-7	16 hours	EC_{10} EC_{50} LL_{10}	>1000 >1000 >1000	Safepharm Laboratories 1994b; IUCLID 2000

Abbreviations: EL_{50} – median effective loading rate, NOELR – no observed effect loading rate, LOELR – lowest observed effect loading rate.

Table E.2. Modelled toxicity data for DAE CAS RN 64742-05-8 (C_{15}–C_{50}) to aquatic organisms (PetroTox 2012)

Test species	Common name	Acute LL_{50} (mg/L)[a] 65:35 aromatic:aliphatic[b]	Acute LL_{50} (mg/L) 85:15 aromatic:aliphatic
Daphnia magna	Water flea	1.6	0.64
Oncorhynchus mykiss	Rainbow trout	0.30	0.16
Pseudokirchneriella subcapitata	Green alga	0.83	0.46
Palaemonetes pugio	Grass shrimp	0.22	0.12
Menidia beryllina	Inland silverside	>1000	>1000

[a] Median lethal loading (LL_{50}) used in place of median lethal concentration (LC_{50}) because of insolubility of petroleum products in water. It does not imply dissolved components.

[b] PetroTox input data: PetroTox v3.06, low resolution mode, one hydrocarbon block with boiling point range of 250 to 640 °C (CONCAWE 2010); 85:15 or 65:35 ratio of aromatics to aliphatics (CONCAWE 1992, API 2012b).

Table E.3. Modelled toxicity data for DAE CAS RN 64742-05-8 (C_{15}–C_{30}) to aquatic organisms (Petrotox 2012)

Test species	Common name	Acute LL_{50} (mg/L)[a] 65:35 aromatic:aliphatic[b]	Acute LL_{50} (mg/L) 85:15 aromatic:aliphatic
D. magna	Water flea	1.1	0.47
O. mykiss	Rainbow trout	0.22	0.12
P. subcapitata	Green alga	0.70	0.40
P. pugio	Grass shrimp	0.16	0.09
M. beryllina	Inland silverside	>1000	>1000

[a] Median lethal loading (LL_{50}) used in place of median lethal concentration (LC_{50}) because of insolubility of petroleum products in water. It does not imply dissolved components.

[b] PetroTox input data: PetroTox v3.06, low resolution mode, one hydrocarbon block with boiling point range of 288 to 534 ^{o}C (API 2012b), 85:15 or 65:35 ratio of aromatics to aliphatics (CONCAWE 1992, API 2012b).

Table E.4. Modelled toxicity data for DAEs CAS RN 64742-04-7 and 64742-11-6 (C_{20}–C_{50}) to aquatic organisms (Petrotox 2012)

Test species	Common name	Acute LL_{50} (mg/L)[a] 65:35 aromatic:aliphatic[b]	Acute LL_{50} (mg/L) 85:15 aromatic:aliphatic
D. magna	Water flea	2.1	0.78
O. mykiss	Rainbow trout	0.32	0.17
P. subcapitata	Green alga	1.0	0.56
P. pugio	Grass shrimp	0.22	0.12
M. beryllina	Inland silverside	>1000	>1000

[a] Median lethal loading (LL_{50}) used in place of median lethal concentration (LC_{50}) because of the insolubility of petroleum products in water. It does not imply dissolved components.

[b] PetroTox input data: PetroTox v3.06, low resolution mode, one hydrocarbon block with boiling point range of 289 to 584°C based on boiling point ranges of the two CAS RNs (API 2012b), 85:15 or 65:35 ratio of aromatics to aliphatics (CONCAWE 1992, API 2012b).

Appendix F. Ecological exposure calculations for DAEs

AF.1 Calculation for exposure via water for manufacturing of rubber and other products

Exposure to DAEs in water is expected if the substance is released from industrial activities via wastewater treatment to receiving water. The concentration of the substance in the receiving water near the discharge point can be used in evaluating the aquatic risk of the substance. It can be calculated using the equation:

$$C_{aquatic-ind} = \frac{1000 \times Q \times L \times (1 - R)}{N \times F \times D}$$

where

$C_{aquatic-ind}$: concentration in water resulting from industrial releases, mg/L
Q: total substance quantity used annually at an industrial site, kg/yr
L: loss to wastewater, fraction
R: wastewater system removal rate, fraction
N: number of annual release days, d/yr
F: wastewater system effluent flow, m^3/d
D: receiving water dilution factor, dimensionless

As DAEs are used by industrial facilities and are expected to be released to water, conservative aquatic industrial release scenarios were developed to cover a range of different potential industrial activities in Canada. For DAEs, the relevant sectors and scenarios include manufacturing of rubber and other products. Inputs used to determine exposure are summarized in Table F.1. Additional information on these scenarios as well as on inputs is available in supporting documentation (Environment Canada 2015).

Table F.1. Summary of input values used for scenarios estimating concentrations in water resulting from industrial releases of DAEs

Input	Value for rubber manufacture	Value for manufacturing of other products	Justification and reference
Annual use quantity for a small and a large user(kg/year)	1 000 000 10 000 000	1 000 000	CEPA s. 71 survey (Environment Canada 2011, 2012)
Loss to wastewater (kg/d)	3.3–33	10	Based on emission factor to wastewater (0.1% for manufacturing of rubber and 0.3% for other products) (ECB 2003) and conservative assumption of no on-site wastewater treatment
Wastewater system removal efficiency (%)	83.5	83.5	Average of removal of oil and grease (79%) and biochemical oxygen demand (88%) from municipal wastewater treatment systems (CWWA 2001)
Number of annual release days (days/year)	300	300	ECB 2003
Daily dilution volume for small and large users (million L/d)	10–10 000 100–500	30–10 000	Based on users identified in the CEPA s. 71 survey (Environment Canada 2011, 2012)

Total concentrations in water near the point of discharge, resulting from the above calculations for the rubber manufacturing scenario, vary between 5.4 × 10^{-5} and 0.054 mg/L and between 1.7 × 10^{-4} and 0.055 mg/L for the other products manufacturing scenario.

AF.2 Calculation for exposure via water for runoff from tire wear and road care products

The PEC in water for the DAEs is estimated based on the combined mass of the DAEs leaching out from tire particles as a result of tire wear and from roads repaired with DAE-containing emulsions. This combined mass is conservatively estimated based on the quantities of DAEs present in tires and road care emulsions. It then yields a conservative estimate for the PEC distribution across 300 Canadian urban areas.

Calculations used to derive the PEC are available in the supporting document (Environment Canada 2015), and the key values used for calculations are listed in Table F.2.

Table F.2. Summary of input values used for scenarios estimating concentrations in water resulting from runoff from tire wear and road washout

Input	Value	Justification and reference
Total annual car tire and light truck tire loss from tire wear (kg/year)	35,289,000	Estimated from a mass balance method (Environment Canada 2012). The calculation used market data for 2006. Parameters are available in Environment Canada 2015.
Total annual heavy truck tire loss from tire wear (kg/year)	8,536,550	Estimated from a mass balance method (Environment Canada 2012). Parameters are available in Environment Canada 2015.
Proportion of tire loss to urban roads, or proportion of road washout on urban roads (%)	81	Assumed to be equal to the proportion of Canadians living in urban areas (Statistics Canada 2011)
Fraction of tire wear particles taken by runoff and entering aquatic streams (%)	66.7	Blok 2005
Proportion of DAE-free tires (%)	>32.5[a]	Proportion derived on the basis of Cheminfo 2012 and communication with the Canadian tire industry 2014, unreferenced
Concentration of DAEs in car tire tread (wt%)	13.5	European Commission 2003
Concentration of DAEs in truck tires (wt%)	4.5	European Commission 2003
Annual quantity of DAEs used in road care emulsions (kg/year)	1,000,000	Environment Canada 2011, 2012
Proportion of DAEs in road care products entering runoff (%)	24	Watts et al. 2010
Canadian population in 2010	34,005,000	Statistics Canada 2011
Number of annual release days via urban runoff (d/year)	91	The number of days in a year for a river to have a flow at or above the 75th percentile flow ((1-75%) of 365 days/year)

[a] Proportion derived only for the purpose of creating a conservative ecological risk assessment.