Screening Assessment for the Challenge

Dodecamethylcyclohexasiloxane
(D6)

Chemical Abstracts Service Registry Number
540-97-6

Environment Canada
Health Canada

November 2008

Synopsis

Pursuant to section 74 of the Canadian Environmental Protection Act, 1999 (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment on dodecamethylcyclohexasiloxane (D6), Chemical Abstracts Service Registry Number 540-97-6. During the categorization process, this substance was identified as a high priority for screening assessment and included in the Ministerial Challenge because it had been initially found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity (PBiT) to non-human organisms and it is known to be in commerce in Canada.

Although the categorization exercise did not determine D6 to be a priority for assessment of potential risks to human health, a human health assessment of D6 was also conducted due to its structure and use pattern similarity to octamethylcyclotetrasiloxane (also known as D4), a high priority for assessment for both human health and ecological risks under CEPA 1999.

D6 is an industrial chemical which was not manufactured in Canada in 2006 in a quantity above the reporting threshold of 100 kg, but which is imported into the country in mixtures with other cyclic siloxanes, as a residual in silicone polymers, and in finished consumer products. From responses to a notice published under section 71 of CEPA 1999, it was determined that between 100 000 and 1 000 000 kg of D6 were imported into Canada in 2006.

D6 may be released to the environment from industrial processes such as blending, formulation and packaging and from its use as an industrial defoamer and degreaser. It is also released from the use and disposal of personal care products. Air, wastewater, and agricultural soil are the principal receiving environmental media for D6 based on its physical-chemical properties and its use patterns.

In air, D6 is persistent with calculated atmospheric half-lives of more than 2 days. D6 has the potential to be transported over long-distances in the atmosphere. However, it has a low potential to be deposited in water or soil in remote regions. The hydrolysis half-life for D6 is expected to be longer than that of its structurally similar analogues, D4 and D5. A half-life of ~401 days was extrapolated for D6 based on the experimental hydrolysis half-lives of D4 and D5 at neutral pH and ambient temperature. D6 is therefore considered persistent under typical Canadian water conditions. In sediment, D6 is expected to have a half-life longer than 49 to 588 days under realistic Canadian sediment conditions (temperature of 5-25^{o}C), indicating that D6 may be persistent in sediment. D6 is not considered persistent in soil, based on evidence of clay-catalysed degradation, with dimethylsilanediol being the stable hydrolysis product. It is therefore concluded that D6 meets the persistence criterion as set out in the *Persistence and Bioaccumulation Regulations*.

The empirical bioconcentration factor is less than 2000, consistent with decreased bioavailability of the substance due to its high log K_{ow} value. The read-across laboratory biomagnification factor values from D4 and D5 indicate that D6 does not biomagnify in the test fish from dietary uptake. Although a modelled bioaccumulation factor over 5000 suggested that the bioaccumulation potential of D6 is high, the predicted bioaccumulation factor alone is not considered to provide sufficient weight to conclude that D6 has a high bioaccumulation potential due to a high degree of uncertainty in this prediction. Thus, while D6 may have some bioaccumulation potential in biota, it is concluded based on empirical bioconcentration factor data and read-across evidence, that D6 does not meet the bioaccumulation criterion as set out in the *Persistence and Bioaccumulation Regulations*.

Information on the toxicity of D6 to sediment-dwelling organisms is not available; a conservative read-across from D5 was applied and it is concluded that the no-effect concentration for D6 to the benthic community is above 69 mg/kg. The experimental toxicity data showed no adverse effects to pelagic aquatic organisms at concentrations up to 0.0046 mg/L, its approximate water solubility limit. However, reduced bioavailability compared to its close analogues, D4 and D5, suggests that no toxic threshold for adverse effect is expected for D6 at its water solubility limit. Given the low bioavailability and low potential for effects, it is concluded that D6 has low potential to cause ecological harm.

With respect to human health, the liver was identified as a target organ for oral exposures and potentially inhalation exposures of D6. The critical effect level for repeated-dose toxicity was based on increased liver weight, periportal lipidosis and thyroid follicular cell hypertrophy in a 4-week rat study. Comparison of the critical effect level for repeated dose effects via the oral route and the upper-bounding estimates of daily intake of D6 by the general population in Canada results in an adequate margin of exposure. Based on an independent review of a refined exposure assessment for personal care products, an adequate margin of exposure was derived by comparison of the critical effect level for repeated dose effects via the oral route and the conservative upper-bounding estimate of daily intake of D6 via personal care products.

Based on the available information on its potential to cause ecological harm, it is concluded that D6 is not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity, or that constitute or may constitute a danger to the environment on which life depends.

Based on the available information on its potential to cause harm to human health, it is concluded that D6 is 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.

This substance will be included in the upcoming *Domestic Substances List* inventory update initiative. In addition and where relevant, research and monitoring will support verification of assumptions used during the screening assessment and, where appropriate,

the performance of potential control measures identified during the risk management phase.

Based on the information available, it is concluded that D6 does not meet any of the criteria set out in section 64 of the *Canadian Environmental Protection Act, 1999*.

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Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that have met the categorization criteria set out in the Act to determine whether these substances present or may present a risk to the environment or human health. Based on the results of a screening assessment, the Ministers can propose to take no further action with respect to the substance, to add the substance to the Priority Substances List (PSL) for further assessment, or to recommend that the substance be added to the List of Toxic Substances in Schedule 1 of the Act and, where applicable, the implementation of virtual elimination.

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

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

The Ministers therefore published a notice of intent in the *Canada Gazette*, Part I, on December 9, 2006 (Canada 2006), that challenged industry and other interested stakeholders to submit, within specified timelines, specific information that may be used to inform risk assessment, and to develop and benchmark best practices for the risk management and product stewardship of those substances identified as high priorities.

The substance dodecamethylcyclohexasiloxane, also known as D6, was identified as a high priority for assessment of ecological risk as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is in commerce in Canada. The Challenge for this substance was published in the *Canada Gazette* on May 12, 2007 (Canada 2007). A substance profile was released at the same time. The substance profile presented the technical ecological information available prior to December 2005 that formed the basis for categorization of this substance. As a result of the Challenge, more than 100 submissions of information were received for this substance pertaining to its physical and chemical properties, bioaccumulation potential, persistence, ecotoxicology, quantity in commerce and so on.

Although the categorization exercise did not determine D6 to be a priority for assessment with respect to risks to human health, it was recommended that a human health assessment also be conducted due to its structure and use pattern similarity to D4, also

known as octamethylcyclotetrasiloxane, a high priority for assessment for both human health and ecological risks under CEPA 1999, and due to the increased use of D6 as an alternative to D4. Therefore, this assessment focuses on information relevant to the evaluation of ecological risks and to the evaluation of risks to human health.

Under CEPA 1999, screening assessments focus on information critical to determining whether a substance meets the criteria for defining a chemical as toxic as set out in section 64 of the Act, where

> "64. […] a substance is toxic if it is entering or may enter the environment in a quantity or concentration or under conditions that
>
> (*a*) have or may have an immediate or long-term harmful effect on the environment or its biological diversity;
>
> (*b*) constitute or may constitute a danger to the environment on which life depends; or
>
> (*c*) constitute or may constitute a danger in Canada to human life or health."

Screening assessments examine scientific information and develop conclusions by incorporating a weight-of-evidence approach and precaution.

This screening assessment includes consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches, up to August 2008 for both human health and ecological sections of the document. Key studies were critically evaluated; modelling results may have been used to reach conclusions. When available and relevant, information presented in hazard assessments from other jurisdictions was considered. The screening assessment does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies and lines of evidence pertinent to the conclusion.

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

This screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. This assessment has undergone external written peer review/consultation. Comments on the technical portions relevant to human health were received from Toxicology Excellence for Risk Assessment (TERA). While external comments were taken into consideration, the final content and outcome of the screening

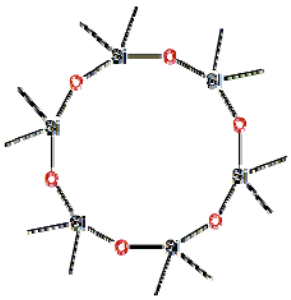
risk assessment remain the responsibility of Health Canada and Environment Canada. Additionally, the draft of this screening assessment was subject to a 60-day public comment period. The critical information and considerations upon which the assessment is based are summarized below.

Substance Identity

For the purposes of this document, dodecamethylcyclohexasiloxane will be referred to as D6, an abbreviated name derived from the siloxane notation developed by General Electric (Hurd 1946).

D6 belongs to a group of cyclic volatile methyl-siloxanes (cVMS) with relatively low molecular weight (<600 g/mol) and high vapour pressure. These cVMS are volatile, low-viscosity silicone fluids consisting of $[-Si(CH_3)_2O-]_x$ structure units in a cyclic configuration. D6 consists of six of these $[-Si(CH_3)_2O-]$ structure units (x = 6) as shown in the chemical structure below (Table 1).

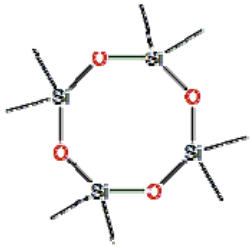
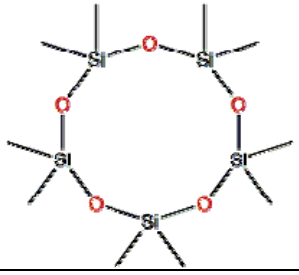
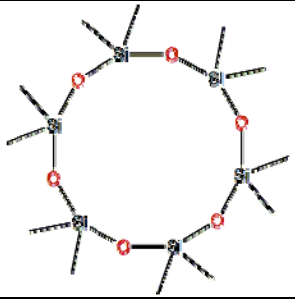
Table 1. Substance identity for D6

Chemical Abstracts Service Registry Number (CAS RN)	**540-97-6**
Name on Domestic Substances List (DSL)	**Cyclohexasiloxane, dodecamethyl-**
National Chemical Inventories (NCI) names[1]	Cyclohexasiloxane, 2,2,4,4,6,6,8,8,10,10,12,12-dodecamethyl- (TSCA) Cyclohexasiloxane, dodecamethyl- (AICS, PICCS, ASIA-PAC, NZIoC) Dodecamethylcyclohexasiloxane (EINECS, ECL)
Other names	D6; Dodecamethylhexacyclosiloxane; Cyclic hexamer: D6; 2,4,6,8,10,12-Dodecamethylcyclohexasiloxane
Major chemical class or use	Organosilicon compounds
Major chemical sub-class	Cyclic volatile methyl-siloxanes (cVMS)
Molecular formula	$C_{12}H_{36}O_6Si_6$
Chemical structure	
Simplified Molecular Input Entry Line System (SMILES)	C[Si]1(O[Si](O[Si](O[Si](O[Si](C)(C)O[Si](O1)(C)C)(C)C)(C)C)(C)C)C
Molecular mass	444.93 g/mol

1 National Chemical Inventories (NCI). 2006: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Commercial Chemical Substances); PICCS (Philippine Inventory of Chemicals and Chemical Substances); NZIoC New Zealand Inventory of Chemicals; and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

It should be noted that D6 is also contained under another Chemical Abstracts Service Registry Number. This registry number, CAS RN 69430-24-6, refers to a mixture of dimethyl-substituted cyclosiloxanes of the general structure $[-Si(CH_3)_2O-]_x$ in a cyclic configuration, where x is generally less than 8, and more commonly x is 3–7 (SEHSC 2007a). This CAS number is associated with the following names: cyclopolydimethylsiloxane, cyclopolydimethylsiloxane (DX), cyclosiloxanes di-Me, dimethylcyclopolysiloxane, polydimethyl siloxy cyclics, polydimethylcyclosiloxane, cyclomethicone and mixed cyclosiloxane. In this report it will be referred to as cyclomethicone, a term commonly used for the mixture in the cosmetics industry.

For this assessment, data from analogue D4 and D5 have also been used based on structural similarity as shown in the table below:

D4	**D5**
	
D6	
	

Physical and Chemical Properties

Table 2 contains experimental and modelled physical and chemical properties of D6 that are relevant to its environmental fate.

Table 2. Physical and chemical properties of D6

Property	Type	Value[1]	Temperature (°C)	Reference
Melting point (°C)	Experimental	-3*		PhysProp 2006
	Modelled	-8.69		MPBPWIN 2000
Boiling point (°C)	Experimental	245*		PhysProp 2006
	Modelled	226.77		MPBPWIN 2000
Density (kg/m^3)	Experimental	963	25	SEHSC 2005
Vapour pressure (Pa)	Experimental	4.6* (0.0345 mm Hg)	25	SEHSC 2005
		4 (0.03 mm Hg)	25	Flaningam 1986
	Modelled	4.73 (0.0355 mm Hg)	25	MPBPWIN 2000
Henry's Law constant ($Pa \cdot m^3/mol$)	Extrapolated from experimental log K_{aw} of D4 and D5	4 950 000* (48.9 $atm \cdot m^3/mol$)		Xu and Kropscott 2007
	Experimental	14 667 (0.145 $atm \cdot m^3/mol$)	26	Kochetkov et al. 2001
		6712 (0.066 $atm \cdot m^3/mol$)	26	Kochetkov et al. 2001
	Modelled	16 212 (0.16 $atm \cdot m^3/mol$)	25	HENRYWIN 2000
Log K_{aw} (Air-water partition coefficient) (dimensionless)	Extrapolated from experimental log K_{aw} of D4 and D5	3.3*		Xu and Kropscott 2007
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)	Experimental	9.06*	22	SEHSC 2007d
		4.36	22.5	Miller 2006
		5.86		Bruggeman et al. 1984
	Modelled	6.33		KOWWIN 2000
	Modelled	6.07		PCKOCWIN 2000
Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)	Modelled	6.1*		PCKOCWIN 2000
Water solubility (mg/L)	Experimental	0.005 13*	23	Varaprath et al. 1996
	Modelled	0.005	25	WSKOWWIN 2000
Log K_{oa} (Octanol-air partition coefficient) (dimensionless)	Experimental	5.76*	24	Xu 2006
	Modelled	5.50		Calculated from modelled $LogK_{ow}$-$LogK_{aw}$

[1] If different, values and units in parentheses represent the original values as reported by the authors or as estimated by the models.

* Values used in modelling for this screening assessment.

Recently, empirical log K_{ow} values were received and were critically evaluated. The experimental log K_{ow} of 4.36 for D6 was determined by using the slow stir method following OECD Guideline 123 (Miller 2006). A radio-labelled ^{14}C-D6 was used in the test. The measurement of K_{ow} was carried out in triplicate with one blank control. The temperature was maintained constant at 22.5 ± 0.5ºC throughout the study. Equilibrium was achieved in 7 days and the weighted average K_{ow} was calculated based on the sampling from the last four days. A log K_{ow} of 4.36 was calculated. The analysis of radio-labelled ^{14}C-D6 in water and octanol was conducted by using liquid scintillation counting (LSC). LSC analysis does not distinguish between a parent compound and its potential hydrolysis products. The author suggested that potential water-soluble hydrolysis products may have been the cause for overestimation of the D6 concentrations in water. However, the hydrolysis potential for D6 is expected to be low under the test conditions that were used (Xu 2006). D6 is expected to have a higher log K_{ow} value compared to its close analogues D4 and D5 due to its lower water solubility. Considering that acceptable log K_{ow} values of 4.45–6.49 and 4.76–8.03 have been reported for D4 and D5 respectively, the above value reported for D6 was considered unreliable and was not considered further in this assessment.

A log K_{ow} value of 9.06 for D6 was estimated by Xu (SEHSC 2007d), extrapolated from the experimental K_{ow} values from D4 (Kozerski and Shawl 2007) and D5 (Kozerski 2007) and is used in this screening assessment.

The log K_{ow} value of 5.86 was determined by Bruggeman et al. (1984) using a high-performance liquid chromatography (HPLC)-retention time method. The measurement was performed on an octadecylsilyl-bonded silica column with 90:10 methanol:water as the mobile phase. Homologous series of n-alkylbenzenes with known log K_{ow} values were used as reference compounds to calibrate the method. The experimental details of this study are currently unavailable.

Recent experiments on the air-water partition coefficient for D4 and D5 were conducted by Xu (Xu and Kropscott 2007). The partitioning equilibrium among air, water and an organic phase (octanol) was simultaneously achieved during the experiment. The calculated log K_{oa} and log K_{ow} values for D4 and D5 were reasonably consistent with the measured experimental values for D4 and D5 reported by Xu (2006) and Kozerski (2007) and are in good agreement with the equilibrium of log K_{ow} = log K_{oa} + log K_{aw}. The study is therefore considered acceptable for this screening assessment report. The average log K_{aw} of 2.69 and 3.13 for D4 and D5, respectively, were determined by the total D4 and D5 radioactivity in air and water. The log K_{aw} of D6, therefore, can be extrapolated as 3.3 in accordance with log K_{aw} = log K_{ow} - log K_{oa}. The extrapolated K_{aw} gives a Henry's Law constant of 4 950 000 Pa•m^3/mol.

For D6, other modelled physical and chemical properties are in good agreement with its measured experimental data. Except for the data discussed above, the most conservative experimental data, when applicable, are used in various model predictions in this screening assessment report.

Sources

There are no known natural sources of D6.

D6 is an industrial chemical which was not manufactured by any company in Canada in 2006 in a quantity above the reporting threshold of 100 kg, but which is imported into the country in mixtures with other cyclic siloxanes, as a residual in silicone polymers, and as an ingredient in finished consumer products. From responses to a notice published under section 71 of CEPA 1999, it was determined that between 100 000 and 1 000 000 kg of D6 were imported into Canada, as raw materials for formulation and in finished products, in 2006 (Environment Canada 2007). The quantities of D6 imported into Canada have increased significantly since the DSL nomination (Environment Canada 1988).

D6 is a constituent of CAS RN 69430-24-6, termed cyclomethicone in the cosmetics industry. Although cyclomethicone was not directly surveyed under CEPA section 71 by Environment Canada and Health Canada in 2007, it is evident that in some cases, responses to the notice published under section 71 of CEPA 1999 for the 2006 calendar year contained data on the quantity of D6 used or imported as CAS RN 69430-24-6 (Environment Canada 2007).

The quantity of CAS RN 69430-24-6 reported in commerce in Canada during the 1986 calendar year was 2 220 000 kg (Environment Canada 1988). In 2005, Canada was a net importer of 11 500 000 kg of all types of silicone polymers and siloxanes (Will et al. 2007).

D6 is an intermediate in the production of polydimethylsiloxanes (PDMS) silicone polymers, and all PDMS contain residual amounts of volatile cyclosiloxanes, including D6. The lower molecular weight (and consequently lower viscosity) polymers may contain from < 0.1% to 0.5% volatile cyclosiloxanes, and higher molecular weight (and consequently higher viscosity) polymers may contain 1-3% volatile cyclosiloxanes. The proportion of the volatile cyclosiloxanes that consists of D6 is highly product-specific. Release of D6 from some applications of PDMS is expected to occur once the PDMS product is in use (SEHSC 2007b).

D6 has been identified as a high production volume (HPV) chemical by the Organisation for Economic Co-operation and Development (OECD 2007) and the US Environmental Protection Agency (US EPA 2007).

In the United States, there is a trend toward the increased use of volatile methyl-siloxanes, including D6, because of their exemption from volatile organic compound (VOC) legislation in 1994 (US EPA 1994a). Volatile methyl-siloxanes were used as an alternative to chlorofluorocarbons (CFCs) as a means of reducing the regulated VOC content in products (specifically, precision and electronic cleaning applications). According to information from the US EPA, the import/production of D6

in the United States was in the range of 4.5–225 tonnes in 1986, increasing to 450–4500 tonnes in 1990, 1994 and 1998, and then increasing again to 4500–45 000 tonnes in 2002.

In Europe, D6 has been identified as a low production volume (LPV) chemical, with Dow Corning Limited of the United Kingdom as the only producer/importer of D6 (ECB 2007). Currently, there are no controls on D6 in Europe. The quantity of D6 used in the European Union as a site-limited intermediate during 2003-2004 is confidential information.

Uses

The most important use, worldwide and in Canada, of D6 is as an ingredient in the formulation of personal care products and as an intermediate in the production of polydimethylsiloxanes (PDMS) silicone polymers. As indicated above, D6 is also a constituent of CAS RN 69430-24-6, termed cyclomethicone in the cosmetics industry. Cyclomethicone is a mixture of low molecular weight volatile cyclic siloxanes, the principal ingredients of which are octamethylcyclotetrasiloxane (D4), decamethylcyclopentasiloxane (D5), and dodecamethylcyclohexasiloxane (D6), in varying proportions. In Canada, the most important uses of the mixtures of low molecular weight volatile cyclic siloxanes, which may contain a certain percentage of D6, are in the preparation of personal care products including hair and skin care products, and antiperspirants (Environment Canada 2007).

All silicone polymers contain trace residual amounts of volatile cyclosiloxanes, including D6. Silicone polymers that contain trace amounts of D6 can be grouped as fluids, gums and resins. Uses of such polymers are described below.

Important uses of silicone fluids include as a formulation component of personal care products for hair and skin care, antiperspirants and deodorants; pharmaceuticals; processing aids such as defoamers; surfactants and mould release agents; lubricants; polishes and coatings on a range of substrates including textiles, carpeting and paper; sealants; architectural coatings; mechanical, heat transfer and dielectric fluids; and reprography (Will et al. 2007).

While it is anticipated that higher molecular weight polymers are used in most of these applications, D6 was reported for use as a defoamer (Environment Canada 2007). Defoamers are employed often at parts per million levels in a range of processing industries including pulp and paper, food, petrochemical, petroleum, and chemical manufacture as well as water treatment. Silicones are also used as defoamers in household products such as cleaners and detergents (Will et al. 2007).

The use of silicone formulants containing D6 in certain pesticide products is regulated in Canada under the *Pest Control Products Act* (PMRA 2007).

Silicone fluid/gel mixtures are used for several types of cosmetic and medical devices. Silicone fluids have been approved as active and non-active ingredients in pharmaceuticals in Canada (DPD 2007), the most common use being in anti-flatulence drugs. Other biomedical uses of silicone fluids in Canada are in blood-handling equipment, as a blood defoaming agent, as protective barriers and lubricants, and for surface treatment of wound dressings.

Silicone gums are used in the production of elastomers that are used as sealants and adhesives, and in moulded silicone rubber, coatings and encapsulation. Silicone elastomers are used in the manufacture of consumer products such as pacifiers. Silicone elastomers are also used in a large number of biomedical applications including short- and long-term implants and prostheses, catheters, contact lenses and dentures (Will et al. 2007).

Silicone resins are primarily used in specialty coatings applications, and in the production of silicone-modified polymers (Will et al. 2007). Consumers may be exposed to D6 through the use of these products and by occupying enclosed spaces where coatings, caulking, sealants and silicone rubber are used as building materials or are present in consumer products.

Releases to the Environment

D6 is not reported as part of Environment Canada's National Pollutant Release Inventory. This substance belongs to a chemical group used in various industry and consumer applications that are associated with the potential for widespread releases.

D6 will be released to the environment during the use of personal care products such as hair and skin care products, antiperspirants and others and these releases will be to air and wastewater. It is estimated that more than 90% of D6 used in personal care products enters the atmosphere (Allen et al. 1997). D6 may also be emitted from industrial processes in which it is used in blending, formulation and packaging operations, and as intermediate in producing PDMS polymers. All of these operations take place in Canada (Environment Canada 2007). Industrial releases of D6 may also occur when silicone polymers are used in process industries as foam control agents, as mould release agents, as lubricants, and in other applications (Environment Canada 2007). The releases from industrial processes are expected to be to the atmosphere and wastewater. The release of D6 to sewage treatment plants as wastewater can lead to its association with sludges that may then be sent to landfills, incinerated or be applied to agricultural soils as soil enrichment. Disposal of consumer and industrial products containing D6 can also lead to the transfer of D6 to landfills.

Detection of D6 at sewage treatment plants, landfills and near industrial plants as well as in indoor and ambient air away from industrial activity is evidence that both point sources and disperse sources contribute to the concentration of D6 in the environment (Norden

2005, Kaj et al. 2005). The application of D6-containing pesticides on crops and the disposal of sewage sludge on agricultural lands or in landfills will result in the release of D6 to environmental media. There is some evidence that D6 is a transient degradation product of PDMS in contact with soil, while the principal degradation products are silanols (Xu et al. 1998). Thus, in addition to release of residual D6 from PDMS manufacture, there may be *de novo* synthesis of D6 occurring in landfills and agricultural lands where sewage sludge containing PDMS is spread, although the overall contribution of PDMS degradation is not considered significant under environmental conditions.

Mass Flow Tool

To estimate the potential release of D6 to the environment at different stages of its life cycle, a Mass Flow Tool was used. Empirical data concerning releases of specific substances to the environment are seldom available. Therefore, for each identified type of use of the substance, the proportion and quantity of release to the different environmental media are estimated, as are the proportions of the substance chemically transformed or sent for waste disposal. Assumptions and input parameters used in making these estimates are based on information obtained from a variety of sources including responses to regulatory surveys, Statistics Canada, manufacturers' websites and technical databases. Of particular relevance are emission factors, which are generally expressed as the fraction of a substance released to the environment, particularly during its manufacture, transformation, and use associated with industrial processes. Sources of such information include emission scenario documents, often developed under the auspices of the Organisation for Economic Co-operation and Development (OECD), and default assumptions used by different international chemical regulatory agencies. It is noted that the level of uncertainty in the mass of substance and quantity released to the environment generally increases further down the life cycle.

Table 3. Estimated releases and losses of D6 to environmental media, transformation and distribution to management processes, based on the Mass Flow Tool[1]

Fate	Proportion of the mass (%)[1]	Major life cycle stage involved[2]
Releases to environment:		
To soil	0	-
To air	77.7	Industrial use and consumer use
To sewer*	12.3	Formulation, industrial use and consumer use
Chemically transformed	0.2	Industrial use
Transferred to waste disposal sites (e.g., landfill, incineration)	9.8	Waste management

* Wastewater before any form of treatment

[1] For D6, information from the following OECD emission scenario documents was used to estimate releases to the environment and distribution of the substance as summarized in this table: OECD 2004; OECD 2006. Values presented for releases to environmental media do not account for possible mitigation measures that may be in place in some locations (e.g., partial removal by sewage treatment plants). Specific assumptions used in the derivation of these estimates are summarized in Environment Canada 2008a.

[2] Applicable stage(s): production, formulation, industrial use, consumer use, service life of article/product, waste disposal.

Based on the Mass Flow Tool (Table 3), the substance is mainly released to air and wastewater (sewer). Air receives the highest potential of releases (77.7%) as a result of the use of consumer products such as skin creams or sun creams and also volatilization of residues in silicone polymers, especially during the first year of use. Releases to wastewater are estimated to be approximately 12.3% from industrial use during on-site formulation and from consumer use of the personal care products. Another 9.8% of the substance is transferred for waste disposal.

Environmental Fate

Based on its physical and chemical properties (Table 2) and the results of Level III fugacity modelling (Table 4; model input parameters are listed in Appendix 5 of this screening assessment), D6 may partition in significant quantities to any environmental medium, depending on the compartment of release.

Table 4. Results of the Level III fugacity modelling for D6 (EQC 2003)

	Fraction of substance partitioning into each compartment			
Substance released to	**Air**	**Water**	**Soil**	**Sediment**
Air (100%)	99.9	0.0	0.1	0.0
Water (100%)	0.9	16.0	0.0	83.0
Soil (100%)	31.8	0.0	68.1	0.1

Based on the information available (Table 3), the environmental release of D6 is estimated to be mainly to air (77.7%). A vapour pressure of 4–4.73 Pa and a Henry's Law constant of 4 950 000 $Pa \cdot m^3/mol$, as well as a long half-life in air, indicate that when D6 is released to air it will remain there (>99%) (Table 4).

When D6 is released to water (12.3%, Table 3), it is expected to adsorb to suspended solids, such as sewage sludge and sediments, based on its high estimated log K_{oc} values (>6). Results of the Level III fugacity simulation for release to water show that approximately 83% will reside in the solid phase (suspended sediment and bed sediments) and 16% will reside in the aqueous phase (water column). Although volatilization from water surfaces is also expected based upon the air-water partition coefficient (K_{aw}), the high sorption of D6 by solid matter significantly reduces D6's volatilization (0.9%, Table 4).

When D6 is released to moist soils through, for example, application of sewage sludge on agricultural lands, it is expected to adsorb strongly to soil (i.e., expected to be immobile), which reduces the potential for volatilization and further partitioning. The results of the Level III fugacity model support this idea, showing that if D6 is released to soil, 68.1% will remain in soil associated with solids, for the same reasons as described for sediment. Approximately 31.8% of the mass fraction is estimated to partition to air. This estimate is consistent with the observation by Xu (1999) that volatilization is the major loss process

of cyclic siloxanes from moist soils. However, the percent volatilization of D6 is less than that of D5 (~71%) due to its high absorptivity to solid matter (K_{oc}>6). In dry soil, D6 is expected to be quickly hydrolyzed by clay minerals to form dimethylsilanediol as the final breakdown product (Xu 1999, Xu and Chandra 1999).

Persistence and Bioaccumulation Potential

Environmental Persistence

Atmospheric Degradation

The Level III fugacity model results indicate that D6, when released to air, will mainly remain in air, where it is expected to be slowly oxidized by the gas-phase reaction with photochemically produced hydroxyl (OH) radicals. No experimental data are available, but the atmospheric oxidation half-life for D6 is predicted to be ~6 days based on a model calculation assuming hydroxyl radical concentrations of 1.5 x 10^6 OH/cm^3 (Table 5b). The half-lives of 2.6–12.8 days can be estimated by AOPWIN based on a measured daily average hydroxyl concentration of 3.5 x 10^6 OH/cm^3 and 0.7 x 10^6 OH/cm^3 (daily average concentration = maximum concentration/2), in summer and winter respectively (Ren et al. 2003, 2006). It is therefore concluded that D6 could be degraded more rapidly in urban centers in summer seasons when the atmospheric hydroxyl radicals are highest. However, when a yearly average removal half-life is estimated, it is consistent with the half-life of ~6 days estimated with hydroxyl radical concentration of 1.5 x 10^6 OH/cm^3. D6 is not expected to react, or react appreciably, with other photo-oxidative species in the atmosphere, such as O_3, nor is it likely to degrade via direct photolysis (Atkinson 1991). Therefore, it is expected that reactions with hydroxyl radicals will be the most important fate process in the atmosphere for the substance. Therefore, the degradation half-life of 5.69 days is considered critical and will be used for D6 in environmental fate modelling.

Navea et al. (2007) have investigated the effects of ozone, aerosols and solar radiation on the fate of D4 and D5 in a simulated environment chamber. They concluded that mineral aerosols such as kaolinite and hematite can significantly accelerate the removal of D4 and D5 from the gas phase of the atmosphere, especially under daytime conditions. The finding also indicated that ozone can further accelerate these removal processes for D4 and D5. Although obtained data suggested that mineral aerosols, combined with ozone, may have significant effects on the environmental fate of cVMS in the air, it is difficult to quantitatively extrapolate the results of the simulations to realistic environmental conditions. First, it should be noted that the study was conducted under unrealistically high concentrations of cVMS, mineral aerosols and ozone. Second, mineral and carbon black samples used in the study were high-purity (>99%) analytical samples that provided maximum surface area and thus, maximally available sorption sites, i.e., ideal conditions for D4/D5 absorption. The degree to which these pure minerals are representative of the particulate matter in air is questionable. Third, it is reasonable to

believe that minerals such as kaolinite and hematite can be found in atmospheric particular matter (PM); however, they are unlikely to be the most common and abundant components in atmospheric dust. In addition, it should be mentioned that the study was conducted in a simulated environment chamber and involved reacting the mineral aerosols with only one cVMS (D4 or D5) at a time. Under actual environmental conditions, thousands of chemicals compete for aerosols' adsorption sites. Therefore, in such conditions, the "effectiveness" of D4/D5 removal from the ambient air could be significantly lower than that observed in the chamber's mono-component atmosphere.

Thus, it may be concluded that the degree to which aerosols and ozone accelerate the degradation of cVMS in air under realistic environmental conditions is uncertain.

Thus, the data demonstrate that this substance is persistent in air (half-life > 2 days) in accordance with the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Table 5a. Empirical data for persistence data of D6

Medium	Fate process	Degradation value	Degradation endpoint /Units	Reference
Water	Biodegradation	4.47%	28 d degradation	Springborn Smithers Laboratories 2005
Water	Hydrolysis	401	Extrapolated from D4 and D5 hydrolysis half-life (days) neutral pH; 25°C	Xu 2007
Water	Hydrolysis	0.9–733	Read-across half-life (days) pH 6-9; 5–25°C	Durham 2006 Kozerski 2008 Bidleman 2008
Water/sediments	Abiotic degradation	49–588	Read-across half-life (days) from D4 neutral pH; 5–25°C	Xu and Miller 2008
Soil (Wahiawa soils from Hawaii)	Clay-catalyzed hydrolysis	1.38 days (32% relative humidity)	Half-life (days)	Xu 1999 Xu and Chandra 1999
Soil (Londo soils from Michigan)	Clay-catalyzed hydrolysis	3.54 days (32% relative humidity); 5.25 days (93% relative humidity)	Read-across half-life (days) from D4	Xu and Chandra 1999

Table 5b. Modelled data for persistence of D6

Medium	Fate process	Degradation value	Degradation endpoint / Units	Model
Air	Atmospheric oxidation	5.96	Half-life (days)	AOPWIN 2000
Air	Atmospheric oxidation	2.6–12.8 [2]	Half-life (days)	AOPWIN 2000
Water	Biodegradation	60	Half-life (days)	BIOWIN 2000 Ultimate survey
Water	Biodegradation	0 (does not biodegrade fast)	Probability	BIOWIN 2000, MITI Linear probability
Water	Biodegradation	0 (does not biodegrade fast)	Probability	BIOWIN 2000, MITI Non-linear probability
Water	Biodegradation	2.0	Percent biochemical oxygen demand (BOD) (MITI 301C)[1]	CATABOL c2004-2008
Water	Biodegradation (anaerobic)	0.1 (does not biodegrade fast)	Probability	BIOWIN 2000

[1] Results from CATABOL biodegradation simulation show that D4 is in the global parameter domain and metabolic domain, but out of the structural domain. The most important of these domains is the metabolic domain and CATABOL suggests that the substance will not be degraded, as the probability of stable methyl group and aromatic ring oxidation products is low.

[2] Atmospheric oxidation half-lives re-calculated with measured OH radical concentrations from New York City in summer and winter, respectively.

Degradation in Water and Sediment

Empirical hydrolysis data are not available for D6. Therefore, a read-across approach was applied using data from other similar siloxanes. Experimental hydrolysis studies were available for its structurally similar analogues D4 (Durham and Kozerski 2005) and D5 (Durham 2006) and were critically reviewed by internal experts (Bidleman 2008); the results of these studies and critical reviews are summarized below. The hydrolysis kinetics of D4 and D5 were determined by measuring the disappearance of radio-labelled parent compounds as a function of time based on OECD Guideline 111. Reactions were investigated in flame-sealed borosilicate glass tubes at pH of 4, 7 and 9 and temperatures of 10˚C, 25˚C and 35˚C. Additional tests were performed for D5 at pH of 5.5 and 8, and temperature of 25˚C. The hydrolysis rates of D4 and D5 were reported to be pH-dependent and followed pseudo first-order kinetics. Both D4 and D5 were found to undergo hydrolysis, with half-lives ($t_{1/2}$) of 0.04–45 days for D4 and 0.9–733 days for D5 under realistic Canadian environmental conditions (pH 6–9, temperature 5–25˚C) (GEMStat 2008, NOAA 2008). The hydrolysis half-lives increased from D4 to D5. Therefore D6, structurally similar to D4 and D5, will be expected to undergo hydrolysis in the Canadian environment (pH 6–9, temperature 5–25˚C) with half-lives of > 0.9-733 days. A half-life of ~401 days was extrapolated for D6 at neutral pH and under ambient temperature based on the hydrolysis data of D4 and D5 (Xu 2007).

Recent information received on microbial degradation indicates that D6 is not likely to be biodegraded in water. The 28-day ready-biodegradability test was performed in sealed

vessels in accordance with OECD Draft Guideline 310 and data showed limited biodegradation (4.47%) of D6 over 28 days in a ready-biodegradation test (Springborn Smithers Laboratories 2005). This is approximately equal to a half-life of 411 days assuming first-order rate kinetics. These data are further supported by two of the models in Table 5b. These models indicate that the probability of biodegradation of D6 in water is effectively zero. Therefore, D6 is expected to be persistent in water ($t_{1/2}$ > 180 days). Also, BIOWIN (2000) reported an overall weighted conclusion of "not readily biodegradable" based on the combined results of the BIOWIN3 and BIOWIN5 models.

Experimental and modelled biodegradation data indicate that D6 has little potential to biodegrade in aqueous environments. Therefore, hydrolysis is likely the major degradation process for D6 in water. The read-across data based on D4 and D5 hydrolysis half-lives and the extrapolated half-life for D6 suggest that D6 is expected to persist for long periods under Canadian water conditions. It is therefore concluded that D6 meets the criterion of persistence in water ($t_{1/2}$ > 182 days) under the *Persistence and Bioaccumulation Regulations* (Canada 2000).

No sediment degradation information was available for D6. However, a preliminary degradation study for D4 in a water/sediment system has been received recently (Xu and Miller 2008). A modified OECD 308 guideline was followed. The study was conducted at ambient temperature (22–25ºC) with natural sediment (sandy silt, high OC content, ~70% water content and 11% organic matter, pH ~7) and water collected from deep under an uncontaminated lake. Radio-labelled D4 in diethylene glycol methyl ether was added via syringe at 10–15 locations on the surface sediment in each flask after the overlying water was carefully removed. Overlying water was again added onto the spiked sediment with minimum disturbance of sediment. Spiking of sediment instead of water ensured the substance's distribution in sediment. This properly addressed the substance's specific physical and chemical properties (high volatility and potential hydrolysis) and improved the reproducibility of the study. The concentrations of D4 measured from day 6 to day 22 (test termination) indicated that a steady state had been reached between water and sediment, with more than 95% D4 and radioactivity being detected in sediment. As demonstrated in the hydrolysis study of D4, the degradation products in sediment/water were oligomer diol intermediates, $HO(Me2SiO)_nH$ (n=2-4), while dimethylsilanediol (DMSD) was the final degradation product. The calculated half-life for D4 degradation in sediment was 49 days at 22–25ºC. The same degradation products observed in the study and in the hydrolysis study of D4 suggested that hydrolysis was the major degradation process in the sediment/water system. The major uncertainty in the study is the lack of test replicates. Since no data were available for degradation half-lives at lower temperatures, a read-across approach using the D4 hydrolysis data was applied. The hydrolysis half-lives of D4 in water were ~ 6–12 times longer when water temperatures were decreased to 5–10ºC from 25ºC. Assuming a similar trend of decreases in sediment, the estimated half-lives for D4 in sediment are 294 and 588 days, at 10ºC and 5ºC, respectively.

The sediment degradation half-lives of D4 are considered as read-across for D6 based on the similarity of the two substances. It is therefore concluded that D6 under some (colder)

Canadian environmental conditions will have a half-life in water of > 182 days and in sediment of > 365 days. D6 is thus considered persistent in water and sediment in accordance with criteria defined under the *Persistence and Bioaccumulation Regulations* (Canada 2000). The extrapolation from D4 sediment degradation at lower temperatures based on hydrolysis, however, is not without uncertainty.

Degradation in Soil

Although no empirical data on biodegradation in soils are available, biodegradation of D6 in water is negligible as noted above, based on the ready-biodegradation test (Springborn Smithers Laboratories 2005) and predictions of five of the six biodegradation models (Table 5b).

Xu (Xu 1999, Xu and Chandra 1999) has extensively investigated potential degradation pathways of cyclosiloxanes, including D4, D5 and D6, in Wahiawa soil from Hawaii at room temperature and 32% relative humidity. He concluded that the ring-opening polymerization reaction to form polydimethylsiloxane (PDMS) and the demethylation for cyclosiloxanes were insignificant in soils at concentrations < 200 mg/kg dry weight. Clay-catalyzed hydrolysis of D6 was observed in highly weathered Wahiawa soils under dry soil conditions. The degradation half-life of D6 on Wahiawa soil (high clay content of 55% with water content of 2.1%) was 1.38 days under dry soil conditions. It was suggested that the dryness of soil severely limits biological activity but promotes abiotic reactions such as surface-acid-catalyzed hydrolysis of PDMS, a polymer with the same dimethylsiloxane backbone as cyclosiloxanes (Xu 1999). The degradation rates of cyclosiloxanes were determined by soil moisture, clay type and clay content, as well as the size of the siloxane molecules that determine the rate of diffusion to the surface catalytic sites. The degradation rate of D6 was much slower than that of D4 and D5 under the same soil conditions (~1 and ~2 hours half-life, respectively for D4 and D5) and supported the statement that degradation rates among the three cyclosiloxanes were expected to decrease as the molecular weight increases: D4 > D5 >> D6. The degradation half-lives of D4 on Londo soil were 3.54–5.25 days at relative humidity of less than 93%. A slower degradation half-life would be expected for D6 in the temperate Londo soil. The weight of evidence suggests that D6 may undergo clay-catalyzed hydrolysis and may not be persistent under dry soil conditions. The lack of hydrolysis degradation of D4 in water-saturated Londo soil also suggests that degradation of D6 is negligible under the same conditions. Volatilization becomes the major loss mechanism for D6 under such soil conditions in an open system, and at a slower rate than D4 and D5.

While investigating the influences of clay types on the degradation potential of polydimethylsiloxanes (PDMS), Xu et al. (1998) demonstrated that PDMS were degraded by clay minerals even though their catalytic activities varied. The widespread presence of these clay minerals suggests that D6 will undergo clay-catalyzed degradation in soil as long as critical soil conditions such as low moisture content are present, despite the tremendous diversity of Canadian soils.

Based on the available empirical studies that show the potential for rapid clay-catalyzed hydrolysis in surface soils, D6 is not considered persistent in soil, since its degradation half-life is less than the criterion of $t_{½} > 182$ days stated in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

The available empirical and modelled data indicate that D6 meets the persistence criteria for air (half-life ≥ 2 days), water (half-life ≥ 182 days) and sediments (half-life ≥ 365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000), but that it does not meet the half-life criterion for soil (i.e., its half-life is < 182 days).

Long-range Transport Potential

The Transport and Persistence Level III model (TaPL3 2000), a regional model, was used to estimate the characteristic travel distance (CTD) of D6. CTD is defined as the maximum distance travelled in air by 63% of the substance. Beyer et al. (2000) have proposed that CTDs of >2000 km represent high long-range atmospheric transport potential (LRATP), those of 700–2000 km represent moderate LRATP, and those of <700 km represent low LRATP. Based on the CTD estimate of 2966 km, the long-range atmospheric transport potential of D6 is judged to be high. This means that D6 is subject to atmospheric transport to remote regions such as the Arctic.

Table 6. Model-predicted characteristic travel distance for D6

Characteristic travel distance	Model (reference)
2966 km	TaPL3 v. 2.10 (TaPL3 2000)
2963 km	OECD LRTP POPs Tool v.2.0 (Scheringer et al. 2006)

The OECD POPs Screening Model can be used to help identify chemicals with high persistence and long-range transport potential (Scheringer et al. 2006). The OECD model is a global model which compartmentalizes the earth into air, water and soil. This model is "transport-oriented" rather than "target-oriented," as it simply identifies the CTD without indicating specifically where a substance may be transported (Fenner et al. 2005). Klasmeier et al. (2006) have suggested that a threshold of 5098 km, based on the model's CTD estimate for 2,2′,3′,4,4′,5,5′-Heptachlorobiphenyl (PCB-180), can be used to identify substances with high long-range transport potential. PCB-180 has been found in remote regions. The CTD calculated for D6 using the OECD model is 2963 km, indicating that D6 still has a significant potential for transport in air, but is below the boundary suggested for global pollutants by Klasmeier et al. (2006).

The OECD POPs Screening Model also calculates the transfer efficiency (TE), which is the percentage of emission flux to air that is deposited to the surface (water and soil) in a remote region (TE = D/E x 100, where E is the emission flux to air and D is the deposition flux to surface media in a target region). The TE for D6 was calculated to be 1.6E-06%, which is well below the boundary of 4.65E-04% (2,4,4'-trichlorobiphenyl, or PCB-28) established for the model's reference substances that are empirically known to be deposited from air to soil or water. The low TE means that D6 has the potential for

long-range travel in the atmosphere without being deposited to Earth's surface in any particular remote region. In addition, the log K_{oa} and log K_{aw} of D6 suggest that it will also have a low Arctic contamination potential (ACP) when examined using chemical partitioning space plots as described by Wania (2003, 2006).

A preliminary monitoring study of a remote ecosystem was conducted in Lake Opeongo, the largest lake in Algonquin Provincial Park, Ontario, Canada. The lake is relatively remote from potential sources of cVMS from sewage and runoff. Therefore, it was assumed that the only significant source of cVMS to the lake would be from atmosphere deposition (Powell 2008). Preliminary analysis of sediments and zooplankton samples for cVMS found no D6, suggesting that atmospheric deposition is not a significant source of D6 to Lake Opeongo. Limits of detection were 19.0 ng (background corrected mass) for both sediments and zooplankton.

It is therefore concluded that D6 has the potential to be transported over long distances in the atmosphere. However, the modelled TE for D6 is low, which suggests that it lacks the potential to be deposited in water or soil in remote regions. The monitoring results of Lake Opeongo also supported the low atmospheric deposition potential for D6. It is expected that airborne D6 will be eventually degraded by hydroxyl radicals in air.

Potential for Bioaccumulation

The empirical and modelled log K_{ow} values for D6 (Table 2) suggest that this substance has the potential to bioaccumulate in biota.

In the Aquatic Compartment

New experimental data were received on bioconcentration studies in aquatic organisms. A bioconcentration study of ^{14}C-D6 (radiochemical purity 99.57%) in fathead minnows (*Pimephales promelas*) was carried out in a flow-through system at concentrations of 4.4 µg/L and 0.41 µg/L for 49 days, followed by 98 days of depuration (Drottar 2005). The mean measured steady-state bioconcentration factor (BCF_{ss}) was calculated to be 1160 L/kg wet weight based on concentrations measured from day 35 to day 49. The kinetic bioconcentration factor (BCF_k) was calculated to be 1660 L/kg based on the uptake and depuration rates (k_1/k_2) for the 0.41 µg/L treatment groups. Fish tissue analysis also indicated that the depuration half-life for radio-labelled D6 was 30 days. The low BCF values for D6 (compared to D4 BCF_{ss} at 12 600 and BCF_k at 13 400; and D5 BCF_{ss} at 7060 L/kg and BCF_k at 13 300) could contribute to the low bioavailability of D6 (higher molecular weight and log k_{ow} ~9 compared to its structurally similar analogues, D4 and D5) and may also be caused by D6 adsorbing onto suspended particles (unconsumed food and feces).

Experimental data have been received on dietary bioaccumulation studies of D4 and D5 (Drottar 2006, 2007; Domoradzki 2008a, 2008b; SEHSC 2008b). The resultant lipid-normalized BMF values for D4 and D5 are in the range of 0.6–0.9. It is therefore

considered that D6, a close analogue of D4 and D5, may have similar low biomagnification potential as suggested by the laboratory fish dietary studies of D4 and D5.

Another bioconcentration study was carried out for invertebrates (Dow Corning Corporation 1985). *Daphnia magna* were exposed to a concentration of 4 µg/L of [^{14}C] D6 for 32 days. The steady state was achieved after 21 days of exposure and the BCF_{ss} was calculated as 2400 L/kg wet weight. The study was not well documented. The sources and acclimation of the test organisms, test conditions, and the test system design were not detailed in the study. A critical review of the study indicated the reliability of the study to be low.

The Arnot-Gobas model (Arnot and Gobas 2003) can be used to predict the bioaccumulation factor (BAF) of this substance, while taking into account any potential metabolism using a metabolic rate constant (k_M). The available BCF *in vivo* test data were used to derive an *in vivo*-based metabolic rate constant according to the method of Arnot et al. (2008a). In this method, k_M is derived according to the following equation:

$$k_M = (k_1\varphi/BCF) - (k_2 + k_E + k_G) \quad (1)$$

where

k_M = the metabolic rate constant (1/days)
k_1 = the uptake rate constant (Arnot and Gobas 2003)
φ = fraction of freely dissolved chemical in water (Arnot and Gobas 2003)
BCF = the available empirical bioconcentration factor
k_2 = the elimination rate constant (Arnot and Gobas 2003)
k_E = fecal egestion rate constant (Arnot and Gobas 2003)
k_G = growth rate constant (Arnot and Gobas 2003)

The method of Arnot et al. (2008a) provides for the estimation of confidence factors (CF) for the k_M to account for error associated with the *in vivo* data (i.e., measurement variability, parameter estimation uncertainty and model error). A mean CF of ± 2.7 was calculated for the available BCF data.

Because metabolic potential can be related to body weight and temperature (e.g., Hu and Layton 2001, Nichols et al. 2007), the k_M was further normalized to 15°C and then corrected for the body weight of the middle trophic level fish in the Arnot-Gobas model (184 g) (Arnot et al. 2008b). The middle trophic level fish was used to represent overall model output as suggested by the model developer (Arnot, personal communication with Bonnell M. of Environment Canada 2008; unreferenced) and is most representative of fish weight likely to be consumed by an avian or terrestrial piscivore. After normalization routines, the k_M ranges from ~0.002 to 0.01 with a median value of ~0.005.

Table 7. Metabolism-corrected BCF and BAF estimates using Arnot and Gobas (2003)

k_M (middle trophic level normalized) day^{-1}	log K_{ow} used	Arnot-Gobas BCF	Arnot-Gobas BAF
1.70E-03 (2.5%)	9.1	302	323 594
4.60E-03 (average)	9.1	138	109 648
1.25E-02 (97.5%)	9.1	56	26 303

The calculated k_M values based on *in vivo* experiments suggest that the rate of metabolism of D6 is quite low (≤ 0.01 day^{-1} at best). The experimental BCF study on fathead minnows (Drottar 2005) demonstrated certain metabolism, even though limited, of D6. The calculated BCF of 302 using the lower percentile rate constant (~0.002) is considerably lower than the BCF values reported by Fackler et al. (1995); this rate constant is therefore considered a best case. A corresponding BAF of 323 594 was calculated for D6 for fish in Canadian waters (Table 7) using this metabolic rate constant.

In the Sediment Compartment

No bioaccumulation information for D6 was available for the sediment compartment. However, biota-sediment accumulation factor (BSAF) studies on benthic organisms are available for its structurally close analogues, D5 (Springborn Smithers Laboratories 2003) and D4 (Kent et al. 1994). The read-across data were used in the weight-of-evidence approach to determine the sediment accumulation potential of D6, even though D6 is expected to be even less bioavailable (greater sorption to organic matter) in sediments than D5 and D4, and consequently may exhibit lower accumulation potential.

The biota-sediment accumulation factors (BSAFs) for D4 were calculated using data from a *Chirononmus tentans* (midge) sub-chronic toxicity study (Kent et al. 1994). Midge were exposed to D4 in sediment of low (LOC), medium (MOC), and high (HOC) organic carbon content ranging from 0.27% to 4.1%. The average BSAFs were calculated (BSAF = $C_{organism\ tissue}$ mg/kg /$C_{sediment}$ mg/kg) to be 0.7, 1.3 and 2.2, respectively, for the HOC, MOC and LOC phases. Biota-sediment accumulation factors were calculated for D5 using data from a midge (*Chironomus riparius*) acute/chronic toxicity study (Springborn Smithers Laboratories 2003). The midge larvae were exposed to D5 concentrations ranging from 13 to 180 mg/kg. Tests were conducted with sediments of 2.0% organic carbon content. The midge BSAFs were calculated to be 1.2, 1.1, 0.83 and 0.46 at treatment levels of 13, 30, 73 and 180 mg/kg dry weight, respectively.

The empirical results indicate that both D4 and D5 may have some potential, though limited (BSAF <2), to bioaccumulate from sediment exposures. The BSAF data of D5 may be used as read-across values for D6 as a worst-case conservative scenario. D6 is therefore considered to have some potential to bioaccumulate through exposure to sediment, although it is likely that D6 would exhibit a lower BSAF due to its reduced bioavailability. However, neither sediment accumulation study specified whether the gut contents of test organisms had been purged before calculation of BSAF values. The BSAF value may thus be over-estimated due to the presence of test substances on sediments within the gut of the invertebrates.

In the Soil Compartment

No bioaccumulation information for D6 was available for the soil compartment.

In the Terrestrial Compartment

The Gobas mass-balance bioaccumulation model for terrestrial organisms (Gobas et al. 2003) uses a chemical's octanol-air and octanol-water partition coefficient (K_{oa} and K_{ow}) to estimate the chemical's biomagnification (BMF) potential in terrestrial food chains. It was estimated that chemicals with a log $K_{oa} > 5$ can biomagnify in terrestrial food chains if log $K_{ow} > 2$ and the rate of chemical transformation or metabolism is low. A log K_{oa} of 5.76 indicates that D6 may have the potential to biomagnify in terrestrial food chains. However, the metabolism of cVMS demonstrated in laboratory mammals could reduce the biomagnification potential in the terrestrial food web.

Summary of the Bioaccumulation Potential of D6

Overall, there is conflicting evidence for the bioaccumulation potential of D6. Empirical bioconcentration testing has shown that the BCF is < 5000, likely a result of the lower aquatic bioavailability of D6 compared with D4 and D5 (as suggested by the physical and chemical properties of cVMS). The bioconcentration potential in other aquatic and benthic organisms at other trophic levels is also expected to be low based on the low reported BCF for fish and expected low bioavailability.

The predicted BCF, corrected for metabolism, is also relatively low compared with D4 and D5. The predicted BAF, also corrected for metabolism, is quite high and exceeds 5000. The mass-balance kinetic model used is based on "first principles," meaning that the most important domain of the model is that a chemical obeys the principal mechanism of the model, in this case passive diffusion. D6 meets this domain and is within the model's log K_{ow} and molecular weight boundaries as well. Therefore, the predictions for bioaccumulation are considered to be applicable to D6. However, there is less agreement between metabolism-corrected BCF values and empirical BCF values, suggesting that BCF and BAF model results for D6 have a high degree of uncertainty due to the relative absence of empirical BCF and BAF values at D6's range of log K_{ow} used in the model (i.e., ≥ 9). Also, the possibility that super-hydrophobic chemicals do not reach steady state in the environment (which the model assumes), adds to the uncertainty (Arnot and Gobas 2006).

Sediment BSAF values for D4 and D5 would suggest a relatively low level of accumulation in sediment macroinvertebrates for D6 as well. As this is the only sediment bioaccumulation test available for cVMS and there are no predictive models for sediment organisms, testing or field evidence at more realistic environmental loadings would help verify these values. No fish BMF studies have been conducted for D6. Using D4 and D5 BMF testing for read-across purposes, it is likely that the biomagnification factor in fish

for D6 would also be low, given its lower bioavailability. However, there is currently no evidence to suggest that this may be the case for other trophic levels. Field mesocosm studies are currently underway to examine trophic transfer of cVMS in aquatic food webs, but these data are not yet available for full evaluation and have not currently been considered for this assessment.

Currently, there is only a modelled BAF >5000 to suggest that the bioaccumulation potential of D6 is high. This value used alone as the only measure of high bioaccumulation potential presents some degree of uncertainty when other evidence suggesting low bioaccumulation potential is considered. Given the conflicting evidence, the predicted BAF alone is not considered to provide sufficient reliable weight to conclude that D6 has a high bioaccumulation potential. It is, however, reasonable to conclude that D6 has some bioaccumulation potential in biota, but this potential is likely to be lower than that of D4 and D5. It is therefore concluded that based on the lack of high bioconcentration potential as well as read-across evidence for low bioaccumulation via dietary exposures in fish, D6 does not meet the bioaccumulation criterion (BCF or BAF $\geqq$ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

A - In the Aquatic Compartment

New empirical ecotoxicity data have been received for D6 and are discussed in detail below (Table 8a). Both studies indicate this substance does not exhibit adverse effects on fish and *Daphnia* exposed at concentrations up to its water solubility limit (~0.005 mg/L).

Juveniles of *Daphnia magna* were exposed to D6 concentrations of 0.27, 0.57, 1.2, 2.5 and 4.6 µg/L (measured) for 21 days under static-renewal conditions, and the test solutions were renewed every 24 hours (Springborn Smithers Laboratories 2006). Acetone was used as a solubilizer at a concentration of 0.1 mg/L. The pH was maintained between 7.4 and 8.4, temperature oscillated between 18 and 21°C, and dissolved oxygen remained at > 60% of saturation. The test water had a hardness of 120–190 mg $CaCO_3$/L. No mortality, reduced reproduction or other biologically significant effects were observed at the highest test concentration of 4.6 µg/L (no-observed-effect concentration ≥ 4.6 µg/L). The temperature control and water hardness deviated from OECD Guideline 211, but were not considered to significantly limit the test. However, feeding during the test was 0.3 mg C/daphnid/day—higher than the OECD guideline of 0.1–0.2 mg C/daphnid/day—which is likely to favour the health of the test organisms and increase their resistance to toxic effects. A higher carbon load to the test system may also act to reduce bioavailability of D6 by providing a sorption substrate. Nonetheless, these

experimental data were considered acceptable for the purposes of this screening assessment, noting possible test limitations as mentioned.

Table 8a. Empirical aquatic toxicity values for D6

Organism	Type of test	Duration	Endpoint[1]	Value (mg/L)	Reference
Water flea *Daphnia magna*	Chronic	21 d	NOEC	0.0046	Springborn Smithers Laboratories 2006
Fathead minnow *Pimephales promelas*	Chronic	49 d	NOEC	0.0044	Drottar 2005

[1] NOEC: no-observed-effect concentration

The aquatic toxicity of D6 to fathead minnow (*Pimephales promelas*) was examined during a BCF study as described in the "Potential for Bioaccumulation" section (Drottar 2005). Juveniles of fathead minnow were exposed to concentrations of 0.41 and 4.4 µg/L (measured) for 49 days under flow-through conditions. No biologically significant effects were observed at the highest test concentration of 4.4 µg/L (NOEC ≥ 4.4 µg/L) during the 49-day fish uptake phase. Although the fish toxicity was determined as part of a BCF study; the test design is not equivalent to a long-term fish early-life stage toxicity test. No experimental data on the toxicity of D6 to early-life stages of fish is available. However, a 93-day fish early life-stage toxicity study with D4 was reported by Sousa et al. (1995). Rainbow trout embryos were exposed to D4 at concentration levels of 0.00025 – 0.0044 mg/L. No adverse effects were observed to embryo viability, hatching success, larval survival, and growth at all treatment levels. Therefore, the chronic NOEC for D4 93-day fish early life-stage is 0.0044 mg/L, the highest concentration tested. It is reasonable to conclude that due to its reduced bioavailability, D6 would also not exhibit adverse effects at the concentration of 0.0044 mg/L.

The acute and chronic toxicity of D6 was predicted using ECOSAR (2004) model. Predicted results are given in Table 8b.

Table 8b. Modelled aquatic toxicity values for D6

Organism	Type of test	Endpoint[1]	Duration	Concentration (mg/L)	Reference
Fish	Acute	LC_{50}	14 d	0.0004	ECOSAR 2004
Fish	Chronic	ChV	30 d	0.00003	ECOSAR 2004
Daphnia	Chronic	EC_{50}	16 d	0.0001	ECOSAR 2004

[1] LC50: the lowest concentration causing 50% mortality; EC50: the lowest concentration causing 50% effects; ChV is the geometric mean of the NOEC (no-observed-effect concentration) and LOEC (lowest-observed-effect concentration).

The modelled results for D6 using ECOSAR suggest that there is a possibility of a high level of chronic adverse effects (i.e., chronic NOEC < 0.1 mg/L) in aquatic organisms at the limit of solubility. However, the reliability of the predicted toxicity values is considered to be low. The log K_{ow} for D6 (9.07) is higher than the recommended ECOSAR log K_{ow} cut off (8.0) for prediction of chronic toxicity using the neutral organic structure-activity relationships and the lack of empirical siloxane data in the model's

training set limit their consideration in this assessment. The model predicted aquatic toxicity data were therefore not considered further.

The empirical evidence suggests that D6 does not exhibit adverse effects to pelagic biota at concentrations below its solubility limit (0.005 mg/L). Nonetheless, the NOEC of 0.0046 mg/L from the 21-day *Daphnia* toxicity test was selected for comparison to predicted environmental concentrations in water.

B – In Other Environmental Compartments

In the Sediment Compartment

No toxicity studies for sediment organisms were found for D6. However, chronic toxicity studies on benthic organisms are available for its structurally close analogue, D5 (Springborn Smithers Laboratories 2003, Krueger et al. 2007, 2008). These experimental data were used in the weight-of-evidence approach to determine the sediment toxicity potential of D6. However, D6 is expected to be even less bioavailable (greater sorption to organic matter) in sediments than D5 and consequently may exhibit lower toxicity potential.

Chronic toxicity studies of D5 (Springborn Smithers Laboratories 2003, Krueger et al. 2008) were carried out on midge (*Chironomus riparius)*. The no-effect concentration for male development rate in these 28-day studies was 69-70 mg/kg dry weight. The lowest-effect concentration for growth and male development rate observed at 160-180 mg/kg dry weight.

The chronic toxicity of D5 was also tested on blackworms (*Lumbriculus variegates)* in a 28-day study (Krueger et al. 2007). The no-effect concentration for survival and reproduction for D5 was 1272 mg/kg dry weight.

Based on the chronic data on D5, *Chironomus riparius* populations are considered to be more sensitive than blackworm populations to cyclosiloxanes. Although it is likely that D6 would exhibit a lower toxicity towards benthic organisms due to reduced bioavailability and hydro-availability, the chronic D5 toxicity values may be used as read-across data for D6 sediment toxicity as a reasonable worst-case exposure and bioavailability potential. A conservative NOEC (no-observed-effect concentration) of 69 mg/kg dry weight and a conservative LOEC (lowest-observed-effect concentration) of 160 mg/kg dry weight can thus be derived for D6.

In the Soil Compartment

No effects studies for soil organisms were found for D6 or its analogues.

In the Terrestrial Compartment

No ecological studies were identified for terrestrial wildlife. Laboratory studies on mammals are discussed under the "Potential to Cause Harm to Human Health" section in this screening assessment.

Ecological Exposure Assessment

In Air

In Canada, preliminary environmental measurements of volatile methyl-siloxanes, including D6, were conducted in the Great Lakes region during February and March of 2006 (personal communication, Environment Canada, Canadian Centre for Inland waters, 2007, unreferenced). Eighteen outdoor air samples were collected from rural and urban areas in Ontario and D6 was present in almost all the samples at concentration levels of < 1 μg/m^3, with the exception of one relatively high D6 concentration detected at ~16 μg/m^3 in the Toronto urban area. This result is in agreement with what has been reported in other jurisdictions (Table 9a).

It is, however, possible that the detection of D6 in ambient air is in part a result of sample contamination. Volatile cyclosiloxanes are present in a wide variety of commercial products, and both Canadian and Nordic monitoring programs have reported problems of high levels of cyclosiloxanes in sample blanks. The methodology for measuring and analyzing air concentrations at ng/m^3 to the low μg/m^3 level is still under development. Very few duplicate measurements are available for outdoor air monitoring and the few that are available exhibit poor reproducibility (personal communication, Environment Canada, Canadian Centre for Inland waters, 2007, unreferenced).

Table 9a. Concentrations of D6 in air

Medium	Location; year	Concentration	Reference
Air	Great Lakes region, Canada; February and March 2006	< 1 – 16 μg/m^3	see footnote 2
Air	Nordic countries[1]; 2004–2005	< d.l. – 2.1 μg/m^3	Norden 2005

[1] Outdoor samples (n=24) were collected in Nordic countries. The detection limit for D6 was 0.03 μg/m^3.
[2] personal communication, Environment Canada, Canadian Centre for Inland waters, 2007, unreferenced.

In Water

In Canada, water from a total of nine sewage treatment plants (STPs), including conventional secondary and tertiary water treatment plants and lagoons, in large urban centres in southwestern Ontario was sampled in October 2005 and winter 2005 (Backus 2007). D6 was detected at concentrations of 0.49–27.33 μg/L and 0.97-2.71 μg/L, respectively, in the influents and effluents. Seasonal differences in D6 concentrations in influents at STPs were only present in the three lagoon influents, while seasonal

differences of D6 in effluents were more significant (from 0.97–1.00 in fall to 2.32-2.71 in winter).

Similar monitoring results have been reported in other jurisdictions (Table 9b). In the United States, D6 was detected in drinking water concentrates from two cities—New Orleans, Louisiana and Cincinnati, Ohio (Lucas 1984, as cited in US EPA 1992).

Table 9b. Concentrations of D6 in water

Medium	Location; year	Concentration	Reference
Water	Great Lakes, Canada; 2006	< 17 ng/g (d.l.)	See footnote 4
STP influents	Southwestern Ontario, Canada; 2006	0.49–27.33 µg/L	See footnote 4
STP effluents	Southwestern Ontario, Canada; October 2005	0.97–2.71 µg/L	See footnote 4
Drinking water	United States	Qualitatively detected	Lucas 1984, as cited in US EPA 1992
Water	Background and urban sites,[1] Nordic countries	< 0.07 µg/L (d.l.)	Norden 2005, Kaj et al. 2005, NILU 2007
STP influents	Nordic countries[2]	0.12–3.7 µg/L	Norden 2005, Kaj et al. 2005, NILU 2007
STP effluents	Nordic countries[3]	< 0.02 (d.l.) – 0.1 µg/L	Norden 2005, Kaj et al. 2005, NILU 2007

[1] A total of 28 sampling sites excluding STP influents and effluents
[2] 7 STP influent sampling sites
[3] 12 STP effluent sampling sites
[4] personal communication, Environment Canada, Canadian Centre for Inland waters, 2007, unreferenced.
d.l. = detection limit

In Sediments

In Canada, surface sediments and sediment cores were collected from Lake Ontario in July 2006 and analyzed for D4, D5 and D6 (Powell and Kozerski 2007). Surface sediments consisting of the upper 5 cm of sediment were collected from Toronto Harbour and the Kingston Basin. Sediment cores, which were sectioned into strata 5 mm thick, were collected from the Rochester, Mississauga and Niagara basins. The surface sediments from Toronto Harbour and Kingston Basin contain moderate total organic carbon (TOC = 2.1–2.4% dw), while sediment cores contain high TOC (4–5% dw). Loss-on-ignition analysis of sediments also demonstrated lower water contents in surface sediments (55–70% ww) than in sediment cores (80–89%). Sediments in Toronto Harbour and the four sedimentary basins are known to be contaminated with a variety of organic compounds that enter the lake through direct discharges of treated wastewater, flow from the upper Great Lakes (Erie, Huron and Michigan) and the Niagara River, and atmospheric deposition. Surface sediments from Toronto Harbour contained the highest concentration of D6, at 0.2 µg/g dry weight. In contrast, concentrations of the cyclic siloxane materials in the surface sediments and sediment cores from the four sedimentary basins were all less than the analytical method detection limit, which was 0.01 µg/g for D6. Similar monitoring results have been reported in other jurisdictions, where D6 was detected in surface sediments from urban areas and point sources (Table 9c).

A preliminary monitoring study of a remote ecosystem was conducted in Lake Opeongo, the largest lake in Algonquin Provincial Park, Ontario, Canada. The lake is relatively remote from potential sources of cVMS from sewage and runoff (Powell 2008). Preliminary analysis of surface sediment and sediment core samples found no D6, with a limit of detection of 19.0 ng (background corrected mass).

The sediment monitoring results from Lake Opeongo and the Lake Ontario area suggest that D6 contamination is more likely to be found near urban centres and point sources.

Table 9c. Concentrations of D6 in sediments

Medium	Location; year	Concentration	Reference
Surface sediments	Toronto Harbour, Canada; July 2006	0.2 µg/g dw	Powell and Kozerski 2007
Surface sediments	Kingston Basin, Canada; July 2006	< 0.01 µg/g dw (d.l.)	Powell and Kozerski 2007
Sediment cores	Rochester, Mississauga and Niagara basins, Canada; July 2006	< 0.01 µg/g dw (d.l.)	Powell and Kozerski 2007
Surface sediments	Lake Opeongo, Algonquin Provincial Park, Ontario, Canada; October 2007	< 19.0 ng (d.l.)[2]	Powell 2008
Sediment cores	Lake Opeongo, Algonquin Provincial Park, Ontario, Canada; October 2007	< 19.0 ng (d.l.)[2]	Powell 2008
Sediments	Nordic countries[1]	< d.l. (varied from sample to sample) – 0.196 µg/g dw	Norden 2005, Kaj et al. 2005, NILU 2007

[1] A total of 30 sediment sampling sites
[2] Background corrected mass as reported in the preliminary study
dw = dry weight, d.l. = detection limit

In Soil

D6 may enter soil from land application of sewage sludge. No monitoring data for D6 in sewage sludge are available for Canada. In Europe, D6 is present in sewage sludge at levels ranging from the low mg/kg dry weight level up to 14.0 mg/kg dry weight (Norden 2005, Kaj et al. 2005, NILU 2007).

No monitoring data are available for D6 in Canadian soil. D6 concentrations in two soil samples from the Faroe Islands were below detection limit (< 4 ng/g dw) (Norden 2005).

In Biota

A preliminary monitoring study of a remote ecosystem was conducted in Lake Opeongo, the largest lake in Algonquin Provincial Park, Ontario, Canada. The lake is relatively remote from potential sources of cVMS from sewage and runoff (Powell 2008). Preliminary analysis of zooplankton samples found no D6. Bulk zooplankton samples were pooled into a single sample for each of the two locations from the lake without

being sorted into species. The limit of detection was 19.0 ng (background corrected mass).

In Europe, D6 was detected in livers of marine fish but not freshwater fish, and mainly from areas representing urban or diffuse sources. Concentrations generally ranged from < 5 to 10 ng/g wet weight (ww), except for one sample from Norway of cod liver with extremely high siloxane concentrations (74 ng/g ww D6). The follow-up environmental monitoring program conducted by the Norwegian government confirmed the originally reported levels of D6 (NILU 2007; see Table 9d of this assessment). D6 was also found in common mussels, flounder livers and fillets, and in cod stomach contents from Norway in the same monitoring program. The concentrations varied with species, gender and age. Among marine mammals monitored, D6 was detected in seal blubber in Denmark at the level of 7.9 ng/g ww (Norden 2005). D6 was not detected in fish muscle samples in Sweden (Kaj et al. 2005).

The presence of D6 in European biota indicates that despite the low detected concentrations or even non-detection of the substance in or near fish habitats, D6 is available in the environment for biota to take up and accumulate.

Table 9d. Concentrations of D6 in biota

Organism	Location; year	Concentration	Reference
Zooplankton	Lake Opeongo, Algonquin Provincial Park, Ontario, Canada; October 2007	< 19.0 ng (d.l.)	Powell 2008
Marine fish liver	Nordic countries[1]; 2002–2004	< 5 (d.l.) – 74 ng/g ww	Norden 2005
Freshwater fish liver	Nordic countries[2]; 2002	< 5 ng/g ww (d.l.)	Norden 2005
Marine mammals	Nordic countries[3]; 2002	< 5 (d.l.) – 7.9 ng/g ww	Norden 2005
Seabird eggs	Nordic countries[4]; 2000–2005	< 5 ng/g ww (d.l.)	Norden 2005
Common mussels	Norway[5]; 2006	1.3–1.8 ng/g ww	NILU 2007
Flounder livers	Norway[6]; 2006	1.4 ng/g ww	NILU 2007
Flounder fillets	Norway[6]; 2006	0.9 ng/g ww	NILU 2007
Cod stomach contents	Norway[7]; 2006	1.8–3.3 ng/g ww	NILU 2007
Cod livers	Norway[7]; 2006	109.1–151.5 ng/g ww	NILU 2007

[1] A total of 11 sampling matrices for marine fish
[2] A total of 10 sampling matrices for freshwater fish
[3] A total of 7 sampling matrices for marine mammals
[4] A total of 17 sampling matrices for seabird eggs
[5] A total of 3 sampling matrices for mussel
[6] A total of 2 sampling matrices for flounder
[7] A total of 3 sampling matrices for cod
ww = wet weight, d.l. = detection limit

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine various supporting information and develop conclusions based on a weight-of-evidence approach and using precaution as required under subsection 76.1 of CEPA 1999. Particular consideration was given to risk quotient analysis, persistence, bioaccumulation potential, toxicity, sources and fate in the environment.

Based on the information available, D6 is highly persistent in water; it also has some bioaccumulation potential in aquatic organisms as suggested by the experimental BCF and its presence in certain European biota. A quantitative risk quotient evaluation of exposure and of ecological effects was therefore conducted as part of the weight-of-evidence evaluation of D6's potential to cause harm.

In the aquatic compartment, two experimental chronic toxicity studies—one with *Daphnia magna* and the other with fathead minnow—were critically reviewed and accepted. D6 exhibited no adverse effects at 0.0044 to 0.0046 mg/L, a concentration that is very close to the water solubility limit of the substance (~ 0.005 mg/L). No application factor was applied to the chronic NOEC of 0.0046 mg/L. The PNEC is therefore 0.0046 mg/L. A risk quotient (RQ) analysis, integrating level of exposure with a toxicity threshold, was performed for D6. In order to address the potential risk of D6 on a national scale in Canada, a distribution profiling risk quotients in water at multiple release sites where the substance can be released by industry or by consumers (i.e., municipal sewage treatment plants) was determined. This type of analysis provides a line of evidence for the risk assessment of a substance when the full range of geographic locations of the industrial and consumer releases of the substance cannot be fully established.

Specifically, when a substance is used by a number of industry sectors but the actual facilities involved cannot be identified, the aquatic exposure can be estimated for all sites where facilities related to these sectors are located. In addition to this, information on potential releases from consumer use can be integrated into the calculations. A predicted environmental concentration (PEC) for the water compartment is determined based on the use quantities identified from the section 71 survey submissions and estimates of releases from individual industrial sites and from consumers. The receiving water is either a watercourse or a lake, and a dilution factor based on the size of the receiving water—up to a maximum of 10—is used to estimate the PEC. The risk quotient at each site is then determined for the water column. The distribution indicates not only the proportion or number of threshold-exceeding sites, but also the magnitude of the exceedence at each of these sites. Further details on the approach are provided in Environment Canada (2008b).

The consumer releases used a database of approximately 1000 municipal discharge sites accounting for about 2/3 of the Canadian population. The industrial release analysis was done for 27 sites relating to 87 industrial facilities identified by NAICS code as possible users of D6. Under these scenarios, a total of 31 (~3.2%) of all evaluated municipal

discharge sites across Canada showed a risk to aquatic organisms, with RQs exceeding 1 (Figure 1). The equation and inputs used to calculate the PEC in the receiving watercourses are described in Environment Canada (2008c).

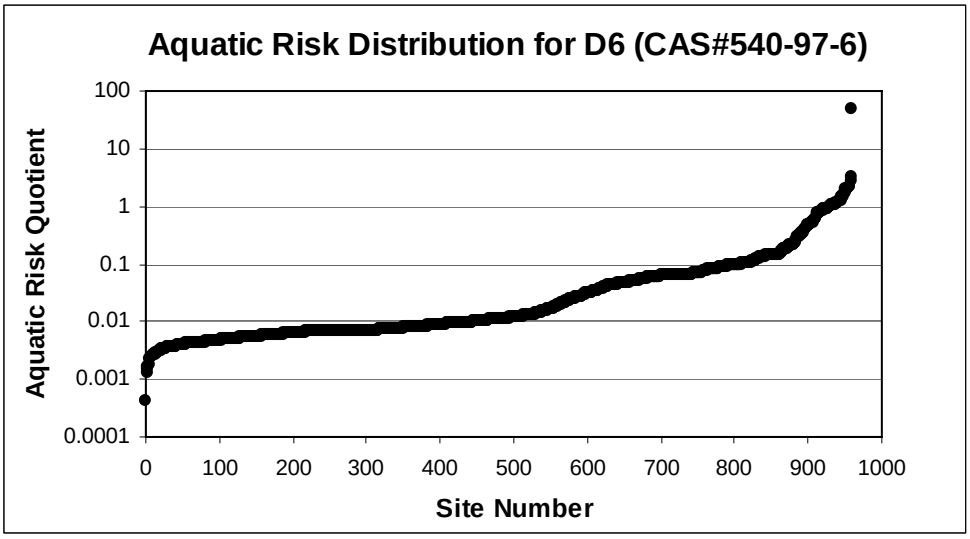


Figure 1. Aquatic risk distribution for D6 (Environment Canada 2008b, 2008c)

Although a risk quotient analysis was conducted for D6, the empirical ecotoxicity evidence suggests that the threshold at which adverse effects in pelagic biota is expected to occur has not been observed in available toxicity tests. Therefore, the RQs calculated in the above scenario are essentially "unbounded" and do not represent "real" observable effects expected at the above sites.

The very high $\log K_{ow}$ for D6 would suggest that it is well into the class of "super-hydrophobic" chemicals which are often associated with low bioavailability to pelagic and benthic biota. Lack of appreciable bioconcentration in test organisms and relatively low tissue residue values from available field monitoring data also suggest that the potential for body burdens reaching critical internal levels from water and sediment exposures is mitigated by low bioavailability.

D6 has been determined to be persistent in the environment, and has a relatively low potential to bioaccumulate in biota. Therefore, because the physical-chemical property, bioconcentration and ecotoxicity profiles for D6 provide a consensus basis for a weight of evidence, it can be reasonably concluded that D6 has a low potential to cause ecological harm in the Canadian environment.

Uncertainties in Evaluation of Ecological Risk

D6 is imported into Canada in significant quantities. Based on the information available, the quantities of D6 imported and used in Canada have increased significantly since the DSL nomination (Environment Canada 1988). Given the trend of increasing use, its environmental release and potential for environmental exposure will increase. D6 is also one of the major components in CAS RN 69430-24-6. It is also present in PDMS at up to

3%. The Challenge to industry and other stakeholders issued by the Government of Canada (Canada 2007) did not survey CAS RN 69430-24-6 (cyclomethicone, the mixture) or PDMS. Even though there is evidence that some companies did report individual cVMS in the mixture under the survey, the quantities of these substances imported into Canada and their uses in 2006 are not completely known, and their releases into the Canadian environment are not considered fully in this assessment report.

For the risk distribution analysis, the PNEC was derived from a concentration that is very close to its water solubility limit (~ 0.005 mg/L), and no application factor was applied to extrapolate laboratory data into the field due to the lack of observed adverse effects at this concentration. Since no release information from industrial operations was available for the risk distribution analysis, it is assumed that releases to wastewater were uniformly distributed among 27 industrial sites evaluated. In reality, certain industrial sites may use higher quantities of D6 than others, resulting in higher releases to the municipal discharging sites associated with these industrial sites and therefore a higher risk than predicted. The distribution concentrations in the analysis applied instantaneous dilution of the effluent from sewage treatment plants (STP) into the receiving water. However, under realistic environmental conditions, instantaneous dilution may not be achieved over a certain distance from the discharge point, and the area near the discharge point of an STP may present a higher risk than predicted.

Sediment is an important media of concern for D6. The D4 sediment degradation studies were used as read-across values for D6 and those studies are not without uncertainties. In addition, extrapolation of half-lives at low temperature in sediment based on hydrolysis data may also contribute to the overall uncertainty in sediment persistence.

The available bioconcentration study and read-across biomagnification factor and sediment accumulation values from the D6 analogues showed a low potential for D6 to bioaccumulate in laboratory tests. There are a lack of field data on bioaccumulation potential via the food web and in non-aquatic organisms.

Model predictions were also included in this screening assessment as a line of evidence. There are higher uncertainties associated with predicted values, as few siloxanes or chemicals with high log K_{ow} values (> 8), as for D6, have been studied and included in the models.

Environmental monitoring data in Canada and elsewhere are limited. Sample contamination is a potential problem in environmental monitoring due to D6's widespread uses. Data on environmental concentrations of D6 in biota and surface water in Canada are lacking and few environmental concentrations have been reported outside of urban areas in Canada. Consequently, monitoring data from European countries have been presented in this report. However, monitoring has been identified as a key component in the Chemicals Management Plan in Canada and D6 is being considered for environmental monitoring under the Plan. Environmental monitoring will contribute to a better understanding of the environmental presence and "true" environmental accumulation potential of the substance in the environment.

Potential to Cause Harm to Human Health

Exposure Assessment

The data on levels of D6 found in environmental media including ambient air near and away from point sources, surface waters, sediments, sewage sludge and biota are described in this report in the section entitled "Ecological Exposure Assessment." Unpublished data from Canada include measurements taken of air near and away from point sources (personal communication, Environment Canada, Canadian Centre for Inland waters, 2007, unreferenced); air, influent and effluent water at wastewater treatment plants (personal communication, Environment Canada, Canadian Centre for Inland waters, 2007, unreferenced); and Great Lakes sediment (Powell and Kozerski 2007). Many analyses of volatile siloxanes have been confounded by sample contamination during collection and analysis, resulting in siloxanes being detected in blanks at levels comparable in some cases to those in samples taken near point sources. Results of extensive sampling and measurement of siloxanes in environmental media in Scandinavia have been published by the Nordic Council of Ministers and the Swedish Environmental Research Institute (Norden 2005, Kaj et al. 2005). Data from these reports were considered reliable and were used to produce the upper-bounding estimates of exposure to siloxanes in air, water and soil by the general population in Canada.

The upper-bounding estimates of daily intake of D6 for six age groups in the Canadian population are shown in Appendix 1. The estimates of intake from environmental media and diet range from 28.7 µg/kg body weight/day (µg/kg-bw/day) for adults aged 60 years and older to 87 µg/kg-bw/day for children aged 6 months to 4 years. The most significant contribution to daily intake from environmental media is inhalation of indoor air, based on a study of 400 homes in Sweden in which D6 was detected in 142 samples, approximately twice as many as for D4. The mean concentration of D6 in indoor air measured in children's bedrooms in this study was 7.9 µg/m^3 and the maximum was 164 µg/m^3 (Kaj et al. 2005).

Confidence in the upper-bounding estimate of exposure to D6 through environmental media and diet is moderate. No Canadian data were used, but data from studies in Scandinavia were available for ambient and indoor air, water and soil. The maximum concentration of D6 measured in indoor air in the Swedish residential study is higher than the maxima measured for D4 and D5 in Swedish homes (Kaj et al. 2005)—a result not readily explained, given that D6 has a lower vapour pressure compared to its lower molecular weight analogues and given the expected relative prevalence of use of the three cyclosiloxanes in 2004. The use of a regulatory limit for DMPS (CAS RN 9006-65-9, dimethylpolysiloxane) in one quarter of dairy products and one half of processed food may overestimate the dietary contribution to total exposure, but the estimated contribution from all food to exposure of the general population from environmental media and diet is less than five percent of the contribution from air.

Using ConsExpo 4.1, software developed to estimate exposure to consumer products, the potential systemic dose of D6 through the use of personal care products was estimated for women that use skin care products, hair care products and antiperspirants (RIVM 2006). Similar calculations for D4 showed that the estimated adult female dose was much higher than that for adult males, chiefly because of leave-on skin care products. Therefore, an estimated systemic dose for adult women only is presented.

Manufacturers of personal care products are required to notify Health Canada of the concentration, within broad ranges, of siloxanes, including D6 and polydimethylcyclosiloxanes, termed cyclomethicone in personal care products.[1] Health Canada has been notified of approximately 530 cosmetic products that contain D6 as the sole siloxane or in mixtures with other specified siloxanes, and that department has also been notified of approximately 6000 cosmetic products that contain cyclomethicone or cyclomethicone mixtures which may contain D6 (CNS 2007). The data on the concentration of D6 in personal care products were obtained principally from the information provided by Canadian industry (Environment Canada 2007, CNS 2007) and were supplemented by information from other sources noted in Appendix 2. Market share data were not used to determine the concentration of D6 in the dominant products in each use category. In cases where the concentration for a product category reported in response to a notice published under section 71 of CEPA 1999 was higher than concentrations reported in the CNS database, a lower concentration of D6 for that product category, consistent with the range reported to the CNS, was used in estimating the systemic dose (Environment Canada 2007, CNS 2007).

It was assumed that 20% of the D6 in a product left on the skin evaporated and the remaining 80% was available for dermal absorption. This approach maintains the conservative bias of screening assessments while considering the relative vapour pressure of D6 compared to D4 for which evaporation data are available (Zareba et al. 2002). Experimental data to provide guidance on partitioning of personal care products arising from evaporation on skin were not located.

Studies of oral dosing of F344 rats showed that approximately 12% of ^{14}C-D6 was absorbed systemically (Dow Corning 2004). Of ^{14}C-D5 applied topically, 0.17% was absorbed across rat skin (Jovanovic et al. 2008). In a 6-hr inhalation study in rats, 1–2% of ^{14}C-D5 was retained in the body (Tobin et al. 2008). It was proposed to use figures of 12% absorption by ingestion, 0.17% absorption via the dermal route and 2% absorption by inhalation for the purpose of estimating dose from personal care products. The dermal and inhalation absorption figures used for D6 are those determined for D5, as shown above. This approach was deemed to be consistent with a conservative bias in screening assessments while avoiding an overestimation of absorption factors. A distinction was made between products that are washed off and those that are left on the body. Other assumptions are noted in Appendix 2.

[1] *Cosmetic Regulations* C.R.C., c. 869.

The results of a sample calculation for the application of hair styling lotion are shown in Appendix 2, and summaries of the estimated systemic dose arising from the use of personal care products by women are shown in Table 1. For adult women, the upper-bounding estimate of daily systemic dose from the modelled personal care products, aggregated over inhalation, dermal and oral exposure, is 0.10 mg/kg-bw/day. In the screening assessment of octamethylcyclotetrasiloxane (D4) it was shown that the systemic dose received by women from the use of personal care products was higher than the dose received by men and this is expected to be the case for D6.

An exposure assessment for use of D6, including personal care product uses, was submitted to the Government of Canada under the Challenge Program (SEHSC 2008a). The methodology is different from that shown in Appendix 2, Table 1, as a Monte Carlo probabilistic analysis was conducted and aggregate general population exposures from all sources (including personal care products) and routes (inhalation, dermal, ingestion) were derived. The contribution of the use of personal care products to total exposure via separate exposure routes (inhalation, dermal, oral) was characterized and then summed to arrive at an aggregated exposure estimate. Due to the fact that D4 and D6 were used as analogues to determine oral toxicity of D5, D5 is used here as a surrogate for validation of the D6 probabilistic exposure assessment. Thus, a probabilistic exposure assessment for use of D5 was also submitted to the Government of Canada under the Challenge Program (SEHSC 2008b). Independent review of the submitted probabilistic assessment showed that this assessment evaluated exposure to both user and non-user groups (see Appendix 4). The data were re-analyzed based on just user groups to allow comparison with the deterministic exposure assessment in this screening assessment. Based on user groups only, the probabilistic exposure values for adult females (most highly exposed adult group) were 10–16 times lower than the deterministic values shown for D5. Therefore, based on D5 used as an analogue to determine probabilistic exposure values for D6, it is expected that probabilistic exposure values for adult females (most highly exposed adult group) will be 10–16 times lower than the deterministic values shown in Appendix 2, Table 1. Note that due to the requirement for detailed analysis and validation of probabilistic exposure assessments, such assessments are normally outside the scope for conducting the exposure component of a screening assessment.

Based on user groups only in the D5 probabilistic exposure assessment, the exposure values for children aged 0–6 months (most highly exposed children's group) were in the range of 0.016–0.032 mg/kg-bw/day (see Appendix 4). A comparison with a deterministic exposure assessment for children was not possible due to the lack of sufficient product use data required for modelling children's exposure in a deterministic exposure assessment. When the children's probabilistic exposure values are compared with the adult female deterministic exposure values, they are 5–10 times lower for D5. Therefore, based on D5 used as an analogue to determine probabilistic exposure values for D6, it is expected that if the children's probabilistic exposure values for D6 were compared to the adult female deterministic exposure values, they would be 5–10 times lower for D6.

Other types of consumer products such as surface coatings, caulking, polishes and cleaners were deemed to contribute significantly less to daily exposure through daily use and were not further considered in the modelling of daily dose through consumer exposure scenarios. Both personal care products and other consumer products contribute to the concentration of D6 in indoor and ambient air and thus exposure by inhalation. Their contribution to total exposure of non-occupationally exposed individuals is estimated via indoor air in the multi-media environmental exposure model discussed in the preceding text of this section.

Confidence in the estimate of systemic dose of D6 through the use of personal care products is low. All estimates were made by the use of models, and the use pattern data were not from Canadian studies. The extent of use of D6 in personal care products and the concentration of D6 in products on the market currently may be lower than used in estimating the systemic dose reported above and in Appendix 2 (Environment Canada 2007, SEHSC 2007a). Consequently, these values are expected to be overestimates of exposure to D6 from use of personal care products.

Health Effects Assessment

Appendix 3 contains a summary of the available health effects information for dodecamethylcyclohexasiloxane (D6).

No international agency has classified D6 for carcinogenicity, genotoxicity or reproductive/developmental toxicity. Only one national review on the health effects of cyclosiloxanes was identified to date, that of the Danish Environmental Protection Agency (EPA). They reviewed health effects for D4 and D5 but not D6 (Lassen et al. 2005).

No carcinogenicity data for D6 were identified. Results of mutagenicity assays using *Salmonella typhimurium* or *Escherichia coli* (NOTOX 1990c) were negative. No other genotoxicity studies were identified.

With regard to reproductive toxicity, a lowest-observed-effect level (LOEL) of 1000 mg/kg-bw/day was determined based on an increased number (non-statistical) of sperm-positive, non-gravid females in a repeated-dose reproductive and developmental toxicity study. No developmental effects were observed at any dose. In this study, male and female Sprague-Dawley (SD) rats were administered 0, 100, 330 or 1000 mg/kg-bw/day of D6 in corn oil by oral gavage daily, seven days/week for up to 45 consecutive days (Dow Corning 2006).

In the repeated-dose portion of this study, a LOEL of 100 mg/kg-bw/day was determined based on increased liver weights and periportal lipidosis in the liver of females and follicular cell hypertrophy of the thyroid in both sexes of rats (dose-related in females) when they were administered the same daily oral doses of D6 for 28 days (Dow Corning 2006). The value of 100 mg/kg-bw/day is considered to be the critical level for

repeated-dose toxicity in this assessment based on both the liver and thyroid effects. Note that for D4 (octamethylcyclotetrasiloxane) and D5 (decamethylcyclopentasiloxane), the liver was also identified as a target organ for oral exposures. The Danish EPA identified the liver as a target organ for D4 exposures, and liver effects were observed in both oral and inhalation studies using D5 (Lassen et al. 2005).

Only one other repeated-dose study was identified. In that study no systemic toxicity was observed in SD rats treated by oral gavage to 0 or 1500 mg/kg-bw/day of D6 for four weeks (Dow Corning 1990).

No published studies on the toxicokinetics of D6 were identified.

The confidence in the toxicity database is low. There was limited information on acute, short-term, developmental, reproductive and genotoxicity data based mainly on oral exposure, but there was a lack of subchronic and chronic toxicity/carcinogenicity data. In addition, no data were identified based on inhalation or dermal (except for one acute study) exposures.

Characterization of Risk to Human Health

The critical effect level for repeated-dose toxicity of D6 is considered to be 100 mg/kg-bw/day via the oral route. This is based on increased periportal lipidosis and dose-related increases in liver weights and thyroid follicular cell hypertrophy in a 4-week rat study. Although repeated-dose inhalation data were not identified, it is also expected that the liver would be a target organ for inhalation exposures to D6 because liver effects were also observed upon inhalation exposures to the structurally similar compounds, D4 and D5 (see Health Effects Assessment section).

Comparison of the critical effect level for repeated dosing via the oral route (100 mg/kg-bw/day) and the upper-bounding estimate of daily intake of D6 by the general population in Canada results in a margin of exposure of approximately 40 000. This is based on adjusting the inhalation contribution to daily intake by an inhalation absorption value of 2.0%, resulting in a systemic exposure of 2.5 µg/kg-bw/day. The margins of exposure for repeated-dose effects and exposure via environmental media to the general population are considered to be adequate to account for uncertainties in the databases on exposure and effects. .

The apparent intake dose of 0.09 mg/kg-bw/day from personal care products which incorporates absorption factors for dermal, inhalation and oral exposure (Table 1, Appendix 2) was corrected by applying the reciprocal of the oral absorption factor to calculate the equivalent systemic dose of 0.19 mg/kg-bw/day. Using this calculated upper-bounding estimate of 0.19 mg/kg-bw/day, a comparison with the critical effect dose level for repeated dosing via the oral route (100 mg/kg-bw/day) resulted in a margin of exposure of approximately 500 from use of personal care products. However, it is considered that the exposure estimates presented above are overestimates of actual

exposure based on a submitted probabilistic assessment and information indicating that the percentage of personal care products containing D6 on the Canadian market may be lower than assumed in deriving exposure estimates. Based on values derived from an independent review of the probabilistic exposure assessment for D5, which is considered to be a surrogate for the D6 probabilistic exposure assessment, it appears that the margin of exposure from use of personal care products would be at least 10 times higher for adults and at least 5 times higher for children from that shown above (i.e. > 2000). On the basis of the above considerations, including consideration for the extent of its database, D6 is considered not to meet the criteria under paragraph 64(c) of CEPA 1999.

Uncertainties in Evaluation of Risk to Human Health

The scope of this screening assessment does not take into consideration a full analysis of the mechanism of action of dodecamethylcyclohexasiloxane and it does not take into account possible differences between humans and experimental species in sensitivity to effects induced by this substance.

There is uncertainty regarding the estimation of exposure and systemic dose because of the use of modelling and a lack of Canadian data. There is uncertainty associated with the use of models and the choice of variables related to the use of consumer products including quantity and frequency of use, absorbed fraction and environmental parameters.

The cumulative exposures of the other cyclosiloxanes in polydimethylsiloxanes (PDMS) are not considered in this assessment. However, D4 and D5 are considered in separate assessments.

Conclusion

Based on the information presented in this screening assessment, it is concluded that dodecamethylcyclohexasiloxane (D6) is not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity or that constitute or may constitute a danger to the environment on which life depends.

Based on the available information on its potential to cause harm to human health, it is concluded that dodecamethylcyclohexasiloxane is not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

It is therefore concluded that dodecamethylcyclohexasiloxane does not meet the definition of toxic as set out in section 64 of CEPA 1999. Additionally, dodecamethylcyclohexasiloxane does not meet the criteria for persistence and bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

The conclusion in this screening assessment is based on the available information at this time and acknowledges that there are uncertainties associated with this assessment. Research on cVMS is currently being conducted to help address these uncertainties, but some of this research has not been completed at this time. In the context of the Challenge program, any new information provided after the final screening assessment may be considered during the risk management phase.

Monitoring has also been identified as a key component in the Chemicals Management Plan in Canada and D6 is being considered for environmental monitoring under the Plan. Field level data will contribute to a better understanding of the distribution of D6 in the environment and its bioaccumulation potential in relevant food webs.

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Appendices

Appendix 1

Table 1. Upper-bounding estimates of daily intake of D6 by the general population in Canada

Route of exposure	Estimated intake (µg/kg-bw per day) of D6 by various age groups							
	0–6 months[1]			0.5–4 years[5]	5–11 years[6]	12–19 years[7]	20–59 years[8]	60+ years[9]
	Breast fed[2]	Formula fed[3]	Fed solid food[4]					
Ambient air[10]	0.03			0.07	0.05	0.03	0.02	0.02
Indoor air[11]	40.2			86.1	67.1	38.2	32.8	28.5
Drinking water[12]	0.47	0.01	.002	.005	.002	.002	.001	.001
Food and beverages[13]			1.48	0.81	0.46	0.25	0.16	0.14
Soil[14]	<.001			<.001	<.001	<.001	<.001	<.001
Total intake	40.7	40.2	41.7	87.0	67.6	38.5	33.0	28.7

1 Assumed to weigh 7.5 kg, to breathe 2.1 m^3 of air per day, to drink 0.8 L of water per day (formula fed) or 0.3 L/day (fed solid food) and to ingest 30 mg of soil per day (Health Canada 1998).

2 The highest concentration of D6 detected in human breast milk was 4.8µg/L in Sweden (Kaj et al. 2005). Breast-fed children 0–6 months of age are assumed to have an intake rate of 0.75 kg of breast milk per day (Health Canada 1998).

3 For exclusively formula-fed infants, intake of water is only that required to reconstitute formula. No data on detectable concentrations of D6 in drinking water were located. No data on concentrations of D6 in formula or baby food were identified for Canada. Approximately 50% of infants are introduced to solid foods by 4 months of age and 90% by 6 months of age (NHW 1990).

4 The dietary intake is based on consumption of 0.3 litres of water and up to 1.18 kg of food daily. This intake pattern is presented as a hypothetical extreme case and does not reflect recommended infant feeding practice.

5 Assumed to weigh 15.5 kg, to breathe 9.3 m^3 of air per day, to drink 0.7 L of water per day and to ingest 100 mg of soil per day (Health Canada 1998).

6 Assumed to weigh 31.0 kg, to breathe 14.5 m^3 of air per day, to drink 1.1 L of water per day and to ingest 65 mg of soil per day (Health Canada 1998).

7 Assumed to weigh 59.4 kg, to breathe 15.8 m^3 of air per day, to drink 1.2 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

8 Assumed to weigh 70.9 kg, to breathe 16.2 m^3 of air per day, to drink 1.5 L of water

per day and to ingest 30 mg of soil per day (Health Canada 1998).

[9] Assumed to weigh 72.0 kg, to breathe 14.3 m^3 of air per day, to drink 1.6 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

[10] D6 has been measured in ambient air near point sources in Canada, the United States and Europe. The highest measured concentration not near a point source, 0.87 $\mu g/m^3$ in Oslo, Norway, was used for the level of D6 in ambient air (Norden 2005).

[11] D6 was detected in 142 of 400 air samples taken in bedrooms in homes in Sweden. The maximum value of 164 $\mu g/m^3$ was used for the level of D6 in indoor air (Kaj et al. 2005). The data set considered includes a survey of homes in Syracuse, New York, in which D6 was detected in 15% of 130 homes and at a maximum concentration of 106 $\mu g/m^3$ (NYIEQ 2005). Canadians are assumed to spend 21 h per day inside (Health Canada 1998).

[12] No data on levels of D6 in Canadian drinking water were identified. D6 was not detected in two samples of surface water away from point sources in Norway. The higher limit of detection of 0.05 µg/L was used (Norden 2005).

[13] No data were identified for the concentration of D6 in foods in Canada. A value of 0.05 ppm D6 was used for dairy and two groups of processed foods. The maximum concentration of DMPS (CAS RN 9006-65-9, dimethylpolysiloxane) in certain processed food is limited by regulation to 10 ppm.* A value of 0.5% D6 in DMPS was assumed and it was further assumed that one quarter of dairy and one half of processed food had been treated with antifoaming agents containing D6. The concentration of D6 in whole flounder filets in the Oslofjord area was measured at 0.9 ng/g wet weight (NILU 2007). The probable intake of D6 from food packaging for an adult was estimated to be less than 0.01 µg/kg-bw/day (as per email from Food Packaging and Incidental Additives Section, Health Products and Food Branch of Health Canada, dated 27 Feb 2008 unreferenced).
Amounts of foods consumed on a daily basis by each age group are described by Health Canada (1998).

[14] No Canadian data were available for D6 levels in soil. No D6 was detected in two soil samples from the Faroe Islands taken at an abandoned and an operating landfill. The higher limit of detection of 4 µg/kg was used (Norden 2005).

* *Food and Drug Regulations*, Division 16. C.R.C., c. 870.

Appendix 2

Consumer Exposure Modelling **Sample ConsExpo 4.1 Report**

Product

D6 hair styling – women – partitioning 20/80

Compound

Compound name	Dodecamethylcyclohexasiloxane	
CAS RN	540-97-6	
molecular weight	445	g/mol
vapour pressure	4.5	Pascal
K_{ow}	9.06	10Log

General exposure data

exposure frequency	0.6	1/day
body weight	69	kilogram

Inhalation model: exposure to vapour – constant rate

weight fraction compound	0.35	fraction
exposure duration	12	hour
room volume	80	m^3
ventilation rate	1	1/hr
applied amount	0.9	gram
release duration	12	hour

Uptake model: fraction

uptake fraction	0.02	fraction
inhalation rate	22	m^3/day

Dermal model: direct dermal contact with product – instant application

weight fraction compound	0.35	fraction
exposed area	1.44E3	cm^2
applied amount	3.8	gram

Uptake model: fraction

uptake fraction	0.0017	fraction

Output

Inhalation (point estimates)

inhalation mean event concentration	1.3	mg/m^3
inhalation mean concentration on day of exposure	0.15	mg/m^3
inhalation air concentration year average	0.09011	mg/m^3/day
inhalation acute (internal) dose	0.000958	mg/kg
inhalation chronic (internal) dose	0.0005753	mg/kg/day

Dermal : point estimates

dermal load	0.924	mg/cm^2
dermal external dose	19.3	mg/kg
dermal acute (internal) dose	0.0328	mg/kg
dermal chronic (internal) dose	0.0197	mg/kg/day

Integrated (point estimates)

total external dose	19.3	mg/kg
total acute dose (internal)	0.0337	mg/kg

total chronic dose (internal)	0.0202	mg/kg/day

Table 1		D6	Systemic Dose by Exposure to Personal Care Products – 69-kg woman								
Product	Amount per application grams	Authority	Frequency per day	Authority	Weight fraction VMS	Authority	Retention factor	Inhalation mg/kg-bw/day at 2.0% abs	Dermal mg/kg-bw/day at 0.17% abs	Oral mg/kg-bw/day at 12% abs	Total mg/kg-bw/day
antiperspirant roll-on	0.8	RIVM	1	Maxim	0.01	NMI	1	0.00001	0.00016		
body lotion	8	RIVM	1.5	RIVM	0.125	Section 71	1	0.00091	0.0296		
sunscreen	6.1	RIVM	0.2	RIVM	0.444	NMI	1	0.00001	0.0107		
face moisturizer	2.5	RIVM	2	RIVM	0.125	Section 71	1	0.00038	0.0123		
face makeup	0.8	RIVM	1	RIVM	0.45	Section 71	1	0.00022	0.0071		
lipstick	0.01	Maxim	4	RIVM	0.25	Maxim	1	0	0.00020	0.0139	
hair spray	6.8	RIVM	1.2	RIVM	0.3	CNS	0.1	0.00146	0.00479		
hair shampoo	20	RIVM	0.7	RIVM	0.03	CNS	0.01	0	0.00008		
hair conditioner	20	RIVM	0.3	RIVM	0.35	Section 71	0.01	0	0.00041		
hair styling	4.7	Maxim	0.6	Maxim	0.35	Section 71	0.1	0.00058	0.00197		
Totals								0.00357	0.06731	0.0139	0.085

Consumer exposure modelling based on ConsExpo (RIVM 2006).
Basic assumptions:

Body weight 69 kg

Absorption by inhalation 2.0%; dermal absorption 0.17%; absorption by ingestion 12% (Dow Corning 2004).

For products left on skin except lipstick, 80% of applied amount is available to be dermally absorbed, 20% evaporates.

For lipstick, 20% is available for dermal absorption and 80% is available for absorption by ingestion.

Authorities:
- NMI: see in references NMI 2007
- RIVM: see in references RIVM 2006
- CNS: see in references CNS 2007
- Section 71: see in references Environment Canada 2007
- Maxim: see in references Maxim 1998

Appendix 3.

Summary of Health Effects Information for Dodecamethylcyclohexasiloxane (D6)

Endpoint	Lowest effect levels[1]/Results
Acute toxicity	**Lowest oral LD_{50}:** > 2000 mg/kg-bw in Wistar rats (NOTOX1990a). **Lowest dermal LD_{50}:** > 2000 mg/kg-bw in Wistar rats (NOTOX1990b). Other studies: US EPA 1994b. No inhalation studies identified.
Short-term repeated-dose toxicity	**Lowest-observed-effect level (LOEL) – oral:** 100 mg/kg-bw/day based on dose-related increase in female liver weights (absolute and relative liver weights statistically significant at 1000 mg/kg-bw/day) and increased periportal lipidosis in the liver of females (but not dose-related in incidence or severity) and follicular cell hypertrophy of the thyroid in both sexes (dose-related in females) in Sprague-Dawley (SD) rats administered D6 at 0, 100, 330 or 1000 mg/kg-bw/day in corn oil by oral gavage, 7 days/wk for 28 days (combined repeated-dose/reproductive and developmental study). Prothrombin time increased in males at 330 mg/kg-bw/day and higher (but no clinical indications of clotting abnormalities). At 1000 mg/kg-bw, there was significantly increased absolute and relative liver weight in females (Dow Corning 2006). Other oral studies: Dow Corning 1990 (Oral NOAEL: 1500 mg/kg-bw/day based on lack of any effects in SD rats exposed by oral gavage, 5 days/week for four weeks to 0 and 1500 mg/kg-bw/day. At the end of the study, liver, kidneys, testes or ovaries, brain, heart, and spleen were examined histopathologically). No dermal or inhalation studies identified.
Subchronic/Chronic toxicity	No data identified.
Carcinogenicity	No data identified.
Developmental toxicity	**Highest no-observed-adverse-effect level (NOAEL) – oral:** 1000 mg/kg-bw/day for developmental toxicity based on lack of developmental effects in SD rats administered D6 at 0, 100, 330 or 1000 mg/kg/day in corn oil by oral gavage daily, 7 days/week for up to 45 days [females exposed from 14 days prior to mating, throughout mating and gestation to post-partum day 3] (combined repeated-dose/reproductive and developmental study) (Dow Corning 2006). No dermal or inhalation studies identified.
Reproductive toxicity	**Lowest oral LOEL:** 1000 mg/kg-bw/day for reproductive toxicity based on increased number (non-statistical) of sperm-positive, non-gravid females in SD rats administered D6 at 0, 100, 330 or 1000 mg/kg-bw/day in corn oil by oral gavage daily, 7 days/week for up to 45 days [females exposed from 14 days prior to mating, throughout mating and gestation to post-partum day 3] (combined repeated-dose/reproductive and developmental study) (Dow Corning 2006). No dermal or inhalation studies identified.
Endocrine disruption *in vitro*	No data identified.
Genotoxicity and related endpoints: *in vivo*	No *in vivo* data identified.
Genotoxicity and mutagenicity: *in*	**Mutagenicity:** **Negative in bacterial reverse mutation**: *Salmonella typhimurium* TA98, TA100,

Endpoint	Lowest effect levels[1]/Results
vitro	TA1535, TA1537 with and without activation and *Escherichia coli* strain WP2 uvrA with and without activation (NOTOX 1990c).

[1] LD_{50} = median lethal dose
LOEL = lowest observed effect level
NOAEL = No observed adverse effect level

Appendix 4: Review of D5 Probabilistic Exposure Assessment

PROJECT	D5 Probabilistic Exposure Assessment
TASK	Review D5 Probabilistic Exposure Assessment conducted by Silicones Environmental, Health and Safety Council (SEHSC)
FOR	Health Canada (Healthy Environments and Consumer Safety Branch)
BY	infoscientific, Henderson, Nevada, USA
PERIOD	August–September, 2008

EXECUTIVE SUMMARY

A review of the D5 probabilistic exposure assessment submitted by SEHSC was done and comments to assist in preparing the screening assessment report for D5 is provided in this report.

"User Only" daily exposures were estimated based on a Monte Carlo analysis using Crystal Ball. Mean exposure and 90th percentile exposure summaries were generated for different subpopulations (children and adults).

For dermal and inhalation exposure routes, the current assessment resulted in higher exposures than the assessment done by SEHSC. The primary reason was the consideration of "user only" subpopulation in the current assessment compared to the "user" and "non-user" subpopulations considered in the SEHSC assessment. The dermal exposure route had higher exposures for both children and adults. Diaper cream, body lotion and sunscreen contributed to higher exposures in the dermal route; soothing vapour in the inhalation route and antifoam and fish in the ingestion route.

INTRODUCTION

As a part of Canada's Chemicals Management Program, Decamethylcyclopentasiloxane (D5) has been identified by Health Canada as a material to be reviewed and considered in a screening level assessment.

SEHSC submitted information on D5 to assist Health Canada in preparing the screening assessment report for D5. The information provided included toxicity information not readily available in the literature and a comprehensive exposure assessment utilizing Monte Carlo analysis. The exposure assessment included information on the levels of D5 in different environmental media and on consumer product use patterns.

Health Canada contracted with infoscientific, USA to review the D5 probabilistic exposure assessment submitted by SEHSC and to provide comments to assist in preparing the screening assessment report for D5.

DESCRIPTION

SEHSC's Monte Carlo-based probabilistic assessment for D5 included the following age-dependent and exposure-route-dependent scenarios:

- Children – dermal route: body lotion, conditioner (leave in), conditioner (rinse off), diaper cream, shampoo (2-in-1), soothing vapour, spray detangler, sunscreen
- Children – ingestion route: antifoam, baby bottle nipple, fish (general population), fish (subsistence population), human milk, leafy vegetables (greens), meat, milk, pacifier, root vegetables, sipper tube, soil, straws, water
- Children – ingestion route: OTC (over-the-counter) drugs
- Children – inhalation route: indoor air, outdoor air, soothing vapour
- Adults – dermal route: after shave, body lotion, conditioner (leave in), conditioner (rinse off), foundation, hair spray, mascara, moisturizer, nail care, roll-on antiperspirant, shampoo, solid antiperspirant, soothing vapour, sunscreen, under-eye cream
- Adults – ingestion route: antifoam, fish (general population), fish (subsistence population), leafy vegetables (greens), lipstick, meat, milk, root crops, soil, water
- Adults – ingestion route: OTC drugs
- Adults – inhalation route: indoor air, outdoor air, soothing vapour

Separate route-specific and total exposure estimates were made for the following subpopulations:

- Children: ages 0 to 6 months, breastfed
- Children: ages 0 to 6 months, non-breastfed
- Children: ages 0 to 6 months, males
- Children: ages 0 to 6 months, females
- Children: ages 7 to 11 months, breastfed
- Children: ages 7 to 11 months, non-breastfed
- Children: ages 1 to 2 years, breastfed
- Children: ages 1 to 2 years, non-breastfed
- Children: ages 2 to 4 years
- Children: ages 6 months to 4 years, males
- Children: ages 6 months to 4 years, females
- Children: ages 4 to 11 years, males
- Children: ages 4 to 11 years, females

- Adults: ages 12 to 19 years, males
- Adults: ages 12 to 19 years, females
- Adults: ages 20 to 59 years, males
- Adults: ages 20 to 59 years, females
- Adults: ages 60+ years, males
- Adults: ages 60+ years, females

The following documents and data files were provided to assist with the review process:

- D5_Kids, an Excel file, compatible with Crystal Ball, that contained all the exposure calculations for children
- D5_Adults, an Excel file, compatible with Crystal Ball, that contained all the exposure calculations for adults
- UPDATED Final Submission for Health Canada – D5, a Word file that contains information related to toxicity and exposure for D5
- Attachment 1 – Exposure Assessment for D5, a Word file that is a report explaining the probabilistic exposure assessment, including inputs used and outputs generated

The following steps were taken during the process of reviewing the D5 probabilistic assessment submitted by SEHSC:

- reviewed documents provided by Health Canada
- identified product-based exposure scenarios, exposure pathways and exposure subpopulations
- used the Excel files provided by Health Canada (D5_Kids.xls and D5_Adults.xls; files created by SEHSC) as starting points
- assured the quality of Crystal Ball-based probabilistic calculations
- generated Crystal Ball-based probabilistic Monte Carlo outputs and compared them with those listed in documents submitted by SEHSC
- commented on the robustness of industry's (SEHSC) probabilistic assessment and recommended whether it should be considered further in the screening assessment for D5

It must be mentioned that the review process did not

- validate the list of scenarios that cover all D5 exposures to children and adults
- validate the input values used in the SEHSC assessment
- validate the sources of the input values

However, the review process did

- check cells designated as Crystal Ball Assumptions (check the assignment of distributional parameters for inputs)
- check cells designated as Crystal Ball Forecasts (check the assignment of results)
- check formulas for the different calculations

A few errors were detected in the calculations. All these errors, which appeared in the formula cells, were incorrect references to formula inputs (incorrect cell references were provided).

Each exposure scenario—dermal, ingestion or inhalation—has two use-related parameters associated with it: frequency of use/occurrence (number of times per day) and percentage of population engaged in scenario. For the parameter "frequency of use/occurrence," the values used in the SEHSC assessment were also used in the current assessment, except when the value was less than 1.0; in this case, a value of 1.0 was assigned.

The SEHSC assessment relies heavily on the parameter "percentage of population engaged in scenario" to estimate exposures for the general population, which includes users and non-users. The current assessment ignores this parameter completely. For example, in the case of a scenario where 20% of the population is engaged, in a probabilistic Crystal Ball run with 200 000 simulations, the SEHSC assessment will have 160 000 estimates with zero values and 40 000 estimates with values greater than zero. On the other hand, the current assessment will have 200 000 estimates with values greater than zero. As a result, both mean exposure estimates and 90^{th} percentile exposure estimates generated by the current assessment will be greater than those generated by the SEHSC assessment. Conclusion: "user-only" exposures make a significant difference when comparing results generated by SEHSC and by infoscientific.

Exposure summary results were generated for 1) individual scenarios by specific exposure routes, 2) multiple scenarios by specific exposure routes (total exposure by specific exposure route) and 3) multiple scenarios aggregated over multiple routes (total exposure).

Total exposure within an exposure route is estimated by summing exposures for each scenario. Then total exposure across multiple exposure routes is estimated by summing exposures for each exposure route. Let us consider single Monte Carlo simulations within two separate probabilistic assessments: (1) a "user only" assessment (similar to the current assessment) and (2) a "user/non-user" assessment (similar to the SEHSC assessment).

In case (1), for each scenario, there is a finite probability that the individual represented in the simulation engages in that scenario. Thus, for multiple scenarios, the individual is involved only in a fraction of the scenarios and not all the scenarios considered. For those scenarios in which the individual engages, exposure estimates are generated. Total exposure is the sum of individual scenario exposures. This case can be extended to represent individuals in a general population.

By contrast, in case (2), for all scenarios, the probabilities for the individual represented in the simulation engaging in each equal 1.0 (100%). And, in this case, for multiple scenarios, the individual is involved in all the scenarios. Total exposure, which is the sum of individual scenario exposures, represents all the scenarios. The probability of an individual in a general population engaging in all the scenarios is unlikely.

Based on the above explanations for the two cases, in the current assessment, the "user only" summaries generated for individual scenarios are valid results. However, the summaries generated for total exposures, either within individual exposure routes or across exposure routes, are improbable and should be interpreted with caution. For total exposures, the estimates generated by SEHSC would be more applicable than the ones generated by the current assessment.

Adding exposures across exposure routes should be done after consideration of route-specific toxicological endpoints. If the route-specific toxicological endpoints are unequal, route-specific total exposures cannot be added without applying appropriate absorption/penetration factors and/or potency factors.

EXPOSURE RESULTS AND DISCUSSION: CHILDREN

Table 1. Children's mean exposures (based on 200 000 Crystal Ball simulations)

Mean exposures		Ages 0–6 months		6 m – 4 yrs		4 yrs – 11 yrs	
		M	F	M	F	M	F
DERMAL	2-in-1 shampoo	3.636E-07	2.178E-07	1.760E-07	1.038E-07	2.358E-07	1.417E-07
	Body lotion					3.625E-03	3.517E-03
	Conditioner leave in					2.498E-04	1.492E-04
	Conditioner rinse off					7.513E-06	4.497E-06
	Soothing vapour			1.447E-05	1.495E-05	6.662E-06	6.464E-06
	Diaper cream	5.665E-03	5.944E-03	2.742E-03	2.832E-03		
	Spray detangler			1.654E-07	9.776E-08	7.617E-08	4.228E-08
	Sunscreen	2.409E-03	2.529E-03	2.915E-03	3.011E-03	2.684E-03	2.605E-03
	Total Dermal	8.075E-03	8.473E-03	5.672E-03	5.858E-03	6.573E-03	6.282E-03
INHALATION	Indoor air	2.403E-04	2.523E-04	2.251E-04	2.326E-04	1.515E-04	1.362E-04
	Outdoor air	4.775E-06	5.006E-06	4.472E-06	4.619E-06	3.012E-06	2.707E-06
	Soothing vapour			2.921E-03	3.017E-03	1.965E-03	1.767E-03
	Total Inhalation	2.451E-04	2.573E-04	3.151E-03	3.255E-03	2.119E-03	1.905E-03
INGESTION	Antifoam					9.252E-04	8.539E-04
	Baby bottle nipple						
	Fish, general					4.499E-04	3.883E-04
	Greens					2.069E-08	2.126E-08
	Human milk						
	Meat					7.121E-08	6.347E-08
	Milk					1.027E-07	8.833E-08
	Pacifier						
	Root vegetable					1.129E-05	1.051E-05
	Sipper tube					5.176E-05	5.176E-05
	Soil					2.181E-06	2.116E-06
	Straws					2.133E-05	2.069E-05
	Fish, subsistence					3.770E-04	3.657E-04
	Water					1.461E-07	1.418E-07
	OTC drugs	5.434E-03	5.701E-03	1.316E-03	1.359E-03	2.213E-06	2.146E-06
	Total Ingestion, Subsistence	4.372E-03	4.372E-03	2.794E-03	2.794E-03	1.389E-03	1.305E-03
	Total Ingestion, General	2.654E-03	2.654E-03	2.428E-03	2.428E-03	1.462E-03	1.328E-03
TOTAL	***Total, Subsistence Population***	1.813E-02	1.880E-02	1.293E-02	1.327E-02	1.008E-02	9.494E-03
	Total, General Population	1.641E-02	1.709E-02	1.257E-02	1.290E-02	1.016E-02	9.517E-03

Table 1 summarizes all the exposure results for children as mean values. When compared with similar results generated by the SEHSC assessment, all the values are higher in the current assessment. Compared to the SEHSC assessment, the current assessment results in a difference of 1.79 to 2.32 times for total dermal exposures, in a difference of 1.00 to 13.56 times for total inhalation exposures, and in a difference of 0.97 to 1.56 times for total ingestion (general population) exposures. The primary reason for the differences is that the SEHSC assessed users and non-users whereas the current assessment considered users only.

Wherever exposures are estimated for multiple age groups, the estimates for lower age groups are usually greater than the estimates for higher age groups. Within dermal exposure scenarios, diaper cream, sunscreen and body lotion are the highest contributions; within inhalation, soothing vapour is the highest contributor; and within ingestion, the highest contributor is over-the-counter drugs for lower age groups and fish (subsistence) for higher age groups.

Table 2. Mean ingestion exposures for breastfed (BF) and non-breastfed (nBF) infants

Mean exposures		Ages 0–6 months		7–11 months		1–2 years		2–4 years
		BF	nBF	BF	nBF	BF	nBF	all
INGESTION	Antifoam	1.060E-03	2.904E-03	1.145E-03	2.260E-03	1.259E-03	1.821E-03	1.390E-03
	Baby bottle nipple		4.871E-04		3.484E-04		2.900E-04	2.092E-04
	Fish, general	3.341E-06	3.980E-04	1.700E-04	4.794E-04	4.800E-04	4.828E-04	5.023E-04
	Greens	4.889E-08	3.968E-08	1.749E-08	3.329E-08	6.773E-08	2.030E-08	2.718E-08
	Human milk	3.425E-04		2.009E-04		1.124E-04		
	Meat	5.972E-08	4.442E-08	5.182E-08	7.268E-08	5.008E-08	9.237E-08	9.152E-08
	Milk	1.355E-07	1.343E-07	6.381E-08	1.957E-07	1.778E-07	2.985E-07	1.639E-07
	Pacifier	4.873E-04	4.873E-04	3.485E-04	3.485E-04	2.902E-04	2.902E-04	2.093E-04
	Root vegetable	1.961E-05	2.103E-05	2.126E-05	2.799E-05	1.702E-05	1.998E-05	1.571E-05
	Sipper tube	2.436E-04	2.436E-04	1.743E-04	1.743E-04	1.451E-04	1.451E-04	1.046E-04
	Soil	9.959E-06	9.959E-06	7.123E-06	7.123E-06	5.929E-06	5.929E-06	4.277E-06
	Straws	4.873E-04	9.740E-05	6.967E-05	6.967E-05	5.799E-05	5.799E-05	4.184E-05
	Fish, subsistence	1.721E-03	1.721E-03	1.231E-03	1.231E-03	1.025E-03	1.025E-03	7.393E-04
	Water	6.673E-07	6.673E-07	4.773E-07	4.773E-07	3.973E-07	3.973E-07	2.866E-07

Table 2 summarizes all ingestion-related mean exposures specific to breastfed and non-breastfed infants. There are no significant differences in the results generated by the current assessment (shown in Table 2) and the SEHSC assessment. The two highest contributors to ingestion exposure for this subpopulation are antifoam and fish (subsistence).

Table 3. Children's 90th percentile exposures (based on 200 000 Crystal Ball simulations)

90th percentile exposures		Ages 0–6 months		6 m – 4 yrs		4 yrs – 11 yrs	
		M	F	M	F	M	F
DERMAL	2-in-1 shampoo	7.952E-07	4.747E-07	3.847E-07	2.260E-07	5.177E-07	3.132E-07
	Body lotion					7.894E-03	7.662E-03
	Conditioner leave in					5.265E-04	3.203E-04
	Conditioner rinse off					1.608E-05	9.733E-06
	Soothing vapour			2.019E-05	2.085E-05	9.294E-06	9.019E-06
	Diaper cream	1.463E-02	1.535E-02	7.073E-03	7.312E-03		
	Spray detangler			3.192E-07	1.882E-07	1.468E-07	8.138E-08
	Sunscreen	7.264E-03	7.613E-03	8.766E-03	9.062E-03	8.081E-03	7.860E-03
	Total Dermal	1.849E-02	1.942E-02	1.244E-02	1.286E-02	1.391E-02	1.338E-02
INHALATION	Indoor air	5.001E-04	5.262E-04	4.700E-04	4.859E-04	3.185E-04	2.853E-04
	Outdoor air	1.137E-05	1.200E-05	1.071E-05	1.100E-05	7.186E-06	6.495E-06
	Soothing vapour			4.379E-03	4.522E-03	2.964E-03	2.640E-03
	Total Inhalation	5.038E-04	5.298E-04	4.663E-03	4.813E-03	3.155E-03	2.808E-03
INGESTION	Antifoam					1.680E-03	1.567E-03
	Baby bottle nipple						
	Fish, general					1.008E-03	8.716E-04
	Greens					3.873E-09	4.007E-09
	Human milk						
	Meat					1.425E-07	1.276E-07
	Milk					1.991E-07	1.747E-07
	Pacifier						
	Root vegetable					2.966E-05	2.903E-05
	Sipper tube					6.587E-05	6.587E-05
	Soil					4.180E-06	4.056E-06
	Straws					2.715E-05	2.634E-05
	Fish, subsistence					8.404E-04	8.146E-04
	Water					2.901E-07	2.813E-07
	OTC drugs	1.304E-02	1.366E-02	3.627E-03	3.746E-03	5.306E-06	5.150E-06
	Total Ingestion, Subsistence	7.195E-03	7.195E-03	4.406E-03	4.406E-03	2.333E-03	2.203E-03
	Total Ingestion, General	4.326E-03	4.326E-03	3.804E-03	3.804E-03	2.488E-03	2.266E-03
TOTAL	***Total, Subsistence Population***	3.317E-02	3.456E-02	2.201E-02	2.260E-02	1.756E-02	1.673E-02
	Total, General Population	3.102E-02	3.242E-02	2.155E-02	2.215E-02	1.773E-02	1.677E-02

Table 3 summarizes all the exposure results for children as 90th percentile values. When compared with similar results generated by the SEHSC assessment, all the values are higher in the current assessment. Compared to the SEHSC assessment, the current assessment results in a difference of 1.33 to 1.69 times for total dermal exposures, in a difference of 1.00 to 9.83 times for total inhalation exposures, and in a difference of 0.97 to 1.36 times for total ingestion (general population) exposures. The primary reason for the differences is that the SEHSC assessed users and non-users whereas the current assessment considered users only.

Table 4. 90th percentile ingestion exposures for breastfed (BF) and non-breastfed (nBF) infants

90th percentile exposures		Ages 0–6 months		7–11 months		1–2 years		2–4 years
		BF	nBF	BF	nBF	BF	nBF	all
INGESTION	Antifoam	2.706E-03	5.188E-03	2.490E-03	3.981E-03	2.423E-03	3.240E-03	2.487E-03
	Baby bottle nipple		6.202E-04		4.434E-04		3.901E-04	2.663E-04
	Fish, general	6.719E-06	9.746E-04	3.701E-04	1.082E-03	1.146E-03	1.063E-03	1.126E-03
	Greens	1.028E-08	1.011E-08	2.465E-09	6.328E-09	1.852E-08	3.972E-09	4.953E-09
	Human milk	4.587E-04		3.428E-04		1.952E-04		
	Meat	1.471E-07	9.750E-08	1.133E-07	1.476E-07	9.887E-08	1.841E-07	1.825E-07
	Milk	3.244E-07	3.045E-07	1.349E-07	4.601E-07	3.777E-07	5.904E-07	3.267E-07
	Pacifier	6.201E-04	6.201E-04	4.432E-04	4.432E-04	3.907E-04	3.907E-04	2.662E-04
	Root vegetable	5.571E-05	6.142E-05	5.768E-05	7.632E-05	4.353E-05	5.262E-05	4.168E-05
	Sipper tube	3.100E-04	3.100E-04	2.216E-04	2.216E-04	1.953E-04	1.953E-04	1.331E-04
	Soil	1.909E-05	1.909E-05	1.365E-05	1.365E-05	1.146E-05	1.146E-05	8.200E-06
	Straws	6.201E-04	1.240E-04	8.864E-05	8.864E-05	7.805E-05	7.805E-05	5.323E-05
	Fish, subsistence	3.837E-03	3.837E-03	2.744E-03	2.744E-03	2.284E-03	2.284E-03	1.648E-03
	Water	1.325E-06	1.325E-06	9.479E-07	9.479E-07	7.950E-07	7.950E-07	5.691E-07

Table 4 summarizes all ingestion-related 90th percentile exposures specific to breastfed and non-breastfed infants. There are no significant differences in the results generated by the current assessment (shown above) and the SEHSC assessment. The two highest contributors to ingestion exposure for this subpopulation are antifoam and fish (subsistence).

Figure 1. Contribution of scenarios to children's mean and 90th percentile dermal exposures

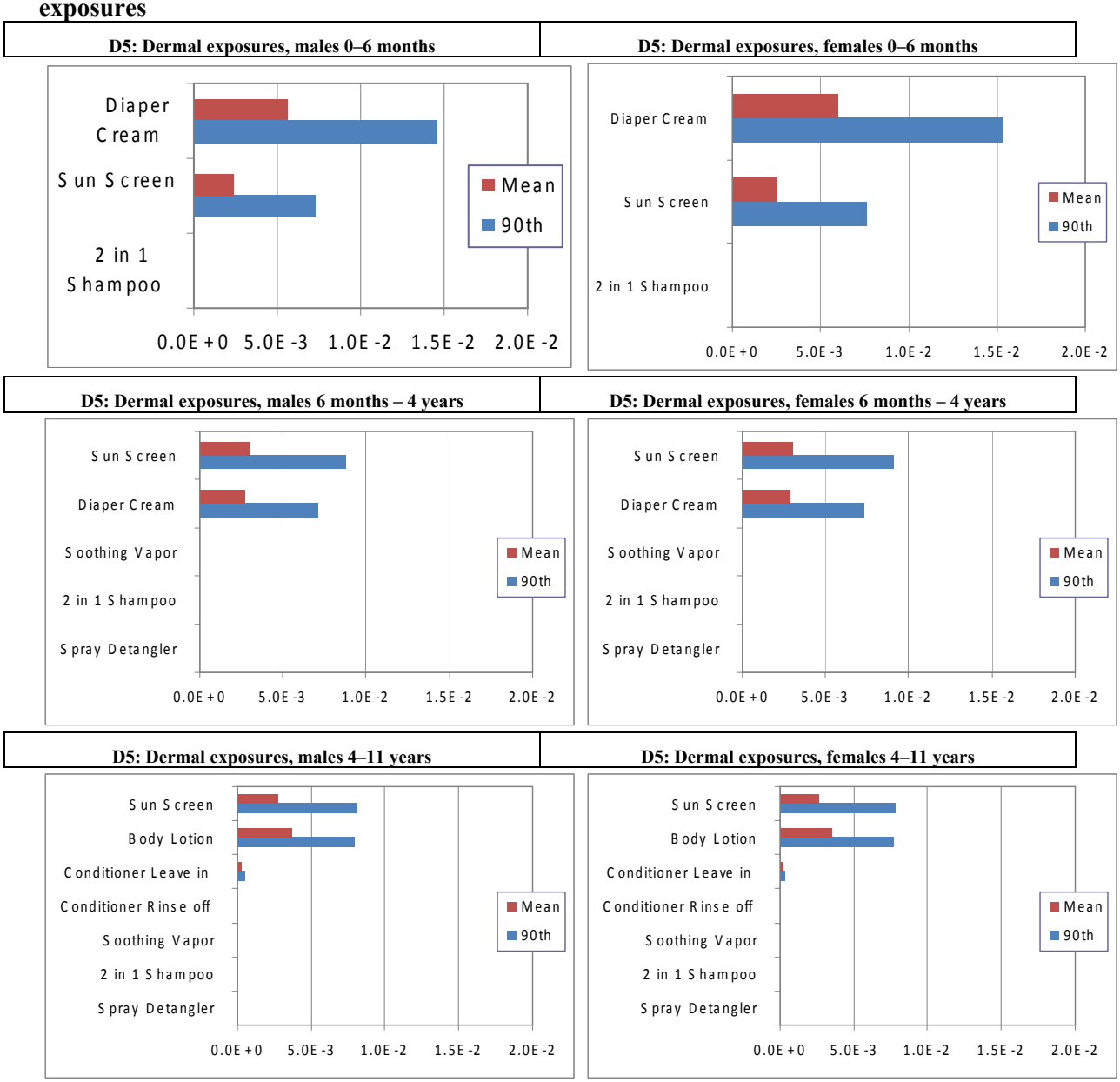

Figure 1 shows the contribution of scenarios to dermal exposures for children's mean and 90th percentile exposures. As seen in the bar charts, diaper cream, sunscreen, and body lotion are the highest contributors to dermal exposures.

Figure 2. Contribution of scenarios to children's mean and 90th percentile inhalation exposures

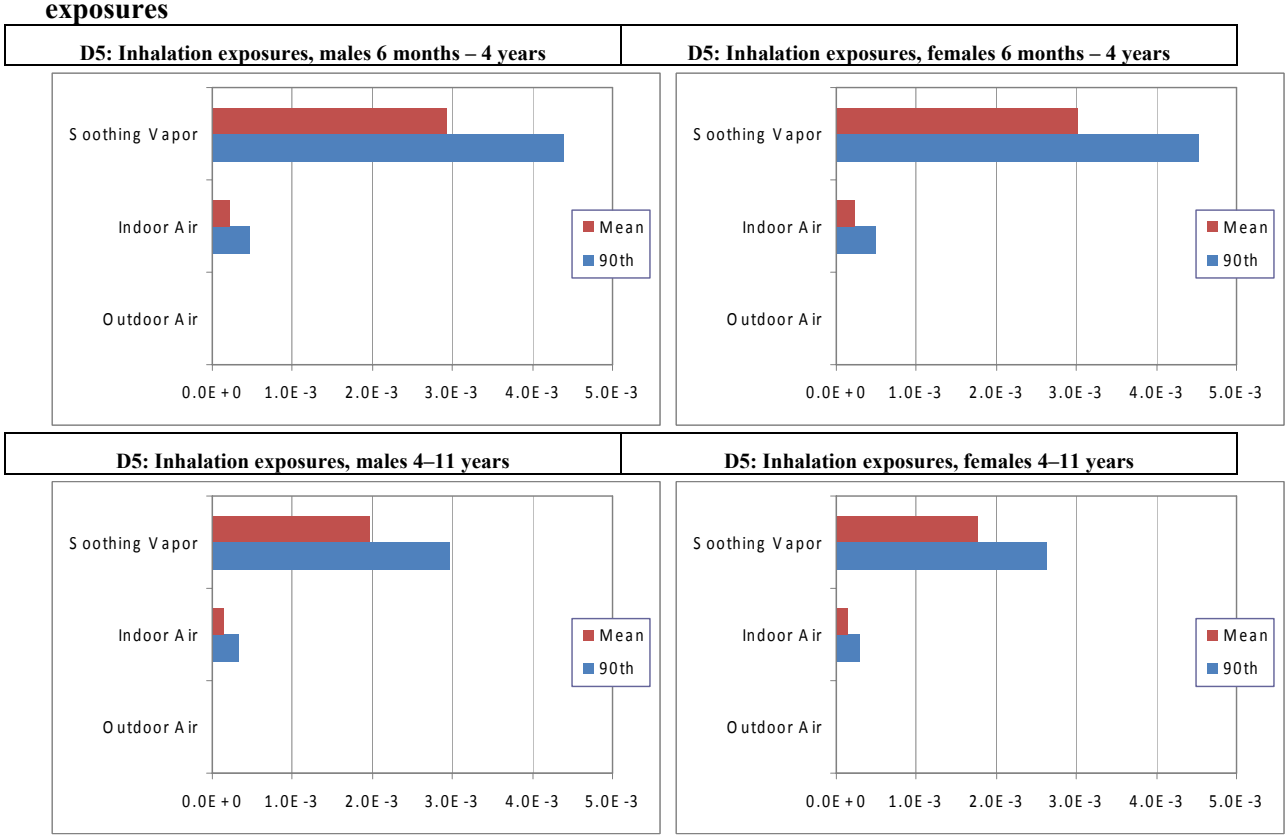

Figure 2 shows the contribution of scenarios to inhalation exposures for children's mean and 90th percentile exposures. As seen in the bar charts, soothing vapour is the highest contributor to inhalation exposures.

Figure 3. Contribution of scenarios to children's (breastfed vs. non-breastfed) mean and 90th percentile ingestion exposures

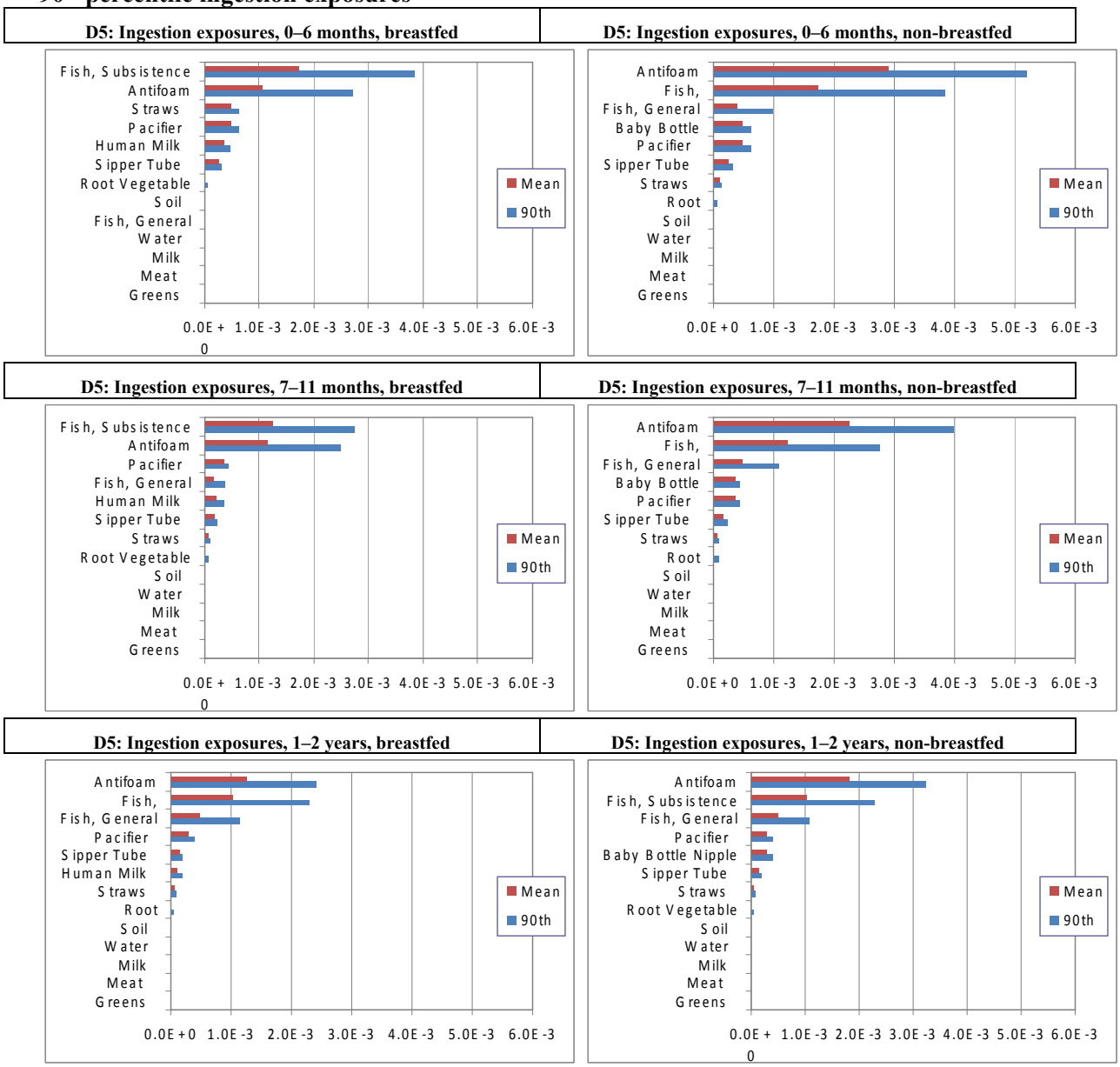

Figure 3 shows the contribution of scenarios to ingestion exposures for children's (breastfed and non-breastfed) mean and 90th percentile exposures. As seen in the bar charts, the highest contributors to ingestion exposures for this subpopulation are antifoam and fish (for the general and subsistence population).

Figure 4. Contribution of scenarios to children's (2–4 and 4–11 years) mean and 90th percentile ingestion exposures

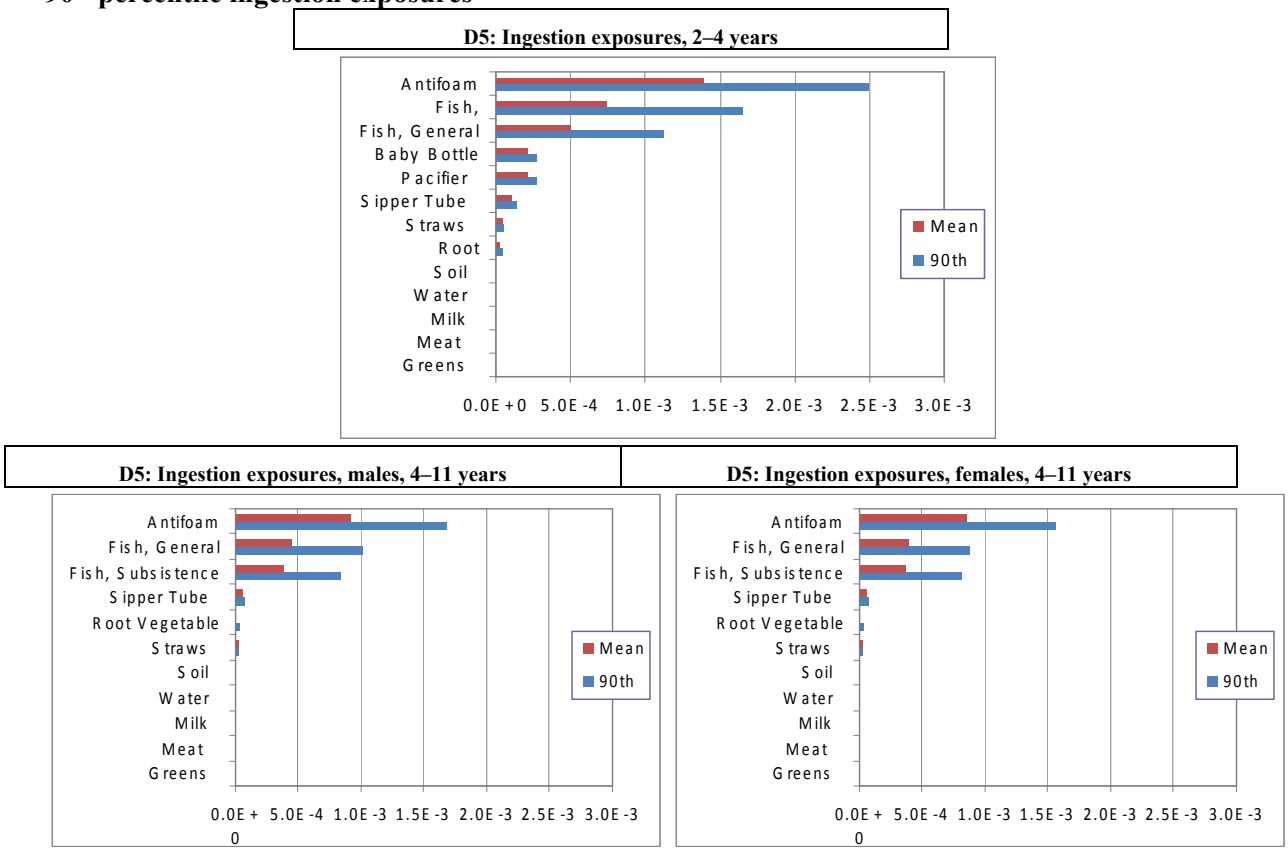

Figure 4 shows the contribution of scenarios to ingestion exposures for children's (2–4 and 4–11 years) mean and 90th percentile exposures. Exposure estimates are based on 200 000 Crystal Ball simulations. As seen in the bar charts, the highest contributors to ingestion exposures for this subpopulation are antifoam and fish (for the general and subsistence population).

Figure 5. Contribution of exposure route to children's mean and 90th percentile total exposure (general population)

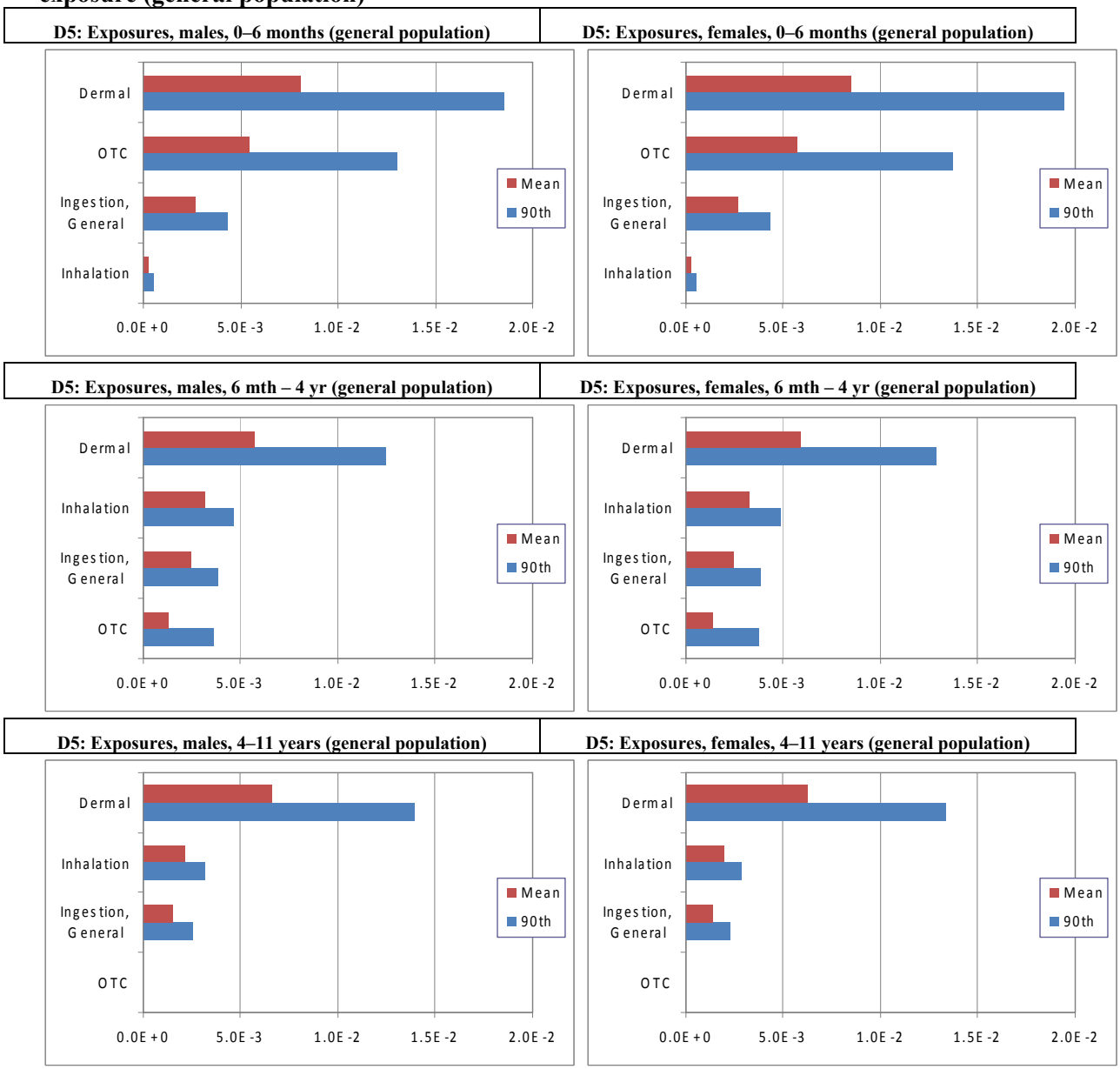

Figure 5 shows the contribution of exposure route to children's mean and 90th percentile total exposures for the general population. The highest exposure route is dermal. In the case of children 0–6 months old, dermal exposure is followed by over-the-counter drugs and then by ingestion; however, in the case of children 6 months – 4 years old and children 4–11 years old, dermal exposure is followed by inhalation and then by ingestion.

Figure 6. Contribution of exposure route to children's mean and 90th percentile total exposure (subsistence population)

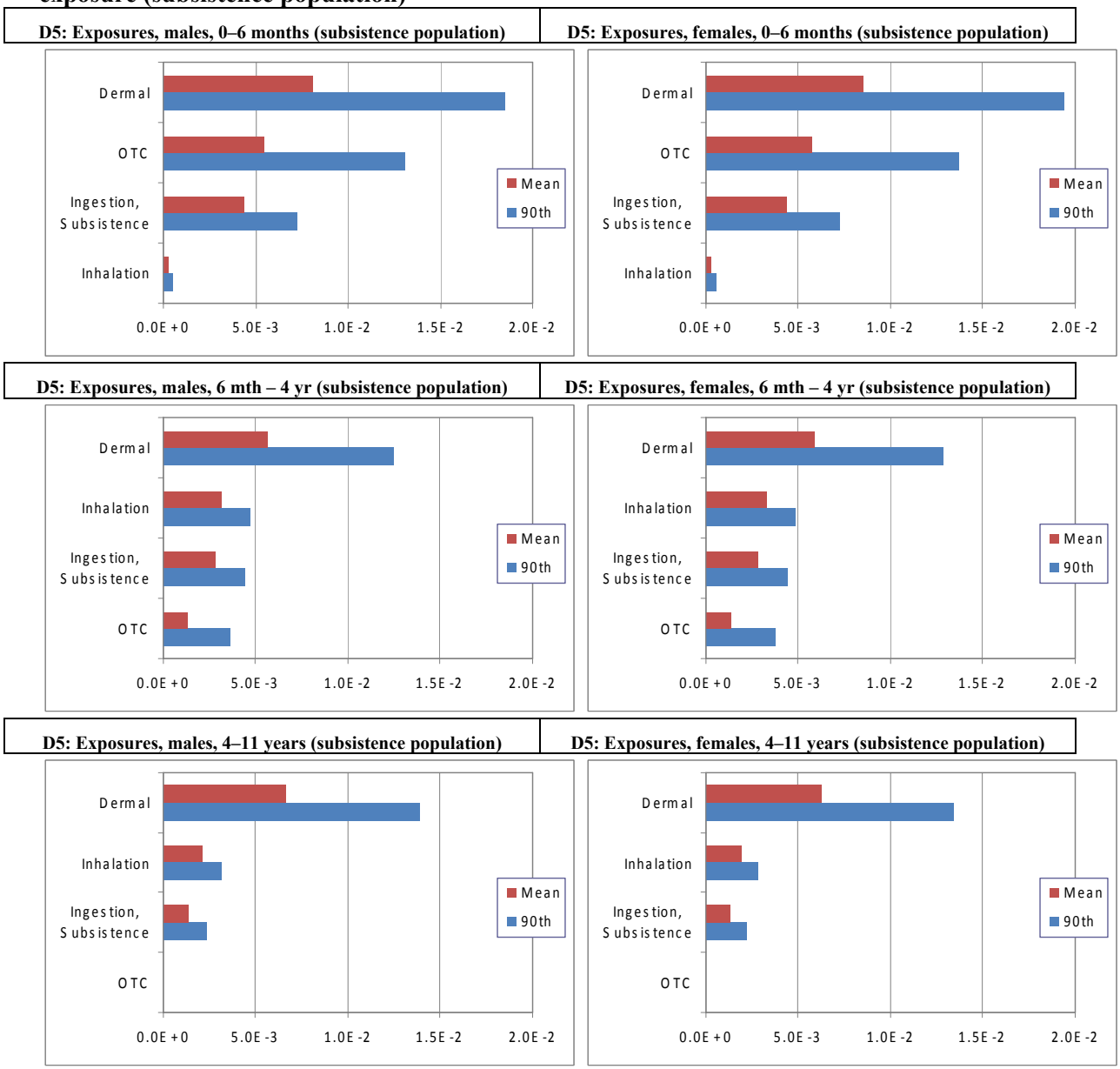

Figure 6 shows the contribution of exposure route to children's mean and 90th percentile total exposures for the subsistence population. The highest exposure route is dermal. In the case of children 0–6 months old, dermal exposure is followed by over-the-counter drugs and then by ingestion; however, in the case of children 6 months – 4 years old and children 4–11 years old, dermal exposure is followed by inhalation and then by ingestion.

EXPOSURE RESULTS AND DISCUSSION: ADULTS

Table 5. Adults' mean exposures (based on 200 000 Crystal Ball simulations)

Mean exposures		12–19 years		20–59 years		60+ years	
		Males	**Females**	**Males**	**Females**	**Males**	**Females**
DERMAL	After shave	1.07E-04		8.25E-05		8.45E-05	
	Body lotion	3.11E-03	3.46E-03	2.40E-03	2.83E-03	2.45E-03	2.93E-03
	Soothing vapour	3.07E-06	3.41E-06	2.37E-06	2.80E-06	2.42E-06	2.90E-06
	Foundation		1.47E-04		1.21E-04		1.25E-04
	Hair spray	1.09E-04	6.44E-05	8.36E-05	5.28E-05	8.56E-05	5.46E-05
	Leave-in conditioner	6.21E-05	3.70E-05	4.78E-05	3.04E-05	4.89E-05	3.14E-05
	Rinse-off conditioner	1.86E-06	1.11E-06	1.43E-06	9.08E-07	1.47E-06	9.40E-07
	Mascara		3.45E-05		2.83E-05		2.93E-05
	Moisturizer		1.18E-03		9.70E-04		1.00E-03
	Nail care		1.14E-04		9.31E-05		9.65E-05
	Roll-on antiperspirant	5.58E-04	4.13E-04	4.29E-04	3.38E-04	4.40E-04	3.51E-04
	Shampoo	1.17E-07	6.95E-08	9.04E-08	5.70E-08	9.26E-08	5.90E-08
	Solid antiperspirant	6.54E-04	4.47E-04	5.03E-04	3.66E-04	5.15E-04	3.79E-04
	Sunscreen	1.88E-03	2.09E-03	1.45E-03	1.71E-03	1.48E-03	1.77E-03
	Under-eye cream				4.24E-05		4.39E-05
	Total Dermal	6.49E-03	7.99E-03	5.00E-03	6.59E-03	5.11E-03	6.83E-03
INHALATION	Indoor air	8.48E-05	6.94E-05	6.13E-05	5.28E-05	5.36E-05	4.91E-05
	Outdoor air	1.69E-06	1.38E-06	1.22E-06	1.05E-06	1.07E-06	9.77E-07
	Soothing vapour	1.10E-03	9.01E-04	7.96E-04	6.86E-04	6.95E-04	6.37E-04
	Total inhalation	1.19E-03	9.72E-04	8.59E-04	7.40E-04	7.50E-04	6.87E-04
INGESTION	Fish, general population	3.08E-04	2.24E-04	2.39E-04	2.36E-04	2.35E-04	2.68E-04
	Leafy vegetables	1.90E-08	1.75E-08	2.21E-08	2.51E-08	2.45E-08	2.71E-08
	Root crops	8.39E-06	6.83E-06	7.49E-06	6.30E-06	7.33E-06	6.59E-06
	Lipstick		1.26E-05		1.03E-05		1.07E-05
	Meat	5.47E-08	3.76E-08	4.68E-08	3.32E-08	3.28E-08	2.86E-08
	Milk	4.63E-08	3.20E-08	1.97E-08	1.89E-08	2.05E-08	1.97E-08
	Soil	5.90E-07	6.55E-07	4.54E-07	5.37E-07	4.65E-07	5.56E-07
	Fish, subsistence population	4.07E-04	4.51E-04	3.13E-04	3.70E-04	3.20E-04	3.83E-04
	Water	1.01E-07	1.13E-07	1.02E-07	1.20E-07	1.04E-07	1.24E-07
	Antifoam	8.09E-04	7.98E-04	7.07E-04	6.38E-04	5.89E-04	5.63E-04
	OTC drugs	1.02E-06	1.13E-06	7.84E-07	9.26E-07	8.02E-07	9.59E-07
	Total Ingestion, General	1.13E-03	1.04E-03	9.55E-04	8.92E-04	8.32E-04	8.49E-04
	Total Ingestion, Subsistence	1.23E-03	1.27E-03	1.03E-03	1.03E-03	9.17E-04	9.65E-04
TOTAL	***General Population***	8.80E-03	1.00E-02	6.81E-03	8.22E-03	6.70E-03	8.36E-03
	Subsistence Population	8.90E-03	1.02E-02	6.88E-03	8.36E-03	6.78E-03	8.48E-03

Table 5 summarizes all the exposure results for adults as mean values. When compared with similar results generated by the SEHSC assessment, almost all the values are higher in the current assessment. Compared to the SEHSC assessment, the current assessment results in a difference of about 2.16 times for total dermal exposures, in a difference of about 13.55 times for total inhalation exposures, and in a difference of about 1.24 times for total ingestion (general population) exposures. The primary reason for the differences is that the SEHSC assessed users and non-users whereas the current assessment considered users only.

Table 6. Adults' 90th percentile exposures (based on 200 000 Crystal Ball simulations)

90th percentile exposures		12–19 years		20–59 years		60+ years	
		Males	**Females**	**Males**	**Females**	**Males**	**Females**
DERMAL	After shave	1.62E-04		1.24E-04		1.27E-04	
	Body lotion	6.77E-03	7.51E-03	5.21E-03	6.16E-03	5.33E-03	6.38E-03
	Soothing vapour rub	4.29E-06	4.76E-06	3.30E-06	3.90E-06	3.38E-06	4.04E-06
	Foundation		3.69E-04		3.02E-04		3.13E-04
	Hair spray	2.70E-04	1.54E-04	2.08E-04	1.26E-04	2.13E-04	1.31E-04
	Leave-in conditioner	1.92E-04	1.07E-04	1.48E-04	8.79E-05	1.51E-04	9.10E-05
	Rinse-off conditioner	5.74E-06	3.18E-06	4.42E-06	2.61E-06	4.52E-06	2.70E-06
	Mascara		6.19E-05		5.08E-05		5.26E-05
	Moisturizer		2.79E-03		2.29E-03		2.37E-03
	Nail care		1.16E-04		9.44E-05		9.75E-05
	Roll-on antiperspirant	1.07E-03	7.92E-04	8.26E-04	6.48E-04	8.45E-04	6.72E-04
	Shampoo	2.50E-07	1.59E-07	1.92E-07	1.30E-07	1.97E-07	1.35E-07
	Solid antiperspirant	8.73E-04	9.63E-04	6.72E-04	7.90E-04	6.87E-04	8.18E-04
	Sunscreen	3.38E-03	3.75E-03	2.60E-03	3.07E-03	2.66E-03	3.18E-03
	Under-eye cream				7.33E-05		7.59E-05
	Total Dermal	1.04E-02	1.29E-02	8.01E-03	1.06E-02	8.20E-03	1.10E-02
INHALATION	Indoor	1.76E-04	1.43E-04	1.27E-04	1.09E-04	1.11E-04	1.01E-04
	Outdoor	4.02E-06	3.31E-06	2.93E-06	2.52E-06	2.56E-06	2.33E-06
	Soothing vapour	1.62E-03	1.29E-03	1.13E-03	9.69E-04	9.93E-04	9.03E-04
	Total inhalation	1.72E-03	1.37E-03	1.20E-03	1.03E-03	1.05E-03	9.58E-04
INGESTION	Fish, general population	6.91E-04	5.20E-04	5.39E-04	5.25E-04	5.20E-04	5.92E-04
	Leafy vegetables	3.75E-09	3.39E-09	4.00E-09	4.47E-09	4.60E-09	4.78E-09
	Root crops	2.24E-05	1.81E-05	2.04E-05	1.75E-05	2.03E-05	1.85E-05
	Lipstick		3.13E-05		2.57E-05		2.66E-05
	Meat	1.08E-07	7.57E-08	9.41E-08	6.64E-08	6.51E-08	5.70E-08
	Milk	9.47E-08	6.81E-08	4.11E-08	4.00E-08	4.14E-08	4.14E-08
	Soil	7.96E-07	8.83E-07	6.12E-07	7.23E-07	6.27E-07	7.49E-07
	Fish, subsistence population	9.09E-04	1.01E-03	6.99E-04	8.27E-04	7.17E-04	8.56E-04
	Water	1.91E-07	2.12E-07	1.74E-07	2.06E-07	1.78E-07	2.13E-07
	Antifoam	1.46E-03	1.24E-03	1.26E-03	1.15E-03	1.03E-03	1.00E-03
	OTC drugs	2.45E-06	2.72E-06	1.88E-06	2.23E-06	1.93E-06	2.31E-06
	Total Ingestion, General	1.94E-03	1.56E-03	1.65E-03	1.54E-03	1.40E-03	1.44E-03
	Total Ingestion, Subsistence	2.09E-03	1.95E-03	1.76E-03	1.76E-03	1.54E-03	1.64E-03
TOTAL	***General Population***	1.28E-02	1.50E-02	9.95E-03	1.23E-02	9.87E-03	1.26E-02
	Subsistence Population	1.30E-02	1.52E-02	1.00E-02	1.25E-02	9.96E-03	1.27E-02

Table 6 summarizes all the exposure results for adults as 90th percentile values. When compared with similar results generated by the SEHSC assessment, almost all the values are higher in the current assessment. Compared to the SEHSC assessment, the current assessment results in a difference of about 1.55 times for total dermal exposures, in a difference of about 9.44 times for total inhalation exposures, and in a difference of about 1.17 times for total ingestion (general population) exposures. The primary reason for the differences is that the SEHSC assessed users and non-users whereas the current assessment considered users only.

Figure 7. Contribution of scenarios to adults' mean and 90th percentile dermal exposures

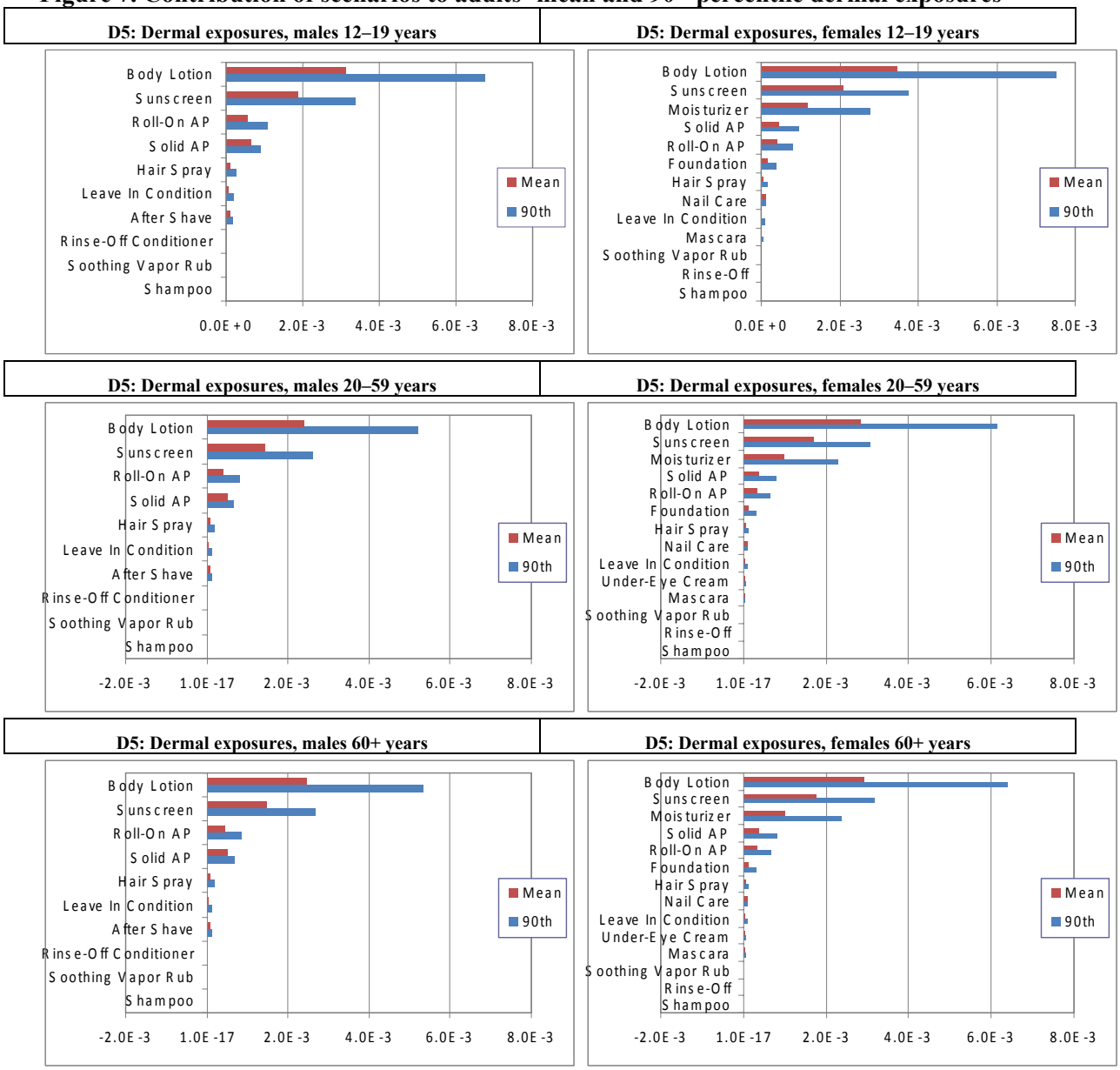

Figure 7 shows the contribution of scenarios to dermal exposures for adults' mean and 90th percentile exposures. As seen in the bar charts, body lotion, sunscreen and moisturizer are the highest contributors to dermal exposures.

Figure 8. Contribution of scenarios to adults' mean and 90th percentile inhalation exposures

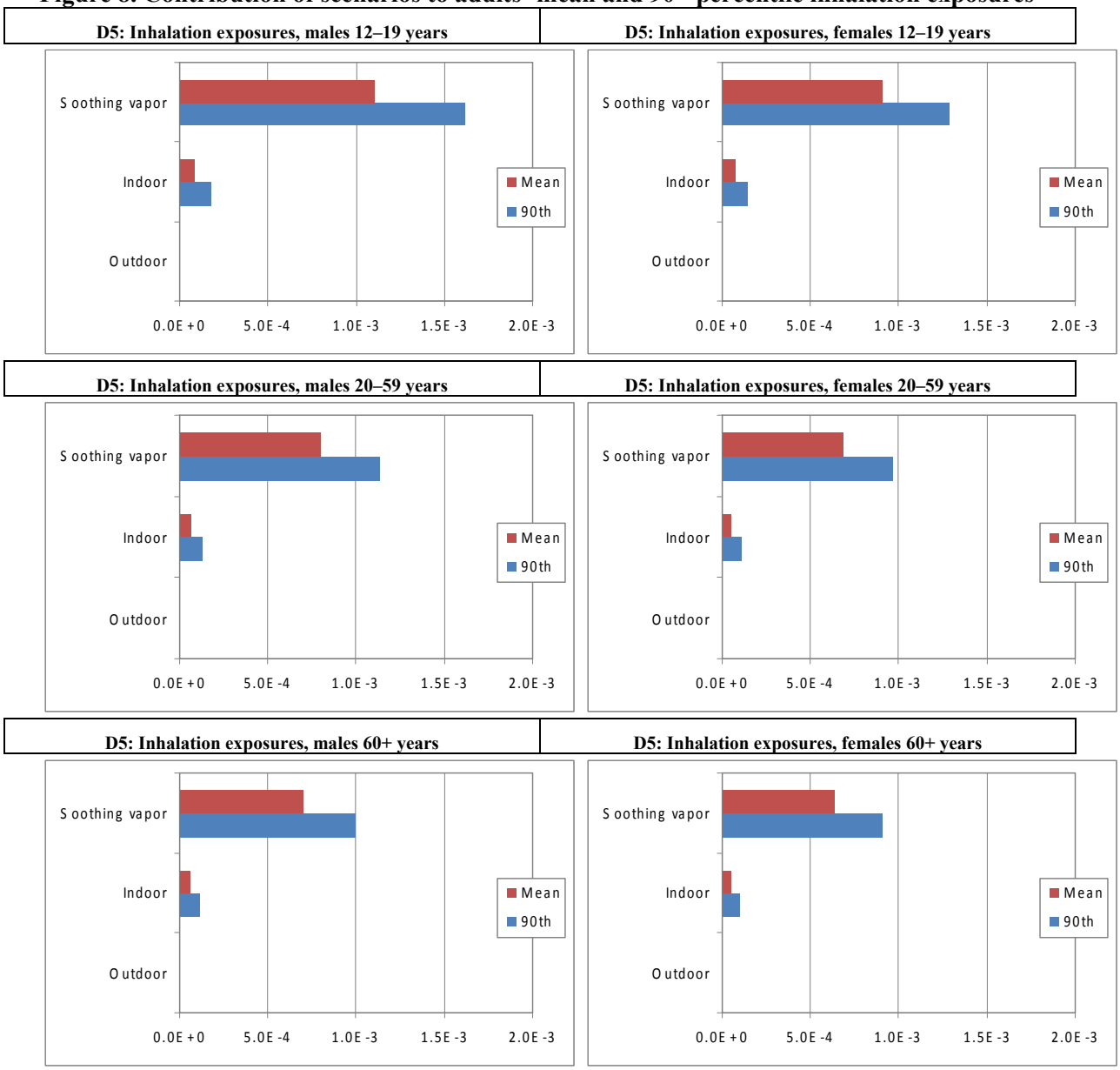

Figure 8 shows the contribution of scenarios to inhalation exposures for adults' mean and 90th percentile exposures. As seen in the bar charts, soothing vapour is the highest contributor to inhalation exposures.

Figure 9. Contribution of scenarios to adults' mean and 90th percentile ingestion exposures

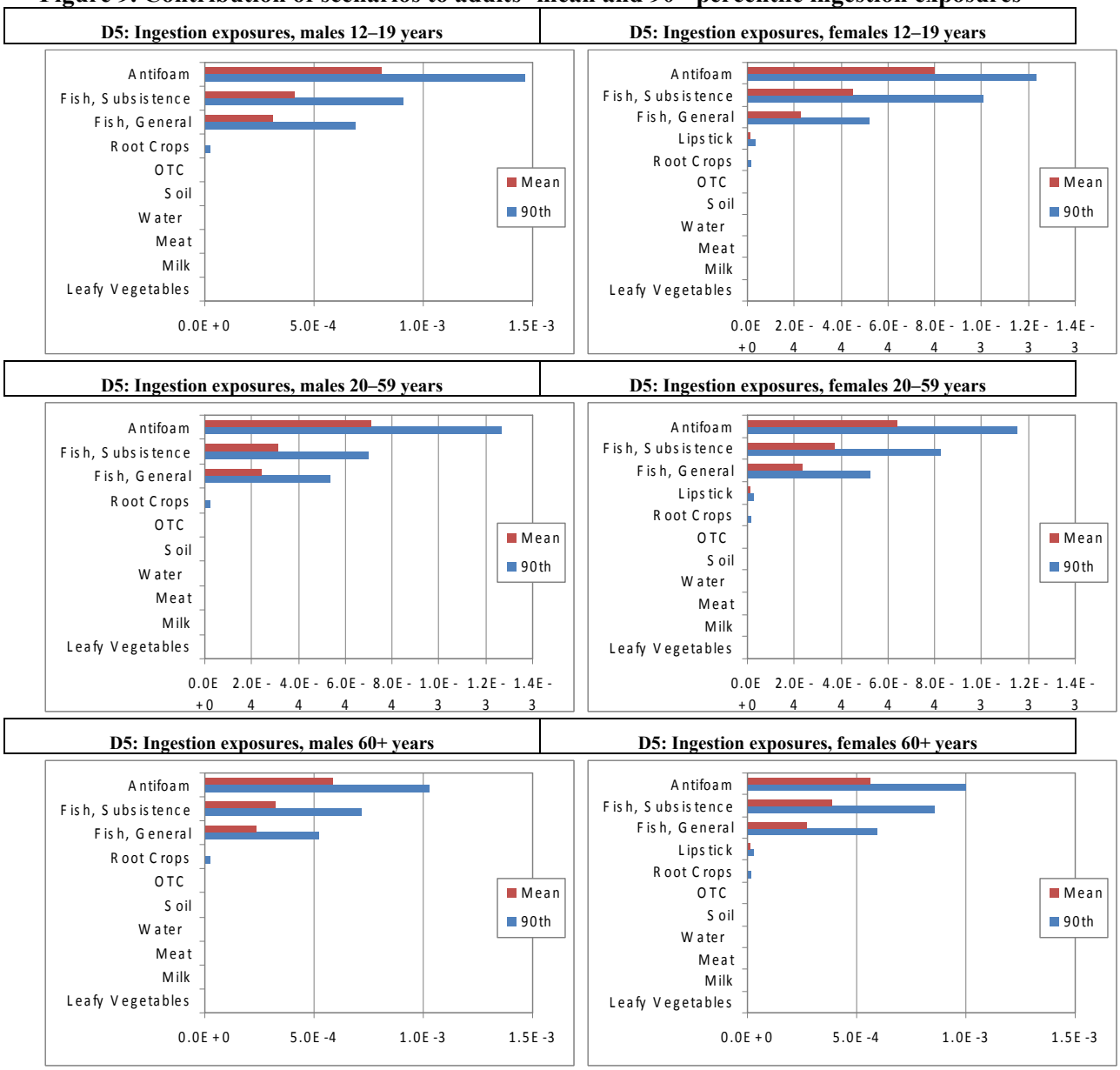

Figure 9 shows the contribution of scenarios to ingestion exposures (general population) for adults' mean and 90th percentile exposures. As seen in the bar charts, antifoam and fish are the highest contributors to ingestion exposures.

Figure 10. Contribution of exposure route to adults' mean and 90th percentile total exposure (general population)

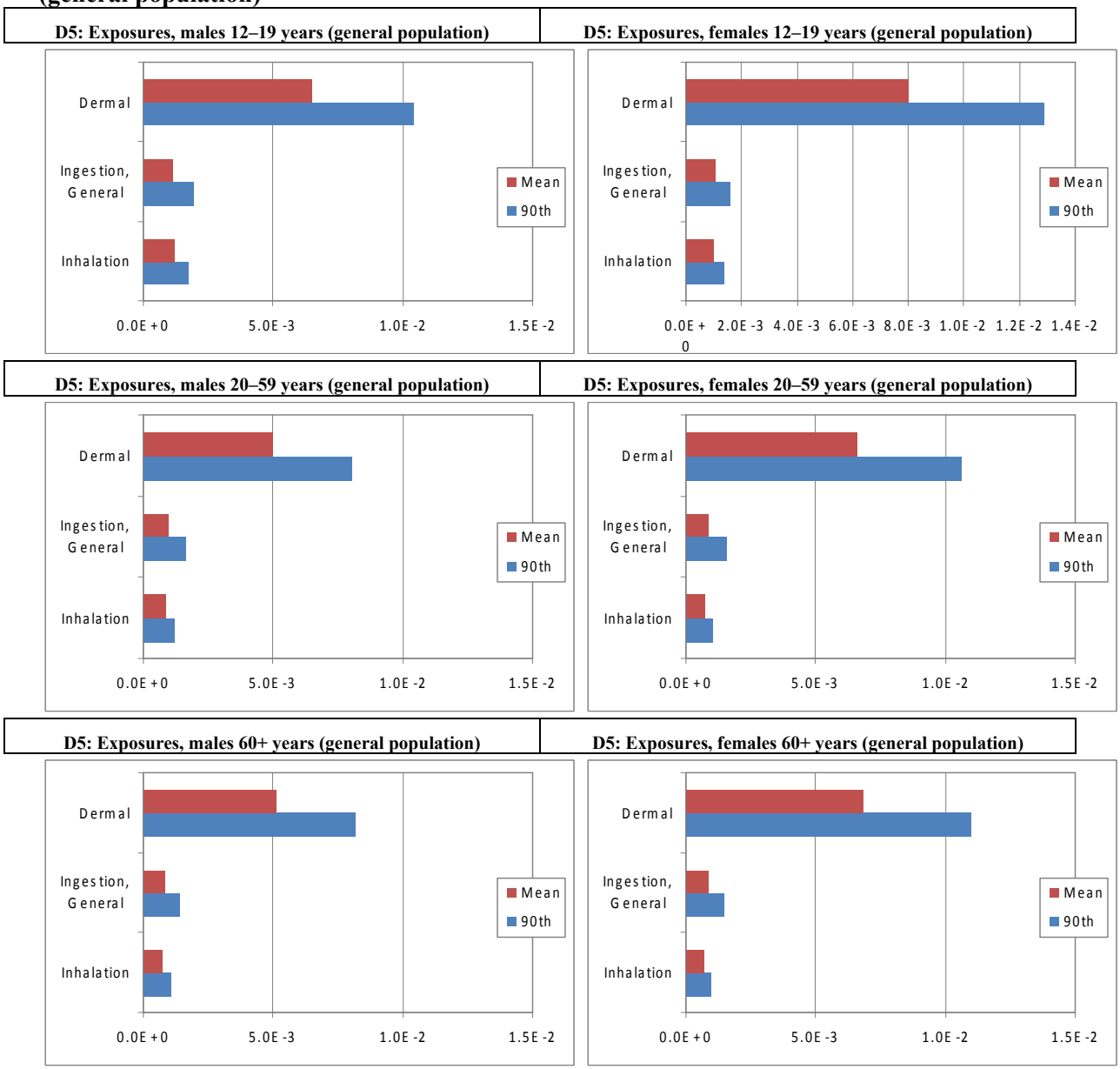

Figure 10 shows the contribution of exposure route to adults' mean and 90th percentile total exposures for the general population. The highest exposure route is dermal. Dermal is followed by ingestion and inhalation.

Figure 11. Contribution of exposure route to adults' mean and 90th percentile total exposure (subsistence population)

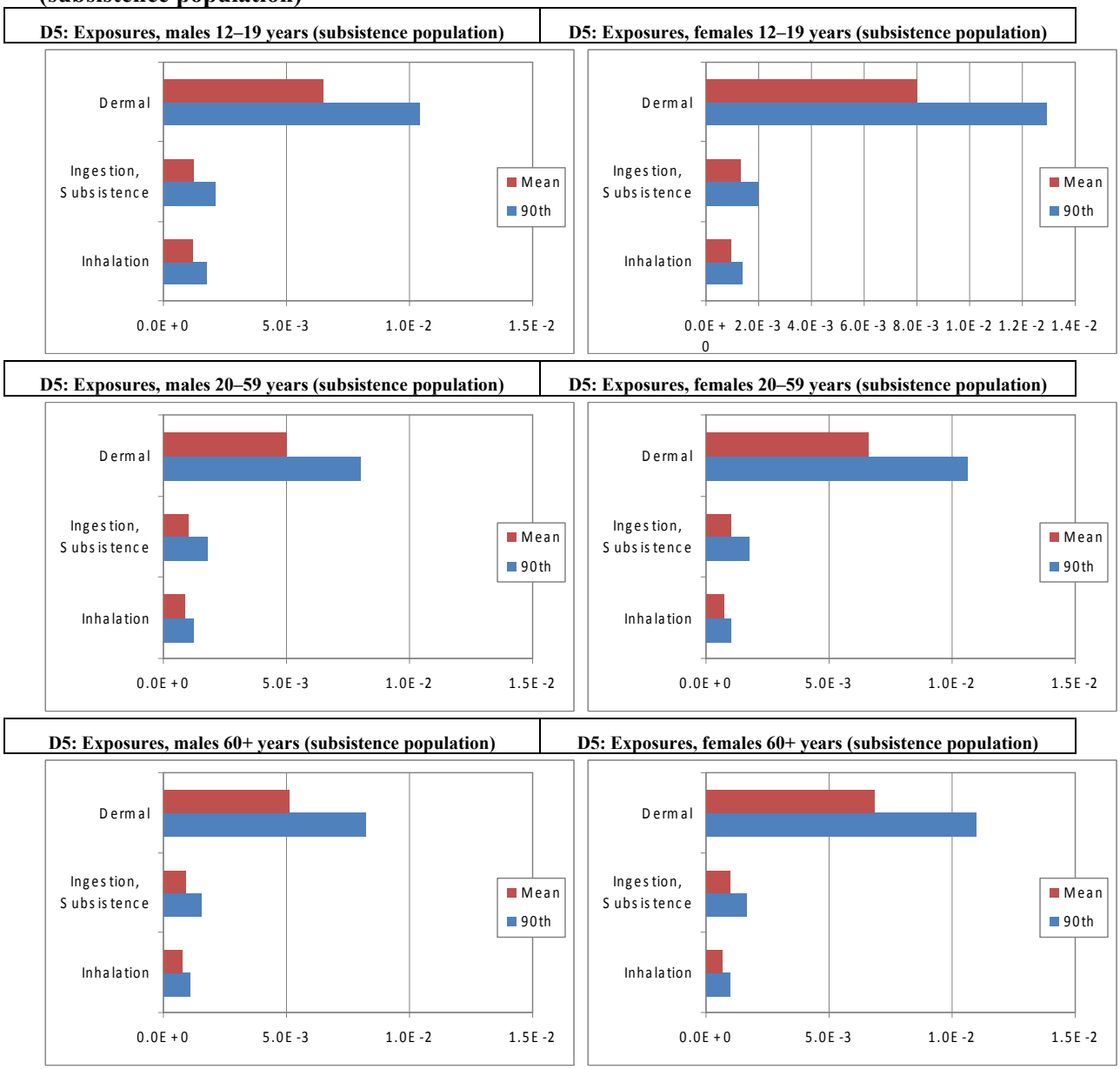

Figure 11 shows the contribution of exposure route to adults' mean and 90th percentile total exposures for the subsistence population. The highest exposure route is dermal. Dermal is followed by ingestion and inhalation.

Appendix 5: Multimedia modelling input parameters for D6 in the ecological screening assessment

Model input parameter	Value
Molecular weight (g/mol)	445
Melting point (ºC)	-3
Boiling point (ºC)	245
Data temperature (ºC)	25
Density (kg/m^3)	963
Vapour pressure (Pa)	4.6 (0.0345 mm Hg)
Henry's Law constant (Pa·m^3/mol)	4 950 000 (48.9 atm·m^3/mol)
Log K_{aw} (Air-water partition coefficient; dimensionless)	3.3
Log K_{ow} (Octanol-water partition coefficient; dimensionless)	9.06
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)	6.1
Water solubility (mg/L)	0.00513
Log K_{oa} (Octanol-air partition coefficient; dimensionless)	5.76
Soil-water partition coefficient (L/kg)	25 178
Sediment-water partition coefficient (L/kg)	50 357
Suspended particles-water partition coefficient (L/kg)	251 780
Fish-water partition coefficient (L/kg)	1660
Aerosol-water partition coefficient; dimensionless	100
Vegetation-water partition coefficient; dimensionless	12 589
Half-life in air (days)	5.96
Half-life in water (days)	401
Half-life in sediment (days)	49
Half-life in soil (days)	5.25
Half-life in vegetation (days)	74