Draft Screening Assessment

Poly(alkoxylates/ethers) Group

Chemical Abstracts Service Registry Numbers

9002-92-0	*61791-24-0*	*68439-45-2*
9002-93-1	*61791-26-2*	*68439-46-3*
9004-82-4	*66455-14-9*	*68439-50-9*
9036-19-5	*67762-19-0*	*68439-72-5*
25322-69-4	*68002-97-1*	*68585-34-2*
28724-32-5	*68131-39-5*	*68603-75-8*
30525-89-4	*68155-39-5*	*68951-67-7*

Environment and Climate Change Canada
Health Canada

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Synopsis

Pursuant to section 68 or 74 of the *Canadian Environmental Protection Act, 1999* (CEPA), the Minister of Environment and Climate Change and the Minister of Health have conducted a screening assessment of 21 substances referred to collectively under the Chemicals Management Plan as the Poly(alkoxylates/ethers) Group. Substances in this group [namely one poly(propylene glycol) (PPG), paraformaldehyde (PF), three alcohol ethoxylate sulfates (AESs), eight alcohol ethoxylates (AEs), two octylphenol ethoxylates (OPEs), and six alkyl amine ethoxylates (ANEOs)] were identified as priorities for assessment as they met categorization criteria under subsection 73(1) of CEPA or were considered a priority on the basis of other concerns. One substance in this group (CAS RN[1] 68155-39-5) was identified as a priority for risk assessment as part of the identification of risk assessment priorities (IRAP) approach's 2015 review.[2] Their Chemical Abstracts Service Registry Numbers (CAS RN), *Domestic Substances List* (DSL) names and subgroups are listed in the table below.

Substances in the Poly(alkoxylates/ethers) Group

CAS RN	Domestic substances list name	Subgroup [a]
25322-69-4	Poly[oxy(methyl-1,2-ethanediyl)], α-hydro-ω-hydroxy-	PPG
30525-89-4	Paraformaldehyde	PF
9004-82-4	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-(dodecyloxy)-, sodium salt	AES
67762-19-0	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-hydroxy-, C10-16-alkyl ethers, ammonium salts	AES
68585-34-2	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-hydroxy-, C10-16-alkyl ethers, sodium salts	AES
9002-92-0	Poly(oxy-1,2-ethanediyl), α-dodecyl-ω-hydroxy-	AE
66455-14-9	Alcohols, C12-13, ethoxylated	AE
68002-97-1	Alcohols, C10-16, ethoxylated	AE
68131-39-5	Alcohols, C12-15, ethoxylated	AE
68439-45-2	Alcohols, C6-12, ethoxylated	AE

[1] The Chemical Abstracts Service Registry Number (CAS RN) is the property of the American Chemical Society and any use or redistribution, except as required in supporting regulatory requirements and/or for reports to the Government of Canada when the information and the reports are required by law or administrative policy, is not permitted without the prior, written permission of the American Chemical Society.

[2] This substance was previously assessed under the rapid screening of substances of lower ecological concern and was concluded in 2013 not to be causing harm to the environment or human health. However, in 2015 the IRAP approach identified it as a priority for further risk assessment based on consideration of more recent information, which indicated a large increase in commercial activity of this polymer in Canada relative to that considered in the 2013 evaluation.

68439-46-3	Alcohols, C9-11, ethoxylated	AE
68439-50-9	Alcohols, C12-14, ethoxylated	AE
68951-67-7	Alcohols, C14-15, ethoxylated	AE
9002-93-1	Poly(oxy-1,2-ethanediyl), α-[4-(1,1,3,3-tetramethylbutyl)phenyl]-ω-hydroxy-	OPE
9036-19-5	Poly(oxy-1,2-ethanediyl), α-[(1,1,3,3-tetramethylbutyl)phenyl]-ω-hydroxy-	OPE
28724-32-5	Poly(oxy-1,2-ethanediyl), α,α'-[(methyloctadecyliminio)di-2,1-ethanediyl]bis[ω-hydroxy-, chloride	ANEO
61791-24-0	Amines, soya alkyl, ethoxylated	ANEO
61791-26-2	Amines, tallow alkyl, ethoxylated (POEA)	ANEO
68155-39-5[b]	Amines, C14-18 and C16-18-unsatd. alkyl, ethoxylated	ANEO
68439-72-5	Amines, C8-18 and C18-unsatd. alkyl, ethoxylated	ANEO
68603-75-8	Amines, N-tallow alkyltrimethylenedi-, propoxylated	ANEO

[a] Abbreviations of subgroup: poly(propylene glycol) (PPG); paraformaldehyde (PF); alcohol ethoxylate sulfates (AESs), alcohol ethoxylates (AEs), octylphenol ethoxylates (OPEs), and alkyl amine ethoxylates (ANEOs).
[b] This substance was not identified under subsection 73(1) of CEPA but was included in this assessment as it was considered a priority on the basis of other concerns.

Various poly(alkoxylate/ether) polymers in this screening assessment are registered active ingredients and formulants used in pest control products, and these uses are regulated by Health Canada's Pest Management Regulatory Agency (PMRA) under the *Pest Control Products Act* (PCPA). This screening assessment only considers the potential effects of poly(alkoxylate/ether) on human health and the environment as a result of non-pesticidal uses of the substance.

These 21 substances were previously evaluated under the Second Phase of Polymer Rapid Screening, which identified PPG and PF as having low potential to cause ecological harm and the AES, AE, OPE, and ANEO subgroups (except POEA; CAS RN 61791-26-2) as having low potential to cause harm to human health. The substances listed above were identified as requiring further assessment for potential human health and/or ecological risks on the basis of structural alerts and/or uses associated with significant consumer exposure. The present assessment further elaborates on the potential for PPG, PF and POEA of the ANEO subgroup to cause harm to human health and for three AESs, eight AEs, two OPEs and all six ANEOs to cause ecological harm, in order to reach an overall conclusion under section 64 of CEPA as to whether they pose an unacceptable risk to the environment or human health.

PPG does not occur naturally in the environment, is prepared industrially, and has widespread applications. In Canada, it is reported to be used in coatings for paper and cans, pulping processes, ultrafiltration/reverse osmosis (UF/RO) water treatment systems, laminated films, inks, textile dyes, paper based materials, paint, food processing, pharmaceuticals, pesticides, toys, and personal care products. It has been reported that more than 1 million kilograms of PPG were imported and/or manufactured in Canada in 2014. PPG does not contain any reactive functional chemical groups or

other structural features associated with human health concerns. PPG has a low hazard profile for human health based on classification guidelines from the United States Environmental Protection Agency (US EPA 2004). Given its physical/chemical properties, both direct exposure (oral, inhalation, dermal) and indirect exposure (through drinking water) of the general population to PPG are expected to be minimal.

PF does not occur naturally in the environment but is prepared industrially from formaldehyde (which can occur naturally in the environment). It has widespread applications, the most important of which is as a formaldehyde-generating substance. However, the PF is consumed during the reaction, and only trace amounts of unreacted PF or formaldehyde are expected to be present. In Canada, PF has been used in adhesives, sealants, agricultural products, coatings, inks, food packaging, pharmaceuticals, pesticides, toys, and other products available to consumers. It has been reported that more than 1 million kilograms of PF were imported and/or manufactured in Canada in 2014. PF does not contain any reactive functional groups or other structural features associated with human health concerns. PF has a moderate hazard profile based on classification guidelines from the US EPA (2004) for human health. Both direct and indirect exposure of the general population to PF is expected to be minimal. Although PF is a potential source for the release of formaldehyde, the release is very slow at ambient temperatures. Therefore, air concentrations of formaldehyde would remain low.

AESs are anionic surfactants that do not occur naturally in the environment. According to available information, the three AESs considered in this assessment are used primarily in products available to consumers. No AESs were reported to be manufactured in Canada, but a combined import quantity of more than 10 million kg was reported in 2014. On the basis of current use patterns, the three AESs are considered unlikely to be causing ecological harm.

AEs are nonionic surfactants that do not occur naturally in the environment. According to available information, the eight AEs considered in this assessment are used in many sectors but are primarily found in products available to consumers, such as cleaners. A combined import quantity of 1 million to 10 million kg was reported in 2014. On the basis of current use patterns, the eight AEs are considered unlikely to be causing ecological harm.

OPEs are nonionic surfactants that do not occur naturally in the environment. According to available information, the two OPEs considered in this assessment are used primarily in paints and coatings, products available to consumers, and a combined import quantity of 0.1 million to 1 million kg was reported in 2014. On the basis of current use patterns, the two OPEs are considered unlikely to be causing ecological harm. It is noted, however, that NPEs (nonylphenol and its ethoxylates) and OPEs are structurally similar and have similar physical-chemical properties. Additionally, both NPEs and OPEs have similar ecotoxicological hazard and their degradation products have similar endocrine (estrogen) disrupting potential. Thus, from an environmental perspective, the two OPE surfactants considered in this assessment would not be considered suitable

alternatives to NPEs.

ANEOs are amine surfactants that do not occur naturally in the environment. According to available information, the six ANEOs considered in this assessment are used primarily in oil and gas extraction, metal working fluids, and products available to consumers. The combined import quantity in 2014 was between 1 million and 10 million kg. On the basis of current use patterns, the six ANEOs are unlikely to be resulting in concerns for the environment in Canada. ANEOs do not contain any reactive functional groups or other structural features associated with human health concerns. The substance POEA within the subgroup ANEO has a moderate hazard profile for human health. Due to its widespread applications, direct and indirect exposure to human from POEA is expected to be moderate.

Considering all available lines of evidence presented in this draft screening assessment, there is low risk of harm to the environment from the 21 substances considered in this assessment. It is proposed to conclude that the 21 substances considered in this assessment 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.

On the basis of the information presented in this screening assessment, it is proposed to conclude that the 21 substances considered in this assessment 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 therefore proposed to conclude that these 21 substances do not meet any of the criteria set out in section 64 of CEPA.

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1. Introduction

Pursuant to section 68 or 74 of the *Canadian Environmental Protection Act, 1999* (CEPA) (Canada 1999), the Minister of Environment and the Minister of Health have conducted a screening assessment of 21 substances referred to collectively under the Chemicals Management Plan as the Poly(alkoxylates/ethers) Group. Substances in this group were identified as priorities for assessment as they met categorization criteria under subsection 73(1) of CEPA or were considered a priority on the basis of other concerns (ECCC, HC [modified 2017]). One substance in this group (CAS RN 68155-39-5) was previously assessed under Rapid Screening of Substances of Lower Concern (Environment Canada, Health Canada [modified 2013]), and was found not to meet any of the criteria under section 64 of CEPA. The polymer was flagged for further assessment on the basis of a 2015 review under the Identification of Risk Assessment Priorities (Canada 2015b) process, which considered information obtained via Phase Two of the DSL Inventory Update (Environment Canada, Health Canada 2014) indicating a large increase in commercial activity of this polymer in Canada relative to that considered in the 2013 evaluation.

Various poly(alkoxylate/ether) polymers in this screening assessment are registered active ingredients and formulants used in pest control products. These uses are regulated by Health Canada's Pest Management Regulatory Agency (PMRA) under the *Pest Control Products Act* (*PCPA*). This screening assessment only considers the potential effects of poly(alkoxylate/ether) polymers on human health and the environment as a result of non-pesticidal uses of the substance.

While the 21 substances considered in this assessment are collectively referred to as the Poly(alkoxylates/ethers) Group, 19 of them were further sub-grouped into AEs, AESs, OPEs, and ANEOs (including Amines, tallow alkyl, ethoxylated (CAS RN 61791-26-2, POEA)). These subgroups have structural similarities that would support a group approach to exposure, hazard and risk characterization; thus, each collective subgroup was assessed for risk. The two remaining individual substances, PPG and PF, are presented in separate chapters. For clarity, this assessment consistently uses the term "class" when referring to the broad range of polymers having similar structure and properties, and "group" or "subgroup" when referring to the sub-set of substances that are being considered under the current assessment.

The 21 substances in the Poly(alkoxylates/ethers) Group have been previously evaluated using a rapid screening approach. The approach and results of its application, are presented in the document "Second Phase of Polymer Rapid Screening: Results of the Screening Assessment" (ECCC, HC 2018). The ecological and human health rapid screening approaches are summarized in the appendix of this screening assessment. Application of these approaches identified PPG and PF as having low potential to be causing ecological harm and identified AESs, AEs, OPEs, and ANEOs (except POEA) as having low potential to cause harm to human health. Results from the screening, in conjunction with any other relevant information that became available after the publication of the report on the second phase of polymer

rapid screening, support the conclusions made under section 64 of CEPA in this screening assessment.

This draft screening assessment includes consideration of additional information on chemical properties, environmental fate, hazards, uses and exposures, including additional information submitted by stakeholders. Relevant data were identified up to September 2017. Empirical data from key studies as well as results from models, when appropriate, were used to reach proposed conclusions. When available and relevant, information presented in assessments from other jurisdictions was considered.

This draft screening assessment was prepared by staff in the CEPA Risk Assessment Program 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 review and/or consultation. Comments on the technical portions relevant to the environment were received from Mr. David Shortt (KAND EHS Services), Mr. Geoff Granville (GC Granville Consulting Corp), and Dr. Karsten Liber (Toxicology Centre, University of Saskatchewan). While external comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Environment and Climate Change Canada and Health Canada.

This draft screening assessment focuses on information critical to determining whether substances meet the criteria as set out in section 64 of CEPA, by examining scientific information and incorporating a weight of evidence approach and precaution.[3] This draft screening assessment presents the critical information and considerations on which the proposed conclusions are based.

2. Polypropylene glycol (PPG)

2.1 Substance identity

Polypropylene glycol (PPG), also known as polypropylene oxide (PPO), is produced by the polymerization of propylene oxide with propylene glycol (Figure 2-1). By choosing the method of polymerization (cationic, anionic, coordination), initiator, reagents, order of addition, and reaction conditions, branched or linear PPG with a variable degree of

[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 to human health associated with exposures in the general environment. For humans, this includes, but is not limited to, exposures from ambient and indoor air, drinking water, foodstuffs, and 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.

polymerization/average number of units (*n*) can be prepared (Herzberger et al. 2016, Gagnon 2000). No residual monomers (i.e., propylene oxide or propylene glycol) are expected to remain, as the process involves several purification stages to remove all impurities. Typically *n* varies from 3 to 69, giving a molecular weight in the range of 200 to 4000 g/mol (MAK 2012). Different naming conventions are used in identifying PPGs. When the official International Nomenclature Cosmetic Ingredient (INCI) name is used, the name is given as PPG along with the average number of units (*n*) (e.g., PPG-3 when *n* = 3). However, the PPGs can also be identified using the average molecular weight as part of the name (e.g., PPG 200 when the molecular weight is about 200 g/mol) (Fiume et al. 2012). PPG contains no reactive functional group associated with adverse human health effects (US EPA 2010). PPGs are non-volatile liquids and vary from miscible to quite insoluble in water from the lowest to the highest molecular weights (Larrañaga et al. 2016; MAK 2012).

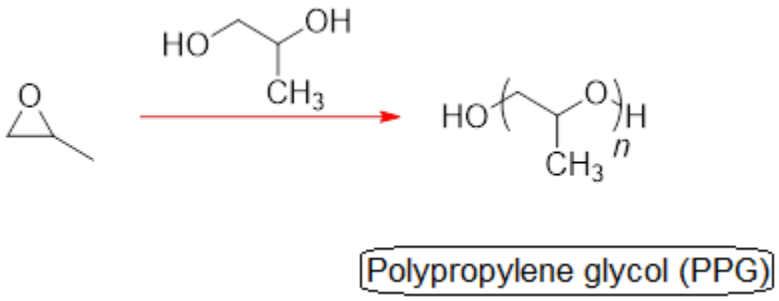


Figure 2-1. Synthesis and representative structure of polypropylene glycol

2.2 Physical and chemical properties

A summary of physical and chemical properties for PPG is presented in

Table 2-1.

Table 2-1. Physical and chemical property values (at standard temperature) for PPG

Property	PPG	Key reference(s)
Physical state	Liquid	Andersen 1994
Molecular weight (g/mol)	200 to 4000	MAK 2012, Andersen 1994
Melting point (°C)	-40 to -35	MAK 2012
Boiling point (°C)	~ 270 (decomposition)	MAK 2012, ECHA 2017
pH	6 to 9	Andersen 1994, FCC 2004
Vapour pressure (Pa)	0.084 Pa	ECHA 2017
Water solubility (w/w)	Miscible to 1.5%	MAK 2012

Property	PPG	Key reference(s)
Water solubility (mg/L)	10 000 to 15 (PPG 425–PPG 2700)	West et al. 2007
Density (g/cm^3)	1.002-1.012	Andersen 1994, ECHA 2017
Octanol/water partition coefficient (log K_{ow})	1.7 to 3.0	Harris and Daugulis 2015, ECHA 2017
Biodegradation	Readily biodegradable 83% to 92% in 28 days (including PPG 425–PPG 2000)	SDS 2017a, SDS 2017b, West et al. 2007

2.3 Sources and uses

PPG is not a naturally occurring substance; it is prepared industrially and has widespread applications.

PPG has been included in a voluntary survey (ECCC 2015) as well as a mandatory survey conducted under section 71 of CEPA (Canada 2015).

Table **2-2** presents a summary of the reported total manufacture, import and use quantities for the substance for 2014. These sources indicate some uses for PPG in Canada as a defoaming agent, absorbency aid, surfactant, lubricant, frothing agent, hardener/resin for adhesive systems, crosslinker, colour concentrate, moisture vapour barrier, flooring adhesive, release agent, and boiler water additive. It has been used in coatings for paper and cans, pulping processes, ultrafiltration/reverse osmosis (UF/RO) water treatment systems, laminated films, inks, textile dye, paper-based materials, paint, food processing, pharmaceuticals, pesticides, toys, and personal care products.

Globally, PPGs are used as additives in metal working fluids, as plasticizers, as antifoaming agents, as additives in the rubber and paint industries, as starting materials for the synthesis of urethane foams and resins, surfactants, polypropylene ethers and esters, and in the production of cosmetic preparations (molecular weight mostly above 1200) (MAK 2012). PPG is used in many polyurethane formulations. It is used as a rheology modifier, wetting agent and dispersant. PPG is listed in the European Commission Regulations as an acceptable substance in plastics used as food contact materials, without restrictions on migration and no specifications on molecular mass (EFSA 2011). In the United States, PPG is an indirect food additive that has been approved for use as a component of resinous and polymeric coatings (21 CFR 175.300), adhesives (21 CFR 175-105), and paper and paperboard in contact with aqueous fatty foods (21 CFR 176.170). PPG with molecular weights above 1000 can be used as boiler water additives (21 CFR 173.310) and defoaming agents (surface active agent; 21 CFR 173.340). PPG is used as a solvent for waxes, resins, cleaning

products, dish care products, and hydraulic fluids and is an ingredient in paintballs, antifreeze and brake fluid (Polymer-search 2017; Larrañaga et al. 2016; ACI 2017).

Table 2-2. Summary of information on Canadian manufacturing, import and use quantities of PPG for 2014 submitted pursuant to a section 71 survey under CEPA

Substance	Total manufacture (kg)	Total imports[a] (kg)	Total manufacture and imports (kg)	Total used[a] (kg)	Survey reference
PPG	NA	1 000 000–10 000 000	1 000 000–10 000 000	1 000 000–10 000 000	Canada 2015, ECCC 2015

Abbreviations: NA, Not Available

[a] Values reflect quantities reported in response to the surveys conducted under section 71 of CEPA (Canada 2015). See surveys for specific inclusions and exclusions (schedules 2 and 3).

A number of domestic government databases were searched to determine other potential uses of PPG in Canada. These uses for PPG are listed in Table 2-3.

Table 2-3. Additional uses in Canada for PPG

Use	PPG
Food additive[a]	N
Food packaging materials and incidental additives[b]	Y
Internal Drug Product Database as medicinal or non-medicinal ingredients in disinfectant, human or veterinary drug products in Canada[c]	Y (NMI)
Natural Health Products Ingredients Database[d]	Y (NMI)
Licensed Natural Health Products Database as medicinal or non-medicinal ingredients in natural health products in Canada[e]	Y
List of Prohibited and Restricted Cosmetic Ingredients[f]	N
Notified to be present in cosmetics, based on notifications submitted under the *Cosmetic Regulations* to Health Canada[g]	Y
Formulant in pest control products registered in Canada[h]	Y
Known toy use[i]	Y

Abbreviations: Y, YES; N, NO; NMI, Non-medicinal ingredient.

[a] Health Canada [modified 2017]; personal communication, email from the Food Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[b] personal communication, email from the Food Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[c] DPD [modified 2017]; personal communication, email from the Therapeutic Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[d] NHPID [modified 2019]; personal communication, email from the Natural and Non-prescription Health Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[e] LNHPD [modified 2018]; personal communication, email from the Natural and Non-prescription Health Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.
[f] Health Canada [modified 2015].
[g] personal communication, email from the Consumer Product Safety Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.
[h] personal communication, email from the Pest Management Regulatory Agency, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.
[i] Toy Industry Association (TIA 2017).

2.4 Potential to cause ecological harm

The critical data and considerations used in the second phase of polymer rapid screening to evaluate the substance-specific potential to cause ecological harm are presented in ECCC (2016).

The above report identified PPG as not containing any reactive functional groups associated with increased ecological concern. This substance was therefore characterized as having a low potential for ecological risk, and so it is unlikely that it results in concerns for organisms or the broader integrity of the environment in Canada.

2.5 Potential to cause harm to human health

2.5.1 Exposure assessment

2.5.1.1 Direct exposure

When used industrially, direct exposure of the general population to PPGs is not expected because these substances are used in a closed system. Furthermore, the release of PPG from end-use applications is limited, as PPGs are mostly combined with other substances into sealed systems that are stable against thermal and hydrolytic breakdown. These products will biodegrade under environmental conditions and will be efficiently removed during treatment in wastewater treatment facilities (Dow 2014).

Oral exposure

As food packaging material, PPG may be used as a defoamer in the manufacture of paper and paperboard, in a coating for paper and paperboard and in adhesives. These are three scenarios where there could be potential for migration of the substance from the food packaging material into food. In theory, adhesives are not direct food contact materials, as there should be a barrier or layer that would prevent migration of the components of the adhesive into food. Even assuming consumer exposure from food pathways, incorporating theoretical worst-case scenarios (i.e., based on 100% migration), the exposure is expected to be very low (personal communication, emails from Food Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated May 2017; unreferenced).

Dermal exposure

Considering the log K_{ow} (1.7 to 3) for PPGs, it is expected that the lower molecular weight PPGs (i.e., those with molecular weights of 200 to 500 g/mol, namely PPG-3 to PPG-7) would have some dermal absorption (WHO 2006). However, for the majority of PPGs (i.e., those with molecular weights above 500 g/mol), dermal absorption is expected to be minimal.

According to notifications submitted under the *Cosmetic Regulations* to Health Canada, PPGs are used in certain cosmetic products in Canada, such as adhesive remover, cleanser, permanent hair colour, moisturizer, shampoo, styling product and toothpaste (emails from the Consumer Product Safety Directorate, Health Canada, to the New Substances Assessment and Control Bureau (NSACB), Health Canada, dated June 2017; unreferenced). The data indicates that approximately 15% of these products contain PPG-3 or PPG-7. The concentration of PPGs in those personal care products is reported to be less than 10%. Using this data, E-FAST (2014) estimates the dermal exposure to PPG-3 (worst case for dermal absorption) as 2.6 µg/kg bw/day (chronic/lifetime) and 43 µg/kg bw/day (acute) for general purposes such as cleansers (E-FAST 2014). Considering the molecular distribution of PPGs (mostly above 500 g/mol), it is expected that the dermal exposure to PPG would be lower than E-FAST estimates.

Inhalation exposure

The low volatility of PPGs makes inhalation improbable except where mists are formed from violent agitation or high temperatures (TOXNET 2017). For general purpose cleaners, E-FAST (2014) estimates the inhalation exposure to PPG-3 (worst case for inhalation) as 13 µg/kg bw/day (chronic/lifetime) and 175 µg/kg bw/day (acute). The peak concentration was estimated to be 2.7 mg/m^3 (E-FAST 2014). Considering the molecular distribution of PPGs (mostly above 500 g/mol) and its low vapour pressure, it is expected that the inhalation exposure to PPG would be lower than E-FAST estimates.

Drug products

PPG is listed as a non-medicinal ingredient in the Natural Health Products Ingredients Database (NHPID [modified 2019]). It can be used as an antifoaming agent or skin-conditioning agent with a dose up to 1.5 mg/kg bw/day as a group tolerable daily intake with 1,2-polypropylene oxide and dipropylene glycol and up to 22% for topical use when formulated to be non-irritating. PPGs are listed in the Licensed Natural Health Products Database (LNHPD) (LNHPD [modified 2018] as being present as a non-medicinal ingredient in a number of currently licensed natural health products, as well as in a limited number of currently approved/marketed non-prescription drugs, in Canada (DPD [modified 2015]). No information regarding the concentration of PPGs in those drugs (including natural health products) is available.

Pesticides

PPG is included on PMRA's pesticide formulants list (Health Canada 2010a). It is present in 255 pesticide products, including herbicides, insecticides, fungicides, nematicides, acaricides, insect growth regulators, insect repellents, adjuvants, plant growth regulators, swimming pool algicides, slimicides, and antifouling paints (personal communication, PMRA, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated May 2017; unreferenced).

Other products

According to the Canadian Consumer Specialty Products Association (CCSPA), PPG is present in 11 products available to consumers (CCSPA communication, dated June 2017; unreferenced).

PPG is used in the forestry industry as a defoamer in the pulping process in the manufacture of paperboard coatings (Environment Canada 2015).

PPG is used as a polymer in toys according to the Canadian Toy Industry Association (TIA 2017).

2.5.1.2 Indirect exposure

PPGs have relatively low volatility and vary in water solubility. When introduced to water, they will tend to remain dissolved in, and transported with, the water to which they are released. However, they will biodegrade under environmental conditions with a rate of degradation around 90% at 28 days (West et al. 2007). PPGs will be efficiently removed during treatment in wastewater treatment facilities (DOW 2014). Consequently, the indirect exposure of the general population to PPG through environmental media such as drinking water is expected to be minimal.

2.5.2 Health effects assessment

During evaluation under the second phase of polymer rapid screening, polypropylene glycol (PPG) was identified as requiring further assessment as a result of a flag for potential toxicity to the central nervous system as well as cardiac toxicity. The polymer does not contain any structural features associated with adverse human health effects. Polymers generally have a lower toxicity than their monomers as they are larger and do not absorb via the dermal or oral route as efficiently as the smaller monomers. Unlike ethylene glycol, propylene glycol has not been associated with nephrotoxicity caused by a metabolite, calcium oxalate, in humans. Propylene glycol is not metabolized to oxalic acid; therefore calcium oxalate is not deposited in the kidneys (ATSDR 2007).

The absorption of PPG in the gastrointestinal tract and its toxicity will depend on its molecular weight. The lower molecular weight species show the greatest toxicity. The toxicity increases initially with molecular weight, reaching a maximum toxicity for PPG 600 and PPG 750 and then decreases with higher molecular weights. PPGs with molecular weights of 2000 or greater have very low acute toxicity (TOXNET 2017). The

symptoms of acute intoxication seen in animal studies with low molecular weight species are excitation of the central nervous system and cardiac arrhythmias (MAK 2012).

The United States Food and Drug Administration (FDA) considers the monomer, propylene glycol (CAS RN 51-55-6), as “generally recognized as safe under the conditions of its intended use” identified in 21 CFR 184.1666 as food grade PPG.

The acute oral toxicity of polypropylene glycol is low, ranging from an LD_{50} of 2910 mg/kg bw for PPG 425 to LD_{50} of 9760 mg/kg bw for PPG 2025 (Shaffer et al. 1951). PPG 425, PPG 1025 and PPG 2025 also have a low acute dermal toxicity in rabbits with an LD_{50} > 10 000 mg/kg bw.

An aqueous solution of PPG 400 was administered intravenously (IV) to dogs at a dose of 20 mg/kg bw. The results of an electroencephalogram (EEG) indicated increased electrical activity in all lobes of the brain. Following intravenous administration of a PPG 750 aqueous solution and an aqueous solution of PPG 1200 (doses 10 mg/kg bw) in dogs, the same EEG pattern was noted. Electrocardiogram patterns following the administration of PPG 400 and PPG 750 indicated changes in cardiac rhythm. However, such responses were not observed after administration of PPG 1200 or PPG 2000 (Andersen 1994’; Shideman and Procita 1951). Manifestations of increased central nervous system activity in the form of enhanced stretch reflexes, muscle tremors, and movements were also noted with PPG 400, PPG 750 and PPG 1200. Convulsant activity was noted at a higher dose (25 mg/kg bw) (Shideman and Procita 1951).

Inhalation of toxic amounts of PPG vapour at room temperature is unlikely because of the low vapour pressure of these substances. PPGs are not skin irritants and at most are slight eye irritants (Andersen 1994). Dermal sensitization was not observed in a study of 300 men who received continuous and repeated dermal application of undiluted PPG 2000 (Andersen 1994).

In a 90-day subchronic study, rats orally administered 275 to 501 mg/kg bw/day of PPG 2000 did not show any evidence of adverse histopathologic, hematologic, or clinical chemistry effects (MAK 2012). Reductions in body weight were noted only at the highest dose. Similar effects were observed in a 90-day study in dogs administered oral doses of PPG in the range of 526 to 810 mg/kg bw/day (MAK 2012; Andersen 1994; AIHA 1980). In another study, PPG 750 was administered to rats over a period of 100 days. Concentrations of 0.1 or 1% were administered at doses of 50 or 500 mg/kg bw/day. PPG 750 (0.1%) did not induce any adverse effects. In the group dosed with 1% PPG 750, a slight increase in liver and kidney weights was noted; however, no histological changes were observed, and therefore a no observed adverse effect level (NOAEL) of 500 mg/kg bw/day was established. Neither of the doses resulted in a central nervous system stimulatory effect (AIHA 1980). In another subchronic oral toxicity study performed in rats, administration of PPG 2000 resulted in a slight reduction in growth and body weight, while administration of PPG 750 to rats and dogs resulted in slight increases in liver and kidney weights in rats (Andersen 1994; TOXNET 2017). No other treatment-related effects were reported. A subchronic dermal study in rabbits did not

show effects at 1 mL/kg bw, but 5 and 10 mL/kg bw caused a slight depression in growth (CIR 2013).

The British Industrial Biological Research Association (BIBRA) reported that PPG of undefined molecular weight and purity was mutagenic in an Ames bacterial test (BIBRA 1990). The European Food Safety Authority (EFSA) Scientific Panel on Contaminants in the Food Chain (CONTAM Panel) considered that this result could be disregarded given the negative genotoxicity information on the monomer propylene glycol. The CONTAM Panel also noted that there was no evidence of a carcinogenic effect of the monomer propylene glycol in two chronic toxicity studies (OECD 2001). Limited information is available on the developmental or reproductive toxicity of PPG. However, the CONTAM Panel noted that the monomer propylene glycol is considered not to have adverse effects on reproduction or developmental effects when evaluated on mice at concentrations of <5% in rats, at doses of ≤ 1600 mg/kg bw/day and in rabbits at doses of ≤ 1230 mg/kg bw/day (CIR 2013).

The Scientific Committee on Food (SCF 1986) established a tolerable daily intake (TDI) of 1.5 mg/kg bw (as a group TDI with polypropylene glycol and dipropylene glycol), which was endorsed by the CONTAM Panel. There are limited toxicological data on PPG, in particular on chronic toxicity and reproductive toxicity. However, the CONTAM Panel considered that information on these endpoints could be read across from the monomer propylene glycol and are considered low (EFSA 2011). PPGs are safe for use in cosmetic products at concentrations up to 50.0% (Fiume et al. 2012; Andersen 1994) considering the TDI established by SCF in 1986 [TDI of 1.5 mg/kg bw] on the basis of a scenario that considered various molecular weights of PPG, including monomers and dimers combined.

2.5.3 Characterization of risk to human health

In this assessment, the human health risks were established through consideration of both the hazard and the direct and indirect exposures of the substance for current uses identified from a voluntary and section 71 surveys conducted under CEPA, as well as from governmental databases.

In general, identified health concerns, such as stimulation of the central nervous system and cardiac arrhythmias, were associated with the low molecular weight oligomers of PPG and are seen primarily through intravenous administration. These effects were not noted when administered orally or dermally for a PPG with a molecular weight greater than 2000. Polydispersity (the molecular weight range in a given product) is typically narrow. Therefore, unreacted low molecular weight oligomers are not anticipated in the products. A NOAEL of 500 mg/kg bw/day was obtained from a subchronic study. However, given that oral exposure is limited to natural health products, drugs and food packaging, the substance would be limited to a molecular weight range for food grade products that do not pose a health risk. The SCF (1986) established a TDI of 1.5 mg/kg bw/day, which was a worst-case scenario obtained with the monomers and dimers. This value also includes uncertainty (safety) factors, but shows that even the monomer can

be tolerated at mg quantities over chronic periods. This value cannot be compared directly with the potential exposure through pharmaceuticals which was estimated at 25 mg/kg bw, as this value is for all glycol products, not just PPG and does not include uncertainty factors. The actual exposure to PPG for medicinal use is expected to be much lower than the exposure to total glycol value above.

Insufficient subchronic dermal studies were available for PPG or the monomer propylene glycol. Therefore, a margin of exposure (MOE) cannot be established on the basis of dermal exposure values. No acute or subchronic adverse health effects are anticipated as a result of dermal exposure to PPG, as both PPG and the monomer (PG) have a low acute dermal toxicity. Studies also show that PPG and PG are non-irritating and are not dermal sensitizers when applied to the skin (CIR 2013). PPGs with molecular weights above 500 are not well absorbed systemically via the dermal route as a result of the large molecular weight. Dermal exposure to PPG through manufactured products available to consumers is expected to be low as it is not easily released once incorporated into a solid matrix and would be poorly absorbed as a result of its molecular size.

No subchronic inhalation studies were available for PPG and therefore no MOE could be calculated using the estimated inhalation exposure values. While inhalation exposure may occur from use of some products available to consumers, PPGs do not have chemical reactivity on mucous membranes. tTherefore, the particles that deposit in the nasopharyngeal or bronchial regions of the respiratory tract during incidental inhalation do not pose a toxicological concern (CIR 2013).

Low molecular weight PPGs have been shown to have transient effects on the central nervous system and heart when administered intravenously. This is generally not a route of anticipated exposure from products available to consumers. There is no reporting of carcinogenicity, genotoxicity or reproductive toxicity in the literature for PPG. Polymeric forms of glycol ethers show a lower toxicity than their monomeric counterparts. The SCF (1986) evaluated PPG (molecular weights greater than 400) in 1996 and established a TDI of 1.5 mg/kg bw/day (EFSA 2011). This value was obtained for the monomer and dimer. However, it may vary depending on the molecular weight range of the polymer.

Taking into consideration the direct and indirect exposures of Canadians to PPG, as well as the low hazard generally associated with PPG, the human health risk for this polymer has been determined to be low.

3. Paraformaldehyde (PF)

3.1 Substance identity

Paraformaldehyde (PF) is a polyether prepared from the polymerization of

formaldehyde in the presence of water (Figure 3-1). The degree of polymerization (*n*) varies depending on the method of preparation, reagents, and reaction conditions (Franz et al. 2016). PF is part of a broader group of formaldehyde polymers called poly(oxymethylenes) (POM). The *n* values of the low-molecular-mass POM are 2 to 8; the *n* values of PF are 8 to 100; the *n* values of the high-molecular-mass POM are > 100. POMs (CAS RN 9002-81-7) are not discussed in this report. PF contains no reactive functional group associated with adverse human health effect (US EPA 2010). It is a solid that slowly decomposes to formaldehyde gas even at ambient temperature, a process which is accelerated by heating. In warm water, PF undergoes hydrolysis and depolymerization to give a formaldehyde solution (Franz et al. 2016).

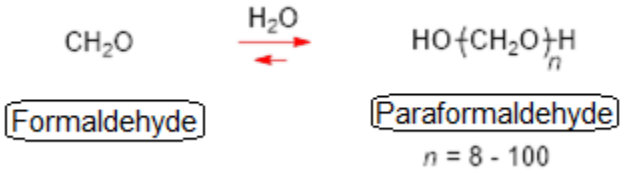


Figure 3-1. Synthesis and representative structure of paraformaldehyde

3.2 Physical and chemical properties

A summary of physical and chemical properties for PF is presented in Table 3-1.

Table 3-1. Physical and chemical property values (at standard temperature) for PF

Property	PF	Key reference(s)
Physical state	Solid	EPA 2008, Rumble 2017
Molecular weight (g/mol)	258 to 3000 (average ~ 900)	EPA 2008, ECCC 2015
Melting point (°C)	120 to 170	EPA 2008, Rumble 2017
Vapour pressure (Pa)	133 to 193	EPA 2008, Health Canada 2010b
Water solubility	Partial (*n* < 15) to insoluble	EPA 2008, SDS 2012, TOXNET 2017a
Octanol/water partition co-efficient (log K_{ow})	< - 4	EPI suite c2000-2012 (estimation)
pH	3.5 to 5.5	EPA 2008, SDS Celanese 2015
Density (g/cm^3)	1.30 to 1.46	EPA 2008, SDS 2017c

3.3 Sources and uses

Although PF is not a naturally occurring substance, it is a source ingredient for formaldehyde, which is abundant in nature (atmosphere and living organisms) (NHPID [modified 2019]). It is also produced industrially in large quantities. Formaldehyde has

previously been assessed under CEPA and is listed on Schedule 1. PF has widespread applications, specifically as a formaldehyde-generating substance. PF is considered a simple means of polymerizing formaldehyde because it can be prepared in a temperature-controlled hydrolysis reaction. Moreover, there are no contaminating residues produced during the evaporation of PF solution (unlike formalin, another source of formaldehyde) (Al-Adham et al. 2013; Kiernan 2000). This is usually performed by the heating of PF solutions (~ 16 hours at 100°C) (Fernandez et al. 1999).

PF has been included in a voluntary survey (ECCC 2015) as well as a mandatory survey conducted under section 71 of CEPA (Canada 2015). Table 3-2 presents a summary of the total manufacture, import and use quantities for the substance in 2014. These sources indicate some uses for PF in Canada are as a chemical intermediate, formulant, polymer component, antimicrobial agent, and drug. It may be used in adhesives, sealants, agricultural products, coatings, inks, food packaging, pharmaceuticals, pesticides, toys and other products available to consumers. PF is also applied by fumigation (granules are heated during application resulting in the release of formaldehyde gas) to materials provided for bee nesting (wood, plastic) and to bee cells during the pre-pupal diapause developmental bee stage (Health Canada 2010b).

Table 3-2. Summary of information on Canadian manufacturing, import and use quantities of PF in 2014 submitted pursuant to a section 71 survey under CEPA

Substance	Total manufacture (kg)	Total imports[a] (kg)	Total manufacture and imports (kg)	Total used[a] (kg)	Survey reference
PF	NA	> 100 000	NA	1 000 000–10 000 000	Canada 2015, ECCC 2015

Abbreviations: NA, Not Available

[a] Values reflect quantities reported in response to the surveys conducted under section 71 of CEPA (Canada 2015). See surveys for specific inclusions and exclusions (schedules 2 and 3).

A number of domestic government databases were searched to determine other potential uses of PF in Canada. These uses for PF are listed in

Table 3-3.

Table 3-3. Additional uses of PF in Canada

Use	PF
Food additive[a]	N
Food packaging materials[b]	Y
Internal Drug Product Database as medicinal or non-medicinal ingredients in disinfectant, human or veterinary drug products in Canada[c]	N

Use	PF
Natural Health Products Ingredients Database[d]	Y
Licensed Natural Health Products Database as medicinal or non-medicinal ingredients in natural health products in Canada[e]	N
List of Prohibited and Restricted Cosmetic Ingredients[f]	N
Notified to be present in cosmetics, based on notifications submitted under the *Cosmetic Regulations* to Health Canada[g]	N
Formulant in pest control products registered in Canada[h]	Y
Known toy use[i]	Y

Abbreviations: Y, YES; N, NO; MI, Medicinal ingredient.

[a] Health Canada [modified 2017]; personal communication, email from the Food Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[b] personal communication, email from the Food Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[c] DPD [modified 2017]; personal communication, email from the Therapeutic Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[d] NHPID [modified 2019]; personal communication, email from the Natural and Non-prescription Health Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[e] LNHPD [modified 2018]; personal communication, email from the Natural and Non-prescription Health Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced

[f] Health Canada [modified 2015].

[g] personal communication, email from the Consumer Product Safety Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[h] personal communication, email from the Pest Management Regulatory Agency, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[i] Toy Industry Association (TIA 2017).

Globally, PF is used in place of aqueous formaldehyde solutions, especially in applications where the presence of water interferes (e.g., in the plastics industry for the preparation of phenol, urea, and melamine resins, varnish resins, thermosets, and foundry resins). These resins are used as moulding powders; in the wood industry as preservative as well as glues for chipboard, plywood and furniture; as bonding resins for brakes, abrasives and foundry dyes; as finishing resins for paper and textiles; as driers and glossing agents for paints; and as insulating varnishes for electrical parts. Other uses include the synthesis of organic substances in the chemical and pharmaceutical industries, in biology labs (as fixative), in the production of textile auxiliaries, and in the preparation of disinfectants and deodorants (Health Canada 2010b; IARC 2012; Franz et al. 2016).

PF is used as a corrosion inhibitor, hydrogen sulfide scavenger, and as a biocide in oil production operations such as drilling, waterflood, and enhanced oil recovery (Gerberich and Seaman 2013). It is used as a fungicide and bactericide in industries as varied as beet sugar refining and warehousing. Hotels and motels, located in humid areas, often use PF, with or without added mothproofing agents, in small bags hung in closets to prevent the formation of mildew. It is used in drawer fumigation of hair cutting

equipment and as a mildewcide in unoccupied vacation homes. In photography, PF is a gelatin hardener and accelerates development stages. It is also the source of formaldehyde in certain fur treatments. PF is a component of certain antiperspirant powders. Shrinkage in wood has been reduced by treatments with the vapours from heated PF (US EPA 2008; Ash and Ash 2004).

PF has been used in lozenges for the treatment of minor throat infections. In dentistry, it has been used as an obtundent (a substance for blunting irritation or lessening pain) for sensitive dentine and as an antiseptic in mummifying pastes and for root canals. PF may be used for the decontamination of equipment thought to be contaminated with the spores of *Bacillus anthracis* (Brayfield 2017). PF is used for disinfecting sickrooms/hospital utensils, clothing, and linen. It is an active ingredient of contraceptive creams (Merck 2013).

About 2% of the PF produced in the United States is used in products available to consumers (US EPA 1991).

3.4 Potential to cause ecological harm

Critical data and considerations used in the second phase of polymer rapid screening to evaluate the substance-specific potential to cause ecological harm are presented in ECCC (2016).

The above report identified PF as not containing any reactive functional groups associated with increased ecological concern. This substance was therefore characterized as having a low potential for ecological risk and so it is unlikely that it results in concerns for organisms or the broader integrity of the environment in Canada.

3.5 Potential to cause harm to human health

3.5.1 Exposure assessment

3.5.1.1 Direct exposure

When used industrially, direct exposure of the general population to PF is not expected because it is used in a closed system and both the PF and resulting formaldehyde are consumed in the reaction.

Given the high vapour pressure of PF, inhalation would be the most critical route of exposure. However, the emitted substance is formaldehyde. Conversion of PF to formaldehyde takes place at room temperature at a very slow rate (Helander 1999). On the basis of the slow liberation of formaldehyde from PF at room temperature, it is expected that the amount of this additional formaldehyde would be minuscule in comparison to the typical levels of formaldehyde in the environment. On average, formaldehyde levels measured over a day in Canadian homes were 20 to 40 µg/m^3 (16 to 32.5 ppb) (Environment Canada, Health Canada 2013).

PF appears on PMRA's pesticide formulants list (with a maximum permitted concentration of 1% in pest control products) as well as on the list of active pesticide ingredients (sanitizer and fumigant). It is present in one pesticide product, a fumigant (personal communication, PMRA, to the New Substances Assessment and Control Bureau, Health Canada, dated May 2019; unreferenced).

PF may be used as a component of adhesives used in food packaging materials and as a component of resins used for the interior coating of cans with direct food contact. Even assuming a theoretical worst-case scenario (i.e., based on 100% migration), the exposure is expected to be very low (personal communication, emails from the Food Directorate, Health Products and Food Branch, to the New Substances Assessment and Control Bureau, Health Canada, dated May 2017; unreferenced).

PF is listed in the NHPID as a source ingredient of formaldehyde (NHPID [modified 2019]). It can be used as a source ingredient for formaldehyde. However, it has not been found as such in currently licensed NHPs (LNHPD [modified 2018], DPD [modified 2017]).

According to the Canadian Consumer Specialty Products Association (CCSPA), PF is present in one product available to consumers (personal communication, from CCSPA, to the New Substances Assessment and Control Bureau, Health Canada, dated May 2017; unreferenced). According to the Canadian Toy Industry Association, PF is used as a polymer/pigment in toys (TIA 2017).

Considering the estimated negligible log K_{ow} (< - 4) and high molecular weight (average ~ 900 g/mole) for PF, meaningful dermal absorption (greater than 10%) is not expected (WHO 2006).

In conclusion, the direct exposure (oral, inhalation, dermal) of the general population to PF is expected to be minimal.

3.5.1.2 Indirect exposure

In the event of an unforeseen environmental release of PF, the substance is not expected to become widely distributed in the aquatic environment because of its low water solubility. PF is biodegradable and would convert to formaldehyde in aqueous media. In soil, the substance would likely volatilize slowly at ambient temperatures as formaldehyde. Consequently, the indirect exposure of the general population to PF through environmental media such as drinking water or air is expected to be minimal.

3.5.2 Health effects assessment

During evaluation under the second phase of polymer rapid screening, PF was identified as requiring further assessment as a result of a flag for potential pulmonary toxicity. Therefore, inhalation is considered the most critical route of exposure.

Because PF has the potential to release formaldehyde, the two substances are often evaluated together, as it is difficult to separate the toxicological effects of PF from those of formaldehyde. There is limited toxicological information on PF, but the toxicity of formaldehyde is well established (Environment Canada, Health Canada 2013).

A safety data sheet (SDS) by Ted Pella, Inc. (SDS 2015) for PF with a purity of 100% indicates that PF has a moderate acute oral toxicity in rats, with an oral LD_{50} of 800 mg/kg bw, and a low acute dermal toxicity in rabbits, with an LD_{50} of 10 000 mg/kg bw. PF has moderate inhalation toxicity with an LC_{50}/4 h of 1070 mg/m^3 (SDS 2012). PF is a skin and eye irritant and may be a sensitizer through inhalation and skin contact. The SDS noted that there may be liver effects based on human evidence. It is not listed as a carcinogen by the International Agency for Research on Cancer (IARC 2018), the National Toxicology Program (NTP 2016) or the National Institute for Occupational Safety and Health (NIOSH 2018).

In contrast, formaldehyde has a higher acute toxicity with a lower acute oral LD_{50} of 100 mg/kg bw in rats, an acute dermal toxicity in rabbits of 270 mg/kg and an acute inhalation toxicity/2 h LC_{50} of 203 mg/m^3 in rats. It is listed as a carcinogen by NTP (2010) and IARC (2012).

An SDS from the company Celanese states that PF was negative in a chromosomal aberration assay in Chinese hamster ovary (CHO) cells. However, PF was positive with and without metabolic activation in an *in vitro* sister chromatid exchange assay using CHO cells and was positive with and without metabolic activation in a mouse lymphoma cell gene mutation assay (SDS 2015a). This suggests that the test substance is mutagenic and clastogenic. However, the contributions of PF rather than formaldehyde to these effects cannot be established with the information provided.

3.5.3 Characterization of risk to human health

In this assessment, the human health risks were established through consideration of both the hazard and the direct and indirect exposure of the substance for current uses identified from a voluntary survey and from section 71 surveys conducted under CEPA, as well as from governmental databases.

There is limited toxicological information on PF. However, acute toxicity for PF is approximately 8 times less than that of formaldehyde. Although there is little subchronic or chronic data on PF, considering the acute results stated above and its larger molecular weight, it is anticipated that it has a lower toxicity than formaldehyde. On the basis of the known uses in Canada, the direct oral and dermal exposure to PF is expected to be minimal. Given that PF is a source material for formaldehyde, it is logical to anticipate that the product of breakdown, formaldehyde, is inherently toxic.

Because of the high vapour pressures of formaldehyde and PF, the US EPA concluded that inhalation would be the most critical route of exposure. Health Canada has assessed the health risks associated with formaldehyde and concluded that

formaldehyde is entering the Canadian environment in a quantity or concentration or under conditions that constitute or may constitute a danger to the environment on which life depends and a danger in Canada to human life or health (Environment Canada, Health Canada 2001). However, the applications for PF are not expected to significantly contribute to the formaldehyde exposure evaluated in the Priority Substances List Assessment Report for Formaldehyde.

The US EPA concluded that formaldehyde and PF were unlikely to affect human health when used in pesticide applications provided that risk reduction measures were implemented (US EPA 2008). Similar proposed measures are being implemented in Canada for the use of formaldehyde and PF in pesticides (Health Canada 2010b).

PF is not expected to pose a health risk as a result of inhalation. Direct consumer exposure to PF from industrial applications is expected to be negligible as only 2% of manufactured PF is used in products directly available to consumers and the resulting formaldehyde is chemically reacted with other components in the reaction mixture and is no longer present in the end use products. Trace quantities of formaldehyde may be present but are not sufficient to pose a health risk as it is not expected to significantly contribute to existing background concentrations of formaldehyde. There were no products containing formaldehyde in the household products database for PF (Household Products Database 2018).

Some direct exposure of users to PF may occur when used commercially by professionals as a fumigant or as a fixative in a laboratory. It is expected that users will wear personal protective equipment and will have only brief exposures during application or preparation. When used as a fumigant, it is expected that individuals are not present in the treatment area until the concentration of formaldehyde has returned to background levels. Exposure for medical applications is expected to be low, and it is anticipated that the benefits will outweigh any of the potential risks associated with the substance.

Given the current use patterns of PF and its low water solubility, significant releases to the environment are not expected. Therefore, there is no anticipated health risks associated with indirect exposure through drinking water.

Although PF has a moderate acute toxicity via the oral route and a moderate toxicity via inhalation, taking into consideration the direct and indirect exposure to PF from known applications in Canada, the overall human health risk from exposure to PF has been determined to be low.

4. Alcohol ethoxylate sulfates (AESs)

4.1 Substance identity

The three substances (see

Table 4-1) considered here are anionic surfactants that are collectively referred to herein as the alcohol ethoxylate sulfates (AESs) subgroup. The AESs subgroup is represented by the structure shown in Figure 4-1. AESs are synthesized through a series of chemical reactions, where a fatty (hydrocarbon) chain alcohol is ethoxylated, followed by a sulfation reaction to introduce the sulfate functionality, and lastly neutralized with a base to yield the final surfactant (Little 1991; Tadros 2012; Cowan-Ellsberry et al. 2014). The three AESs are a part of a broader class of anionic surfactants with different fatty alcohol chain lengths, varying degrees of ethoxylation, and different counter ion salts. This larger collection of AESs is referred to as the chemical class. The AESs class are typically represented using the shorthand notation, "CxEOnS", where x is the alkyl chain-length and n is the degree of ethoxylation (Cowan-Ellsberry et al. 2014). For example, an AESs with a 12 carbon alkyl chain (C) and two ethoxylate (EO) units can be represented by $C_{12}EO_2S$.

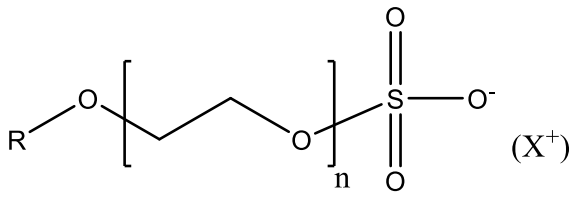
Given the similarities between AESs within this class of substances, read across data from within the class were also utilized where appropriate. However, this assessment will focus only on the three substances listed in

Table 4-1. Depending on the fatty alcohol chain, the degree of ethoxylation, and the counter ion involved, the number average molecular weight can range from 283 to greater than 900. The monomer and reactants for the three AESs surfactants are summarized in Table 4-2, Table 4-3, and

Table 4-4.

Table 4-1. Alcohol ethoxylate sulfates (AESs)

CAS RN	CAS name	Shorthand notation
67762-19-0	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-hydroxy-, C10-16-alkyl ethers, ammonium salts	$C_{10\text{-}16}EO_nS$
68585-34-2	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-hydroxy-, C10-16-alkyl ethers, sodium salts	$C_{10\text{-}16}EO_nS$
9004-82-4	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-(dodecyloxy)-, sodium salt	$C_{12}EO_nS$



n = number of repeating ethoxylate units

CAS RN 67762-19-0: R = C10-16, X^+ = Ammonium salt ($NH4^+$)

CAS RN 68585-34-2: R = C10-16, X^+ = Sodium Salt (Na^+)

CAS RN 9004-82-4: R = C12, X^+ = Sodium Salt (Na^+)

Figure 4-1. Representative structure of AESs

Table 4-2. Reactants composition for CAS RN 67762-19-0

Reactants	CAS RN
Alcohols, C10-16	67762-41-8
Oxirane	75-21-8
Sulfur trioxide	7446-11-9
Ammonium hydroxide ((NH4)(OH))	1336-21-6

Table 4-3. Reactants composition for CAS RN 68585-34-2

Reactants	CAS RN
Alcohols, C10-16	67762-41-8
Oxirane	75-21-8
Sulfur trioxide	7446-11-9
Sodium hydroxide (NaOH)	1310-73-2

Table 4-4. Reactants composition for CAS RN 9004-82-4

Reactants	CAS RN
Dodecanol	27342-88-7
Oxirane	75-21-8
Sulfur trioxide	7446-11-9
Sodium hydroxide (NaOH)	1310-73-2

4.2 Physical and chemical properties

The broader class of AESs are surfactants with variable number average molecular

weight and physical-chemical properties. Information gathered through a voluntary survey (ECCC 2015) as well as a mandatory survey conducted under section 71 of CEPA (Canada 2015) indicates that the three AESs subject to assessment here typically have number average molecular weights between 283 and 900. In addition, the survey data indicates the substances are highly water soluble, which is consistent with the surface active behaviour of surfactants. Vapour pressure data were not available for the three AESs. However, vapour pressure on the broader class of AESs indicates that vapour pressure of AESs is expected to be low. According to Urano et al. (1984), the K_{oc} determined for $C_{12}EO_5S$ is 1.1 L/kg.

4.3 Sources and uses

Information from the HERA (2004) report on AESs indicates that this class of substances is used in a multitude of applications spanning multiple sectors. They are commonly found in household and industrial cleaning products, personal care products, and other industrial products (HERA 2004).

The three AESs under assessment here have been included in a voluntary survey (ECCC 2015) as well as a mandatory survey conducted under section 71 of CEPA (Canada 2015).
Table **4-5** presents a summary of the total manufacture and import quantities for the substance in 2014. These sources indicate that the AESs subgroup is primarily used in products available to consumers and in pulp and paper manufacturing. Minor uses in paints and coatings, oil and gas recovery, and adhesive applications have also been reported.

Table 4-5. **Summary of information on Canadian manufacture and import quantities of the three AESs for 2014 submitted pursuant to a voluntary survey and a section 71 survey under CEPA**

CAS RN	CAS name	Total manufacture[a] (kg)	Total imports[a] (kg)
67762-19-0	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-hydroxy-, C10-16-alkyl ethers, ammonium salts	10 000–100 000	100 000–1 000 000
68585-34-2	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-hydroxy-, C10-16-alkyl ethers, sodium salts	100 000–1 000 000[b]	10 000 000–100 000 000
9004-82-4	Poly(oxy-1,2-ethanediyl), α-sulfo-ω-(dodecyloxy)-, sodium salt	100 000–1 000 000[b]	1 000 000–10 000 000

[a] Values reflect quantities reported in response to a voluntary survey (ECCC 2015) and a mandatory survey conducted under section 71 of CEPA (Canada 2015). See surveys for specific inclusions and exclusions (schedules 2 and 3).

[b] According to follow-up communications with industry, a major Canadian manufacturer ceased manufacturing operations in 2016.

4.4 Releases to the environment

According to the survey information, the three AESs were both manufactured in and imported into Canada in 2014. According to follow-up information, manufacturing of the AESs subgroup in Canada has mostly ceased, and these substances have been primarily imported into Canada since 2016. They are formulated in Canada into various products, such as cleaning products and personal care products. Depending on the application, substances in the AESs class in general may be formulated into various products at concentrations ranging from 1% to more than 50% (Robinson et al. 2010).

On the basis of the survey information, the three AESs are imported into Canada and reformulated into various products available to consumers, including shampoo, laundry detergents, soaps, and cleaners. Therefore, they could be released during formulation and through end-use applications.

4.5 Environmental fate and behaviour

4.5.1 Environmental distribution

As the three AESs in the subgroup being assessed are expected to behave similarly to the broader class of AESs, environmental distribution of the three AESs are based on read-across behaviour from the broader class. The AES class of substances comprises low molecular weight surfactants that are expected to have low vapour pressure (HERA 2004) and high water solubility. They are primarily used in down-the-drain products, such as cleaning products and personal care products. Literature studies of different AESs found that these surfactants are efficiently removed during wastewater treatment (WWT) (Little 1991; McAvoy et al. 1998; Matthijs et al. 1999; Scott and Jones 2000).

Once released to the environment, AESs in general are not expected to volatilize into the air compartment as they have low vapour pressure (HERA 2004). It is anticipated that they will undergo environmental biodegradation and be removed from the water column (Little 1991; McAvoy et al. 1998; Matthijs et al. 1999; Scott and Jones 2000).

If released to soil, the resulting polymer is expected to dissolve into soil pore water and to undergo biodegradation. Volatilization from the soil or soil pore water is not expected because of the expected low vapour pressure.

4.5.2 Environmental persistence

The broader class of AESs has been thoroughly studied over the years. In particular, the biodegradability of different AESs has been studied under various environmental conditions. Sibila et al. (2008) found that $C_{10\text{-}16}EO_3S$ reached a biodegradation level of 25% in 9 days and greater than 96% in 124 days in sea water. It was also reported that alcohol ethoxylate sulfates will undergo significant biodegradation under aerobic and

anaerobic conditions (Swisher 1970; Little 1991; Scott and Jones 2000; HERA 2004; Cowan-Ellsberry et al. 2014). Information submitted in mandatory and voluntary surveys (ECCC 2015; Canada 2015) indicated that the three AESs are readily biodegradable. Biodegradation of AESs may occur through a combination of three different pathways, namely i) ω-/β-oxidation of the alkyl chain, ii) enzymatic cleavage of the sulfate substituent leaving an alcohol ethoxylate, and iii) cleavage of an ether bond in the AESs molecule producing either the alcohol (central cleavage) or an alcohol ethoxylate and an oligo(ethylene glycol) sulfate (Swisher 1987; Steber and Berger 1995; HERA 2004). Complete biodegradation of AESs will yield CO_2, H_2O, and sulfate anions (Paulo et al. 2017), which are not expected to pose an ecological risk. On the basis of available biodegradation studies, the three AESs are expected to undergo extensive environmental biodegradation and are not expected to be persistent in the environment.

4.5.3 Bioaccumulation potential

According to summary information from Black and Howes (1992), different ^{14}C-labelled AESs ($C_{16}EO_{3,9}S$, $C_{11}EO_3S$, $C_{12}EO_3S$) orally administered to rats were eliminated from the body in urine, feces and CO_2. This suggests that the tested AESs will be eliminated from the body and have limited bioaccumulation potential.

Alcohol ethoxylates (AEs) are a class of nonionic surfactants that are structurally similar to the broader class of AESs. The difference between the two classes of substances is the presence of sulfate functionality in AES surfactants, which may cause differences in bioaccumulation potential between substances in the two classes. However, the results of AEs are considered to be indicative of the bioaccumulation potential of the broader class of AESs. AEs are taken up by fish and are eliminated from fish through rapid metabolism (Bishop and Maki 1980; Wakabayashi et al. 1987; Tolls et al. 1994; Environment Canada 2013). According to Tolls et al. (2000), AEs exhibited high biotransformation in fathead minnows (*Pimephales promelas*) and are expected to have a bioconcentration factor between < 5 L/kg and 390 L/kg. Comber et al. (2003) concluded that alkyl chains of surfactants can undergo ω- and β-oxidation in fish and rats with a number of anionic, nonionic and cationic surfactants, which includes AEs and AESs.

Considering that AES ($C_{16}EO_{3,9}S$, $C_{11}EO_3S$, $C_{12}EO_3S$) and structurally similar AEs surfactants are eliminated from biological organisms through biotransformation, the three AESs are not considered to have significant bioaccumulation potential.

4.6 Potential to cause ecological harm

4.6.1 Ecological effects assessment

Modelling of the three AES polymers was not performed, as there are sufficient ecotoxicological data available.

As noted in Section 4.1, the broader class of AESs are surfactants that are composed of different alkyl chain lengths, varying number of ethoxylate repeating units, and different

counter ion salts. Owing to the differences above, the toxicity for AESs can vary even for two polymers with the same CAS RN. For example, Dyer et al. (2000) reported 48-h LC_{50} acute toxicity for the freshwater invertebrate *Ceriodaphnia dubia* to range from 0.76 mg/L for $C_{15}EO_1S$ to 167.31 mg/L for $C_{15}EO_8S$. The differences in toxicity could be attributed to the changes in solubility of the surfactant as the ethoxylatelength increases.

Environmental toxicological effects of different AESs have been reported in various journal articles and risk assessment reports (RIVM 1995; Dyer et al. 2000; HERA 2004; Cowan-Ellsberry et al. 2014). The effects data are summarized in Table 4-6. Ecotoxicological effects studies for the three AESs considered here, were also submitted in response to the voluntary (ECCC 2015) and mandatory surveys (Canada 2015). The toxicity of the three AESs surfactants is similar to those reported in literature and falls within the typical toxicity range for other AESs.

The toxicity data reported are for different AESs surfactants with different counter ions, alkyl chain lengths, and varying degree of ethoxylate units. According to Little (1991), the sodium salt of $C_{12\text{-}14}EO_3S$ AES appears to be less toxic than for the same AESs with the ammonium salt. This could be the effect of the ammonium ions and not due to the AES. In addition, it was observed that AESs appear to be more toxic with increasing alkyl chain lengths (Little 1991; Dyer et al. 2000). Little (1991) further reported that for AESs with the same alkyl chain lengths (up to C_{16}), the surfactant becomes less toxic with increasing ethoxylate units. A similar trend was also observed in Dyer et al. (2000).

From Table 4-6, it can be seen that the toxicity of AESs to different species varies widely. Depending on the AES, toxicity can range from low to high in fish, algae, and invertebrates. The available data suggest that fish and invertebrates are the most sensitive species.

Table 4-6. Aggregate ecotoxicity data for AESs surfactants

Organism	Acute result (mg/L)[a]	Chronic results (mg/L)[a]
Algae [b]	EC_{50} = 2.45-1000	NOEC = 0.35–50.5
Invertebrate [b]	EC_{50} = 0.78-350	NOEC = 0.06–6.3
Fish [b]	LC_{50} = 0.3-375	NOEC = 0.1–2.2
Mesocosm (*Corbicula fluminea*) [c]	-	NOEC = 0.075
Mesocosm (*Goniobasis* spp) [c]	-	LOEC > 0.75
Mesocosm (*Periphyton*) [c]	-	NOEC = 0.61
Mesocosm (invertebrate spp) [c]	-	NOEC = 0.25
Mesocosm (Fish, invertebrate and algal taxa) [c]	-	NOEC > 2
Marine algae [d]	EC_{50}=4.68-24.02	NOEC=2.8-16.8
Marine invertebrates [d]	LC_{50}=23.92	-

[a] EC_{50} is the effect concentration for 50% of the population; LC_{50} is the lethal concentration for 50% of the population; NOEC is the no observed effect concentration; LOEC is the lowest observed effect concentration.
[b] Toxicological effects are extracted from summary information in Little 1991; RIVM 1995; Dyer et al. 2000; HERA 2004; Ivanković and Hrenović 2009; Cowan-Ellsberry et al. 2014.

[c] Toxicological effects are extracted from HERA 2004.
[d] Toxicological effects are extracted from Sibila et al. 2008.

Because each study utilizes different AESs the comparison of toxicity between studies is more difficult. Quantitative structure-activity relationship (QSAR) equations have previously been used to normalize the toxicity reported in literature (Cowan-Ellsberry et al. 2014; HERA 2004). The QSAR equations developed by Dyer et al. (2000) were used to normalize the chronic toxicity of invertebrates for each homologue series of AESs. The estimated predicted no effect concentration (PNEC) ranged from 0.035 mg/L to 0.89 mg/L for alkyl chain lengths between 12 and 18 carbons (HERA 2004). Cowan-Ellsberry et al. (2014) also reported the use of QSAR equations developed by Dyer et al. (2000) to normalize the diverse AESs toxicity to one single AES. The first step requires knowledge of which AES is most common in the environment. On the basis of the chronic toxicity, the 5th percentile species sensitivity distribution PNEC was estimated to be 0.073 mg/L for $C_{13.5}E_3S$ (Cowan-Ellsberry et al. 2014).

As there is no information on the most common AES present in Canadian environment, it is not considered feasible to calculate a PNEC value as reported in HERA (2004) and Cowan-Ellsberry et al. (2014). Therefore, the critical toxicity value (CTV), the chronic NOEC of 0.06 mg/L for invertebrate, was selected from the available dataset (Table 4-6).

The aquatic PNEC is derived from the CTV, which is divided by an assessment factor (AF) as shown:

$$\text{Aquatic PNEC} = \text{CTV} / \text{AF}$$

$$\text{Aquatic PNEC} = 0.06 \text{ mg/L} / 1$$

$$\text{Aquatic PNEC} = 0.06 \text{ mg/L or } 60.0 \text{ µg/L}$$

An overall AF of 1 is selected to estimate aquatic PNEC. The AF selected represents 1 for chronic toxicity and 1 for species sensitivity. The selected CTV is already a chronic value, so therefore it is unnecessary to apply a factor greater than 1 to standardize the CTV toxicity value. i.e., acute to chronic toxicity standardization. Also, considering the available ecotoxicity data for AESs (more than 3 categories and more than 7 species), a factor of 1 was selected to represent the species sensitivity variation.

A comparison of the estimated PNEC of 60.0 µg/L to those reported in HERA (2004) and Cowan-Ellsberry (2014) shows that the estimated PNEC falls within the PNEC range estimated using QSAR equations. Thus, the PNEC of 60 µg/L is considered reliable for use in the risk assessment of the three AESs.

4.6.2 Ecological exposure assessment

According to the data collected through the voluntary (ECCC 2015) and mandatory surveys (Canada 2015), the three AESs are used as surfactants in products available to consumers. Follow-up information gathered indicates that, while manufacturing of the three AESs in Canada has ceased, they continue to be imported into Canada. As there are no current manufacturing activities for the AESs subgroup in Canada, environmental exposure for the manufacturing for the AESs subgroup is not considered further.

According to the survey results, there are two major uses that can result in releases to the aquatic environment: formulation of the three AESs in products available to consumers and consumer release of products containing these substances. The following presents a summary of the exposure releases and calculation for the AESs subgroup, and the detailed exposure analyses are presented in the document Supporting Documentation: Ecological Exposure Analysis of Poly(Alkoxylates/Ether) (ECCC 2018).

The broader class of AESs have average removal rates ranging from 69.7% to 98.2%, depending on the WWT type involved (McAvoy et al. 1998). Effluent concentrations after WWT range from 4 µg/L to 58 µg/L, with one site having an effluent concentration of 167 µg/L (McAvoy et al. 1998). The site that reported the highest AESs concentration in the effluent was hydraulically overloaded and exceeded the maximum design capacity. However, the reported removal rate for this site was still 97.7%. It should be pointed out that the measured effluent concentration does not account for the dilution that will occur in surface water. Thus, the overall surface water concentration would be expected to be lower. For the purpose of this assessment, an overall average removal rate of 88%, calculated using the reported removal rate in McAvoy et al. (1998), is assumed for the three AESs.

Products available to consumers formulation

An exposure scenario was developed for the formulation of cosmetics and products available to consumers, such as laundry detergents and cleaners. The facilities involved in these activities discharge their treated or untreated wastewater to wastewater treatment systems[4] for final treatment before it is released to the aquatic environment. As not all formulators will have necessary equipment to pre-treat their wastewater prior to discharge into wastewater treatment systems (WWTS), for the purpose of this assessment, it is assumed that the formulator will discharge untreated wastewater into the WWTS.

The predicted environmental concentration (PEC) for the three AESs in receiving water

[4]In this assessment, the term “wastewater treatment system” refers to a system that collects domestic, commercial and/or institutional household sewage and possibly industrial wastewater (following discharge to the sewer), typically for treatment and eventual discharge to the environment. Unless otherwise stated, the term wastewater treatment system makes no distinction of ownership or operator type (municipal, provincial, federal, indigenous, private, partnerships). Systems located at industrial operations and specifically designed to treat industrial effluents will be identified by the terms “on-site wastewater treatment systems” and/or “industrial wastewater treatment systems”.

is estimated from the amount released to the WWTS, the effluent flow and the dilution factor of the receiving watercourse.

$$PEC = [10^9 \times Q \times E \times (1\text{-}R)] \div [F \times D \times N]$$

Where:

PEC: predicted environmental concentration in receiving water near discharge point, µg/L
Q: total quantity of AESs used per year, kg/y
E: emission factor to wastewater, unitless
R: overall wastewater treatment removal, unitless
F: daily wastewater flow, L/d
D: receiving water dilution factor near discharge point, unitless
N: number of operation days per year, d/y
10^9: conversion factor from kg to µg (µg/kg)

The scenario was based on known formulators, which would purchase surfactant blends from a supplier to formulate into various products. The highest use quantity for one of these formulators is in the range of 100 000 kg to 1 000 000 kg per year (ECCC 2015; Canada 2015). Considering the significant range reported for these formulators, the logarithmic average of this range is used for the calculations. The quantity (Q) of AESs that will be formulated at an individual facility is assumed to be 316 200 kg per year. Furthermore, it is assumed that the facility will operate 300 days per year (N) with an emission rate (E) of 0.3% (European Chemicals Bureau 2003). It is also assumed that the average WWTS removal rate (R) will be 88% for AESs. The 10^{th} percentile daily dilution volume[5] for WWTSs associated with industrial facilities is 2.289×10^7 L/d. This near-discharge-point exposure is taken as the aquatic PEC for AESs. The aquatic PEC is estimated to be 16.58 µg/L.

Down-the-drain consumer release

The three AESs are used primarily as surfactants in cosmetics and products available to consumers, such as cleaners and laundry detergents. AES-containing products are therefore expected to be released by consumers throughout Canada, and the down-the-drain consumer PEC is estimated using the Consumer Release Aquatic Model (CRAM 2017). CRAM is a Canadian population-based probabilistic model used to estimate environmental exposure resulting from down-the-drain release of chemicals present in products available to consumers, considering different wastewater treatment systems

[5] The daily dilution volume (L/d) is defined as the effluent flow of the WWTS or facility (L/d) discharging to the environment multiplied by the dilution factor offered by the receiving water body. Unless otherwise stated, the dilution factor is based on the 10th percentile low flow value of receiving water bodies and is limited to a maximum of 10 near discharge points.

types.

For the three AESs, a total mass in the range of 1 to 10 million kg/yr was reported for 2014 for use in cleaners, laundry detergents and personal care products (Canada 2015). For a conservative estimation, a maximum quantity of 10 million kg/yr was used in the prediction. The distribution of PECs for down-the-drain release of AESs is presented in Table 4-7.

Table 4-7. AESs distribution of PECs and risk quotients calculated by CRAM

Percentile [a]	PEC (µg/L)	Risk quotient
10	54.87	0.91
20	33.92	0.57
30	25.06	0.42
40	20.12	0.34
50	16.63	0.28
60	13.85	0.23
70	11.51	0.19
80	9.22	0.15
90	6.45	0.11
100	0.42	0.01

[a] The percentile is the distribution of the CRAM results.

4.6.3 Characterization of ecological risk

The approach taken in this ecological risk assessment was to examine direct and supporting information and develop conclusions on the basis of a weight-of-evidence approach. Lines of evidence considered include information on sources and fate of the substance, persistence, bioaccumulation, estimated exposure to the substance, and ecological hazard properties. The AESs subgroup comprises anionic surfactants that are used in various applications, including laundry detergents, soaps, and cleaners. On the basis of available information, more than 10 000 000 kg of the three substances in the AESs subgroup were imported into Canada in 2014.

According to the available information, the three AESs are expected to be dispersed in water. Partitioning into the air compartment and sediments is not expected due to low vapour pressure and low log K_{oc}, respectively. Furthermore, the three AESs are anticipated to undergo significant biodegradation under aerobic and anaerobic conditions. Degradants of AESs, namely CO_2, H_2O, and sulfate anions (Paulo et al. 2017), are not expected to pose an ecological risk and therefore were not considered further in this assessment.

Information in the form of bioaccumulation factor or bioconcentration factor test data that could be used to assess the bioaccumulation potential of the three AESs was unavailable. However, a read-across C^{14} elimination study of AESs ($C_{16}EO_{3,9}S$, $C_{11}EO_3S$, $C_{12}EO_3S$) in rats indicates that the studied AESs are rapidly eliminated from the body and do not accumulate. Furthermore, alcohol ethoxylates were reported to

have high metabolism rates in fish (Bishop and Maki 1980; Wakabayashi et al. 1987; Tolls et al. 1994; Environment Canada 2013) and are expected to have bioconcentration factors between < 5 L/kg and 390 L/kg (Tolls et al. 2000). On the basis of available information, the three AESs are expected to have low bioconcentration potential.

According to the ecological hazard profile for different AESs, the three substances could have ecotoxicities ranging from low to high for both acute and chronic toxicity. As a conservative assumption, the lowest chronic CTV was selected to estimate the PNEC. The PNEC for the three AESs is estimated to be 60 µg/L.

On the basis of the PNEC (60 µg/L) and the estimated formulator PEC (16.58 µg/L), the risk quotient (PEC/PNEC) was calculated to be 0.28. Furthermore, a series of risk quotients calculated on the basis of the varying PECs estimated from CRAM are presented in Table 4-7.

On the basis of the risk quotient estimated for environmental releases from industrial formulators and products available to consumers, neither scenario for AESs is expected to result in environmental concern (i.e., risk quotients greater than 1). However, the 10th percentile risk quotient calculated for CRAM is approaching 1. Considering that conservative values, such as the low CTV selected, and high volumes were used to estimate the PNEC and PEC, it is anticipated that the risk quotient is an over-estimation of the potential risk. Overall, the three AESs are not expected to result in ecological concern on the basis of available information.

4.7 Potential to cause harm to human health

Classification of the hazard data and exposure profiles used to develop the potential for human health risks associated with the three AESs are presented in the document ‘Supporting Documentation: Final Risk Matrix Location of Polymers’ (Health Canada 2017).

Although exposure was established as high, the human health hazard associated with the three AESs was determined to be low. Therefore, taking into consideration the available data, it is unlikely that exposure to the substance will pose a human health risk.

5. Alcohol ethoxylate (AEs)

5.1 Substance identity

The eight substances (see Table 5-1) under assessment are nonionic surfactants that are collectively referred to herein as the alcohol ethoxylates (AEs) subgroup. The AEs subgroup is represented by the structure shown in Figure 5-1. AEs are synthesized

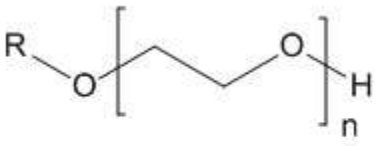
through a series of chemical reactions, where hydrophobic fatty alcohols of various chain lengths are joined to hydrophilic ethylene oxide units (i.e. ethoxylated) by an ether linkage under alkaline reaction conditions to give the final surfactant (Talmage 1994; Tadros 2012; Cowan-Ellsberry et al. 2014). The AEs under assessment are a part of a larger class of nonionic surfactants with different fatty alcohol chain lengths and varying degrees of ethoxylation. This larger collection of AEs is referred to as the chemical class.

Due to the similarity between all of the AEs in the subgroup and between the larger chemical class, data utilized in this screening assessment were obtained from the eight AEs (where available) and from the broader chemical class.

AEs are often represented using the shorthand notation "C_xEO_n", where x is the alkyl chain-length and n is the degree of ethoxylation. The fatty alcohol chain lengths can vary in number of carbons and degree of linearity. In addition, the degree of ethoxylation also varies for this type of surfactant. The carbon chain length is typically 8 to 18 carbons long; the carbon backbone is usually a primary structure, while the number of ethoxylate (EO) repeating unitstypically ranges from 3 to 10-12. Considering the typical fatty alcohol chain and the degree of ethoxylation, the number average molecular weight can range from 174 to 798.

Table 5-1. AEs surfactants

CAS RN	CAS name
9002-92-0	Poly(oxy-1,2-ethanediyl), α-dodecyl-ω-hydroxy- (i.e. C_{12} ethoxy homologue)
66455-14-9	Alcohols, C_{12-13}, ethoxylated
68002-97-1	Alcohols, C_{10-16}, ethoxylated
68131-39-5	Alcohols, C_{12-15}, ethoxylated
68439-45-2	Alcohols, C_{6-12}, ethoxylated
68439-46-3	Alcohols, C_{6-11}, ethoxylated
68439-50-9	Alcohols, C_{12-14}, ethoxylated
68951-67-7	Alcohols, C_{14-15}, ethoxylated



R = C_8 to C_{18} (typical)
n = number of repeating ethoxylate (EO) units

Figure 5-1. Representative structure of AEs

5.2 Physical and chemical properties

Since substances in the AE surfactant subgroup have a range of number average molecular weights with varying amounts of ethoxylation (which is related to hydrophilicity), their physical-chemical properties can vary as well. The primary manifestation of this variation is in their water solubility. The safety data sheets (SDS) for the subgroup of AEs listed in Table 5-1 use a variety of descriptions for water solubility such as completely soluble, soluble, dispersible, miscible, will emulsify, partly soluble and insoluble. The solubility of the alcohol ethoxylates depends on both the alkyl chain length and the number of EO units. Molecules with an average alkyl chain length of 12 or fewer carbon atoms and with 5 or more EO units are usually fully soluble in water at room temperature (Tadros 2012). AEs are surface active and can form micelles at sufficiently high concentrations. Their 'solubility', which would include the critical micelle concentration, is in the single digit milligram per litre range and above. The solubility increases with the number of EO units (HERA 2009).

Vapour pressure data are not available for the eight AEs under assessment. However, the vapour pressure for the broader class of alcohol ethoxylates is expected to be low since the corresponding vapour pressure for the pure alcohols, which would provide an upper bound for vapour pressure, have been measured and are themselves low. Since the water affinity of the AE surfactant class is relatively high, this, combined with their low expected vapour pressures, would suggest that the Henry's law constant is low and hence, evaporation from aqueous media would be insignificant.

For most organic chemicals, the octanol-water partition coefficient (K_{ow}) is a highly useful and relatable property for determining such characteristics as adsorption to organic matter (in soils, sediments, dissolved organic carbon for example) and for determining bioaccumulation and eco-toxicity. However, K_{ow} is difficult to measure for surfactants since they preferentially locate at the octanol/water interface(s). The environmental fate and distribution of surfactants tends to be driven by adsorption and surface effects rather than by traditional K_{ow}-driven partitioning. For these reasons, K_{ow} is not often used as a parameter in environmental risk assessments of surfactants when evaluating environmental fate. Despite this, some collections of K_{ow} exist for the class of AE surfactants (HERA 2009; Cowan-Ellsbury et al. 2014). They have been reported to vary from a log K_{ow} of approximately 8.5 down to about 1. The log K_{ow} value tends to decrease with an increasing EO unit number (higher hydrophilicity) and tends to increase with the longer alkyl chains from the relevant alcohol (higher lipophilicity).

5.3 Sources and uses

Both the subgroup of AEs and the larger class are general nonionic surfactants used in many applications spanning multiple chemical sectors. AEs are predominantly used in laundry and dishwashing detergents as well as in household, industrial and institutional cleaners. They can also be found in personal care products, such as shampoos, body washes, liquid hand soap, and in hand dishwashing detergents. Lesser amounts are found in the pulp and paper, oil and gas, cosmetic, textile and agricultural sectors

(HERA 2009). Large quantities of substances in the AE class are also used as feedstocks in the manufacture of alcohol ethoxysulfates (AES) surfactants by the process of sulfonation.

The eight AE surfactants under assessment have been included in a voluntary survey (ECCC 2015) as well as a mandatory survey conducted under section 71 of CEPA (Canada 2015).
Table 5-2 presents a summary of the total manufacture and import quantities reported for these substances for 2014. These surveys indicate that the AE subgroup members are primarily used in cleaning products and personal care products. Minor uses in paints and coatings, oil and gas recovery, lubricants and adhesive applications have also been reported.

Table 5-2. Summary of information on Canadian import quantities of the eight AE subgroup members in 2014 submitted pursuant to a voluntary survey and a section 71 survey under CEPA

CAS RN	CAS name	Total manufacture[a] (kg)	Total imports[a] (kg)
9002-92-0	Poly(oxy-1,2-ethanediyl), α-dodecyl-ω-hydroxy-	100 000 – 1 000 000[b]	100 000 – 1 000 000
66455-14-9	Alcohols, C_{12-13}, ethoxylated	100 000 – 1 000 000[b]	100 000 – 1 000 000
68002-97-1	Alcohols, C_{10-16}, ethoxylated	100 000 – 1 000 000[b]	100 000 – 1 000 000
68131-39-5	Alcohols, C_{12-15}, ethoxylated	1 000 000 – 10 000 000[b]	1 000 000 – 10 000 000
68439-45-2	Alcohols, C_{6-12}, ethoxylated	1 000 000 – 10 000 000[b]	100 000 – 1 000 000
68439-46-3	Alcohols, C_{6-11}, ethoxylated	1 000 000 – 10 000 000[b]	1 000 000 – 10 000 000
68439-50-9	Alcohols, C_{12-14}, ethoxylated	1 000 – 10 000[b]	1 000 000 – 10 000 000
68951-67-7	Alcohols, C_{14-15}, ethoxylated	0	100 000 – 1 000 000

[a] Values reflect quantities reported in response to a voluntary survey (ECCC 2015) and a mandatory survey conducted under section 71 of CEPA (Canada 2015). See surveys for specific inclusions and exclusions (Schedules 2 and 3).

[b] According to follow-up communications, a major Canadian chemical manufacturer has ceased production of these ethoxylated alcohol surfactants as of the end of 2016. The manufacturing quantities minus the quantity exported from Canada are included in the calculations for predicted environmental concentrations (PECs) thus making them more conservative.

5.4 Releases to the environment

According to survey information, members of the AE subgroup were both manufactured in and imported into Canada in 2014. It was subsequently learned that manufacturing of these AEs in Canada has now ceased and that, as of the end of 2016, they are only

imported into Canada. The eight AEs are formulated in Canada into different products, such as laundry products, various cleaning products and personal care products. Depending on the application, alcohol ethoxylates, as a class, may be formulated into different products at concentrations up to 24% (HERA 2009). Therefore, the AEs under consideration in this assessment could be released during formulation and through end-use applications. Considering the use pattern of these products, it is expected that all members of the AE subgroup would be completely released to wastewater treatment systems during use.

5.5 Environmental fate and behaviour

5.5.1 Environmental distribution

Substances in the AE class are low molecular weight surfactants that are expected to have low vapour pressure (HERA 2009) and a range of water solubilities—from completely water soluble to insoluble—depending on alkyl chain length and degree of ethoxylation. AEs are primarily used in down-the-drain products, such as cleaning products and personal care products. Studies for different AE class members indicates that these surfactants are efficiently removed during wastewater treatment (WWT) (Talmage 1994, McAvoy et al. 1998, Matthijs et al. 1999, Scott and Jones 2000). Once released into the environment, AEs are not expected to volatilize as they are expected to have low vapour pressure (HERA 2009). Substances in the AE class are anticipated to undergo environmental biodegradation and to be removed from the water column (Talmage 1994; McAvoy et al. 1998; Matthijs et al. 1999; Scott and Jones 2000).

AEs can potentially be transferred from the water column to material such as suspended inorganic and organic matter, activated sludge, or sediment by adsorption depending upon the properties of the individual AE homologue (carbon length and degree of ethoxylation) and the properties of the material to which it is adsorbed.

If released to soil, the eight AEs under assessment are expected to dissolve into soil pore water or become adsorbed to organic matter where it is expected that they would then biodegrade. Volatilization from the soil or soil pore water is not expected because of the low expected vapour pressure of AEs.

5.5.2 Environmental persistence

Information submitted in response to voluntary and mandatory surveys (ECCC 2015; Canada 2015) indicates that the eight AEs are readily biodegradable. In addition, the biodegradability of alcohol ethoxylates in the environment has been thoroughly studied over many years. It has been reported that they will undergo rapid biodegradation under both aerobic and anaerobic conditions, under both laboratory and field conditions (Swisher 1987; Talmage 1994; Scott and Jones 2000; HERA 2009; Cowan-Ellsberry et al. 2014). The biodegradability of the different AE homologues is relatively unaffected by the alkyl carbon chain length and the number of EO units. Linear AEs are normally easily degraded under aerobic conditions, with only small differences in the time needed

for their ultimate degradation. Degradation under anaerobic conditions is slower than under aerobic conditions. In addition, the degree of alkyl chain branching increases the time needed for ultimate degradation. The mechanism of biodegradation for the AE class is the same as that of the AES class, described above in section 4.5.2.

On the basis of available biodegradation studies, the eight AEs under assessment are expected to undergo extensive environmental biodegradation and are not expected to be persistent in the environment.

5.5.3 Bioaccumulation potential

Limited bioconcentration data for the AE class in fish are available in the published literature.

The majority of the data available are based on studies using ^{14}C-radiolabelled compounds that do not allow the distinction between the parent compound and metabolites. Therefore, the bioconcentration factors for the parent compound are likely overestimated in these types of experiments (Madsen et al. 2001). By use of these ^{14}C-labelled surfactants, whole body concentration ratios (BCFs) have been estimated for four various AEs in fish. These range from < 5 L/kg to 799 L/kg (Bishop and Maki 1980; Wakabayashi et al. 1987; Tolls et al. 1994, 2000; Environment Canada 2013).

As a class, AEs are taken up by fish but are rapidly metabolized and eliminated (Bishop and Maki 1980; Wakabayashi et al. 1987; Tolls et al. 1994, 2000; Environment Canada 2013). Tolls et al. (2000) found that these surfactants were not stored in fathead minnows (*Pimephales promelas*) because of high biotransformation in the fish and are expected to have bioconcentration factors between < 5 L/kg and 390 L/kg. Comber et al. (2003) concluded that alkyl chains of surfactants can undergo ω- and β-oxidation in fish and rats with a number of anionic, nonionic and cationic surfactants, which includes AEs.

Considering that AE surfactants as a classare eliminated from biological organisms through biotransformation, the eight AEs under assessment are not considered to have significant bioaccumulation potential.

5.6 Potential to cause ecological harm

5.6.1 Ecological effects assessment

As noted in Section 5.1, AEs are a class of surfactants composed of different alkyl chain lengths and varying numbers of ethoxylate repeating units. Because of this structural variation, the toxicity for AE class members can vary significantly even for two polymers of the same CAS RN. In general, the toxicity of individual homologues increases with increasing alkyl chain length and, conversely, toxicity decreases with increasing number of ethoxylate units.

The environmental toxicological effects of various AE class members have been reported in numerous journal articles, review articles and risk assessment reports. In addition, data on the ecotoxicological effects of the eight AEs under assessment were also gathered through voluntary (ECCC 2015) and mandatory surveys (Canada 2015). The toxicity of the eight AE surfactants were found to be similar to those reported in the literature and fall within the reported toxicity range for both acute and chronic toxicity.

Because the various ecotoxicological studies reported in the literature have utilized different mixtures of AEs consisting of different homologue amounts, comparison of toxicity from one study to the next is difficult (Cowan-Ellsberry et al. 2014). Quantitative structure-activity relationship (QSAR) equations have therefore been developed to normalize the toxicity reported. HERA (2009), Cowan-Ellsberry et al. (2014) and Environment Canada (2013) have used QSAR equations to normalize both acute and chronic toxicity of several aquatic species to a set of homologues of specific chain lengths and specific number of ethoxylate units.

A Federal Water Quality Guideline (FWQG) for Alcohol Ethoxylates has been developed for Canada (Environment Canada 2013). The first step in the development of the FWQG was to identify the average homologue distribution in Canadian municipal wastewater effluents based on monitoring data. This was found to be $C_{13.7}EO_5$. A set of $LC_{20}\backslash EC_{20}$ chronic aquatic toxicity data were then obtained for three fish species, eight invertebrate species and six plant species and normalized to the average homologue species, namely $C_{13.7}EO_5$. Finally, a set of species sensitivity distribution (SSD) curves were fitted to this chronic toxicity dataset. A logistic model provided the best fit of the models tested, and the 5^{th} percentile (HC5) of the SSD curve was determined to be 70 µg/L, with lower and upper confidence limits of 50 and 110 µg/L.

This value of 70 µg/L was recommended as the default Canadian FWQG. This value will be used as the critical toxicity value or CTV for the eight alcohol ethoxylates considered in this assessment, in particular as seven of the eight alcohol ethoxylates listed in Table 5-1 are specifically identified as substances to which the FWQG applies.

$$\text{Aquatic PNEC (mg/L)} = \text{CTV} / \text{AF}$$

$$\text{Aquatic PNEC} = (0.070 \text{ mg/L}) / 1$$

$$\text{Aquatic PNEC} = 0.070 \text{ mg/L} = 70 \text{ µg/L}$$

An AF of 1 is selected to obtain the aquatic PNEC. The AF selected represents 1 for chronic toxicity and 1 for species sensitivity. The selected CTV is already a chronic value, so therefore it is unnecessary to apply a factor greater than 1 to standardize the CTV toxicity value (i.e., not necessary to conduct an acute-to-chronic toxicity standardization). Also, considering the large amount of ecotoxicity data available for the AE class (more than 15 different species, covering more than 10 taxonomic groups), a factor of 1 was selected to represent the species sensitivity variation.

Modelling of AEs was not performed, as there are sufficient experimental ecotoxicological data available.

5.6.2 Ecological exposure assessment

According to data collected through voluntary (ECCC 2015) and mandatory surveys (Canada 2015), the eight AEs under assessment are used primarily in the following applications: products available to consumers such as cleaners, oil and natural gas extraction, pulp and paper, adhesives and sealants, lubricants and greases, paints and coatings.

One company has reported the manufacture and import of AEs and surfactant blends (Environment Canada 2015). In December 2016, this facility ceased all production of AEs and currently only imports such products for sale (personal communication, industry stakeholder - ethoxylated surfactants, 2017). No other company manufactures AEs (including the eight substances under assessment) in Canada and, in the future, such nonionic surfactants are expected to be only imported into Canada. Therefore, no exposure scenario for the manufacturing of AEs was developed.

According to survey data, the major uses of the eight AEs that can result in releases to the aquatic environment are through the formulation of various products, such as personal care products, cleaners and laundry detergents, through commercial or consumer release of products containing these surfactants, and through release by the pulp and paper industry. The following presents a summary of the exposure releases of AEs, which are presented in detail in the document ‘Supporting Documentation: Ecological Exposure Analysis of Poly(Alkoxylates/Ethers)’ (ECCC 2018).

Although activities relating to oil and natural gas extraction have been identified, no quantitative scenario has been developed for this sector because process waters used in onshore oil field applications are not normally discarded to sewers or to the freshwater aquatic environment. Under normal onshore oil field applications, the process water is used for oil well stimulation or is disposed of through deep well injection in North America (OECD 2012).

Use of AEs in the pulp and paper sector

According to survey information, one or more of the eight AEs under assessment are used in the manufacture of products by paper mills. They can be used as flocculants, processing aids, retention aids, felt cleaners and otheruses. The products used as retention and drainage aids are expected to be retained at 98% in paper and 2% in sludge. However, any of the eight specific AEs used in the pulp and paper water treatment process could have 100% release to wastewater. The latter is used as a conservative assumption for the calculations.

Although most of the survey submission information stated that products containing the eight AEs are used as retention and drainage aids (i.e. no release to water), an

exposure scenario was developed to account for other possible uses, including processing aids and water treatment in the papermaking process.

The annual use quantity at pulp and paper mills ranged between 1 000 and 10 000 kg/yr, and the upper limit of the range was used. PECs were calculated using a distribution of daily dilution volumes (L/d) based on information relevant to pulp and paper mills (wastewater flow, dilution). The 10^{th} percentile aquatic PEC was calculated as 34 µg/L and is selected as a suitable representative PEC.

In addition to this generic scenario, a second approach was considered for a representative worst-case facility, using the eight AEs in a number of applications, to determine whether this large use site would be of concern.

This second approach is based on the highest quantity of alcohol ethoxylates reported to be used at a single mill. The amount reported was stated for use in pulp and paper applications but did not specify where and how it was used in the process. It was conservatively assumed that it would be 100% released to wastewater. Site-specific information from this mill was used to calculate the PEC. The PEC calculated is 21.5 µg/L.

Formulation for products available to consumers

The formulation scenario is based on reported amounts of substances in the AE subgroup and is estimated using a generic indirect discharge scenario. The scenario considers facilities associated with the blending of these AEs to produce various cosmetics and products available to consumers, such as cleaning products and laundry detergents, as well as formulation facilities for adhesives and sealants, paints and coatings, lubricants, and automotive care products.

The predicted environmental concentration (PEC) of these AEs in receiving water is estimated from the amount released from WWTSs, their effluent flow and the dilution factor for each receiving watercourse.

$$PEC = [10^9 \times Q \times E \times (1\text{-}R)] \div [F \times D \times N]$$

where

- PEC: predicted environmental concentration in receiving water near a discharge point, µg/L
- Q: a substance's annual use quantity at a facility, kg/year
- E: emission factor to wastewater, unitless
- R: wastewater treatment removal, unitless
- F: daily wastewater flow, L/d
- D: receiving water dilution factor near discharge point, unitless
- N: number of annual operation days, d/y
- 10^9: conversion factor from kg to µg (µg/kg)

The wastewater treatment removal of the AE class has been widely studied and reported in the literature. They are known to be highly biodegradable. HERA (2009) presented a series of OECD ready tests (OECD 1992), cited from various references, indicating that the different alcohol ethoxylates are readily biodegradable. The lowest reported removal rate was 97.3% in the reviewed literature. For the purposes of this assessment, a more conservative wastewater removal rate of 95% for all treatment types was used in the PEC calculation.

The generic indirect discharge scenario for the various formulated products is based on the reported import quantity range of the eight AEsunder asssessment. The highest use quantity for one of these formulators is in the range of 1 000 000 kg to 10 000 000 kg per year. Considering the significant range presented, the logarithmic average of this range is used for the calculations. The quantity (Q) of AEs that will be formulated at an individual facility is assumed to be 3.162×10^6 kg per year. Furthermore, it is assumed that a facility will operate 300 days per year (N) with an emission rate (E) of 0.3%. The maximum WWTS removal rate (R) is 95%. The 10^{th} percentile daily dilution volume associated with industrial facilities is 2.289×10^7 L/d. This near-discharge-point exposure is taken as the aquatic PEC for AE. Using these inputs, the aquatic PEC was calculated to be 69.1 µg/L.

In addition to this generic scenario covering formulation activities, the concentration of AE in receiving water resulting from the activity specifically associated with the facility reporting the highest use quantity was also calculated to ensure that this large use site would not represent a risk. The same assumptions, inputs and calculations were used as above, but the actual daily effluent flow and dilution associated with this formulation facility were used in the calculation. This resulted in an aquatic PEC of 10.49 µg/L.

Down-the-drain consumer releases

The consumer use scenario assumes release of products available to consumers to a WWTS since these products are expected to be widely used by many consumers across the country and the quantities released to the sewer are subject to wastewater treatment and discharge.

A “down-the-drain” calculation was developed for the AE subgroup when used as surfactants in such products as cleaners, laundry detergents and personal care products. As consumer releases of AE-containing products are expected to occur throughout Canada, the consumer PEC is estimated using CRAM (CRAM 2017).

For a worst-case scenario, CRAM was run with a quantity of 10 million kg/yr—which is beyond what was reported under the CEPA section 71 survey—in order to account for maximum uses of AEs. This analysis was done to determine those conditions that have potential to cause harm. A wastewater removal rate of 95% was assumed for all wastewater treatment types. The distribution of PECs for down-the-drain analysis is presented in

Table 5-3.

Given the assumptions of the scenario, the 10th percentile of the distribution of the CRAM results is selected as a suitable representative aquatic PEC.

Table 5-3. Distribution of PECs and risk quotients of AEs calculated by CRAM

Percentile [a]	PEC (µg/L)	Risk quotient
10	16.76	0.24
20	10.00	0.14
30	7.47	0.11
40	5.99	0.09
50	5.00	0.07
60	4.18	0.06
70	3.45	0.05
80	2.75	0.04
90	1.98	0.03
100	0.06	0.001

[a] The percentile is the distribution of the CRAM results.

5.6.3 Characterization of ecological risk

The approach taken in this ecological risk assessment was to examine direct and supporting information and develop conclusions on the basis of a weight-of-evidence approach. Lines of evidence considered include information on sources and fate of the substance, persistence, bioaccumulation, estimated exposure to the substance, and ecological hazard properties. On the basis of available information, between 1 million and 10 million kg of any individual AE was used in Canada in 2014. Due to their physical-chemical properties, AE subgroup members are expected to be dispersed in water, but are not likely to partition either to air or sediment. Furthermore, the eight AEs under assessment would be highly biodegradable in the environment and have low bioaccumulation potential. The PNEC for the eight AEs under assessment is estimated to be 70 µg/L, based on the Canadian Federal Water Quality Guideline.

The predicted environmental concentrations for formulation (69 µg/L), use of products available to consumers (17 µg/L) and use in the pulp and pulp sector (34 µg/L) are below the PNEC value (70 µg/L). Consequently, on the basis of any calculated risk quotients (PEC ÷ PNEC) for the environmental release scenarios presented, the eight AEs under assessment are not expected to represent an environmental concern (i.e., risk quotients are less than 1). The generic indirect discharge does show a risk quotient approaching 1. However, considering that conservative values, such as a lower WWTS removal rate, and higher use quantities (typically the upper range of the reported volume range) were used to estimate the PECs, it is reasonable to anticipate that these calculated risk quotients would be an over-estimation of the potential risk. Overall, on the basis of available information, the eight AEs under assessment are not expected to result in an environmental concern.

5.7 Potential to cause harm to human health

Classification of the hazard data and exposure profiles used to develop the potential for human health risks associated with alcohol ethoxylates are presented in the document 'Supporting Documentation: Final Risk Matrix Location of Polymers' (Health Canada 2017).

Although exposure was established as high, the human health hazard for the eight AEs under assessment was determined to be low . Therefore, taking into consideration the available data, it is unlikely that exposure to the eight substances in the AE subgroup will pose a human health risk.

6. Octylphenol ethoxylates (OPEs)

6.1 Substance identity

The two substances (see Table 6-1) under assessment are nonionic surfactants, collectively referred to herein as the octylphenol ethoxylates (OPEs) subgroup. OPEs are represented by the structure shown in Figure 6-1. They are synthesized by first reacting diisobutylene with phenol under acidic conditions. Subsequently the final OPE is produced by reacting the relatively hydrophobic octylphenol with hydrophilic ethylene oxide units (i.e. ethoxylated) via an ether linkage under alkaline conditions, giving the final surfactant (Talmage 1994). The OPE subgroup under assessment is part of a larger collection of nonionic surfactants with various fatty alcohol chain lengths and varying degrees of ethoxylation. This larger collection of OPEs is referred to herein as the OPE class.

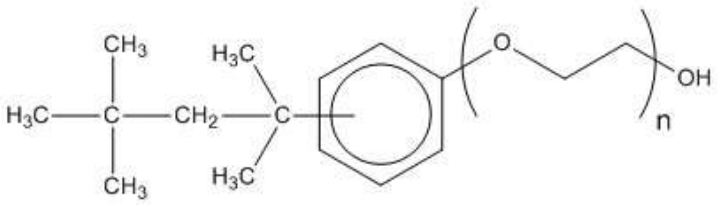
OPEs are often represented by the shorthand notation, "$OPEO_n$" or "OPE_n" or sometimes "OP_nEO", where n is the number of ethoxylate units or degree of ethoxylation. The degree of ethoxylation varies, and it has been reported that similar surfactants (ethoxylated nonylphenol) become completely water soluble when n is greater than 6 (Talmage 1994). For a typical degree of ethoxylation of 9 or 10 for commercial products, the number average molecular weights would be 602 and 646, respectively (Swisher 1987).

The two substances under assessment are members of a broader chemical class of octylphenol ethoxylate surfactants. Given the paucity of test data available for these two substances, read-across was used to derive physical-chemical properties, information on environmental fate and ecotoxicity data. This is a technique for predicting the properties of substance(s) (in this case, the two OPE substances) by using data for the same properties from other substances (in this case, the broader class of OPE surfactants). This approach is possible because the various chemical and environmental properties are consistent across the subgroup and class members. Additionally, this read-across approach was supplemented by data published in the

scientific literature and from reference sources.

Table 6-1. OPE surfactants

CAS RN	CAS registry name
9002-93-1	Poly(oxy-1,2-ethanediyl), α-[4-(1,1,3,3-tetramethylbutyl)phenyl]-ω-hydroxy-
9036-19-5	Poly(oxy-1,2-ethanediyl), α-[(1,1,3,3-tetramethylbutyl)phenyl]-ω-hydroxy-



n = number of repeating ethoxylate (EO) units; i.e. degree of ethoxylation.

The octyl group can be at the *para* position relative to the ethoxylate group for CAS RN 9002-93-1 or it can be at an unspecified position (as shown) for CAS RN 9036-19-5. Typically the *para* position isomer predominates in the mix representing over 90% of all the isomers.

Figure 6-1. Representative structure of OPEs

6.2 Physical and chemical properties

The OPE surfactant subgroup has a range of molecular weights due to varying amounts of ethoxylation (a property related to hydrophilicity). It also has varying amounts of octyl chain branching. A consistent trend is that water solubility increases with the number of ethoxylate (EO) units and degree of octyl branching. The safety data sheets (SDSs) for the compounds listed in Table 6-1 use a variety of descriptions for water solubility, such as soluble, completely soluble, readily soluble and fully miscible. The two OPE substances under assessment will be regarded as fully water soluble considering they are used as aqueous surfactants (see Section 6.3).

For many discrete organic chemicals, the octanol-water partition coefficient (K_{ow}) is the primary factor for determining such properties as adsorption to organic matter (e.g., in soils, sediments, dissolved organic carbon) and for determining bioaccumulation and ecotoxicity. However, K_{ow} is difficult to measure for surfactants since they preferentially locate at the octanol/water interface. Also, the environmental fate and distribution of surfactants tend to be driven by adsorption and surface effects rather than by traditional K_{ow}-driven partitioning. For these reasons, K_{ow} is not often used as a parameter in environmental risk assessments of surfactants when evaluating environmental fate.

However, despite these limitations, there are some reported log K_{ow} values available for

the larger class of OPEs and ethoxylated nonylphenols (NPEO or NPE), a similar surfactant class, which contains one more carbon in the alkyl chain than an OPE. $NPEO_9$ has a reported log K_{ow} value of 3.59 (Environment Canada, Health Canada 2001). A log K_{ow} value of 2.7 (estimated) was listed in the SDS for a commercial product (SDS for Sigma-Aldrich product number N6507, CAS RN 9036-19-5, purity ~95%), but there was no indication of the degree of ethoxylation. In addition, for $OPEO_8$, ECHA has reported log K_{ow} values of 2.94, 3.49 and 3.82 (ECHA 2012). The ECHA report also states that no physical-chemical properties could be found for the four octylphenol ethoxylate compounds considered (including CAS RN 9002-93-1) in accepted databases nor were any registration dossiers available.

The vapour pressure of substances in the OPE subgroup is low: 0.01 mm Hg 20°C (SDS for Nonidet-P40 (NP40), CAS RN 9002-93-1, purity 90-100%), < 1.00 mm Hg at 20 °C (SDS for Sigma-Aldrich Triton™ X-100, CAS RN 9002-93-1, purity <=100%) and 2.75×10^{-12} mm Hg (calculated value) for $OPEO_8$ (ECHA 2012). In addition, for CAS RN 9002-93-1 with one unit of ethoxylation (MW = 250.38), the vapour pressure has been estimated to be 3×10^{-6} mm Hg at 25 °C (SRC 2017). These low vapour pressures, combined with the known high water solubility of OPE surfactants, would suggest that the Henry's law constant is low and hence evaporation from aqueous media would be insignificant.

6.3 Sources and uses

The two substances under assessment were included in a voluntary survey (ECCC 2015) as well as a mandatory survey conducted under section 71 of CEPA (Canada 2015). Table 6-2 presents a summary of the reported total manufacture and import quantities for these two substances for 2014. These same sources indicate that these two substances can have a range of uses functioning as surfactants. The largest uses are found in oil and natural gas extraction, in the coatings sector (additive in paints, coatings, sealants and adhesives), in solvents for cleaning and degreasing, and in chemical manufacturing (emulsion polymerization). Minor uses have been reported in printing ink manufacturing, as part of scaling and corrosion inhibitor products, in soap and cleaning compound manufacturing, as plasticizers, in the manufacture of food packaging containers and also as part of pesticide formulations. Most often the range of concentrations used in these products is low, at around 0.01% to 2%. However, for some uses, the concentration can be significantly higher, such as in oilfield extraction at maximum reported concentrations of 10% to 23% and up to 5% to 15% in cleaners/degreasers.

According to a major manufacturer of OPEs (Dow 2015), the OPE chemical class of surfactants is commonly used in paints, emulsions and wetting agents and are a type of alkylphenol ethoxylate (APE) often sold under the trade name TRITON™ X octylphenol ethoxylate surfactants, where X is a number such as 100. This series of surfactants, i.e. the larger chemical class, has been primarily used in industrial and paint/emulsion applications. However, they can be used for many applications, such as emulsifiers (in the manufacture of emulsion polymers), as stabilizers (in latex polymers), as coatings

(for pigment wetting and stabilization in coatings), in agriculture (as emulsifiers or dispersants) and in cleaning products (minor use), such as liquid, paste, or powdered cleaning compounds, and heavy-duty industrial products.

Table 6-2. Summary of reported information on Canadian manufacturing and import quantities of the two OPE surfactants in 2014 submitted pursuant to a voluntary survey and to a survey under section 71 of CEPA

CAS RN	CAS Registry Name	Total manufacture[a] (kg)	Total imports[a] (kg)
9002-93-1	Poly(oxy-1,2-ethanediyl), α-[4-(1,1,3,3-tetramethylbutyl)phenyl]-ω-hydroxy-	0	10 000 – 100 000
9036-19-5	Poly(oxy-1,2-ethanediyl), α-[(1,1,3,3-tetramethylbutyl)phenyl]-ω-hydroxy-	100 000 – 1 000 000[b]	10 000 – 100 000[b]

[a] Values reflect quantities reported in response to a voluntary survey (ECCC 2015) and a mandatory survey conducted under section 71 of CEPA (Canada 2015). See surveys for specific inclusions and exclusions (schedules 2 and 3).

[b] Further to follow-up communications with a major Canadian manufacturer, it provided manufacturing and import quantities for 5 months and these quantities were then extrapolated over the entire year. Additionally, the manufacturing of OPEs in Canada has ceased since the surveys were conducted.

6.4 Releases to the environment

Survey information indicates that the two OPEs under assessment could be released during formulation and through end-use applications in Canada. Considering the use pattern of the products mentioned above, it is expected that the two OPEs would be released primarily to wastewater treatment systems. However, it is also possible they could be released to agricultural soil from chemical use or from cleaning and degreasing operations. Additionally, these two OPEs may be deep-well injected as part of waste disposal from petroleum extraction procedures or could form part of petroleum feedstocks in refineries.

6.5 Environmental fate and behaviour

6.5.1 Environmental distribution

Given their physical and chemical properties, the two OPEs under assessment are expected to have low vapour pressure, high water solubility, and varying levels of affinity for organic carbon, based on read-across information from the broader OPE chemical class, as described below.

Modelling of 4-tert-octyphenol ethoxylates with varying degrees of ethoxylation (ECHA 2012) suggests that the affinity of the OPE class for organic phases (soil, sediment, organic matter) can be expected to increase with lower degrees of ethoxylation since shorter chain species would have relatively high log K_{ow} and log K_{oc} values.

Consequently, it can be expected that all OPEs with higher degrees of ethoxylation (~9-10), which are the more commonly observed surfactants, would remain in the aqueous phase, while the lower chain length species would sorb to available organic material.

As surfactants, substances in the OPE subgroup would primarily be released to the environment through industrial and consumer use via municipal wastewater treatment systems (WWTSs). Considering the expected low vapour pressure, volatilization to air is not expected from WWTSs. Biodegradation of the class, including the two OPEs under assessment, would be a significant removal mechanism in WWTSs due to the presence of large amounts of microbiota. Generally, biodegradation of alkylphenols (including OPEs) leads to loss or reduction of the ethoxylate chain and not in rapid mineralization (Staples et al. 2008). As a result, various stable degradation products would be formed.

Loss of lipophilic degradation products and shorter-chain OPEs occurs by adsorption onto suspended solids, which are then removed from water in WWTSs by physical methods such as sedimentation. Shorter-chain OPEs and lipophilic degradants would also partition to sewage sludge. Sludge is physically removed from WWTSs and then typically undergoes anaerobic digestion (i.e. further degradation) before being disposed of by application to soil, incineration or landfilling.

The more hydrophilic degradants and residual amounts of longer-chain OPEs would remain in the water and be released to the aquatic environment after wastewater treatment.

6.5.2 Environmental persistence

All alkylphenol ethoxylates, including the two OPE subgroup members under assessment, undergo transformation to less complex structures in both sewage treatment plants and surface waters as a result of biodegradation. The mechanism involves first the loss of the ethoxy groups to produce various intermediates including octylphenol and eventually, over a long time period, mineralization (UK 2005).

The chemical class of OPEs produce primarily octylphenol monoethoxylate (OP_1EO) and octylphenol diethoxylate (OP_2EO) under anaerobic conditions and primarily octylphenoxy acetic acid (OP_1EC) and octylphenol monoethoxy acetic acid (OP_2EC) under aerobic conditions (UK 2005; Frazee et al. 1964; Ball et al. 1989; Ahel et al. 1996; Field and Reed 1996; Lee and Peart 1998). OP_1EC is the carboxylic acid of mononethoxylated octylphenol (i.e. OP_1EO) formed by oxidation of the terminal OH group on the ethoxylate chain; OP_2EC is the corresponding carboxylic acid of the diethoxylate (OP_2EO), also formed by oxidation of the terminal OH group. These intermediates are themselves converted to octylphenol, albeit at a slower rate than the rapid initial degradation of OPE polymers.

Generally, alkylphenols containing eight or more ethoxylate units (the most common chain length in commercial products) are removed from sewage treatment systems at over 90% efficiency. Test results of nonylphenols in freshwater found 99% primary

degradation after 100 hours (Jonkers et al. 2001) for NP_4EO (ethoxylate range of 2-9) and $NP_{10}EO$ (ethoxylate range of 4-15). Given these results, it can expected that OPEs would show a similar level of degradation as there is only one carbon difference between NPEs and OPEs.

Although there is discrepancy in the published literature about whether OPEs meet the criteria for readily biodegradable, it is generally accepted that the entire class of OPEs degrade rapidly, producing more persistent and stable intermediates, as identified above. Often the cause of failing to meet the more stringent criteria for a ready biodegradation screening test is not due to sufficient levels of observed degradation (>60%) but rather to not meeting the “10-day window” i.e., failing to show sufficient degradation within 10 days after reaching 10% degradation level. Usually, this results when the inoculum has not been acclimatized to OPEs.

Overall, OPEs are expected to be similar to NPEs, i.e. they are conservatively considered to be not readily biodegradable using standard biodegradation test methods. However, as substantial degradation generally occurs after acclimation, they would be considered inherently biodegradable. The aerobic degradation of OPEs initially results in the formation of stable intermediates, mainly OP_1EO, OP_2EO, OP_1EC, OP_2EC and, in lesser amounts, octylphenol (UK 2005).

Therefore, it is expected that the two OPE substances under assessment would have degradation properties similar to those of the broader class of OPEs, and hence these two OPEs are inherently biodegradable but not readily biodegradable.

6.5.3 Bioaccumulation potential

The results of a bioconcentration study conducted according to the OECD 305 test guideline are available for CAS RN 9036-19-5 using the fish (*Cyprinus carpio*) as the test species (J-CHECK 2010). The test substance was described as poly(oxyethylene) octylphenyl ether n=7-11 (average number of polymerization is 9). This material was also described as being 98.93% pure with a water solubility greater than or equal to 100 g/L. Bioconcentration factors (BCFs), the ratio of the concentration in fish to the concentration in water, were determined at two test substance concentrations, namely 0.2 mg/L and 0.02 mg/L, both nominal values. A preliminary range finding test was conducted for rice fish (*Oryzias latipes*) with the 96-hr LC_{50} determined to be 28 mg/L.

The maximum measured BCF (L/kg) value over the 28-day study period was reported for each peak, or chemical species containing a specified degree of ethoxylation, for each of the two concentration levels. The results are as follows:

Peak A (n=11 or $OPEO_{11}$): BCF < 3, at 0.2 mg/L; BCF < 30 at 0.02 mg/L

Peak B (n=10 or $OPEO_{10}$): BCF < 3, at 0.2 mg/L; BCF < 30 at 0.02 mg/L

Peak C (n=9 or $OPEO_9$): BCF < 3, at 0.2 mg/L; BCF < 31 at 0.02 mg/L

Peak D (n=8 or $OPEO_8$): BCF < 3, at 0.2 mg/L; BCF < 30 at 0.02 mg/L

Peak E (n=7 or $OPEO_7$): BCF < 3, at 0.2 mg/L; BCF < 31 at 0.02 mg/L

Given these results, the two OPEs under assessment are not considered to have significant potential for bioaccumulation.

6.6 Potential to cause ecological harm

6.6.1 Ecological effects assessment

The acute ecotoxicological effects of octylphenol (OP) and the class OPEs have been studied and reviewed previously. Substances in the OPE class are nonionic surfactants that are acutely toxic to various organisms (UK 2005). Summary data for OP and OPE (UK 2005; Environment Canada 2002) show that OPEs generally exhibit less chronic toxicity than OP. In addition, the acute toxicity of OP is generally similar to that of nonylphenol (NP), and the LC\EC_{50} values are within a factor of 3 of one another (UK 2005). This is not unexpected as OP and NP are similar in structure (OP has one less carbon in the alkyl chain than NP, and the alkyl structure in both OP and NP comprise similarly branched chains) and are likely to act through a similar mode of action (CCME 2002). A Canadian Water Quality Guideline (CWQG) for the Protection of Aquatic Life is available from the Canadian Council of Ministers of the Environment (CCME) for NP for water exposures. The CWQG reviewed available information on NP and NPEs to develop a recommended NP\NPE water concentration (CCME 2002). Additionally, NP and NPEs were previously assessed through a Priority Substance List (PSL) risk assessment (Environment Canada, Health Canada 2001). The PNEC developed in the PSL assessment of NP\NPE and the recommended CWQG guideline value for NP\NPE in freshwater are both 1.0 µg/L.

OP and OPEs hazard data, as reported in the UK assessment of OP (UK 2005), and supporting documentation for the PSL assessment of NP\NPE (Environment Canada 2002), are generally above the NP/NPE PNEC of 1.0 µg/L (Environment Canada, Health Canada 2001). There is one exception, where a 108 day LOEC for rainbow trout (*Oncorhynchus mykiss*) was reported to be 1.0 µg/L. As OPEs are expected to have lower acute and chronic hazard than OP, and OP is expected to have similar toxicological properties to NP, the PNEC from previous risk assessment characterization work on NP and NPEs was also used for OPEs.

It is known that alkylphenol ethoxylates and alkylphenols (APEs\APs) - including NP, NPE, OP, and OPE - have weak estrogenic activity (Porter et al. 2011; Acir and Guenther 2018) where the substance can disrupt the normal functioning of the endocrine system of various organisms. For instance, exposure of APEs\APs can induce the production of vitellogenin, a precursor chemical of egg yolk protein, present in the blood plasma of sexually mature female fish, in male fish (Environment Canada, Health Canada 2001; Genovese et al. 2014). Furthermore it has been reported that

exposure to low concentrations of OP resulted in shifting of sex ratios, suppressions of ovarian development, and reduced reproduction and growth of zebrafish (*D. rerio*) (Mahgiubi 2011). Exposure of zebrafish embryo to OP resulted in increased cardiovascular system defect development, as well as changes in gene expression and transcription factor suppression (Saputra et al. 2016).

Estrogenic effects were also reported for other taxonomic groups. Arslan et al. (2007) and Arslan and Parlak (2007), reported that sea urchins (*Arbacia lixula* and *Paracentrotus lividus*) exposed to low levels of OP demonstrated growth inhibition and malformation of the skeletal systems. Roepke et al. (2005) further reported that the OP negatively impacted the development of sea urchin (*Strongylocentrotus purpuratus* and *Lytechinus anamesus*) embryos. Duft et al. (2003) reported increase in unshelled (under developed) embryos of mudsnail (*Potamopyrgus antipodarum*) after OP exposure.

OPEs with more than two ethoxylate units generally have low estrogenic activity and appear to be less toxic than OP (UK 2005). According to the NP\NPE PSL report (Environment Canada, Health Canada 2001), OP may be more estrogenically active than NP. However, a document for OPE (ECHA 2012) suggests that 4-*tert*-nonylphenol and 4-*tert*-octylphenol have very similar endocrine activity. Thus, it is assumed that OPE and NPE will have similar estrogenic activity (ECHA 2012). Considering the above information, it is expected that OP would have greater estrogenic activity than OPE, but similar estrogenic activity to NP. The final PNEC of 1.0 µg/L, as used in the PSL assessment, takes into account the potential estrogenic effect of NP and so will be employed to account for the estrogenic activity of OP.

Based on Canada's Water Quality Guideline (WQG) for nonylphenols and its ethoxylates (NPEs) and Canada's PSL report on NPEs, the final PNEC of 1.0 µg/L was selected as the critical toxicity value or CTV for the two members of the OPE subgroup under assessment. This was done as a conservative estimate of their potential endocrine-disrupting effects. The WQG and supporting documentation indicates that the OPE class is very similar in structure and behaviour to NPEs and likely acts through a similar mode of action. The CTV would therefore likely be similar and applicable to the two members of the OPE subgroup as well.

6.6.2 Ecological exposure assessment

According to data collected through voluntary (ECCC 2015) and mandatory surveys (Canada 2015), these two OPEs are used in the following industries or sectors: paints and coatings, polymer production (emulsion polymerization), adhesives and sealants, and cleaning products.

The mandatory survey data indicated some manufacture of the two OPEs in Canada. However, Canadian production has now ceased and currently only imports of the two OPEs occur (personal communication with an industry stakeholder - ethoxylated

surfactants, 2018). Therefore, no exposure scenario for the manufacturing of the OPE subgroup was developed.

According to the two surveys, the following four major activities involving the two OPEs can result in releases to the aquatic environment: (a) the formulation of OPEs to produce surfactant blends; (b) the formulation of paints and coatings; (c) the formulation of various products available to consumers, such as cleaners; and (d) the consumer release of products in a “down-the-drain” scenario. The following is a summary of the exposure releases of the two specific OPEs being assessed, which are presented in detail in the document ‘Supporting Documentation: Ecological Exposure Analysis of Poly(Alkoxylates/Ethers)’ (ECCC 2018).

The exposure scenarios outlined below, i.e. for the remainder of section 6.6.2, were developed for the two OPE surfactants under assessment on the basis of their quantity ranges in Canada and associated use patterns.

Product formulation – surfactant blends

An exposure scenario has been developed to represent a large product formulator who may import pure or nearly pure OPEs and who blends them to produce various products at lower concentrations. The facilities involved in these activities are determined to discharge their treated or untreated wastewater to wastewater treatment systems (WWTSs) for final treatment prior to their release to the aquatic environment. As not all formulators have the necessary equipment to pre-treat their wastewater prior to discharge to WWTSs, it is assumed for the purpose of OPE assessment that the formulator will discharge untreated wastewater into a WWTS.

Again, the predicted environmental concentration (PEC) in receiving waters is estimated from the amount released to the WWTS, the effluent flow and the dilution factor of the receiving watercourse.

$$PEC = [10^9 \times Q \times E \times (1-R)] \div [F \times D \times N]$$

where

- PEC: predicted environmental concentration in receiving water near a discharge point, µg/L
- Q: a substance’s annual use quantity at a facility, kg/year
- E: emission factor to wastewater, unitless
- R: wastewater treatment removal, unitless
- F: daily wastewater flow, L/d
- D: receiving water dilution factor near discharge point, unitless
- N: number of annual operation days, d/y
- 10^9: conversion factor from kg to µg (µg/kg)

Based on literature, the WWTS removal rate was estimated to be between 80 and 90%

(Melcer et al. 2007). To be conservative the lower end of this range (80%) was selected for use in all wastewater treatment types.

The highest use quantity for the largest formulator is in the range of 10 000 to 100 000 kg per year. Considering the significant range presented, the logarithmic average of this range is used in the calculations. The maximum quantity (Q) of OPEs that will be formulated at an individual facility is assumed to be 31 620 kg per year. Furthermore, it is assumed that the facility will operate 300 days per year (N) with an emission rate (E) of 0.1%. The WWTS that receives the discharge from the facility with the highest quantity use of OPEs has a daily dilution volume of 1.711×10^9 L, which is used to estimate the level of exposure near the discharge point of WWTSs; this near-discharge-point exposure is taken as the aquatic PEC. Using these inputs, the aquatic PEC was calculated to be 0.0123 µg/L.

Formulation of paints and coatings

A paint and coatings formulation scenario was selected to estimate the environmental concentrations using representative worst-case assumptions. This scenario is based on the largest amount of these OPEs used at a facility for paint formulation, which is 10 000 kg. For facilities handling this amount of substance, the number of operating days is estimated at 300 days per year (N), with an emission rate (E) of 0.5%. The WWTS that receives the discharge from this large paint formulating facility has a daily dilution volume of 5.2934×10^8 L. This near-discharge-point exposure is taken as the aquatic PEC. Using these inputs, the aquatic PEC was calculated to be 0.064 µg/L.

Formulation of cleaning and similar products available to consumers

A cleaning products formulation scenario was selected to estimate the environmental concentrations using representative worst-case assumptions. This scenario is based on the high end of the quantity range reported for the two OPEs when used at a facility for cleaning product formulation, which is 10 000 kg. For facilities handling this amount of substance, the number of operating days is estimated at 300 days per year (N), with an emission rate (E) of 0.3%. A distribution of daily dilution volumes for the personal care and cleaning products sector was created; it covers about 35 facilities in Canada engaged in this activity. For the calculation, the 10^{th} percentile of the lowest daily dilution volume was selected. This value corresponds to 3.8014×10^7 L/d and is used to estimate the level of exposure near the discharge point of WWTSs; this near-discharge-point exposure is taken as the aquatic PEC. Using these inputs, the aquatic PEC was calculated to be 0.526 µg/L.

Down-the drain consumer release

A “down-the-drain” calculation was developed for substances in the OPE subgroup when used as surfactants in products such as cleaners, laundry detergents and personal care products. As consumer releases of OPE-containing products are expected to occur across Canada, the consumer PEC is estimated using CRAM (CRAM

2017.

The CRAM model was run with a quantity of 100 000 kg/yr, which is at the upper end of the range of the total reported quantities under the CEPA section 71 survey. A wastewater removal rate of 60% was used for primary treatment facilities, 80% was used for secondary treatment facilities and 92.4% was used for lagoons. The distribution of PECs for down-the-drain analysis is presented in

Table 6-3.

Given the assumptions of the scenario, the 10th percentile of the distribution of CRAM results is selected as a suitable representative aquatic PEC.

Table 6-3. OPEs distribution of PECs and risk quotients calculated by CRAM

Percentile [a]	PEC (µg/L)	Risk Quotient
10	0.70	0.70
20	0.38	0.38
30	0.25	0.25
40	0.19	0.19
50	0.14	0.14
60	0.11	0.11
70	0.09	0.09
80	0.07	0.07
90	0.05	0.05
100	0	0

[a] The Percentile is the distribution of the CRAM results

Monitoring and surveillance information

Octylphenol and nonylphenols were included in a Chemicals Management Plan monitoring and surveillance program for surface water and biosolids. The concentrations of octylphenol were sampled for three consecutive weekdays in the raw influent, final effluent and biosolids of 12 Canadian wastewater treatment systems during the years 2010-11 and 2011-12. The 12 WWTSs are representative of typical Canadian treatment systems (primary, secondary, aerated lagoon, facultative lagoon, advanced systems). The median concentration of octylphenol in aquatic effluents was <3.6 ng/L. Additionally, the maximum measured concentration of octylphenol was 7.67 ng/L. For these measurements, octylphenol was detected in only 1 of 84 samples. For biosolids, the median and maximum concentration of octylphenol was measured at 64.7 ng/g and 271 ng/g respectively, and OP was detected in 9 of 65 samples (Environment Canada 2013a).

6.6.3 Characterization of ecological risk

The approach taken in this ecological risk assessment was to examine direct and supporting information and develop conclusions on the basis of a weight-of-evidence

approach. Lines of evidence considered include information on sources and fate of the substance, persistence, bioaccumulation, estimated exposure to the substance, monitoring and surveillance data, and ecological hazard properties. On the basis of available information, between 0.01 and 0.1 million kg of the two OPEs under assessment were used in Canada in 2014. The PNEC for the OPE subgroup was estimated to be 1.0 µg/L, based upon the Canadian Water Quality Guideline for the Protection of Aquatic Life as developed by the Canadian Council of Ministers of the Environment for nonylphenol and its ethoxylates, a closely related ethoxylated polymer.

With respect to the long-term persistence of these polymers, available biodegradation data for the OPEs under assessment suggests that they will not be readily biodegradable in the environment. However, as substantial degradation occurs after acclimation, they would be considered inherently biodegradable. The degradation of OPE polymers initially results in the formation of stable intermediates including octylphenol. It is likely that these polymers are not hydrolyzable. This is consistent with the absence of readily hydrolyzable groups in the representative polymer structure.

The empirical data used to assess the bioaccumulation potential support the low bioaccumulation potential of the two OPE polymers for aquatic organisms.

The predicted environmental concentrations for the four major activities involving OPEs (ranging from 0.0123 to 0.70 µg/L) are below the PNEC value. Consequently, on the basis of any calculated risk quotients (i.e. PEC/PNEC) for the environmental release scenarios considered, the two OPEs under assessment are not expected to represent an environmental concern (i.e., risk quotients are less than 1). Considering that conservative values, such as a conservative WWTS removal rate, and high use quantities (volumes) were used to estimate the PECs, it is anticipated that any risk quotients would be an over-estimation of the potential risk. Overall, the two OPEs under assessment are not expected to result in an environmental risk on the basis of available information and the conservative estimation of PEC and PNEC values.

It is noted that the properties and ecological hazards of both NPEs (nonylphenol and its ethoxylates) and OPEs have been reviewed and found to be similar, particularly their structural and physical-chemical properties (Environment Canada, Health Canada 2001 and references therein; CCME and references therein). Additionally, both NPEs and OPEs have similar ecotoxicological hazard levels, and their degradation products have similar endocrine (estrogen) disrupting potential. Accordingly, from an environmental perspective, the two OPE surfactants considered in this assessment would not be considered suitable alternatives to NPEs.

6.7 Potential to cause harm to human health

Classification of the hazard data and exposure profiles used to develop the potential for human health risks associated with octylphenol ethoxylates are presented in the document ‘Supporting Documentation: Final Risk Matrix Location of Polymers’ (Health

Canada 2017).

Although exposure was established as high, the human health hazard for the substance was determined to be low for the two OPEs under assessment. Therefore, taking into consideration the available data, it is unlikely that exposure to the substance(s) will pose a human health risk.

7. Alkylamine ethoxylates (ANEOs)

7.1 Substance identity

The six substances (see

Table 7-1) considered in this chapter are cationic surfactants that are collectively referred to herein as the alkylamine ethoxylates (ANEOs[6]) subgroup. They consist of amine alkoxylate surfactants with a range of alkyl chain lengths and alkoxylation levels. ANEOs are represented by the structures shown in Figure 7-1 and Figure 7-2.

All six ANEOs considered in this screening assessment have similar alkyl chain lengths, namely between C8 and C18. In addition, available compositional information suggests that ANEOs typically have between 2 and 25 alkoxylate repeating units.

Given the overlapping alkyl chain lengths and differences in alkoxylation level between the six substances, they are expected to have similar properties. Therefore, for the purpose of this screening assessment, a read-across approach for physical and chemical properties and hazard properties was taken.

Amines, tallow alkyl, ethoxylated (CAS RN 61791-26-2), also known as polyethoxylated tallow amine or POEA, is used as surfactant in glyphosate herbicide formulation, which has been widely studied. POEA is synthesized using tallow oil typically composed of C_{14}-C_{18} alkyl chains (Table 7-2).

As POEA is used as a surfactant in glyphosate formulation, it has been reported in more studies than other ANEOs. POEA has also been thoroughly reviewed by the Pest Management Regulatory Agency (PMRA) as part of the glyphosate re-assessment.

Table 7-1. ANEO surfactants

CAS RN	CAS name
68155-39-5	Amines, C14-18 and C16-18-unsatd. Alkyl, ethoxylated
68439-72-5	Amines, C8-18 and C18-unsatd. Alkyl, ethoxylated

[6] ANEO is commonly used as the abbreviation for alkyl (A) amine (N) ethoxylates (EO) in literature.

61791-24-0	Amines, soya alkyl, ethoxylated
61791-26-2	Amines, tallow alkyl, ethoxylated (POEA)
28724-32-5	Poly(oxy-1,2-ethanediyl), α,α'-[(methyloctadecyliminio)di-2,1-ethanediyl]bis[ω-hydroxy-, chloride
68603-75-8	Amines, N-tallow alkyltrimethylenedi-, propoxylated

Table 7-2. Typical fatty acid composition of tallow and soya oil

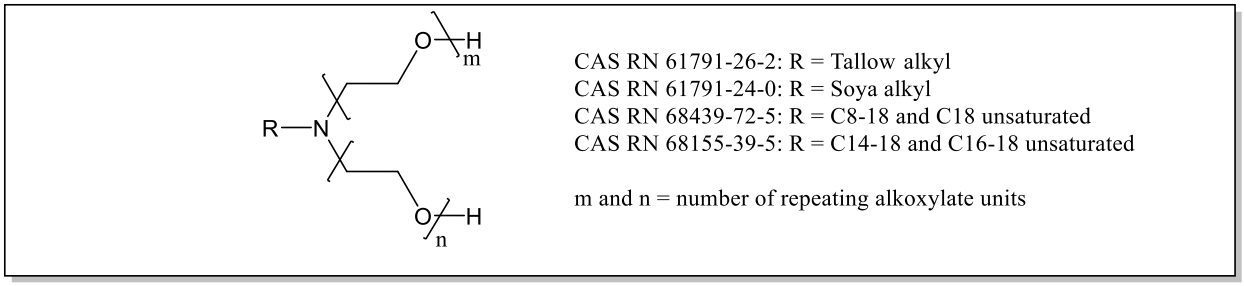
Fatty acid	Chain length: number of Unsaturation	Tallow oil % Composition [a, b]	Soya oil % Composition [a,b]
Myristic	14:0	1-6	0.9
Palmitic	16:0	20-37	7-12
Stearic	18:0	14-21	2-5.5
Palmitoleic	16:1	3-9	--
Oleic	18:1	35-46	20-50
Linoleic	18:2	4-10	35-60
α-Linolenic	18:3	0-3	2-13

[a] CIR 2015.
[b] Visek 2003.

According to the Cosmetic Ingredient Report (CIR 2015) and Rodriguez (2015), ANEOs are synthesized through a series of chemical reactions, where fatty acids or long carbon chain acids undergo amination to produce primary amine (Figure 7-3). The amine then reacts with ethylene oxide or propylene oxide to generate the simple ANEOs with two alkoxylate units (CIR 2015, Visek 2003). Further reaction with ethylene oxide/propylene oxide in the presence of a catalyst will yield ANEO with a higher degree of alkoxylation. The resulting ANEO contains an amine core with one branch consisting of a long carbon chain moiety and one or more branches of repeating alkoxylate units with terminal alcohol groups (Tush and Meyer 2016). Typically, ANEOs are nonionic surfactants; however, ANEOs can form cations when quaternized. For example, CAS RN 28724-32-5 is quaternized with methylene chloride to generate quaternary ANEOs.

The six ANEOs currently under assessment are a part of a larger class of amine surfactants with different alkyl chain lengths and varying degree of alkoxylation. However, this assessment will focus only on the substances listed in

Table 7-1. Considering alkyl carbon chain length and the degree of alkoxylation, the number average molecular weight can range from 350 to greater than 900 (Canada 2015; ECCC 2015).



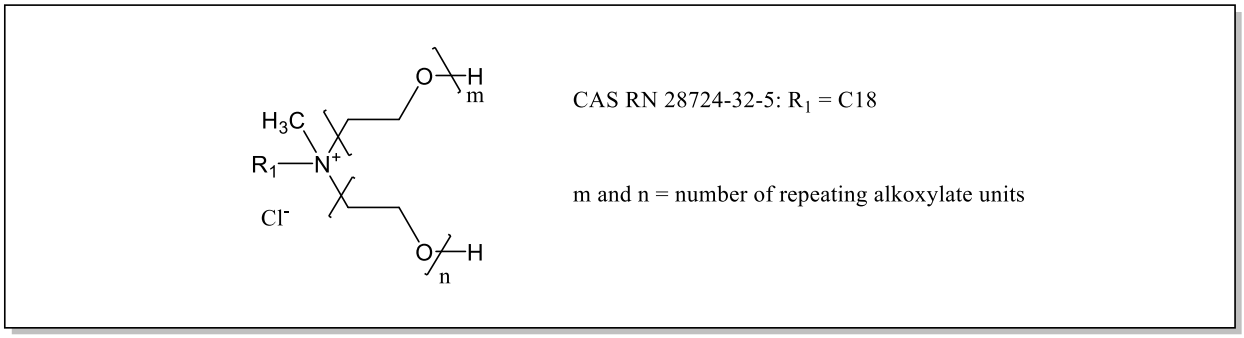


Figure 7-1. Representative structure of ANEOs

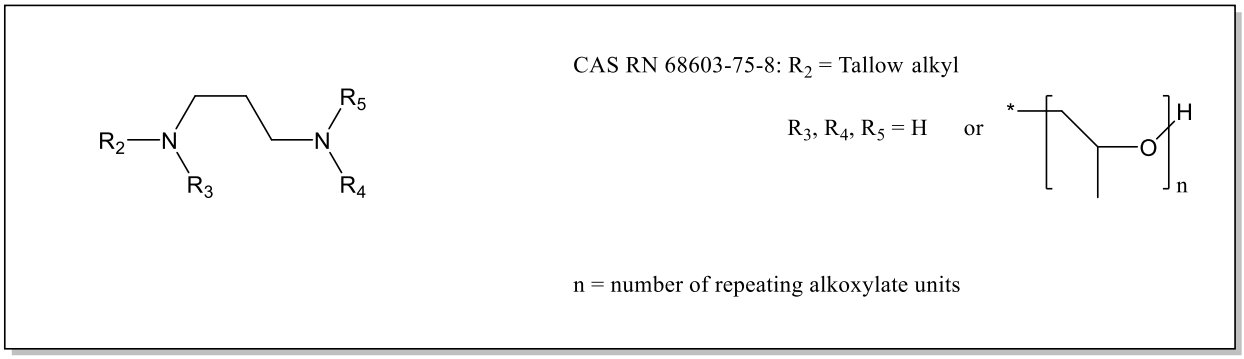


Figure 7-2. Representative structure of 68063-75-8

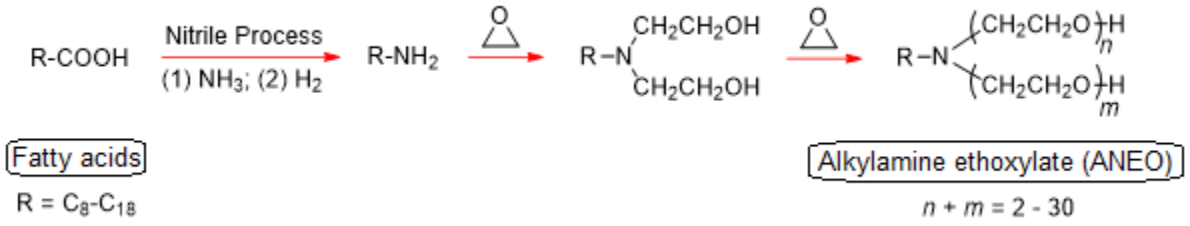


Figure 7-3. ANEOs synthesis (CIR 2015; Tush and Meyer 2016; Visek 2003)

7.2 Physical and chemical properties

ANEOs are surfactants with variable number average molecular weight and physical-chemical properties. A range of properties was found through literature searches, a

voluntary survey (ECCC 2015) as well as a mandatory survey conducted under section 71 of CEPA (Canada 2015). The data gathered are presented in Table 7-3, which is an aggregation of that available for the six ANEOs.

Table 7-3. Physical and chemical property values for ANEOs

Property	Values	Key reference(s)
Physical state	Liquid	Canada 2015, ECCC 2015, Health Canada 2015
Molecular weight (g/mol)	350 to >900	Canada 2015, ECCC 2015
Vapour pressure (mmHg)	5.1×10^{-14} to <1	Canada 2015, ECCC 2015, Health Canada 2015
Water solubility	Water available	Canada 2015, ECCC 2015, Health Canada 2015,
Organic carbon/water partition coefficient (log K_{oc})	3.4 to 4.2	Health Canada 2015
Adsorption-desorption distribution coefficient (log K_d)[a]	2.88 to 3.77	ECCC 2018

[a] log K_d are calculated based on the log K_{oc} using the following equation: log K_d = log (Koc x Foc), where Foc is 0.37 and 0.3 for activated sludge and raw sewage, respectively.

The data indicate that ANEOs typically have number average molecular weights from 350 to > 900. Given the surface active behaviour of ANEOs, different water solubility values have been reported. However, as ANEOs can form stable emulsions in water, they are considered to be water available. Some experimental data on log octanol/water partition coefficient (log K_{ow}) were found. However, test guidelines, including OECD 107 and 117, indicate that these methods are not applicable to substances with surface active properties. For this reason, the data are not presented.

7.3 Sources and uses

The six ANEOs have been included in a voluntary survey (ECCC 2015) as well as a mandatory survey conducted under section 71 of CEPA (Canada 2015).

Table 7-4 is a summary of the reported total manufacture, and total import quantities for the substances for 2014. These sources indicate that the six ANEOs are primarily used in oil and gas extraction applications, metal working applications, and cleaners and personal care applications. Minor uses in food packaging and fuel additives applications have also been reported. Depending on the application, ANEOs may be formulated at different concentrations. For example, POEAs are formulated at < 20% concentration in pesticide formulations (Health Canada 2015). Also, current formulation practices for cocoalkyl amine ethoxylate in cosmetic or personal care products are typically less than 3.5% (CIR 2015).

Table 7-4. Summary of information on Canadian manufacturing and import quantities of the six ANEOs in 2014 submitted pursuant to a voluntary survey and to a survey under section 71 of CEPA

CAS RN	CAS name	Total manufacture[a] (kg)	Total imports[a] (kg)
68155-39-5	Amines, C14-18 and C16-18-unsatd. Alkyl, ethoxylated	0	100 000 – 1 000 000
68439-72-5	Amines, C8-18 and C18-unsatd. Alkyl, ethoxylated	0	100 000– 1 000 000
61791-24-0	Amines, soya alkyl, ethoxylated	0	10 000 – 100 000
61791-26-2	Amines, tallow alkyl, ethoxylated	1 000 000 – 10 000 000[b]	100 000 – 1 000 000
28724-32-5	Poly(oxy-1,2-ethanediyl), α,α'-[(methyloctadecyliminio)di-2,1-ethanediyl]bis[ω-hydroxy-, chloride	0	100 000 – 1 000 000
68603-75-8	Amines, N-tallow alkyltrimethylenedi-, propoxylated	0	10 000 – 100 000

[a] Values reflect quantities reported in response to a voluntary survey (ECCC 2015) and a mandatory survey conducted under section 71 of CEPA (Canada 2015). See surveys for specific inclusions and exclusions (schedules 2 and 3).

[b] According to follow-up communications with industry, a major Canadian manufacturer ceased its manufacturing operation in 2016.

7.3.1 Uses of amines, tallow alkyl, ethoxylated (CAS RN 61791-26-2; POEA)

Amines, tallow alkyl, ethoxylated (CAS RN 61791-26-2), also known as POEA, was identified for further human health screening through the second phase of polymer rapid screening (2017). Therefore, a number of domestic government databases were searched to determine other potential uses of POEA in Canada that could result in human exposure. They are listed in Table 7-5.

Table 7-5. Additional uses in Canada for POEA

Use	POEA
Food additive[a]	N
Food packaging materials[b]	N
Internal Drug Product Database as medicinal or non-medicinal ingredients in disinfectant, human or veterinary drug products in Canada[c]	N
Natural Health Products Ingredients Database[d]	N
Licensed Natural Health Products Database as medicinal or non-medicinal ingredients in natural health products in Canada[e]	N
List of Prohibited and Restricted Cosmetic Ingredients[f]	N

Use	POEA
Notified to be present in cosmetics, based on notifications submitted under the *Cosmetic Regulations* to Health Canada[g]	N
Formulant in pest control products registered in Canada[h]	Y
Known toy use[i]	N

Abbreviations: Y, YES; N, NO

[a] Health Canada [modified 2017]; personal communication, email from the Food Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[b] personal communication, email from the Food Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[c] DPD [modified 2017]; personal communication, email from the Therapeutic Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[d] NHPID [modified 2019]; personal communication, email from the Natural and Non-prescription Health Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[e] LNHPD [modified 2017]; personal communication, email from the Natural and Non-prescription Health Products Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[f] Health Canada [modified 2015].

[g] personal communication, email from the Consumer Product Safety Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[h] personal communication, email from the Pest Management Regulatory Agency, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, dated June 2017; unreferenced.

[i] Toy Industry Association (TIA 2017).

POEA is used in the manufacture of food packaging materials as a surfactant and antistatic agent.

Certain glyphosate products (pesticides) contain POEA, which functions as a surfactant. No risk or concerns to human health or the environment were identified provided that these products contained no more than 20% POEA by weight and that the proposed label directions (including larger spray buffer zones for products that contain POEA) are followed. All currently registered glyphosate end-use products in Canada meet the 20% limit (Health Canada 2015). Any pesticide product containing POEA that has been registered since the completion of the glyphosate re-evaluation must also meet the 20% limit. A valid scientific rationale accompanied by acceptable data is required when requesting registration for a pesticide product containing more than 20% POEA by weight.

7.4 Releases to the environment

According to the survey information, the six ANEOs were imported into Canada in 2014, with POEA being the only substance manufactured in Canada. Current information indicates that manufacturing of POEA in Canada ceased in 2016, but that it continued to be imported into Canada. On the basis of survey data, the six ANEOs are formulated into various industrial and commercial products. Products containing the six ANEOs are used in oil and gas extractions applications, metal working application, cleaning and personal care applications. ANEOs are typically formulated into products available to consumers at concentrations of 1% to 5% (SDS 2015b; CIR 2015).

Although activities relating to oil and natural gas extraction have been identified, no quantitative scenario has been developed for this sector because process waters used in onshore oil field applications are not normally discarded to a sewer or the freshwater aquatic environment.

On the basis of survey information, the six ANEOs could be released during formulation and through end use applications in Canada. Considering the use pattern of the products mentioned above, it is expected that the six ANEOs would be released primarily to wastewater treatment (WWT) systems.

7.5 Environmental fate and behaviour

7.5.1 Environmental distribution

Based on the physical and chemical data presented in Table 7-3, the six ANEOs are expected to have low vapour pressure, high water solubility, and strong affinity for organic carbon (high log K_{OC}). Furthermore, it was found that POEA has a strong affinity for soil and suspended solids (Rodriguez 2015; Tush and Meyer 2016).

Depending on the use patterns, the six ANEOs could be released into the environment through WWTS discharges. Given their physical and chemical properties, ANEO polymers that go through waste treatment facilities are anticipated to primarily adsorb onto suspended solids and be removed from the water column.

If released to soil, the polymer is expected to adsorb onto soil (Tush and Meyer 2016) and to undergo some biodegradation over time. Volatilization from the soil or soil pore water is not expected due to expected low vapour pressure.

7.5.2 Environmental persistence

Considering that ANEOs do not contain any known functional groups that would readily undergo hydrolysis, they are anticipated to be hydrolytically stable in the environment. This is supported by the information reported by Health Canada (2015) for POEA with a hydrolysis half-life > 140 days.

Depending on the degree of alkoxylation and duration of the biodegradation study, biodegradation of ANEOs can range from < 25% to over 60%. According to Van Ginkel et al. (1993), POEA biodegradation can range from 22% to 60% over 28 days for POEA with 50 ethoxylate units and 2 ethoxylate units, respectively. Furthermore, it was reported that biodegradation is a two-stage process, with ANEOs initially undergoing rapid biodegradation, followed by a significantly slower biodegradation process. The initial biodegradation process involves bond scission between the amine-alkyl bond, after which the free alkyl chain can be biodegraded (Van Ginkel et al. 1993). The slower biodegradation of the second phase suggests that the residual amine ethoxylate biodegrades at a much slower pace. This was attributed to the possibility that the amine-ethoxylates are strongly adsorbed to soil/sediments where bioavailability is significantly decreased (Rodriguez 2015).

In their risk assessment, Giesy et al. (2000) referred to some unpublished work on biodegradation of POEA in various soils and in aquatic environments, which showed that POEA is primarily degraded through microbial activities in both soil and aquatic environments. Based on mineralization of POEA, the estimated half-lives for POEA in soil and water were < 1 week and < 4 weeks, respectively (Giesy et al. 2000).

Overall, the six ANEOs are expected to be hydrolytically stable, but can undergo biodegradation in less than 4 weeks. On the basis of available biodegradation information, the six ANEOs are not expected to significantly persist in the environment.

Table 7-6. Hydrolysis and biodegradation of POEAs

Endpoint	Results	Source
Hydrolysis half-life	> 140 days	Health Canada 2015
Biodegradation	20% to > 60% after 28 days	Canada 2015
Biodegradation half-life (aquatic environment)	< 4 weeks	Giesy et al. 2000
Biodegradation half-life (soil)	< 1 week	Giesy et al. 2000

7.5.3 Bioaccumulation potential

ANEOs are amine surfactants that could become cationically charged in the environment, which would enhance their adsorption to an anionic surface, such as fish gills, algal cells or the negatively charged components of organic particles. The strong association of ANEOs to suspended solids, soils, and humic substances has been reported in various studies (Andersson 2012; Chen et al. 2014; Deese et al. 2016; Ishiguro et al. 2007; Rodriguez 2015; Tush and Meyer 2016). These authors report strong association of POEA to suspended solids in water as well as to soils, which would reduce bioavailability. This will limit uptake as well as passage of the polymers through biological membranes. Furthermore, the six ANEOs are not considered persistent in the environment, which means its bioaccumulation potential would be

limited. A similar conclusion was proposed by Health Canada (2015) for POEA. Given the strong association of the six ANEOs towards anionic surfaces in the environment and given that they are non-persistent in the environment, the six ANEOs are not considered to have significant bioaccumulation potential.

7.6 Potential to cause ecological harm

7.6.1 Ecological effects assessment

As noted in Section 7.1, ANEOs are surfactants that are composed of varying alkyl chain lengths and alkoxylate units. Owing to the differences described earlier, the ecotoxicity for different ANEOs in the class can vary significantly even for two polymers with the same CAS RN. For example, Moore et al. (1987) reported 48-h LC_{50} acute toxicity to a freshwater invertebrate (*Daphnia pulex*) from POEA with 15 and 150 ethoxylate repeating units to be 2.35 mg/L and 66.09 mg/L, respectively. The authors attributed the toxicity differences to the increase in ethoxylate units. Furthermore, Brausch and Smith (2006) reported toxicity to a freshwater invertebrate (*Thamnocephalus platyurus*) ranging from 5.17 µg/L to 2.01 µg/L for POEA with 2 and 15 ethoxylate repeating units, respectively. The two studies highlight the fact that the toxicity trends that are observed in one species may not be observed in another species.

The ecotoxicological effects of the six ANEOs were gathered through voluntary (ECCC 2015) and mandatory surveys (Canada 2015) and various literature sources. The majority of hazard data were gathered for POEA, with a small number of data stemming from the other five ANEOs. As referenced in Section 7.1, POEA is widely used in glyphosate herbicide formulations and thus has been extensively studied. The hazard data for other ANEOs demonstrate similar hazard profiles as POEA. Considering the variability in alkyl chain lengths (
Table 7-1 and
Table 7-2) and ethoxylate units, the effects data from PEOA and other ANEOs are deemed to be appropriate to perform a read across analysis for the six ANEOs. All effects data are summarized in Table 7-7.

Table 7-7. Aggregate ecotoxicity data summary for six ANEOs surfactants[a]

Organism	Acute result (mg/L)[b]	Chronic results (mg/L)[b]
Algae	EC_{50}=0.0282-4.1	NOEC=0.16-1.22
Invertebrates	EC_{50}/LC_{50}=0.00201-66.09	NOEC=0.0032-20.0
Fish	LC_{50}=0.0789-13.0	-
Amphibians	LC_{50}=0.68-2.2	-
Marine Algae	EC_{50}=3.35	-
Marine Invertebrate	LC_{50}=0.6	-
Marine Fish	LC_{50}=1.4-4.5	-

[a] Toxicological effects are extracted from Benijts-Claus and Persoone 1987; Brausch and Smith 2006; Canada 2015; ECCC 2015; ECHA 2018; Giesy 2000; Moore et al. 1987; Moore et al. 2000; Health Canada 2015; Rodriguez-Gil 2015; Servizi et al. 1987; Wan et al. 1989.

[b] EC_{50} is the effect concentration for 50% of the population; LC_{50} is the lethal concentration for 50% of the population; NOEC is the no observed effect concentration.

The ecotoxicity data summary in
Table 7-7 indicates toxicity ranging from moderate to high for all species. Freshwater and marine invertebrates appear to be most sensitive to exposure.

Rodriguez-Gils (2015) conducted a review of the hazard data available for POEA and performed a battery of ecotoxicity testing on the substance. Using the results, along with available literature data, an acute species sensitivity distribution (SSD)[7] approach was taken to characterize the hazard of POEA. The 5th percentile[8] or HC_5 concentration was determined to be 0.17 mg/L on the basis of the SSD. Similarly, the Pest Management Regulatory Agency (Health Canada 2015) conducted a thorough review of the available hazard data in the literature for POEA and generated acute SSDs for three taxonomic groups. The HC_5 values for freshwater invertebrates, amphibians, and marine fish were estimated to be 0.0041 mg/L, 0.35 mg/L and 2.6 mg/L, respectively. An SSD analysis combining data from all taxonomic groups was not performed by PMRA (Health Canada 2015).

For this assessment, a multispecies SSD was generated using available data. However, the reliability of the result could not be ascertained as the SSD curve produced did not effectively fit the data set and hence the HC_5 was not used. The poor data fit is likely the result of the disproportionate distribution of data points, where the majority of the data have LC_{50} or EC_{50} values that are greater than 0.1 mg/L, and only four data points have toxicity less than 0.05 mg/L. As there are no indications that the low LC_{50} or EC_{50} values are erroneous, these data endpoints were included in the data set. Given that Health Canada (2015) has completed an SSD analysis for three taxonomic groups, a conservative approach was taken. The POEA HC_5 (0.0041 mg/L) for freshwater invertebrates—representing the highest hazard—was selected as the overall critical toxicity value (CTV) for the six ANEOs. It is recognized that the CTV chosen would likely be more conservative than an HC_5 derived from a multispecies SSD as determined by Rodriguez-Gils (2015) or the HC_5 reported by PMRA (Health Canada 2015) for amphibians and marine fish. However, considering the structural and molecular weight variability of ANEOs, the chosen CTV is anticipated to be protective of the different species considered regardless of the six ANEOs.

Ishiguro et al. (2007) studied the interaction of cationic surfactants with different humic substances. The study concluded that the binding of cationic surfactant to humic substances is driven by both electrostatic and hydrophobic attractions, which would

[7] SSD are a cumulative distribution of toxicity endpoints for multiple species to a toxicant. SSD attempts to account for variations in sensitivity of different species to the same toxicant. From an SSD, a critical toxicity value (CTV) can be estimated for a given percentile.

[8] The 5th percentile or HC_5 concentration is determined through SSD, which is the concentration that is protective of 95% of the species.

significantly affect the fate of cationic substances in the environment. Furthermore, Andersson (2012) reported that in the presence of humic acids, the toxicity of several alkylamine surfactants to daphnia was reduced. Chen et al. (2014) reported toxicity reductions of up to five fold to daphnia in the presence of humic acids for quaternary surfactants. Deese et al. (2016) reported similar findings, where the toxicity of quaternary amine surfactants to a marine invertebrate (*Artemia franciscana*) was significantly reduced in the presence of humic acids. Based on the available data, the invertebrate HC_5 chosen from the PMRA (Health Canada 2015) is expected to be primarily driven by the toxicity endpoint for *Thamnocephalus platyurus* (Brausch and Smith 2006). According to Brausch and Smith (2006), the test was conducted using synthetic freshwater, which suggest that humic acid would not be present in the test water. The chosen CTV is therefore not expected to account for the strong adsorptive behaviour of the six ANEOs to humic substances. It is anticipated that when ANEOs are released to the environment, their toxicity would be reduced in the presences of humic substances. For the purpose of considering the mitigating effect of humic acids typically found in the environment, a five-fold mitigation is applied to the CTV to account for the strong adsorption potential of the six ANEOs to suspended matter in the environment. The mitigation factor was chosen after considering the strong adsorption potential of ANEO to suspended solids and soils and was selected on the basis of the results of Chen et al. (2014).

The aquatic PNEC is derived from the CTV, which is divided by an assessment factor (AF) as shown:

$$\text{Aquatic PNEC} = [\text{CTV} \times 5] / \text{AF}$$

$$\text{Aquatic PNEC} = [0.0041 \text{ mg/L} \times 5] / 1$$

$$\text{Aquatic PNEC} = 0.0205 \text{ mg/L or } 20.5 \text{ µg/L}$$

An AF of 1 is selected to estimate the aquatic PNEC. It represents the species sensitivity. The selected CTV is based on the acute studies; however, an acute-to-chronic factor was not considered necessary due to the fact that the six ANEOs are expected to be rapidly removed from the water column through adsorption to suspended solids and biodegradation (Health Canada 2015; Rodriguez-Gils 2015). Also, considering the available ecotoxicity data for the six ANEOs (greater than 3 categories and greater than 7 species), a factor of 1 was selected to represent the species sensitivity.

7.6.2 Ecological exposure assessment

According to the data collected through the voluntary (ECCC 2015) and mandatory surveys (Canada 2015), the six ANEOs are used as surfactants in various industrial products and products available to consumers. As none of the six ANEOS are manufactured in Canada, an exposure scenario for this activity was not considered.

Although activities relating to oil and natural gas extraction have been identified, release of ANEOs to the aquatic environment through oil and gas extraction is not expected to result in an increase in ANEO concentrations in the aquatic environment. Under normal onshore oil field applications, the process water is used for oil well stimulation or is disposed of through deep well injection in North America (OECD 2012). Therefore, this activity is not considered further.

The other major use of the six ANEOs is in metal working applications and cleaners and personal care products, where the substance is formulated into different products for industrial, commercial, and consumer use. The following presents a summary of the exposure releases of the six ANEOs from different sources. The detailed exposure estimates are presented in the document 'Supporting Documentation: Ecological Exposure Analysis of Poly(Alkoxylates/Ethers)' (ECCC 2018).

Wastewater removal rate predictions for the six ANEOs using Simple Treat 3.1 (SimpleTreat 2003) indicate removal efficiency of 90% through secondary treatment and 45% for primary treatment (ECCC 2018). Residual amounts of ANEOs could be released into the environment after WWT via effluent. In the environment, they are expected to adsorb to suspended solids and settle to the sediments (Rodriguez 2015). Furthermore, they are anticipated to biodegrade over time (Van Ginkel et al. 1993). Considering the strong affinity of ANEOs for organic matter and suspended solids in WWTS, the predicted removal rates are likely an underestimation of the true removal rate of the six ANEOs from wastewater. However, for the purpose of this assessment, a maximum removal rate of 90% is assumed.

Products formulation

A generic discharge scenario has been developed for the formulation of the six ANEOs into different products. The facilities involved in these activities discharge their treated or untreated wastewater to wastewater treatment systems for final treatment prior to its release to the aquatic environment. As not all formulators will have the necessary equipment to pre-treat their wastewater prior to discharge into wastewater treatment systems (WWTS), for the purpose of this assessment, it is assumed that the formulator will discharge untreated wastewater into WWTS.

The predicted environmental concentration (PEC) of the six ANEOs in receiving water is estimated from the amount released to the WWTS, the effluent flow and the dilution factor of the receiving watercourse, as follows:

$$PEC = [10^9 \times Q \times E \times (1\text{-}R)] \div [F \times D \times N]$$

Where:

PEC: predicted environmental concentration in receiving water near discharge point, µg/L
Q: total quantity of ANEOs used per year, kg/y

E: emission factor to wastewater, unitless
R: overall wastewater treatment removal, unitless
F: daily wastewater flow, L/d
D: receiving water dilution factor near discharge point, unitless
N: number of operation days per year, d/y
10^9: conversion factor from kg to µg (µg/kg)

The scenario is based on a generic formulation facility utilizing any of the six ANEOs to formulate different products. Survey information indicates that a typical industrial facility would utilize 1 000 kg to 10 000 kg per year to formulate various products (ECCC 2015; Canada 2015). For the purpose of this assessment, it is assumed that the maximum quantity (Q) of 10 000 kg per year will be used per site. Furthermore, it is assumed that the facility will use these substances over 20 days per year (N) with an emission rate (E) of 0.3% (European Chemicals Bureau 2003). The overall WWTS removal rate (R) is estimated to be 90% based on predicted removal rate. The 10th percentile[9] daily dilution volume for WWTSs associated with industrial facilities is 1.776×10^7 L/d. This near-discharge-point exposure is taken as the aquatic PEC for ANEOs. The aquatic PEC is estimated to be 8.45 µg/L.

Industrial use

ANEOs have been reported to be used in metal working fluids. According to information from the mandatory survey (Canada 2015), spent working fluids are sent to approved off-site treatment facilities for treatment prior to discharge into WWTS. It was reported that up to 10 000 kg of the substance could be sent to off-site treatment facilities per year. However, the information gathered does not indicate the number of days on which the transfer would occur. In addition, it could be expected that the metal working facility would generate other waste that would be mixed with the metal working fluid prior to being sent for treatment. Considering the uncertainties associated with the release pattern from the metal working facilities and the removal rates from the off-site facilities, any scenarios developed for metal working fluid may not be a realistic representation of the release potential of ANEOs in metal working fluid. For that reason, no quantitative estimation is presented.

Down-the-drain consumer release

The six ANEOs are used as surfactants in cosmetics and products available to consumers, such as cleaners and laundry detergents. Therefore, ANEOs containing products are expected to be released by the consumer throughout Canada. The down-

[9]As opposed to the other calculations presented in this assessment, the 2.5th percentile low flow of receiving water bodies was used to determine the dilution factor of the receiving environment instead of the usual 10th percentile low flow value. This value was used as ANEOs are not expected to remain in the water column for long duration. The 2.5th percentile is meant to account for lower flow events that can occur over a short period of time (in terms of days). Since the PNEC for ANEOs are calculated to represent acute toxicity events, the 2.5th percentile flow value of receiving water bodies reflects a suitable parameter to calculate concentration at the acute exposure level.

the-drain consumer PEC is estimated using CRAM (CRAM 2017).

A total mass between 100 000 kg and 1 000 000 kg per year for the six ANEOs was reported for use in various products, including cleaners, laundry detergents and personal care products (Canada 2015). As a worst-case assumption, a maximum quantity of 1 million kg/yr was used in the prediction. The distribution of PECs for down-the-drain release of ANEOs is presented in

Table 7-8. Furthermore, as the six ANEOs are not expected to remain in the water column for long durations, a PEC reflective of acute exposure conditions was used instead of a PEC reflective of chronic exposure conditions. This results in a slightly higher PEC.

Table 7-8. ANEOs distribution of PECs and risk quotients calculated by CRAM

Percentile [a]	PEC[b] (µg/L)	Risk quotient
10	8.15	0.40
20	4.33	0.21
30	2.74	0.13
40	2.03	0.10
50	1.62	0.08
60	1.30	0.06
70	1.06	0.05
80	0.83	0.04
90	0.60	0.03
100	0.05	0.002

[a] The percentile is the distribution of the CRAM results.
[b] PEC results were calculated based on acute exposure.

7.6.3 Characterization of ecological risk

The approach taken in this ecological risk assessment was to examine direct and supporting information and develop conclusions on the basis of a weight-of-evidence approach. Lines of evidence considered include information on sources and fate of the substance, persistence, bioaccumulation, estimated exposure to the substance, and ecological hazard properties. The six ANEOs are surfactants used in various applications including oil and gas extraction, metal working fluid, laundry detergents, soaps, and cleaners. On the basis of available information, more than 1 000 000 kg of ANEOs was manufactured and imported into Canada in 2014.

Considering the available information, when the six ANEOs are released into the soil compartment, they are expected to adsorb strongly (log K_{oc} 3.4 to 4.2) to soil and will have limited migration potential from the point of release. Similarly, when they are released into the aquatic compartment, they are expected to partition to sediments. Partitioning of the six ANEOs into the air compartment is not expected because of their low vapour pressure. Furthermore, the six ANEOs are anticipated to undergo some biodegradation. Degradants of ANEOs are anticipated to pose a lower ecological risk

than ANEOs as the hazard is primarily due to the surface activity. Therefore, the degradants of the six ANEOs were not considered further in this assessment.

Information in the form of bioaccumulation factor or bioconcentration factor test data which could be used to assess the bioaccumulation potential of the six ANEOs was unavailable. The strong association of POEA to anionically charged substances in the environment would reduce bioavailability for uptake across biological membranes. Furthermore, the six ANEOs are not considered persistent in the environment, which means its bioaccumulation potential would also be limited. PMRA (Health Canada 2015) concluded that POEA is non-bioaccumulative on the basis that the components can be broken down easily and that it is not persistent in soil or water. Given that ANEOs are anticipated to have similar properties as POEA, the six ANEOs are expected to have low bioconcentration potential.

According to the ecological hazard profile of the six ANEOs, ecotoxicity ranges from moderate to high for both acute and chronic effects. As they are not expected to persist in the water column when released, the POEA HC_5 for freshwater invertebrates estimated by Health Canada (2015) was selected as the CTV for the six ANEOs. In addition, the toxicity of the six ANEOs is anticipated to be mitigated by humic substances and suspended solids in the environment. Thus, a toxicity mitigation factor of 5 is applied to the CTV. The PNEC for the six ANEOs is estimated to be 20.5 µg/L.

For industrial use in metal working fluids, the information gathered indicates that up to 10 000 kg of the substance could be transferred to off-site treatment facilities per year, but the number of days of transfer is unknown. In addition, it is possible that the metal working facility could generate other waste that would be mixed with the metal working fluid. This would further dilute the ANEOs during each transfer. Given the uncertainty associated with metal working fluids, quantitative estimation of a PEC through metal working fluid exposure was not considered.

On the basis of the estimated PNEC (20.5 µg/L) and the estimated formulator PEC (8.45 µg/L), the risk quotient (PEC/PNEC) for the product formulation scenario is estimated to be 0.41. A series of risk quotients for consumer release(s), estimated using the varying PECs obtained from the CRAM (2017) model, is presented in Table 7-8.

Considering the risk quotient estimated for environmental releases from product formulation and products available to consumers, neither scenario for the six ANEOs is expected to result in environmental concern (i.e., risk quotients greater than 1). Given that conservative values (such as the low CTV) and high volumes were used to estimate the PNEC and PEC, it is anticipated that the risk quotients are an over-estimation of the potential risk. Overall, taking the available information, the six ANEOs are not expected to result in ecological concern.

7.7 Potential to cause harm to human health

The six ANEOs were previously screened through the second phase of polymer rapid screening. Through this rapid screening process, five ANEOs (see Table 7-9) were identified as not requiring further human health assessment. The five ANEOs were found to have either a low exposure or low human health hazard. Therefore, taking into consideration the available data, it is unlikely that exposure to those substances will pose a human health risk.

Classification of the hazard data and exposure profiles used to develop the potential for human health risks associated with the five ANEOs are presented in the document 'Supporting Documentation: Final Risk Matrix Location of Polymers' (Health Canada 2017).

Table 7-9. Human health assessments on ANEOs

CAS RN	CAS name
68155-39-5	Amines, C14-18 and C16-18-unsatd. Alkyl, ethoxylated
68439-72-5	Amines, C8-18 and C18-unsatd. Alkyl, ethoxylated
61791-24-0	Amines, soya alkyl, ethoxylated
28724-32-5	Poly(oxy-1,2-ethanediyl), α,α'-[(methyloctadecyliminio)di-2,1-ethanediyl]bis[ω-hydroxy-, chloride
68603-75-8	Amines, N-tallow alkyltrimethylenedi-, propoxylated

The substance 'Amines, tallow alkyl, ethoxylated' (POEA; CAS RN 61791-26-2) was found to have high exposure as well as high human health hazard through the second phase of polymer rapid screening (2017). It was therefore identified for further human health assessment.

7.7.1 Exposure assessment of amines, tallow alkyl, ethoxylated (CAS RN 61791-26-2)

7.7.1.1 Direct exposure

When used industrially for the manufacture of food packaging materials, direct exposure of the general population to POEA is not expected as the substance is trapped within a solid matrix from which it is not expected to be significantly released.

The worst-case aggregate exposure (the sum of dietary, pesticide residue and occupational applications derived contributions, infrequent, and all incidental exposures related to occasional behaviors) estimates for POEA in children ranged from 26 µg/kg bw/day for chronic exposure, to 91 µg/kg bw/day for acute exposure. For adults, those values ranged from 32 µg/kg bw/day for chronic exposure to 163 µg/kg bw/day for acute exposure (Williams et al. 2000).

Dietary exposure to POEA residues in food is not expected to be significant based on the assumption that residues would occur in proportion to active pesticide residue exposures, based on the relative amount of each in the formulation (*e.g.* 2:1, glyphosate: POEA). Using this ratio, the Theoretical Maximum Daily Intake (TMDI)

exposures for POEA are estimated as 12 and 26 µg/kg bw/day for the U.S. population and for children (1-6 years), respectively (Williams et al. 2000).

A screening level assessment for acute dietary exposure was conducted by the US EPA for four alkyl amine polyalkoxylates (ANEOs) including POEA. Based on the maximum amounts of ANEOs (inert ingredients such as surfactant) as well as the highest tolerance level residue for all food forms, including meat, milk, poultry and eggs, and default processing factors for dried foods, the chronic and acute dietary exposures to ANEOs for the adult U.S. population were estimated to be 40 and 114 µg/kg bw/day, respectively. For children 1-2 years old (the most highly exposed population subgroup) these values were reported as 127 and 315 µg/kg bw/day, respectively (US EPA 2009). Reasonably, these values for POEA would be proportionally lower (since several ANEOs were examined).

Although predicted dermal absorptions for the representative ANEO chemicals (such as POEA) using models ranged from negligible to 1.1%, EPA considered a conservative scenario with dermal absorption of 5% for ANEOs (US EPA 2009).

The concentration of POEA ranges from <1% in ready-to-use glyphosate pesticide formulations (such as Roundup®) to 21% in some concentrated professional products (Bradberry et al. 2004).

POEA is on the Pest Management Regulatory Agency (PMRA) pesticide formulants list (Health Canada 2010a). It is present in 176 pesticide products including herbicides, insecticides, fungicides, and slimicides, and in material preservatives (personal communication, PMRA, the New Substances Assessment and Control Bureau, Health Canada, dated May 2017; unreferenced).

According to Canadian Consumer Specialty Products Association (CCSPA), POEA is present in eight products available to consumers (personal communication, CCSPA, to the New Substances Assessment and Control Bureau, Health Canada dated May 2017; unreferenced).

According to notifications submitted under the *Cosmetic Regulations* to Health Canada, POEA is not used in registered cosmetic products (personal communication, emails from the Consumer Product Safety Directorate, Health Canada, to the New Substances Assessment and Control Bureau, Health Canada, December 2016; unreferenced).

POEA is not listed as a medicinal or non-medicinal ingredient in the NHPID, the LNHPD, or the DPS. Therefore, it is not expected to be present in such approved or licensed products in Canada (NHPD [modified 2019]; LNHPD [modified 2018]; DPD [modified 2017]).

The Water and Air Quality Bureau (WAQB) of Health Canada confirmed that there is no limit for POEA in drinking water (personal communication, emails from the WAQB, Health Canada, May 2017; unreferenced).

Given the negligible vapour pressure of POEA, no inhalation exposure is expected.

In summary, no inhalation exposure of the general population to POEA is expected. The dermal exposure is considered minimal. The oral exposure was estimated to be 12 to 32 µg/kg bw/day for adults, a maximum of 26 µg/kg bw/day for children (1-6 years), and no more than 127 µg/kg bw/day for children (1-2 years).

7.7.1.2 Indirect exposure

Surfactants are expected to bind tightly to soil and sediment particles and to degrade quickly via microbial degradation. Acute exposure to POEA from drinking water was calculated to be 1.8×10^{-2} µg/kg bw (for adults) and 5.5×10^{-2} µg/kg bw (for children). The chronic exposures, calculated in the same manner, were 1.0×10^{-3} and 3.0×10^{-3} µg/kg bw/day for adults and children, respectively (Williams et al. 2000).

The US EPA estimated that the acute drinking water concentrations for ANEOs (such as POEA) ranged from 0.001 to 41 µg/L. The concentrations for chronic drinking water ranged from 0.0002 to 19 µg/L (US EPA 2009).

POEA is expected to be non-volatile, non-persistent in soil and water, and immobile in soil and sediment. It is not likely to leach to groundwater because of its rapid microbial transformation and strong adsorption to soil particles (Health Canada 2015).

A Canadian study showed that, under real-world environmental conditions, unintended exposure of aquatic systems to POEA will most likely result in short, single-pulse exposures. These are due to rapid (< 24 h) partitioning of POEA into sediment and onto suspended particulates, where it will likely remain strongly bound, with low bioavailability (Rodriguez 2015).

In summary, the indirect exposure of the general population to POEA through environmental media such as drinking water is expected to be minimal (in the ng/kg bw range).

7.7.2 Health effects assessment

During evaluation under the Second Phase of Polymer Rapid Screening assessment, POEA was identified as requiring further assessment as a result of potential pulmonary toxicity. POEA does not contain any reactive functional groups which are known to be associated with adverse human health effects.

Alkyl amine polyalkoxylates are not acutely toxic by the oral and dermal routes of exposure, or via inhalation under normal use conditions, but can show moderate toxicity in animal studies. Concentrated materials are generally corrosive, are eye and skin irritants at lower concentrations, and may be dermal sensitizers. There is no evidence that alkyl amine polyalkoxylates are neurotoxic, mutagenic, or clastogenic (US EPA 2009).

An SDS by Stepan indicates that POEA has a moderate acute oral toxicity in rats with an LD_{50} > 1437 mg/kg bw in males and 1316 mg/kg bw in females, as well as a moderate dermal toxicity in rabbits with an LD_{50} > 1260 mg/kg bw. It can cause severe skin burns and eye damage but is not expected to be a dermal sensitizer. It is not considered to be carcinogenic by IARC, ACGIH, NTP or OSHA. Prolonged inhalation may be harmful (SDS 2017d).

The acute inhalation toxicity (4 h) of POEA was tested in Wistar rats (5/sex) via nose-only liquid aerosol at concentrations of 0.27, 0.6, 2.3 and 5.7 mg/L. One of 5 males and 3 of 5 females died at 0.27 mg/L, and 2 of 5 males and 2 of 5 females died at 0.6 mg/L. All animals died when exposed to concentrations of 2.3 or 5.7 mg/L. Histopathological examination of 2 females that died shortly after exposure showed various lung lesions, including lung congestion, alveolar edema and multifocal suppurative (partly necrotic) bronchopneumonia (document provided by BASF to Environment Canada in response to a CEPA section 71 survey on April 18, 2013). The LC_{50} was established at 0.473 mg/L, which is indicative of very high inhalation toxicity. An EFSA document reported an inhalation NOAEL of 1.66 mg/kg bw/day from a whole body inhalation study performed in rats (6 h/day, 5 d/wk) (EFSA 2015).

POEA was administered to Sprague–Dawley rats in the diet for 1 month at concentrations of 0, 800, 2000, or 5000 ppm. Body weight gains were reduced in males at the 2000 ppm level and in both sexes at the high-dose level. Prominent/enlarged lymphoid aggregates in the colon of high-dose females were associated with direct irritation/inflammatory effect of the test material. In a subsequent 3-month study with rats, POEA was administered in the diet at concentrations of 0, 500, 1500, and 4500 ppm. In animals from the high-dose group, effects noted included intestinal irritation, decreased food consumption and decreased body weight gain, as well as alterations in serum hematology/clinical chemistry parameters. Intestinal irritation was also observed in some animals from the 1500 ppm dosage level. Therefore, the NOAEL was established at 500 ppm in the diet (36 mg/kg bw/day, males and females combined) (Williams et al. 2000). Another 90-day subchronic study in rats generated a NOAEL of 19.9 mg/kg bw/day in males and 24.1 mg/kg bw/day in females based on histological lesions of the intestinal mucosa (EFSA 2015). POEA was administered in gelatin capsules to beagle dogs daily for 14 weeks. Because gastrointestinal intolerance (as evidenced by emesis and diarrhea) was observed at a preliminary stage, dosages were decreased during the first 4 weeks of the study and then maintained at 0, 30, 60, or 90 mg/kg bw/day for the final 10 weeks of the study. A NOAEL of 21 mg/kg bw/day was established on the basis of clinical chemistry findings of lower blood calcium and protein concentrations (EFSA 2015).

POEA was administered by gavage to pregnant Sprague–Dawley rats on gestation days 6 through 15 at dosages of 0, 15, 100, or 300 mg/kg bw/day. Significant maternal toxicity, including mortality, was noted at the highest dosage tested, while minimal effects occurred at the mid-dose level. There were no effects in fetuses at any dosage. The NOAELs for maternal and developmental toxicity were shown to be 15 and 300 mg/kg bw/day, respectively. The POEA surfactant is not a teratogen or a developmental

toxin in rats (Williams et al. 2000).

7.7.3 Characterization of risk to human health

In this assessment, human health risks were established through consideration of both the hazard and the direct and indirect exposure of the substance for current uses identified from voluntary surveys and mandatory surveys conducted under section 71 of CEPA, as well as from governmental databases.

POEA has moderate acute and subchronic toxicity and high inhalation toxicity in animals. However, the health effects are more associated with the surfactant properties of the substance causing cellular membrane damage and not a result of intrinsic systemic toxicity of the substance. The majority of observed effects were the result of irritation of the gastrointestinal tract. POEA is not expected to be a developmental toxicant, as maternal toxicity was observed at lower dose levels than those observed for developmental toxicity. Although a low MOE of <118 was obtained for oral exposure associated with children 1-2 using chronic exposure values, the MOE is the sum of the toxicity of four substances, only one of which is POEA. Since the proportions of each substance were not available, a more refined calculation could not be performed, but it can logically predicted that the MOE for POEA alone would be greater.

Table 7-10. Risk Characterization of POEA

Exposure scenario	Estimated exposure per event	Critical effect level	Critical health effect endpoint (systemic effect)	MOE
Oral, adults	12–32 µg/kg bw	NOAEL of 15 mg/kg bw/day	Gastrointestinal intolerance	1250–469
Oral, children (1-2 years)	<127 µg/kg bw	NOAEL of 15 mg/kg bw/day	Gastrointestinal intolerance	>118
Oral, children (1-6 years)	26 µg/kg bw	NOAEL of 15 mg/kg bw/day	Gastrointestinal intolerance	577

POEA has a high toxicity via inhalation that is associated with its surfactant properties and their effects on the alveoli. Inhalation exposure resulting from products available to consumers is not anticipated as the vapour pressure is negligible and products generating aerosols are not expected. Therefore, the health risk is low.

Taking into consideration the routes of consumer exposure as well as moderate health hazard associated with POEA, through characteristics that are common to all surfactants, the human health risk has also been determined to be low on the basis of the current exposure scenarios.

8. Uncertainties in evaluation of ecological risk

AESs, AEs, OPEs, and ANEOs are low molecular weight surfactants. There are various uncertainties related to the ecological assessment of AESs, AEs, OPEs, and ANEOs. It is recognized that a given CAS RN can describe polymers that have different number average molecular weights and composition, and hence a different range of physical-chemical properties and hazard properties. Furthermore, there are uncertainties in the exposure scenarios, such as the maximum quantity that a formulation could utilize in a year, the flow and dilution of the receiving water bodies, and the emission factor. However, considering that conservative assumptions were used to determine the hazard and exposure potentials for the four groups of substances, changes in molecular weight, quantities, or other factors are not expected to result in a significant change in ecological risk.

9. Uncertainties in evaluation of risk to human health

The degree of polymerization (*n*) and molecular weight of polymers (including those in this report) are rarely characterized by exact values, but by a range. Consequently, physical and chemical properties vary (sometimes considerably), resulting in different behaviour in environmental and physiological media.

These polymers within this grouping can be synthesized at different molecular weights. The smaller molecular weight substances can have a different toxicity profile and potential to absorb than the higher molecular weight polymers. Information on the size of the polymer for each application is not always available which adds uncertainty to the risk evaluation.

Because PF releases formaldehyde in an aqueous environment, it is difficult to separate the toxicological effects of PF from those of formaldehyde.

In some situations, a value could be calculated for a particular route of exposure, but there was insufficient toxicological information to calculate the MOE for aggregate exposures, thereby leaving some uncertainty in the risk assessment.

10. Conclusion

Considering all available lines of evidence presented in this draft screening assessment, there is low risk of harm to the environment from PPG, PF, and the three AESs, eight AEs, two OPEs and six ANEOs considered in this assessment. It is proposed to conclude that PPG, PF, and the three AESs, eight AEs, two OPEs and six ANEOs considered in this assessment 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.

On the basis of the information presented in this draft screening assessment, it is proposed to conclude that PPG, PF, and the three AESs, eight AEs, two OPEs and six ANEOs 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 therefore proposed to conclude that PPG, PF, and the three AESs, eight AEs, two OPEs and six ANEOs considered in this assessment do not meet any of the criteria set out in section 64 of CEPA.

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Appendix. Assessment approaches applied during the second phase of polymer rapid screening

The approaches applied during the second phase of polymer rapid screening are outlined in this section. The detailed analyses, as well as the results of the second phase of polymer rapid screening for the individual substances, are presented in Chapter 2 to 7.

Characterization of ecological risk for PPG and PF

The ecological risks of PPG and PF were characterized using the approach described in detail in the report *Second Phase of Polymer Rapid Screening: Results of the Screening Assessment* (ECCC, HC 2018). The approach consisted of multiple steps that addressed different factors related to the potential for a polymer to cause ecological harm. At each step in the rapid screening process, any substance that appeared to present a potential for harm was identified as requiring further assessment. The approach was intended to be pragmatic, protective of the environment, and fairly rapid, largely making use of available or easily obtainable data. It is summarized below.

The ecological component of the second phase of polymer rapid screening approach consisted of four main steps to identify polymers that warrant further evaluation of their potential to cause harm. The first step involved identifying polymers which are not likely to be of ecological concern based on low reported import and manufacture quantities according to Phase Two of the Domestic Substances List Inventory Update (Canada 2012), a voluntary survey (ECCC 2015) and a mandatory survey conducted under section 71 of CEPA (Canada 2015). Polymers with import and/or manufacture volumes less than 1000 kg per year are not likely to be of ecological concern. This is consistent with the notifying trigger quantity of 1000 kg for polymers under section 7 of the *New Substances Notification Regulations (Chemicals and Polymers)* (Canada 2005).

The second step involved determining whether the polymer will likely have water extractability greater than 2% by weight. Water extractability greater than 2% by weight indicates that the polymer may be more bioavailable to aquatic organisms. The increased potential for exposure to aquatic organisms may present higher ecological risk. Literature, online safety data sheet (SDS) databases, the internal New Substances database for polymers, data gathered through a voluntary survey (ECCC 2015) and a mandatory section 71 survey under CEPA (Canada 2015), and other reliable sources and databases (e.g. QSAR toolbox, ECHA chemical database) were searched for water extractability and solubility information.

The third step in the ecological component involved identifying polymers with reactive functional groups (RFGs). RFGs are groups with chemical functionality that are considered to be reactive and may have damaging effects on the biological community. These groups are well described in Schedule 7 of the *New Substances Notification Regulations (Chemicals and Polymers)* (Canada 2005), and polymers containing RFGs may be of increased ecological concern and require further screening. The RFGs

include, among others, potentially cationic or cationic functionalities, alkoxy silanes, and phenols with unsubstituted ortho or para positions. To determine the presence of RFGs, structural information was gathered through a voluntary survey (ECCC 2015) and a mandatory survey under section 71 of CEPA (Canada 2015). For polymers where no representative structures were provided, structural representations were derived from information available for similar polymers obtained from the internal New Substances program database or the Chemical Abstract Services (CAS) name and based on professional knowledge of likely polymerization mechanisms.

The final step for ecological considerations involved applying environmental release scenarios to estimate environmental exposure. Two generic aquatic exposure scenarios were applied to identify potential concerns near the point of discharge of a polymer into the environment. These scenarios involved comparing conservative (i.e., ecologically protective) estimates of exposure in receiving waters (predicted environmental concentrations [PEC]) with an effects threshold (predicted no-effect concentration [PNEC]) in order to evaluate whether a polymer is likely to cause harm to the local aquatic environment. The approaches made use of quantity information from each reporting company gathered through Phase Two of the DSL Inventory Update (Canada. 2012), and import and/or manufacture volumes through a voluntary survey (ECCC 2015) and a mandatory survey conducted under section 71 of CEPA (Canada 2015). The aquatic PNEC for each of the scenarios was derived from the critical toxicity value (CTV), which was divided by an assessment factor (AF) as shown:

$$\text{Aquatic PNEC (mg/L)} = \text{CTV} / \text{AF}$$

CTVs were based on empirical or modelled data (where appropriate). Experimental ecotoxicity data were gathered through the voluntary survey and polymer survey under section 71 of CEPA, literature information, as well as read-across data from polymers that have been assessed by the New Substances program. If the scenarios indicated a low likelihood of harm to aquatic organisms (i.e., ratio of PEC/PNEC is less than 1), the polymer is anticipated to present low ecological concern.

It is recognized that conclusions resulting from the use of the second phase of polymer rapid screening have associated uncertainties, including commercial activity variations. However, the use of both a wide range of information sources (relating to both exposure potential and hazard concerns identified for a polymer) and conservative exposure scenarios increases confidence in the overall approach that the polymers identified as not requiring further assessment are unlikely to be of concern.

Information on the decision taken at each step for each polymer is presented in a document titled *Information on the Decision Taken at Each Step for Rapid Screening II of Polymers* (ECCC 2016).

On the basis of the available information, PPG and POEA were identified in the second phase of polymer rapid screening as being unlikely to cause ecological harm.

Characterization of risk to human health for polyalkoxylates (other than POEA)

The human health risks of polyalkoxylates (other than POEA) were characterized using the approach outlined in the report *Second Phase of Polymer Rapid Screening: Results of the Screening Assessment* (ECCC, HC 2018). This process consisted of determining the location of each polymer in a health risk matrix, assigning a low, moderate or high level of potential concern for substances based on their hazard and exposure profiles. The matrix has three exposure bands that represent different exposure potentials, increasing from band 1 to 3, and three hazard bands that represent different hazard potentials, increasing from band A to C.

The first step involved identifying the degree of direct and indirect exposure for each polymer based on its human exposure potential derived through its use pattern, its import, manufacture or use quantity, and its water extractability. To determine whether a polymer is used in or is present in a product available to Canadians, numerous additional sources of information related to both domestic and international use and product information were searched and consulted.

The highest exposure band (3) is designated for polymers that are expected to have high direct exposure resulting from their use in products available to consumers intended for consumption or application to the body, such as personal care products. **The middle exposure band (2)** is designated for polymers that are anticipated to have moderate direct or indirect exposure resulting from the use of polymers in household products not intended to be applied to the body or consumed, such as cleaning products, household paint and sealants. **The lowest exposure band (1)** is designated for polymers that are anticipated to have low direct or indirect exposure. This exposure band includes polymers that are used in the industrial sector to form manufactured articles and that are often contained within or reacted into a cured or hardened polymer matrix during industrial manufacturing.

The second step involved identifying the hazard potential and corresponding hazard band for each polymer based on the presence of reactive functional groups (RFGs) and available toxicological data. Identification of a hazard band was performed independently of the identification of an exposure band. **The highest hazard band (C)** is associated with polymers that are known or suspected to have a RFG or metals of concern to human health. The highest hazard band is also assigned to polymers for which toxicological data on the polymer or a structurally-related polymer shows or suggests that the polymer may pose a human health risk. **The middle hazard band (B)** is associated with polymers that do not contain any RFGs or metals of concern to human health but may contain other structural features, such as ethylene glycol, aliphatic and aromatic amines or maleic acid anhydrides, that may be associated with human health effects. **The lowest hazard band (A)** is associated with polymers that do not contain a RFG or other structural feature or metals that are known to be associated with human health concerns and for which available toxicological data indicates a low concern for human health.

The final step combined the exposure and hazard potentials to determine the overall risk potential as represented by the location in the risk matrix. Polymers that have a moderate-to-high exposure potential and the highest hazard potential (cells 2C or 3C) are identified as requiring further assessment to determine their risk to human health.

Polymers that are placed in all other cells of the risk matrix are considered unlikely to cause harm to human health at current levels of exposure. As a result, these polymers are not identified as requiring further human health assessment.

It is recognized that conclusions resulting from the use of this polymer rapid screening approach have associated uncertainties, including commercial activity variations and limited toxicological information. However, the use of a wide range of information sources (relating to both exposure potential and hazard concerns identified for a polymer), as well as the use of conservative exposure scenarios, increase confidence in the overall approach that the polymers identified as not requiring further assessment are unlikely to be of concern.

Information on the decision taken at each step for the substances in this assessment is presented in Health Canada (2017).

Based on available information, substances in the polyalkoxylates group; propylene glycols, paraformaldehyde and alkylamine ethoxylates, were identified in the second phase of polymer rapid screening as potentially resulting in significant direct or indirect exposure or posing a health hazard as a result of exposure. Based on available information, substances in the polyalkoxylates group; alcohol ethoxylates sulfates, alcohol ethoxylates and octylphenol ethoxylates are not anticipated to result in significant direct or indirect exposure or pose a health hazard as a result of exposure. It is therefore unlikely that exposure to these substances will result in a human health risk for the general population.