Substance Profile for The Challenge
Decamethylcyclopentasiloxane (D5)
CAS No. 541-02-6

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) required the Minister of Health and Minister of the Environment to categorize the approximately 23,000 substances on the Domestic Substances List (DSL). Categorization involved identifying those substances on the DSL that are a) considered to be persistent (P) and/or bioaccumulative (B), based on criteria set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada, 2000), and "inherently toxic" (iT) to humans or other organisms, or b) that present, to individuals in Canada, the greatest potential for exposure (GPE).

Further to this activity, the Act requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that meet the categorization criteria. A screening assessment involves a scientific evaluation of available information for a substance to determine whether the substance meets the criteria set out in section 64 of CEPA 1999. Based on the results of a screening assessment, the Ministers can propose taking no further action with respect to the substance, adding the substance to the Priority Substances List (PSL) for further assessment or recommending the addition of the substance to the List of Toxic Substances in Schedule 1 of CEPA 1999 and, where applicable, the implementation of virtual elimination of releases to the environment.

A number of substances have been identified by the Ministers as high priorities for action based on the information obtained through the categorization process. This includes substances:

- that were found to meet all of the ecological categorization criteria, including persistence, bioaccumulation potential and inherent toxicity to aquatic organisms (PBiT), and that are known to be in commerce, or of commercial interest, in Canada, and/or
- that were found either to meet the categorization criteria for GPE or to present an intermediate potential for exposure (IPE), and were identified as posing a high hazard to human health based on available evidence on carcinogenicity, mutagenicity, developmental toxicity or reproductive toxicity.

Based on a consideration of the ecological and/or human health concerns associated with these substances, and the requirement under section 76.1 of CEPA 1999 for the Ministers to apply a weight of evidence approach and the precautionary principle when conducting and interpreting the results of an assessment, sufficient data are currently available to conclude whether these substances meet the criteria under section 64 of CEPA 1999.

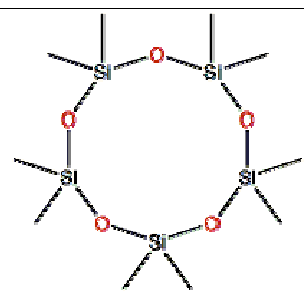
As such, the Ministers have issued a Challenge to industry and other interested stakeholders through publication in Canada Gazette Part I December 9, 2006 to submit, within the timelines stated in the Challenge section of this document, specific information that may be used to inform risk assessment and to develop and benchmark best practices for risk management and product stewardship.

The substance decamethylcyclopentasiloxane (D5) was identified as a high priority for action as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The technical human health and ecological information that formed the basis for concern associated with this substance is contained in Appendices I and II, respectively.

Substance Identity

For the purposes of this document, decamethylcyclopentasiloxane will be referred to as D5, an abbreviated name derived from the General Electric's siloxane notation (Hurd 1946).

D5 belongs to a group of cyclic volatile methyl-siloxanes (VMS) with relatively low molecular weight (< 600) and high vapour pressure. These cyclic VMS are volatile, low-viscosity silicone fluids consisting three to six -$(CH_3)_2SiO$- structure units in a cyclic configuration. D5 consists of five of these -$(CH_3)_2SiO$- structure units as shown in the chemical structure below.

CAS Registry Number	541-02-6
Inventory names	Cyclopentasiloxane, decamethyl-; Decamethylcyclopentasiloxane (English, French); Decamethylcyclopentasiloxan (German); decametilciclopentasiloxano (Spanish); Decamethyl cyclopentasiloxane
Other names	Cyclic dimethylsiloxane pentamer; Cyclo-decamethylpentasiloxane; D5; DC 2-5252C; DC 245; DC 345; DC 345 Fluid; Dimethylsiloxane pentamer; Dow Corning 2-5252C; Dow Corning 245; Dow Corning 245 Fluid; Dow Corning 345; Dow Corning 345 Fluid; Dow Corning 345EU; Execol D 5; KF 995; LS 9000; Mirasil CM 5; NUC Silicone VS 7158; Pentacyclomethicone; SF 1202; SH 245; SH 245 (siloxane); Silbione 70045V5; Silbione V 5; Silicone SF 1202; TFS 405; TSF 405; TSF 465; Union Carbide 7158 Silicone Fluid; Volasil 245; VS 7158
Chemical group	Discrete organics
Chemical sub-group	Cyclic Volatile Methyl Siloxanes (VMS)
Chemical formula	C10H30O5Si5
Chemical structure	
SMILES	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
Molecular mass	370.78 g/mol

It should be noted that D5 is also present under another CAS No. 69430-24-6 (dimethylcyclosiloxane, or cyclomethicone). Dimethylcyclosiloxane is a compound made up of octamethylcyclotetrasiloxane (D4) and decamethylcyclopentasiloxane (D5) (Danish EPA 2004). The relative proportions of the two substances in this compound are not known.

Based on information submitted in response to a legal Notice published in 2006 under section 71 of CEPA 1999 (Environment Canada 2006a), D5 was not manufactured in Canada in 2005 in a quantity meeting the 100 kg reporting thresholds. In total, fifty-two companies reported import of this substance into Canada in 2005, with twenty-one companies in the 100-1,000 kg range, twenty-five companies in the 1,001 – 100,000 kg range and eight companies reporting in the > 100,000 kg range.

D5 is used in a variety of industry activities in Canada such as construction; chemical industry; textiles; leather and hide tanning and finishing; plastic and rubber products; cleaning compounds, toiletries and pharmaceuticals; and paints, coating and adhesives (Environment Canada 2006a). It is also an ingredient in pesticide formulations (PMRA 2005). Additional and more detailed descriptions of industry activity codes are provided in Appendix II. In other countries, uses include silicone fluids, elastomers and resins (HSDB 2006); cosmetics and other personal care products; detergents and cleaning agents; paint, lacquers and varnishes; polishes; fuel additives; and printing inks (SPIN 2007).

THE CHALLENGE

Respecting direction under section 76.1 of CEPA 1999, and in the absence of additional relevant information as a result of this Challenge, the Ministers are predisposed to conclude, based on a screening assessment, that this substance satisfies the definition of toxic under section 64 of CEPA 1999. As such, the Ministers are prepared to then recommend to the Governor in Council that this substance be added to the List of Toxic Substances in Schedule 1 of CEPA 1999, with the intent of initiating the development of risk management measures taking into account socio-economic considerations.

If it is determined that the substance meets the virtual elimination criteria in subsection 77(4) of CEPA 1999, then subsequent risk management activities will be based on the objective of eliminating the release of any measurable quantity of the substance to the environment. In the absence of further information on existing management practices for a substance, actions would be proposed based on the assumption of worst-case practices. The management actions being considered for such substances at this time include prohibition through regulations, of the manufacture, use, sale, offer for sale and import of this substance, except for those activities controlled under the *Pest Control Products Act* and/or the *Food and Drugs Act.*

Exceptionally, should no information be identified to indicate that this substance is in commerce in Canada, the Ministers will conclude, based on a screening assessment, that this substance does not satisfy the definition of toxic under section 64 of CEPA 1999. However, given the properties of this substance, there is concern that new activities for the substance that have not been identified or assessed under CEPA 1999 could lead to the substance meeting the criteria set out in section 64 of the Act. Therefore it would be recommended that this substance be subject to the Significant New Activity provisions specified under subsection 81(3) of the Act, to ensure that any new manufacture, import or use of this substance in quantities greater than 100 kg/year is notified, and that ecological and human health risk assessments are conducted as specified in section 83 of the Act prior to the substance being introduced into Canada.

Section 71 Notice

Under the Challenge, information deemed necessary for improved decision making may be gathered by the Minister of Environment using section 71 of CEPA 1999. This information may be used for the purpose of assessing whether a substance is toxic or is capable of becoming toxic as defined under section 64 of CEPA 1999, or for the purpose of assessing whether to control, or the manner in which to control a substance.

The information mandated through the notices may relate to, among other things; quantity of the substance imported, manufactured, used, or released, concentrations, suppliers, customers, as well as types of uses of the substance.

Copies of the section 71 notice and guidance on how to comply with it are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca), or from the contact provided below.

Opportunity to Submit Additional Information to Inform Screening Assessment

The Ministers of Health and Environment are inviting the submission of additional information for consideration during screening assessment of this substance. Data of the types described in the following paragraphs are considered most relevant, although other submitted information will be considered.

Data on the persistence, bioaccumulation, and potential for toxicity of the substance to organisms in different environmental media – Through the categorization exercise, available experimental data were collected up to December 2005. Where acceptable experimental data were not available, Quantitative Structure Activity Relationships (QSARs) or read across data were used to fill the data gaps. Since experimental data are preferred, interested parties have an opportunity to provide new or additional relevant experimental study information on the persistence, bioaccumulation, and potential for toxicity of this substance to organisms in different environmental media (air, water, sediment, soil). Efforts should focus on providing data for the endpoints for which quality experimental data does not already exist, as demonstrated by the information summarized in Appendix II of this document. As submitted data will be evaluated for completeness and robustness, it is recommended that stakeholders follow the guidance for test protocols and alternative approaches for test data, as described in Section 8 of the "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers".[1]

Data on the toxicity of the substance to human health - Through the categorization exercise, the high health priorities for action were those substances identified by various agencies as representing a high health hazard on the basis of potential to induce cancer, and/or adversely affect reproduction and development, two critical determinants of the health of Canadians of all ages. The hazard classifications used were those developed by national or international agencies in which large numbers of substances have been classified for endpoint-specific hazard based on original review and critical evaluation of data, assessments of weight of evidence and extensive peer review. Interested parties have an opportunity to provide new or additional relevant experimental study information on the toxicity of the substance to human health which could inform the screening assessment.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

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[1] "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers (version 2005)", Government of Canada, Available from http://www.ec.gc.ca/substances/nsb/eng/cp_guidance_e.shtml

Opportunity to Submit Additional Information on Current Uses and Existing Control Measures to Inform the Risk Management Approach for this Substance

The Ministers of Health and Environment are inviting the submission of additional information that is deemed beneficial by interested stakeholders, relating to the extent and nature of the management/stewardship of substances listed under the Challenge.

Organizations that may be interested in submitting additional information in response to this invitation include those that manufacture, import, export or use this substance whether alone, in a mixture or in a product, including manufactured items.

Additional information is being invited in the following areas:

- Import, manufacture and use quantities
- Substance and product use details
- Releases to the environment and spill management
- Current and potential risk management and product stewardship actions
- Existing legislative or regulatory programs controlling/managing the substance
- Information to support the development of a regulatory impact assessment.

A questionnaire is available which provides a detailed template as an example for the submission of this information. Guidance on how to respond to the challenge questionnaire is also available. Interested stakeholders are invited to provide available additional information, recognizing that not all questions in the questionnaire may be relevant to a particular substance, use, or industrial sector.

Copies of the questionnaire and associated guidance are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca)**,** or from the contact provided below.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

Request for Documents and Submission of Information

Documents and instructions may be requested from the following contact. Information in response to the above Challenge must be submitted to this address:

DSL Surveys Coordinator
Place Vincent Massey, 20th Floor
351 Saint Joseph Boulevard
Gatineau QC K1A 0H3
Tel: 1-888-228-0530/819-956-9313
Fax: 1-800-410-4314 / 819-953-4936
Email: DSL.surveyco@ec.gc.ca

Appendix I
Human Health Information
to Support the Challenge for
Decamethylcyclopentasiloxane (D5)
CAS No. 541-02-6

Introduction

Under the *Canadian Environmental Protection Act, 1999* (CEPA 1999), Health Canada undertook to categorize substances on the Domestic Substances List (DSL) to identify those representing the greatest potential for human exposure (GPE) and those among a subset of substances considered persistent (P) and/or bioaccumulative (B) by Environment Canada that are also considered to be "inherently toxic" to humans.

In order to efficiently identify substances that represent the highest priorities for screening assessment from a human health perspective, Health Canada developed and applied a Simple Exposure Tool (SimET) to the DSL to identify those substances that meet the criteria for GPE, Intermediate Potential for Exposure (IPE) or Low Potential for Exposure (LPE), and a Simple Hazard Tool (SimHaz) to identify those substances that pose a high or low hazard.

Decamethylcyclopentasiloxane (D5) is considered to meet the criteria for IPE under SimET and does not meet the criteria for high hazard under SimHaz. This document summarizes the currently available information on which the SimET and SimHaz results are based.

Exposure Information from Health Related Components of DSL Categorization

SimET was developed and used to identify substances on the DSL considered to represent GPE. This approach was based on three lines of evidence: 1) the quantity in commerce in Canada, 2) the number of companies involved in commercial activities in Canada (i.e., number of notifiers), and 3) the consideration by experts of the potential for human exposure based on various use codes. The proposed approach was released for public comment in November 2003 and also enabled designation of substances as presenting an IPE or LPE, based on criteria for quantity and nature of use (Health Canada 2003).

Results of the Application of SimET

D5 has been determined to be IPE based on a consideration of the DSL nomination information listed below.

Nomination Information for DSL

Quantity in Commerce

The quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 1,110,000 kg.

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was four.

Use Codes and Description

The following DSL use codes have been identified for the substance:

21 Formulation component
60 Cosmetics
76 Organic Chemicals, Industrial
85 Pigment, Dye and Printing Ink
86 Plastics

Potential Uses in Canada

Potential uses in Canada are provided in Appendix II.

Hazard Information from Health Related Components of DSL Categorization

Simple Hazard Tool (SimHaz)

SimHaz is a tool that has been used to identify, among all of the approximately 23 000 substances on the DSL, those considered to present either high or low hazard to human health based on formalized weight of evidence criteria and/or peer review/consensus of experts. This tool has been developed through extensive compilation of hazard classifications of Health Canada and other agencies and consideration of their robustness based on availability of transparent documentation of both process and criteria (Health Canada 2005).

Results of the Application of SimHaz

D5 has not been classified for hazard by any of the agencies considered under the SimHaz tool and therefore does not meet the criteria for high hazard under SimHaz.

Uncertainties

SimET and SimHaz have been developed as robust tools for effectively identifying substances from the DSL considered to be human health priorities for further consideration. It is recognized that they do not include a number of elements normally considered in a human health risk assessment such as a comprehensive characterization of exposure and hazard, a comparison of exposure metrics to hazard metrics and a detailed analysis of uncertainties.

References

Health Canada. 2003. Proposal for Priority Setting for Existing Substances on the Domestic Substances List under the Canadian Environmental Protection Act, 1999: Greatest Potential for Human Exposure. http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs- sesc/pdf/contaminants/existsub/greatest_potential_human_exposure.pdf

Health Canada. 2005. Proposed Integrated Framework for the Health-Related Components of Categorization of the Domestic Substances List under CEPA 1999**.** http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/contaminants/existsub/framework-int-cadre_e.pdf

Appendix II
Ecological Information
to Support The Challenge for
Decamethylcyclopentasiloxane (D5)
CAS No. 541-02-6

The information in this document will form the basis of a screening assessment under section 74 of CEPA, 1999. Data relevant to an ecological screening assessment were identified in original literature, review documents, and commercial and government databases prior to December 2005. Properties and characteristics may also have been estimated using Quantitative Structure Activity Relationship (QSAR) models. In addition, an industry survey was conducted for the year 2005 through a Canada Gazette Notice issued pursuant to section 71 of CEPA 1999 (Environment Canada, 2006b). This Notice requested data on the Canadian manufacture and import of the substance.

Physical and chemical properties

Table 1 contains experimental and modelled physical-chemical properties of D5 which are relevant to its environmental fate.

Table 1. Physical and chemical properties for D5

Property	Type	Value	Temperature ºC	Reference
log K_{ow} (Octanol-water partition coefficient)	Experimental	5.20		Bruggeman et al. 1984
log K_{ow} (Octanol-water partition coefficient)	Modelled	5.71		Kowwin v.1.67
Boiling point ºC	Experimental	210		SRC PHYSPROP Database 2003
Boiling point ºC	Modelled	196.78		MPBPWIN v1.41
Melting point ºC	Experimental	-38		SRC PHYSPROP Database 2003
Melting point ºC	Modelled	-5.19		MPBPWIN v1.41
Vapour Pressure (Pa)	Experimental	26.66 (0.20 mm Hg)	25	Flaningam, 1986
Vapour Pressure (Pa)	Modelled	29.06 (0.22 mm Hg)	25	MPBPWIN v1.41
Henry's Law Constant (Pa·m^3/mol)	Experimental[a]	40530 (0.40 atm-m^3/mol)	25	HSDB 2006
Henry's Law Constant (Pa·m^3/mol)	Modelled	12159 (0.12 atm-m^3/mol)	25	HenryWin v3.10

log K_{oc} (Organic carbon-water partition coefficient)	Modelled	5.16		PCKOCWIN v1.66
Water solubility (mg/L)	Modelled	0.05	25	WSKOWWIN v1.41

[a]estimated using experimental vapour pressure and water solubility data

Manufacture, Importation, and Uses

Manufacture and Importation

In Canada, no manufacture of D5 was reported in response to a CEPA section 71 survey notice for the 2005 calendar year in a quantity meeting the 100kg reporting threshold (Environment Canada 2006a). There were fifty-two Canadian companies reporting import of this substance into Canada in 2005 (Environment Canada 2006a), with twenty-one companies in the 100-1,000 kg/year range, twenty-five companies in the 1,001 – 100,000 kg/yr range and eight companies reporting in the > 100,000 kg/year range (see Appendix I for the quantity of D5 reported in commerce in Canada during the calendar year 1986). D5 is also a constituent of CAS No. 69430-24-6 (dimethylcyclosiloxane); however, dimethylcyclosiloxane was not surveyed under CEPA section 71 by Environment Canada in 2006 (Environment Canada 2006b). In Canada, the quantity of dimethylcyclosiloxane reported in commerce during the calendar year 1986 was 2,220,197 kg/year.

Elsewhere, D5 has been identified as a High Production Volume (HPV) chemical by the Organisation for Economic Co-operation and Development (OECD), the European Chemicals Bureau (ECB), the US Environmental Protection Agency (EPA), and the International Congress & Convention Association (ICCA). According to information from the US EPA, the import/production of D5 was in the range of 4,500 – 22,500 tonnes in 1986, 1990, and 1994. The import/production increased to 22,500 – 45,000 tonnes in 1998, and 45,000 – 225,000 tonnes in 2002.

In Europe, four companies have been identified as producers/importers of D5: Bayer AG of Germany, Dow Corning Limited of the UK, Rhodia Chimie of France, and Amway Europe of Belgium (ECB 2006). In Nordic countries, the SPIN database indicated that the total registered consumption of D5 and dimethylcyclosiloxane (CAS No. 69430-24-6) during 2000 – 2004 was less than 100 and 85 tons per year, respectively (SPIN 2007).

Uses

In response to a CEPA section 71 survey notice for the 2005 calendar year, companies importing D5 identified their business activity as (Environment Canada 2006a) the Retail Trade of Health and Personal Care Items; Footwear Stores; Automotive Parts (including accessories and tires), the Construction Industry; Mining and Oil/Gas Extraction; Transportation, Warehousing and Storage; Health Care and Social Assistance (Offices of Physicians and Other Health Practitioners, Hospitals and Related Services, Facilities for the Elderly); Other Services (except Public Administration) which includes Household Goods Maintenance /Repair and Esthetic Services for Women. Also reported was the Wholesale Trade of: Pharmaceuticals, Toiletries and Cosmetics; New Motor Vehicle Parts and Accessories; and Chemicals (except Agricultural) and Allied Products. Additional activities included the Manufacture of: Basic Chemicals; Converted Paper Products; Textile and Fabric Finishing/Coating; Leather and Hide Tanning/Finishing; Plastic and Rubber Products; Fiber, Yarn, and Threads; Pulp, Paper, and Paperboard; Petroleum and Coal Products; Soap, Cleaning Compounds, and Toiletries; Pharmaceuticals and Medicines; Paint, Coating, and Adhesives; Machine Shops and Metal Parts; Commercial and Service Industry Machinery; Computer Equipment; Electrical Equipment and Components; Medical Equipment and Supplies; Household Appliances; Printer Inks and Cartridges; Motor Vehicle Parts; Other Foods (which may include perishable prepared foods such as fresh pizza and pasta); Other Chemical Products/Preparations; and Other Miscellaneous Items.

The above industrial activities identified through the CEPA section 71 Notice are based on the North American Industry Classification System (NAICS) codes. These codes define the company's sectors and business lines, but do not describe the use of the substance or product within the company. This differs from the DSL Nomination Functional Use Codes utilized during categorization and listed in Appendix I. Use Codes indicate specific applications or uses for the substance or products containing the substance. NAICS has currently defined over 3000 NAICS codes. The Functional Use Codes were defined for the purposes of the DSL Nomination.

The number of industrial activities identified as using D5 in 2005 is considerably greater than the number of DSL Use Codes for this substance identified in 1986. A NAICS defines the activities of a company rather then a substance, so the broad number of activities identified may only be distantly relevant to the substance. As well, there were an increased number of notifiers importing or manufacturing the substance as well as an increase in the amount of this substance being manufactured or imported into Canada.

The following use patterns for D5 have been identified worldwide (SPIN 2007 unless otherwise specified):

- Raw materials, intermediates, or by-products in productions of silicone fluids, elastomers, and resins (HSDB 2006).
- Raw materials for production of cosmetics, or intermediates for cosmetics and hygienic articles
- Paint, lacquers and varnishes
- Surface treatment and polishing agents for motor vehicles and other plastic materials
- Inert ingredient in pesticide formulation (USEPA 2004).
- Impregnation materials in pesticides, paints, textile industry etc.
- Adhesives, binding agents.
- Cleaning/washing agents, softeners, surfactants, detergents
- Construction materials, fillers or sealing compounds in construction industry.
- Fuel additives.

- Process regulators.
- Reprographic agents.
- Printing inks.
- Lubricants and additives.
- Odour agents.

Similar uses are expected in Canada based on the use/activity codes reported by industry during the section 71 survey (as listed previously), and those reported to the DSL during the calendar year 1986 in Canada (see Appendix I). D5 is also used as an inert ingredient in pesticide formulations in Canada (PMRA 2005).

Since D5 belongs to a group of substances used in a variety of industrial applications and consumer products such as personal care, detergents, and fuel additives, etc., it may be released to the environment in a dispersive manner.

Releases, Fate, and Presence in the Environment

Releases

D5 is not naturally produced in the environment. Measured data concerning the environmental releases of this substance in Canada were not collected as part of the s. 71 survey. Its disperse use pattern suggests possible release to several compartments such as air, sewage treatment plants (STPs), and landfills. D5 may enter the environment through evaporation due to its high volatility. When released to STPs, its high log K_{ow} and K_{oc} values indicate partitioning of the compound to the active sludge that may then be applied to agricultural soil as fertilizer or landfilled. Disposal of consumer and industrial products containing D5 can also lead to the release of D5 to landfills. Agricultural, landfill, and STP releases may lead to groundwater, soil and sediment exposure.

Fate

D5 is expected to partition into air based on its high vapour pressure and Henry's law constant. The high log K_{ow} and log K_{oc} values indicate that D5 will also likely partition to soil and sediments. Indeed, the results of the Level III Fugacity modelling indicate that if this substance is released equally to the three major environmental compartments (air, water, and soil), it will partition into all compartments including air, water, soil, and sediments, with the latter two compartments being predominant (Table 2).

Table 2. Results of the Level III fugacity modelling for D5 (EPIWIN v3.12)

Receiving media	% in Air	% in Water	% in Soil	% in Sediment
Air (100%)	98.70	0.01	1.25	0.03
Water (100%)	3.42	21.40	0.04	75.10
Soil (100%)	6.84	0.01	93.10	0.02
Air, water, soil (33.3% each)	8.40	12.10	37.30	42.30

If D5 is released solely to air, a vapour pressure of 26.66 Pa and Henry's Law constant of 40530 Pa·m^3/mol indicate it will remain mainly in air, with only a very small amount partitioning into the other environmental compartments (< 2 %, Table 2).

If released to water, D5 is expected to adsorb to suspended solids and sediment based upon its log K_{oc} value. Although volatilization from water surfaces is also expected based upon the Henry's Law constant of this compound, its high adsorptivity to sediment may reduce the potential for volatilization. Thus, if water is a receiving medium, D5 is expected to remain mainly in water and partition into sediments and, to some extent, air as illustrated by the results of the Level III fugacity modelling (Table 2).

If released to soil, D5 is expected to rapidly volatilize from dry and moist soil to the air based on its vapour pressure (Table 1). The log K_{oc} value of D5 also indicates that this substance will adsorb to and be relatively immobile in soil, thus reducing its potential for volatilization. Thus, if released to soil, D5 will remain mainly in soil, with some partitioning into air, which is illustrated by the results of the Level III fugacity modelling (Table 2).

Presence in the Environment

No monitoring data relating to the presence of the substance in Canadian environmental media (air, water, soil, sediment) have yet been identified. Elsewhere, an environmental monitoring program of volatile methylated siloxanes initiated by Nordic countries found that D5 was present in all sampled media except soil. It was suggested that this substance was distributed in the Nordic environment mainly in urban areas and near or within STPs through its dispersive uses (Norden 2005). D5 was also detected in aquatic organisms in the Nordic countries (Norden 2005) and Germany (SEHSC 2005a). The Swedish National Screening Programme in 2004 indicated that D5 was present near or within STPs and in air, but was not found in surface water, sediment or fish muscles (Kaj et al. 2005).

In Air

D5 was found in air in the Nordic environment during 2003 - 2005. The average air concentration was in the range of 0.05 - 19 µg/cm^3 in urban areas, landfills, and other sampling sites, with the exception of samples taken inside STPs where the concentration was significantly higher (Norden 2005). Sweden also conducted indoor air measurements in children's bedrooms in 400 households. D5 was detected in 250 homes at concentrations of 0.5 – 79.4 µg/m^3 (personal communication, Norbert Schmidbauer, Norweigian Institute for Air Research 2005, as cited in Kaj et al. 2005).
In the US, D5 was detected in 29 indoor air samples (0.3-12.4 µg/m^3) from office buildings located in 7 cities and in three outdoor air samples (0.21-0.9 µg/m^3) (VOC data base 1990, as cited in USEPA 1992).

In Water

In Nordic countries, D5 was not detected in background or urban water samples (detection limit <0.1 µg/L). However, D5 was the predominant cyclosiloxane in samples of incoming water to STPs, with concentrations varying from < 5 µg/L to near 30 µg/L. Concentrations detected in outgoing STP effluents were all below 5 µg/L (Norden 2005). In the US, D5 has been qualitatively detected in drinking water systems (Lucas 1984, as cited in USEPA 1992).

In Soil
D5 was not detected (detection limit < 5 ng/g dry weight) in soil samples taken from two landfills from the Faroe Islands (Norden 2005).

In Sediments
D5 was the predominant cyclosiloxane detected in sediments in the Nordic environment, though variability was great for sediments collected close to urban areas. The measured concentrations generally ranged from <5 – 130 ng/g dw; however, one Danish sample was 2,000 ng/g dw (Norden 2005).

In STPs
D5 was found in all but one of the sludge samples analysed in the Nordic and Swedish screening programmes, and was found to be the predominant cyclosiloxane in STPs, making up 78 – 94% of the total amount in the samples in the Nordic programme. The concentration of D5 was reported to range from approximately 1,000 – 100,000 ng/g dw (averages of approximately 11,000 and 23,000 ng/g dw in the Swedish and Nordic programmes, respectively) (Norden 2005, Kaj et al. 2005).

In Aquatic Organisms
D5 was the predominant cyclosiloxane in fish livers and marine mammals in the Nordic screening programme. The substance was detected in both freshwater and marine fish from sampling sites in urban areas and near STPs in the range of < 5 – 84 ng/g ww, except for one sample of cod liver (9 livers pooled) collected at a location near a city centre in Norway that had an extremely high concentration of D5 (2,200 ng/g ww). The concentrations varied with species, gender, and age. D5 was also detected in the blubber of seals and pilot whales at concentrations ranging from <5 – 24 ng/g ww (Norden 2005). D5 was also detected in fish samples in Germany at concentrations ranged from 0.15– 2.6 mg/kg (SEHSC 2005a).

As concentrations of D5 in Nordic waters were <5 µg/L, except for STP influents, the detection of D5 in biota indicates that D5 has the potential to bioaccumulate (Norden 2005).

Rationale for P, B and iT status

Environmental Persistence

Once released in the environment, D5 appears to be relatively persistent in air, water, soil and sediments. The Level III Fugacity model indicates D5 will partition to air, where it is expected to be oxidized by gas-phase reaction with photochemically produced hydroxyl radicals. The empirical half-life for D5 in the gas-phase hydroxyl radical reaction is 6.9

days (Atkinson 1989) (Table 3a), indicating that this substance is persistent in air (half-life > 2 days). D5 is not expected to react, or react appreciably, with other photo oxidative species in the atmosphere, such as O_3 and NO_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 this substance. The model AOPWIN (v1.91) (Table 3b) also provides evidence supporting the persistence potential of this substance with a predicted atmospheric oxidation half-life of 7 days.

Table 3a. Empirical persistence data for D5

Medium	Fate Process	Degradation Value	Degradation Endpoint	Reference
Air	Photodegradation	6.9	half-life (days)	Atkinson, 1989

Table 3b. Modelled persistence data for D5

Medium	Fate Process	Degradation Value	Degradation Endpoint	Model
Air	atm-oxidation	7.15	half-life (days)	AOPWIN v1.91
Water/soil	Biodegradation	37.5	half-life (days)	BIOWIN v4.02, Ultimate survey
Water/soil	Biodegradation	0	Probability	BIOWIN v4.02, MITI Linear Probability
Water/soil	Biodegradation	0.0003	Probability	BIOWIN v4.02, MITI Non-linear Probability

Empirical persistence data for water, sediment and soil are not available for D5. Therefore, a weight-of-evidence approach (ESD 2006a) was applied by reading across data from similar chemicals and using the models shown in Table 3b.

D5 is structurally similar to, and a close analogue of, both D3 (hexamethylcyclo-trisiloxane, CAS No. 541-05-9) and D4 (octamethylcyclotetrasiloxane, CAS No. 556-67-2) such that it is expected that D5 will exhibit similar biodegradation potential as D3 and D4. Experimental data show no biodegradation of D3 over 28 days in a ready-biodegradation test (SEHSC 2005b), suggesting that it is persistent in water, sediment and soil. As well, no biodegradation of D4 was observed in an aerobic water/sediment system (Silicones Health Council 1991, as cited in HSDB 2006). These data are further supported by two of the models in Table 3b which indicate that the probability of biodegradation of D5 occurring in water or soils is effectively zero. Therefore, D5 is expected to be persistent in water, sediments and soils.

Therefore, based on the above data, D5 is categorized as persistent in air based on empirical data, and is also likely to be persistent in soil, sediment and water based on the weight-of-evidence from the behaviour of similar chemicals and modelled data.

The long-range transport potential (LRTP) of D5 from its point of release to air is estimated to be moderate according to the model prediction presented in Table 4. The TaPL3 model was used to estimate Characteristic Travel Distance (CTD), defined as the maximum distance traveled by 63% of a substance; or in other words, the distance that 37% of the substance may travel beyond. Beyer et al. (2000) have proposed CTD's of >2,000 km as representing high LRTP, 700-2,000 km as moderate, and <700 km as low. Based on the result shown in Table 4, D5 is expected to be able to reach areas far from its emission sources, but unlikely to be found in the Arctic.

Table 4. Model Predicted Characteristic Travel Distance (CTD) for D5

Characteristic Travel Distance	Model (Reference)
1,776 km	TaPL3 (CEMC 2003)

Based on the empirical data (Table 3a) it is concluded that D5 meets the persistence criteria for air (half-life > 2 days), and based on the modelled (Table 3b) and read-across data it is concluded that D5 meets the persistence criteria for soils, sediments and water (half-lives in soil and water ≥ 182 days; in sediments ≥365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada 2000).

Potential for Bioaccumulation

There is no empirical bioaccumulation data available for this substance. However, the empirical and modelled log K_{ow} values for D5 (Table 1) suggest that this substance has the potential to bioaccumulate in the environment (log $K_{ow} > 5$). The Silicones Environmental, Health, and Safety Council of North America reported that D5 has the potential to be taken up by fish as noted in a laboratory bioconcentration study where particles were not present to which D5 could bind and where D5 was not allowed to evaporate (SEHSC 2004). The Nordic environmental monitoring data also indicates that D5 has the potential to accumulate in fish livers and marine mammals (Norden 2005). Read-across data from structurally similar D4 (octamethylcyclotetrasiloxane, CAS No. 556-67-2) also indicate that D5 can bioconcentrate. The experimental BCF value for D4 was 12,400 L/kg in fathead minnows (*Pimephales promelas*).

The qualitative D5 data and read-across data from D4 are supported by the model results (Table 5). The Modified GOBAS BAF middle trophic level model produced a BAF of 34,670 L/kg wet weight, indicating that this substance has the potential to bioconcentrate and biomagnify in the environment. Two other models, the GOBAS BCF middle trophic level model and OASIS model, also provide evidence supporting the bioconcentration potential of this substance. The BCFWIN model prediction, however, was lower. The BCFWIN model may underestimate the BCF value for this type of substance (i.e., cyclosiloxanes), as suggested by D4 data where the BCFWIN modelled BCF (1,698 L/kg) was much lower than an experimentally derived BCF (12,400 L/kg).

Table 5. Modelled bioaccumulation data for D5

Test Organism	Endpoint	Value wet wt	Reference
Fish	BAF	34,670 L/kg	Gobas BAF T2MTL (Arnot and Gobas, 2003)
Fish	BCF	7,244 L/Kg	Gobas BCF T2LTL (Arnot and Gobas, 2003)
Fish	BCF	46,774 L/kg	OASIS 2005
Fish	BCF	1,995 L/kg	BCFWIN v2.15

The modelled bioaccumulation values do not take into account the metabolic potential of D5. However, an experimental BCF study with D4 indicates that metabolism is not likely significant (Fackler et al. 1995). Therefore, D5 is likewise not expected to exhibit significant metabolism based on the similarity in structure of D4 and D5.

The weight of evidence indicates that D5 meets the bioaccumulation criterion (BCF, BAF ≥ 5,000) as set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada 2000).

Ecological Effects

In the Aquatic Compartment

Empirical ecotoxicity data are not available for D5. However D4, a structurally similar substance and close analogue of D5, exhibits extremely high short- and long-term toxicity at concentrations above 0.0044 mg/L to fish and daphnia. Similar modes of action and toxicities to aquatic organisms are expected for D5 and D4 based on their similarity in structure and physical-chemical properties.

There is modelled data that suggest that D5 causes harm to aquatic organisms at relatively low concentrations (e.g., LC50 < 1 mg/L). Table 6 lists those predictions that were considered reliable and were used in the QSAR weight-of-evidence approach for aquatic toxicity (ESD 2006a). Modelled ecotoxicity data for D5 are of the same magnitude as for D4. The lowest values causing 50 % effect (EC50) daphnia and algae are 0.03 and 0.096 mg/L, respectively.

Table 6. Modelled aquatic toxicity values for D5

Organism	Endpoint	Duration	Concentration (mg/L)	Model
Daphnia	EC50	16 d	0.032	ECOSAR v.0.99h
Green Algae	EC50	96 h	0.096	ECOSAR v.0.99h

Both modelled predictions and the category approach indicate that D5 is very toxic to aquatic organisms, with extremely high short- and long-term toxicity within or close to its solubility limit (0.05 mg/L). These results indicate that D5 is highly hazardous to aquatic organisms (i.e. acute LC/EC50 < 1.0 mg/L).

In Other Media

No studies on the effects of this compound on non-aquatic, non-mammalian organisms were found.

Potential to Cause Ecological Harm

Evidence that a substance is highly persistent and bioaccumulative as defined in the *Persistence and Bioaccumulation Regulations* of CEPA 1999 (Government of Canada 2000), together with evidence of commercial activity, provides a significant indication of its potential to be entering the environment under conditions that may have harmful long term ecological effects (ESD 2006b). Substances that are persistent remain in the environment for a long time, increasing the potential magnitude and duration of exposure. Substances that have long half-lives in mobile media (air and water) and partition into these media in significant proportions have the potential to cause widespread contamination. Releases of small amounts of bioaccumulative substances may lead to high internal concentrations in exposed organisms. Highly bioaccumulative and persistent substances are of special concern, since they may biomagnify in food webs, resulting in very high internal exposures, especially for top predators. Evidence that a substance is both highly persistent and bioaccumulative, when taken together with other information (such as evidence of toxicity at relatively low concentrations, and evidence of uses and releases) may therefore be sufficient to indicate that the substance has the potential to cause ecological harm.

The volume of D5 imported into Canada in 2005 is very high, in the order of more than 1000 tonnes. Its large importation volumes and dispersive use, especially its wide application in household products, along with its volatile nature indicate a potential for releases into the Canadian environment. Once released in the environment, because of its resistance to degradation, D5 will remain in the air, water, sediment and soil for a long time, and may be transported relatively long distances. As it persists in the environment, it will likely bioaccumulate and may biomagnify in trophic food chains. It has also been demonstrated to have very high toxicity. This information suggests that D5 has the potential affect to cause ecological harm in Canada.

Uncertainties

Uncertainties exist in the conclusions reached in this document because most P, B, iT evaluations are based either on modelled data, or read-across from structurally similar substances.

Information on environmental concentrations or monitoring data in Canada and long term, low level exposure of D5 is also lacking. The most recent monitoring data in the United States are from the 1980's. The environmental monitoring data from Sweden (Kaj et al. 2005) and Nordic countries (Norden 2005) indicate that D5 concentrations in surface water, sediments, and soil did not reach levels that have been estimated to cause significant adverse effects to aquatic and soil-dwelling organisms. However, use volumes in Sweden and Nordic countries are relatively small compared to those in Canada and the United States.

Another uncertainty arises where D5 is also one of the components in CAS No. 69430-24-6 (dimethylcyclosiloxane), which had an imported quantity of more than 2,220 tonnes in commerce in Canada during the calendar year 1986. The total quantity of D5 being released into the Canadian environment should therefore be considered higher than that from CAS No. 541-02-6 alone. However, the amount of D5 released that is associated with use of dimethylcyclosiloxane can not be estimated as the proportion of D5 in dimethylcyclosiloxane is not known.

Regarding toxicity, based on the predicted partitioning behaviour of the substance, the significance of soil and sediments as important media of exposure is not well addressed by the effects data available for this substance.

Predicted concentrations, associated with the inherent toxicity to aquatic organisms, may be an additional source of uncertainty in some situations, e.g., where these concentrations exceed the solubility of the chemical in water (either experimental or predicted). Given that concentrations for both the toxicity and water solubility often vary considerably (up to several orders of magnitude), it is acknowledged that these uncertainties exist.

There is also uncertainty associated with basing the overall conclusion that D5 may be causing ecological harm solely on information relating to its persistence, bioaccumulation, relative toxicity and use pattern. Typically quantitative risk estimates (i.e., risk quotients or probabilistic analyses) are important lines of evidence when evaluating a substance's potential to cause environmental harm. However, when risks for persistent and bioaccumulative substances such as this cyclosiloxane are estimated using such quantitative methods, they are highly uncertain and are likely to be underestimated (ESD 2006b). Given that long term risks associated with persistent and bioaccumulative substances cannot at present be reliably predicted, quantitative risk estimates have limited relevance. Furthermore, since accumulations of such substances may be widespread and are difficult to reverse, a conservative response to uncertainty (that avoids under-estimation of risks) is justified.

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