

Screening Assessment for the Challenge

Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, reaction products with ammonia, octamethylcyclotetrasiloxane and silica

**Chemical Abstracts Service Registry Number
68937-51-9**

**Environment Canada
Health Canada**

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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 Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, reaction products with ammonia, octamethylcyclotetrasiloxane and silica, Chemical Abstracts Service Registry Number* 68937-51-9. This substance will be referred to by its derived acronym, OMSSA, in the screening assessment. This substance was identified as a high priority for screening assessment and included in the Challenge initiative under the Chemicals Management Plan because it was found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and is believed to be in commerce in Canada.

The substance OMSSA was not considered to be a high priority for assessment of potential risks to human health, based upon application of the simple exposure and hazard tools developed by Health Canada for categorization of substances on the *Domestic Substances List*.

OMSSA belongs to a class of chemicals described as Unknown or Variable Composition, Complex Reaction Products, or Biological Materials (UVCBs). This substance consists of the reaction products of 1,1,1-trimethyl-N-(trimethylsilyl)-silanamine (HMDS) (CAS RN 999-97-3), octamethylcyclotetrasiloxane (D4) (CAS RN 556-67-2) and synthetic amorphous silica (SAS) (CAS RN 7631-86-9). In the present assessment, this substance is represented by its major component (>90%), a surface-treated synthetic amorphous silica (SAS) component. It is noted that D4 is a reaction residual in OMSSA, present at up to 5% of the final composition of this substance. D4, as a discrete substance, has been assessed in 2008 under the Challenge initiative, and it was concluded that the substance posed an ecological risk.

OMSSA is used in Canada and elsewhere in industrial settings as a component in the production of silicone sealant and silicone rubber. No manufacture of OMSSA was reported in response to section 71 survey notices for the 2005 or 2006 calendar years. However, OMSSA imports to Canada were greater than 100 000 kg in 2005 and just under 100 000 kg in 2006.

Based on its physical and chemical properties and the expected lack of biodegradation of the SAS component of OMSSA, it is expected that OMSSA is persistent in air, water, soil and sediments. Based on the available information regarding uptake of the treated SAS, the representative component of OMSSA, through various routes of exposure, OMSSA does not appear to be bioaccumulative in organisms. Therefore, the substance meets the

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persistence criteria but does not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*.

There were no ecotoxicological data identified for OMSSA. Based on the experimental data, both surface-treated SAS and untreated SAS present low toxicity to aquatic organisms.

Available information regarding the ecological risk associated with the current estimated exposure concentrations of OMSSA in water suggests that OMSSA is unlikely to cause ecological harm in Canada. Therefore, considering the available information, it is concluded that OMSSA does not meet the criteria in paragraphs 64(a) and (b) of CEPA 1999, as it 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.

On the basis of the health effects information for an analogue of OMSSA, Silane, dichlorodimethyl-, reaction products with silica (CAS RN 68611-44-9), the possible health effects associated with exposure to OMSSA are mainly on the respiratory system. However, the potential for exposure of the general population to OMSSA from environmental media is expected to be negligible. Exposure to OMSSA from consumer products is not expected because it is only used in industrial settings. Since the exposure of the general population to OMSSA is expected to be low, the risk to human health is expected to be low. It is, therefore, concluded that OMSSA does not meet the criteria in paragraph 64(c) of CEPA 1999, as it 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.

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

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

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that have met the categorization criteria set out in the Act to determine whether these substances present or may present a risk to the environment or to human health.

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

- met all of the ecological categorization criteria, including persistence (P), bioaccumulation potential (B) and inherent toxicity to aquatic organisms (iT), and were believed to be in commerce in Canada; and/or
- met the categorization criteria for greatest potential for exposure (GPE) or 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 2006a), 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, Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, reaction products with ammonia, octamethylcyclotetrasiloxane and silica, had been identified as a high priority for assessment of ecological risk as it had been found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The Challenge for this substance was published in the *Canada Gazette* on December 26th, 2009 (Canada 2009a). A substance profile was released at the same time. The substance profile presented the technical information available prior to December 2005 that formed the basis for categorization of this substance. As a result of the Challenge, submissions of information pertaining to the properties and uses of the substance were received.

Although Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, reaction products with ammonia, octamethylcyclotetrasiloxane and silica was determined to be a high priority for assessment with respect to the environment, it did not meet the criteria for GPE or IPE and high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity.

Screening assessments focus on information critical to determining whether a substance meets the criteria as set out in section 64 of CEPA 1999. Screening assessments examine scientific information and develop conclusions by incorporating a weight-of-evidence approach and precaution[†].

This final 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 2010 for ecological and human health 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 final 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.

This final screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. The ecological portion of this assessment has undergone external written peer review/consultation. Additionally, the draft of this screening assessment was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Health Canada and Environment Canada. Approaches used in the screening assessments under the Challenge have been reviewed by an independent Challenge Advisory Panel.

The critical information and considerations upon which the final assessment is based are summarized below.

[†] A determination of whether one or more of the criteria of section 64 are met is based upon an assessment of potential risks to the environment and/or to human health associated with exposures in the general environment. For humans, this includes, but is not limited to, exposures from ambient and indoor air, drinking water, foodstuffs, and the use of consumer products. A conclusion under CEPA 1999 on the substances in the Chemicals Management Plan (CMP) Challenge Batches 1-12 is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the Controlled Products Regulations, which is part of regulatory framework for the Workplace Hazardous Materials Information System [WHMIS] for products intended for workplace use. Similarly, a conclusion based on the criteria contained in section 64 of CEPA 1999 does not preclude actions being taken under other sections of CEPA or other Acts.

Substance Identity

Substance Name

For the purposes of this document, this substance will be referred to as OMSSA, derived from the domestic substances list (DSL) name, Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, reaction products with ammonia, octamethylcyclotetrasiloxane and silica. The substance under assessment consists of the reaction products under high temperatures (i.e. ~250°C) of 1,1,1-trimethyl-N-(trimethylsilyl)-silanamine (HMDS), Chemical Abstracts Service Registry Number (CAS RN) 999-97-3; octamethylcyclotetrasiloxane (D4), CAS RN 556-67-2; and synthetic amorphous silica (SAS), CAS RN 7631-86-9, with a primary particle size average of 10 nm (range from 4 to 12 nm) (Environment Canada 2010a).

The reactant HMDS (CAS RN 999-97-3) may represent a residual component in OMSSA. HMDS is present at ~15% during the manufacturing of OMSSA prior to the heat activated reaction process that results in surface treated silica >90% in the final OMSSA substance (Environment Canada 2010a). However, HMDS is known to undergo rapid hydrolysis in the presence of water and is expected to produce ammonia (CAS RN 7664-41-7) and trimethylsilanol (CAS RN 1066-40-6). The final treated silica in OMSSA is generally cleaned using a solvent to remove residual ammonia, and thus, these components will likely make up a very small fraction (<1%) if any of the final OMSSA substance. The D4 reactant will react with surface silanols to form linear polydimethylsiloxyl groups on the surface of the SAS particles in OMSSA. However, as D4 is more resistant to hydrolysis, it remains as a residual in OMSSA at a concentration of 1–5%. It is noted that D4 has been previously assessed under the Challenge and it was concluded that it posed an ecological risk (Environment Canada and Health Canada 2008).

As shown in Table 1, surface-treated SAS was selected as representative component for OMSSA in this screening assessment.

Table 1. Substance identity for OMSSA

Chemical Abstracts Service Registry Number (CAS RN)	68937-51-9
DSL name	Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, reaction products with ammonia, octamethylcyclotetrasiloxane and silica
National Chemical Inventories (NCI) names¹	<i>Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, reaction products with ammonia, octamethylcyclotetrasiloxane and silica (TSCA, EINECS, AICS, PICCS, ASIA-PAC, NZIoC); 1,1,1-Trimethyl-N-(trimethylsilyl)silanamine reaction products with ammonia, octamethylcyclotetrasiloxane and silica (ECL)</i>
Other names	<i>Octamethylcyclotetrasiloxane, silica, ammonia, and</i>

	<i>hexamethyldisilazane reaction product; Silicone dioxide; Treated silica</i>
Chemical group (DSL Stream)	Organics UVCB ²
Major chemical class or use	Silicones
Major chemical sub-class	Surface treated synthetic amorphous silica
Chemical formula	O ₂ Si ⁴
Representative chemical structure used to run the estimation model²	No structure available for particulate
Representative SMILES used to run the estimation model³	No SMILES available for particulate
Molecular mass	210 ⁸ – 10 ⁹ g/mol (particulate) ⁴

National Chemical Inventories (NCI). 2009: 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); NZIoC (New Zealand Inventory of Chemicals); PICCS (Philippine Inventory of Chemicals and Chemical Substances); and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

- ² This substance is a UVCB (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products, or **B**iological Materials); i.e., it is not a discrete chemical and thus may be characterized by a variety of structures. To assist with modelling, the structure and corresponding SMILES presented here were chosen to represent the substance.
- ³ Simplified Molecular Input Line Entry System
- ⁴ Elemental composition of amorphous silicon dioxide which exists as a particle and may contain various surface structures not reflected in this elemental composition and molecular weight, including free silanol, hydrogen-bonded silanol, trimethylsilyl, siloxane and organosiloxane groups, among others.

Silica is a silicon-oxygen tetrahedral unit where a silicon atom is central within four oxygen atoms that are shared with adjacent silicon atoms. Various physical forms of silica are caused by differences in the spatial relationships of the tetrahedral that determine its physical characteristics. For example, amorphous silica has an irregular tetrahedral pattern whereas crystalline silica is polymorphic where each variety has a characteristic regular three-dimensional arrangement of the tetrahedral (Heppleston 1969).

There are two main manufacturing methods of SAS. The methods are the wet method (i.e. silica gel or colloidal silica; precipitated silica) and the thermal method (i.e. pyrogenic or fumed silica). The manufacturing process for pyrogenic SAS is based on the hydrolysis of volatile silanes, especially silicon tetrachloride (SiCl₄), in the flame of an oxygen-hydrogen burner (Auner and Weis 1996). Silicon tetrachloride is continuously vaporized, mixed with dry air and then with hydrogen, fed to the reactor and hydrolyzed. Hydrolysis is followed by the growth (nucleation, condensation, coagulation) and agglomeration of pyrogenic SAS particles. The physico-chemical properties of the pyrogenic silica can be controlled by varying the process parameters such as feedstock, flame composition and flame temperature. Various wet methods of manufacturing SAS

exist including precipitate, gel and colloid methods. The precipitate and gel methods involve neutralization of an aqueous solution of an alkali metal silicate (e.g. water glass) with (sulphuric) acid. Only the colloid method results in the production of stabilized discrete silica particles; however, this method represents only a minor fraction of the total production of SAS globally (ECETOC 2006).

As described in ECETOC (2006), a significant proportion of the global production of SAS is rendered hydrophobic to improve its affinity for and dispersion in non-polar materials (e.g. polymers, resins). This is generally done by surface modification using organo-silicon compounds. Surface modified (after-treated) SAS can be obtained either by physical or chemical reaction. The most common Si-organic compounds used for the treatment are hexamethyldisilazane (HMDS; CAS RN 999-97-3), dimethyldichlorosilane (CAS RN 75-78-5) and polydimethylsiloxanes (e.g. CAS RN 9016-00-6). The first compound forms mono-functional moieties upon hydrolysis, whereas the latter two give rise to bi-functional units, as shown below.

- Hexamethyldisilazane $\rightarrow \equiv\text{Si}-\text{O}-\text{Si}(\text{CH}_3)_3$
- Dimethyldichlorosilane $\rightarrow \equiv\text{Si}-\text{O}-[\text{Si}(\text{CH}_3)_2-\text{O}]_{x=1-3}$
- Polydimethylsiloxane $\rightarrow \equiv\text{Si}-\text{O}-[\text{Si}(\text{CH}_3)_2-\text{O}]_{x=3-6(10)}$

The surface treatment does not change the solid properties such as particle size. However, surface treatment does alter physico-chemical properties, e.g. hydrophobicity, reduced moisture uptake depending on the type and amount of surface treatment (ECETOC 2006, Langer et al. 1958).

Specifically, the substitution of structural silanol groups by methylsilyl groups through reactions with appropriate organosilicon compounds substantially moderates the energy of adsorption of polar adsorbates (one can observe a decrease in values of adsorption and heat of adsorption), and the silica surface acquires stable hydrophobic properties. At the same time, such a chemical modification of surface prevents the agglomeration of disperse silica particles and facilitates their more uniform distribution in hydrocarbons and polymeric media (Schwarz et al. 2004).

The treated SAS, representative of OMSSA in this screening assessment, has a primary particle size average of 10 nm (range from 4 to 12 nm) (Environment Canada 2010a). In the production of pyrogenic SAS, molten spheres of primary particles may collide and irreversibly fuse together to form three-dimensional branched aggregates that may be several times larger than the primary particles (Villota and Hawkes 1986). Similarly, primary particles of precipitated SAS form larger aggregates in solution. Furthermore, these aggregates may agglomerate through chemical interaction of the surface silanol groups forming larger clusters[‡] (ECETOC 2006). Finally, the process of surface

[‡] Confusion exists in the use of terms “aggregation” and “agglomeration” in the scientific literature. Some publications refer to aggregates as the larger more loosely assembled particles (Walker 1998). For the purpose of this document however, the convention used by the International Organization for Standardization (ISO) will be followed, using these definitions:

Agglomerate: A group of particles held together by relatively weak forces, including Van der Waals forces, electrostatic forces and surface tension.

treatment may also contribute to further agglomeration of aggregates, resulting in particle sizes of up to 1000 times the primary particle size (i.e. 10 µm) for the treated particles in OMSSA (Environment Canada 2010a). Thus, the treated silica in OMSSA may be defined by a particulate size range from 10 nm to 10 µm with a hydrophobic surface due to silylation process resulting in nonpolar organosilane groups and elevated temperatures used in the treatment process resulting in more siloxane groups on the surface, compared to those silicas with a fully hydroxylated surface.

This screening assessment addresses the entire formulation including the size fraction which may include a nano-size fraction. Given the current level of understanding, it does not make a distinction between the fate, exposure and effects of the nano-scale particles from those of larger particles or aggregates. The Government of Canada is currently in the process of examining methods to assess risks posed by nano-scale materials in Canada, and is also in the process of developing a regulatory framework for nanomaterials. As such, any potential risks posed by OMSSA at the nanoscale may be subject to separate review at a future date.

Finally, although various levels of treatment may be used in the production of OMSSA, the information received under the Challenge (Environment Canada 2010a) indicated that the level of treatment for OMSSA was 3.5–4.5 weight (wt) %, likely measured using the Brunauer Emmet Teller (BET) C Test (Brunauer et al. 1938). Additional calculated range of 1–3 wt% was subsequently provided (Environment Canada 2010a), however the accuracy of this result could not be determined with certainty by the authors. Therefore, the higher range of 3.5-4.5 wt% is considered the more accurate description of the treatment level of OMSSA in the present assessment. The surface treatment results in trimethylsilyl and dimethylsiloxyl surface groups. These characteristics of SAS in OMSSA are imparted by both the mode of manufacture of the untreated silica and the treatment process.

Physical and Chemical Properties

Table 2a contains experimental physical and chemical properties relevant to the treated SAS component of OMSSA that are important to its environmental fate. Key studies from which experimental data were reported for some of these properties were critically reviewed for validity.

Reviewing the pertinent literature on surface-treated silica revealed several forms of treated silica that vary by different surface chemistry types and degrees of coverage. Analogues for OMSSA with measured data for physical-chemical properties used in this assessment included common treated silica substances such as CAS RN 68611-44-9, CAS RN 67762-90-7 and CAS RN 68909-20-6 as well as the untreated SAS (CAS-RN

Aggregate: A heterogeneous particle in which the various components are not easily broken apart.

Hence while an aggregate may be considered to be permanent, agglomerates may break up under certain conditions (Aitken et al. 2004).

7631-86-9) (see Table 2b for analogue comparison table) for the characterisation of the ecological risk as described below, and treated silica CAS RN 68611-44-9 for the characterisation of risk to the human health.

Solubility of a substance influences its mobility and bioavailability in the environment. Therefore, it is one of key parameters in the characterisation of the chemical's fate when it is released into the environment. The use of a range of analogues for OMSSA is of particular importance for the characterisation of ecological risk in the aquatic compartment. The level of treatment of OMSSA is uncertain and may result in a range of physical-chemical properties including rendering the substance more or less hydrophobic. This in turn may impact the bioavailability of OMSSA in the aquatic compartment. Therefore, the use of analogues that captures this range allows for a more complete characterisation of the ecological effects, understanding that the physical-chemical properties of the analogues may represent a broader range of characteristics than those specific to OMSSA.

Modelled values were not available to provide physical-chemical property estimates for the treated silica component of OMSSA as this component could not be represented by a chemical structure within the domain of any available models.

Finally, as the representative component of OMSSA, the treated SAS, exists as a particulate and as such many of the traditional physical-chemical parameters used to predict environmental fate and behaviour may not be applicable. The properties traditionally used in chemical risk assessment that are not generally applicable to particulates which may be governed more by their physical manifestation include boiling point, $\log K_{ow}$, $\log K_{oc}$, vapour pressure and Henry's Law Constant. However, due to the potential presence of volatile organo-silane components vapour pressure was still considered as a potentially significant property for potentially predicting the fate and behaviour of OMSSA (see Table 2a).

Table 2a. Physical-chemical properties for surface treated SAS component (>90% of OMSSA)

CAS RN	Type	Value	Temperature (°C)	Reference
Melting point (°C)				
7631-86-9	Experimental	1700– 1710		ESIS c1995–2009
68611-44-9		1700		MSDS 2010
67762-90-7		1700		MSDS 2008
68909-20-6		1700		MSDS 2007
Boiling point (°C)				
7631-86-9	Experimental	2230		ESIS c1995–2009
67762-90-7		2230		MSDS 2008
68909-20-6		2300		MSDS 2007
Density (kg/m³)				
7631-86-9	Experimental	2200	20	OECD 2004
7631-86-9		50–350 ¹		ESIS c1995–2009
68611-44-9		2000	20	ESIS c1995–2009
68611-44-9		30-50 ¹		ESIS c1995–2009
67762-90-7		2200	20	MSDS 2008
67762-90-7		30–100 ¹		MSDS 2008
68909-20-6		2200	20	MSDS 2007
68909-20-6		100–300 ¹		MSDS 2007
Vapour pressure (neutral form) (Pa)				
7631-86-9	Experimental	0		CDC 2005
68611-44-9		<0.001		US EPA 2009
Water solubility (mg/L)				
7631-86-9	Experimental	15–68 ²		OECD 2004
7631-86-9		120		ECETOC 2006
68611-44-9		<0.001		IUCLID Data Set 2002
Surface pK_a (acid dissociation constant, dimensionless)				
7631-86-9	Experimental	7.1 ⁷		Environment Canada 2010a
Primary particulate diameter (nm)				
68937-51-9 (OMSSA) ⁵	Experimental	4-12 (10) ⁶		Environment Canada 2010a
7631-86-9 ³		5–50		ECETOC 2006
7631-86-9 ⁴		5–100		ECETOC 2006

¹Bulk density;²Measured at pH 5.5-6.6;³Manufactured using a thermal method (i.e. pyrogenic);⁴Manufactured using a wet method (i.e. precipitated);⁵Unagglomerated silica component only;⁶Average particle size;⁷Surface Silanols.

Table 2b. SAS Component Analogue Comparison Table

CAS RN	Name	Surface Chemistry	Characteristics
OMSSA			
68937-51-9	Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, reaction products with ammonia, octamethylcyclotetraasiloxane and silica	Silanol groups, hydrogen-bonded silanol groups, dimethylsilyl, trimethylsilyl, siloxane groups, among others	Occurs in various size ranges (primary particle size 4–12 nm; aggregate/agglomerate size > 10nm and up to 10 µm)
Analogues			
68611-44-9	Silane, dichlorodimethyl-, reaction products with silica	Silanol groups, hydrogen-bonded silanol groups, dimethylsilyl and siloxane groups, among others	Occurs in various size ranges; contains all groups except trimethylsilyl group
67762-90-7	Siloxanes and silicones, di-me, reaction products with silica	Silanol groups, hydrogen-bonded silanol groups, dimethylsilyl and siloxane groups, among others	Various size ranges; contains all groups with except trimethylsilyl group
68909-20-6	Silanamine, 1,1,1-trimethyl-N-(trimethylsilyl)-, hydrolysis products with silica	Silanol groups, hydrogen-bonded silanol groups, trimethylsilyl and siloxane groups, among others	Occurs in various size ranges; contains all groups except dimethylsilyl group
112945-52-5	Pyrogenic SAS (untreated)	Silanol groups, hydrogen-bonded silanol groups and siloxane groups, among others	Occurs in various size ranges (primary particle size 5–50 nm, aggregate size 100 nm–1000 nm, agglomerate 100–250 µm)
112926-00-8	Precipitated SAS (untreated)	Silanol groups, hydrogen-bonded silanol groups and siloxane groups, among others	Occurs in various size ranges (primary particle size 5–100 nm, aggregate size 100 nm –1000 nm, agglomerate 100–250 µm)
7631-86-9	Untreated SAS	Silanol groups, hydrogen-bonded silanol groups and siloxane groups, among others	Occurs in various size ranges, may encompass several polymorphs of silica

Sources

Silicon (Si) is the second most abundant chemical element after oxygen and makes up 28-59% of the earth's crust. Silicon may be present as the oxide (silica, SiO₂) in crystalline silica in rocks, sands and soils, and as biogenic amorphous silica in diatomite and silica fibres or non-biogenic silica in vitreous silica (OECD 2004, ECETOC 2006). However, only the dissolved form of silica is bioavailable. It has been estimated that on a global scale, the level of anthropogenic SAS represents up to 2.4% of the dissolved silica naturally present in the aquatic environment (ECETOC 2006).

Recent information on manufacture and import quantities, as well as uses in Canada, was collected through industry surveys conducted for the years 2005 and 2006 under a *Canada Gazette* notices issued pursuant to section 71 of CEPA 1999 (Canada 2006b, 2009b). No manufacture of OMSSA was reported in response to section 71 survey notices for the 2005 or 2006 calendar years. However, there were imports greater than 100 000 kg in 2005 and just under 100 000 kg in 2006 (Environment Canada 2010a). There were fewer than four notifiers in 2005 and one in 2006. Three stakeholders identified themselves as having an interest in this substance in 2005 and two identified themselves as having an interest in this substance in 2006.

In the past, the quantity reported to be manufactured, imported or in commerce in Canada during the 1984–1986 calendar years was 100 kg. The number of notifiers for the 1984–1986 calendar years was fewer than four. Thus, the import quantities of OMSSA to Canada have increased from the 1980s to 2006.

Uses

Information on the uses for the 2005 and 2006 calendar years was gathered in response to the CEPA section 71 notices (Canada 2006b, 2009b). OMSSA was reported to be used as filler in adhesives and sealants. In addition, the DSL use code identified for OMSSA for the years 1984-1986 was Formulation Component.

According to information submitted as a result of the section 71 survey under CEPA 1999, OMSSA is used in Canada in industrial settings as a component in the production of silicone sealant and silicone rubber (Environment Canada 2010a).

In Canada, OMSSA is not listed in the Drug Products Database (DPD 2010), the Therapeutic Products Directorate's internal Non-Medicinal Ingredients Database, the Natural Health Products Ingredients Database or the Licensed Natural Health Products Database as a medicinal ingredient or non-medicinal ingredient present in pharmaceuticals for human or veterinary use or natural health products (DPD 2010, NHPID 2010, LNHPD 2010, 2010 personal communication from Therapeutic Products Directorate & Veterinary Drugs Directorate to Risk Management Bureau, Health Canada, unreferenced).

OMSSA is not listed as an approved food additive under Division 16 of the Food and Drug Regulations (Canada 1978). It has not been identified as being used/present in formulations of incidental additives or used in food packaging materials (2010 personal communication from Health Canada Food Directorate to Risk Management Bureau, Health Canada, not referenced).

Releases to the Environment

A method has been developed by Environment Canada to estimate a substance's losses during different stages of its life cycle, including its fate within a finished product or article (Environment Canada 2008). This method, referred to as Mass Flow, consists of a life cycle analysis and a spreadsheet tool (Mass Flow Tool or MFT) that integrates information on the manufacturing, importation and use data available for the substance. Starting with an identified mass of the substance, each life cycle stage is subsequently evaluated until no mass remains. Relevant factors are considered, uncertainties recognized and assumptions may be made during each stage, depending on information available. The estimated losses represent the complete mass balance of the substance over the life cycle of the substance and include releases to wastewater and other receiving compartments (land, air), chemical transformation, transfer to recycling activities and transfer to waste disposal sites (landfill, incineration). However, unless specific information on the rate or potential for release of the substance from landfills and incinerators is available, the method does not quantitatively account for releases to the environment from disposal. Ultimately, the estimated losses provide a first tier in the exposure analysis of a substance and help to estimate environmental releases and focus exposure characterization in the assessment.

In general, releases of a substance to the environment depend upon various losses from its manufacture, industrial use, and/or consumer/commercial use. These losses can be grouped into seven types: (1) discharge to wastewater; (2) emission to air; (3) loss to land; (4) chemical transformation; (5) disposal to landfill; (6) loss to incineration; and (7) disposal through recycling (i.e., recycling is deemed a loss and not considered further). They are estimated using regulatory survey data, industry data and data published by different organizations. The discharge to wastewater refers to raw wastewater prior to any treatment, whether it be on-site industrial wastewater treatment or off-site municipal wastewater treatment. In a similar manner, the loss via chemical transformation refers to changes in a substance's identity that may occur within the manufacture, industrial use, and consumer/commercial use stages, but excludes those during waste management operations such as incineration and wastewater treatment. The loss to land includes unintentional transfer or leakage to soil or paved/unpaved surfaces during the substance's use and service life (e.g., from the use of agricultural machinery or automobiles). The loss to land, however, does not include transfers subsequent to a substance's use and service life (e.g., land application of biosolids and atmospheric deposition).

The losses estimated for OMSSA over its lifecycle (based on conservative assumptions) are presented in Table 3 (Environment Canada 2010b). OMSSA is not manufactured in

Canada so estimated losses are based on the import quantities reported for the calendar year 2006 (i.e. just under 100,000 kg).

Table 3. Estimated losses of OMSSA during its lifecycle

Type of Loss	Proportion (%)	Pertinent lifecycle stages
Wastewater	3.9	industrial and commercial use
Air emission	1.3	industrial use
Land	-	-
Chemical transformation	-	-
Landfill	26.1	Industrial and commercial use
Incineration	-	-
Recycling	-	-
Export	68.7	-

OMSSA is estimated to be released to wastewater systems at 3.9% during the industrial and consumer/commercial use stages and air at 1.3% during the industrial use stage only. Assumptions made include losses during container handling, re-formulation operations, and use of products containing the substance (i.e. sealants). A large amount (68.7 %) of OMSSA imported into Canada is exported out of Canada, thus a smaller amount (26.1%) of the substance is estimated to end up in landfills from any associated industrial and consumer uses.

The above loss estimates indicate that OMSSA has potential for releases to the environment. In general, wastewater is a common source for releases of a substance to water and soil through wastewater treatment facilities and the subsequent waste management of sludge. In addition, emissions to air can result in atmospheric deposition to soil and water. Finally, if leachate is not collected and treated, some landfills may have the potential to leach substances into groundwater, or there may be releases of some of the reaction residuals in the substances to the atmosphere. However, as the products containing OMSSA (i.e. rubbers and sealants) would fully encapsulate the substance, there would be minimal, if any, releases to air during use and end-of-life disposal.

Environmental Fate

Based on its physical and chemical properties (Table 2a) OMSSA is expected to predominantly reside in soil and/or sediment, depending on the compartment of release.

When released to air, the SAS component of OMSSA is expected to be deposited to surface waters and soils (based on its tendency to aggregate and agglomerate to several times the primary particle size, its high density and negligible vapour pressure estimates). However, some fine particulate matter in Canada is known to originate from industrial regions of other countries, where the smaller particles are most likely to be transported larger distances (Environment Canada and Health Canada 2000). The low to negligible analogue vapour pressure (≤ 0.001 Pa) for the surface-treated SAS component of OMSSA

is consistent with the fact that it is a large complex molecule (Kirk-Othmer c2010a). Surface treated SAS particles are not expected to volatilize at environmentally realistic temperatures.

The particulate character of the surface-treated SAS component of OMSSA should have a key influence on its fate in the environment. Its particle size (0.01–10 μm) and density (2000–2200 kg/m^3 or 2 – 2.2 times that of water), together with its chemical stability and low aqueous solubility (<0.001 mg/L), indicate that it will partition by gravity to sediments if released to surface waters, and will tend to remain in soils if released to terrestrial environments. However, a small amount of the treated SAS will dissolve to form silicic acid which is expected to remain in solution.

The pK_a of the surface silanols on untreated SAS is around 7.1, Therefore, at pH 6 less than 10% of the surface silanol groups would be dissociated, whereas at pH 9, almost all the surface silanols groups would be dissociated and the untreated silica particle would have a strong negative charge. Negatively charged silica particles may bind cations and remain suspended in aqueous media or may associate and bind with positively charged soil or sediments in the environment. The treated SAS component of OMSSA may also contain surface dimethylsilanol groups that may ionize at a higher pH (e.g. pK_a of trimethylsilanol = 11) than the surface silanols (Tripp and Hair 1995). Nevertheless, at environmentally relevant pH, the treated silica particle would carry a negative charge which would facilitate its suspension in aqueous solution and association with cationic sediments, soil mineral or organic materials.

SAS particles are known to dissolve in aqueous media to form orthosilicic acid [$\text{Si}(\text{OH})_4$] (CAS RN 10193-36-9) as shown in equation (1) along with oligomeric forms of silicic acid (Kirk-Othmer c2010a):



At environmentally relevant pH (6-9), the solubility of SAS is independent of pH (Kirk-Othmer c2010a). Orthosilicic acid has primary pK_a values of >9 (i.e. $\text{pK}_{a1} = 9.9$, $\text{pK}_{a2} = 11.8$, $\text{pK}_{a3} = 12$, $\text{pK}_{a4} = 12$) (Lide 2007–2008), and thus, will be neutral for the most part at environmentally relevant pH (i.e. at pH 9 <15% will be ionized). At pH >9, the solubility of SAS greatly increases due to the ionization of silicic acid. Thus, at environmentally relevant pH, the solubility of SAS will be limited and other parameters such as SAS particle size and ambient temperature/pressure may also influence the solubility. Particles with a diameter less than 5 nm have a progressively greater solubility than do particles of continually increasing diameters. In addition, the aqueous solubility of SAS increases with increasing temperature and pressure (Kirk-Othmer c2010a).

It is expected that the surface treatment may render the surface more hydrophobic than untreated pyrogenic SAS which may have the effect of reducing the solubility of the SAS component in OMSSA in water by reducing surface wetting. However, due to the presence of organic substances such as surfactants, salts, acids and alkalis in the environment, surface-treated silica may wet and then adsorb onto soils or sediments in

the environment (ECETOC 2006). Nevertheless, the flocculation of particles and removal from the water column via sedimentation is more likely as the hydrophobicity of SAS increases (Barthel 1995).

Persistence and Bioaccumulation Potential

Environmental Persistence

No empirical or modelled data were available to provide quantitative estimates of environmental persistence of the treated SAS particles in OMSSA in any environmental media including water.

The surface treated SAS component of OMSSA is present as either coarser agglomerates $\leq 10 \mu\text{m}$ or finer aggregates ($\ll 10 \mu\text{m}$ but $> 10 \text{nm}$) and few, if any, discrete primary particles (10 nm) would exist (Environment Canada 2010a) (see Table 4).

Table 4. Typical particle size distributions for two polymorphs of SAS (ECETOC 2006)

	<i>Pyrogenic SAS</i>	<i>Precipitated SAS</i>
Primary Particle	5-50 nm	5–100 nm
Aggregate	100-1000 nm	100–1000 nm
Agglomerate	1-250 μm	1–250 μm

The primary particles are linked together as aggregates via siloxane bonds formed in the pyrolysis / dehydration process in manufacturing the silica particles, however larger agglomerates may form by hydrogen bonding or van der Waals interactions that are considerably weaker than siloxane bonds (Kirk-Othmer c2010b). The hydrogen bonds between agglomerates may fall apart in the aqueous environment and the siloxane bond holding together the primary particles may be susceptible to hydrolysis in aqueous media. The aggregates may thus break down in aqueous environments; however, break-down will likely occur at a much slower rate than the break-down of the hydrogen bonds. Ding et al. (2010) demonstrated that at a sufficiently high energy input into aqueous dispersions both hydrophobic and hydrophilic agglomerates were broken into aggregates; however even at the highest energy input (i.e. high shear mixer for 4 hours at 8000 rpm), these aggregates could not be broken into single primary particles.

Another potentially important process that may occur is dissolution of the SiO_2 lattice of SAS and the formation of orthosilicic $[\text{Si}(\text{OH})_4]$ acid (equation (1)) along with oligomeric forms (as described previously in the Environmental Fate section), which may lead to the transformation of a fraction of the silica particles to soluble inorganic acids. However, the hydrophobic nature of treated SAS in OMSSA may inhibit the dissolution observed in untreated SAS. Thus, conversion of treated SAS to silicic acid may occur minimally in aqueous environments and the majority of the surface-treated SAS component of OMSSA is expected to persist as aggregated or agglomerated particulate matter in the environment.

Given its physical properties and the lack of expected biodegradation of the treated SAS component of OMSSA, it is expected that OMSSA remains persistent in soil, sediments, and air, as well as water.

The long range atmospheric travel potential of the treated SAS component of OMSSA could not be modelled based on this component's unique particulate properties. It has been determined that there is substantial contribution (50% or more for fine particles) from long-range transport events from industrial regions of the United States to ambient levels of particulate matter, consistent with the fact that it is the smaller particles that are most likely to be transported long distances (Environment Canada and Health Canada 2000). Given that the treated SAS component of OMSSA tends to aggregate/agglomerate to PM_{>0.1-10} (see Table 2b), it is likely that this component does not have a high potential for long range atmospheric transport, rather it may be deposited closer to the emission sources.

Based on the information presented data OMSSA meets the persistence criteria in water, soil, sediment and air (half-lives in soil and water ≥ 182 days; half-life in sediment ≥ 365 days; half-life in air ≥ 2 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

Experimental log K_{ow} values for analogues of the treated SAS component of OMSSA (other surface-treated and untreated SASs – see Table 2b) were not applicable to particulate matter (NOTOX 2002, IUCLID Data Set 2002, OECD 2004).

No experimental data on the whole body accumulation of surface-treated or untreated SAS are available for aquatic or terrestrial species. Moreover, the available quantitative structure-activity relationship (QSAR) models are not suitable for predicting the bioaccumulation potential of OMSSA. As well, bioconcentration factor (BCF) and bioaccumulation factor (BAF) values may not be the most appropriate metrics to evaluate the bioaccumulation potential of metals or other inorganic substances (i.e. O₂Si), as BCFs and BAFs are considered of little usefulness in predicting element hazards (Schlekat et al. 2007). Some elements naturally may be highly accumulated from the surrounding medium because of their nutritional essentiality. The importance of dissolved silica in the development, physiology and skeletal structure of algae, plants and animals is acknowledged (Markert 1994, Martin 2007): dissolved silica (i.e. monomeric or oligomeric silicic acid) can be actively assimilated by freshwater and marine organisms (e.g. diatoms, radiolarians, and sponges). These are natural processes that are, in most cases, related to structural function (OECD 2004, Exley 1998). For example, diatoms, which are probably the most important organisms capable of processing silicic acid in terms of their diversity, ubiquity and biomass, assimilate silicic acid to form a silica frustule surrounding their cell wall (Exley 1998).

The uptake of silica is a natural process that occurs in nearly all plants and has important impacts on their function and productivity (OECD 2004, Sparks et al. 2010). Silica, in the form of silicic acid, is taken up by the roots and is translocated throughout the plant in the form of monomeric silicic acid. In the tissues, silica can be found in the form of amorphous bodies known as phytoliths, but other forms have been identified as well (Sparks et al. 2010). Amounts of silica in plant tissues varies from approximately 0.1 to 10% dry weight, depending on the species. There is extensive evidence indicating a link between silica availability and increased crop yields in rice, wheat and maize (Sparks et al. 2010). In addition, silica content in plant tissue may provide structural support as well as resistance to pathogens, herbivory and translocation of water and salts (Sparks et al. 2010, Exley 1998). Therefore, the uptake of amorphous silica by plants is considered a natural process in the environment.

In summary, the available evidence indicates that OMSSA is expected to have low accumulation potential. Dissolved silica (i.e. silicic acid) can be actively assimilated by terrestrial plants and aquatic species through natural processes that are, in most cases, related to structural function. Based on the available information regarding uptake of OMSSA's major representative component through various routes of exposure, OMSSA does not appear to be bioaccumulative in water-, air- or soil-dwelling organisms and does not meet the bioaccumulation criterion ($BAF \geq 5000$) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

A - In the Aquatic Compartment

The toxicity of OMSSA to aquatic organisms is described by using analogues of the surface treated SAS component of the substance. Specifically, a range of SAS analogs is used for the major component of OMSSA, the surface treated SAS, to capture the potential variability of physico- chemical properties, and in particular the degree of hydrophobicity, that may result from variation in the level of surface-treatment of the substance. Empirical data for aquatic toxicity of the surface-treated SAS (CAS RN 68611-44-9) and untreated SAS (CAS RN 112945-52-5 and 7631-86-9) are presented in Table 5.

Table 5. Empirical aquatic toxicity data for the representative components and analogues of OMSSA

Representative Components (CAS RN)	Particle Size (nm)	Test Organism	Test Type	Endpoint	Value (mg/L)	Reference
Surface treated SAS (68611-44-9)	N/A ⁴	<i>Daphnia magna</i>	Acute (24 hrs)	EL ₅₀ ¹	>10,000	NOTOX 2002, IUCLID Data Set 2002
	N/A	Zebra fish (<i>Brachydanio rerio</i>)	Acute (96 hrs)	LL ₅₀ ²	>10,000	
	N/A	Algae (<i>Scenedesmus subspicatus</i>)	Chronic (72 hrs)	EL ₅₀	>10,000	
Untreated pyrogenic SAS (112945-52-5)	N/A	Zebra fish (<i>Brachydanio rerio</i>)	Acute (96 hrs)	LL ₀	10,000	OECD 2004
		<i>Daphnia magna</i>	Acute (24 hrs)	EL ₅₀	>10,000	
				EL ₀	1000	
Untreated SAS (7631-86-9)	<62000 ⁵	Algae (<i>Pseudokirchneriella subcapitata</i>)	Chronic (72 hrs)	NOEC ³	>1000	Van Hoecke et al. 2008

¹ EL₅₀ – The loading of a substance that is estimated to cause some effect on 50% of the test organisms

² LL₅₀ – The loading of a substance that is estimated to be lethal to 50% of the test organisms

³ NOEC – The No Observed Effect Concentration is the highest concentration in a toxicity test not causing a statistically significant effect in comparison to the controls.

⁴ not available

⁵ particle size of aggregate/agglomerate

The acute toxicity of the surface-treated SAS (dichloromethyl-, reaction products with silica; CAS RN 68611-44-9) to zebra fish (*Brachydanio rerio*), daphnids (*Daphnia magna*) and algae (*Scenedesmus subspicatus*) were described in a High Production Volume Assessment Report prepared by NOTOX (2002) and summarized in the IUCLID Data Set summaries (IUCLID Data Set 2002), both submitted to the United States Environmental Protection Agency (US EPA) in 2002.

Zebrafish and daphnids were tested at two concentrations; dilutions of the test substance at 1000 and 10 000 mg/L were stirred for 20 hours and then allowed to stand for 4 hours before addition of the test organisms (NOTOX 2002, IUCLID Data Set 2002). Concentrations tested were above the solubility limit, and undissolved test substance was observed on the bottom and surface of the suspension (IUCLID Data Set 2002). No mortality to zebra fish was observed up to the highest loading tested (10 000 mg/L). No immobilization in daphnia was observed at either the 1000 or 10 000 mg/L loadings. The 10 000 mg/L loading was filtered through perlon wool before testing in order for the daphnia to be visible (IUCLID Data Set 2002).

The effects of the surface-treated SAS on the growth rate and biomass of algae (*Scenedesmus subspicatus*) were evaluated (NOTOX 2002). Test solutions were prepared by adding 63, 630 and 6250 mg of the substance to 500 mL of ultrapure water, shaking for 24 hours, and filtering. Final nominal concentrations, based on unfiltered solutions, were 101, 1008 and 10 000 mg/L (IUCLID Data Set 2002). No effects on the growth rate or biomass were observed (NOTOX 2002).

The acute effects of the untreated SAS to zebra fish (*B. rerio*) and invertebrates (*D. magna*) were reported in a Chemical Screening Initial Data Set (SIDS) Initial Assessment Report (OECD 2004) prepared by the Organization for Economic Cooperation and Development (OECD). In its summary of untreated SAS studies, CAS RN 7631-86-9, CAS RN 112945-52-5, and CAS RN 112926-00-8 were considered. In two studies investigating the acute effects of SAS to zebra fish (*B. rerio*), excess concentrations (1000 and 10 000 mg/L loadings) of the untreated SAS were stirred for 20 hours in dilution water and allowed to stand for 4 hours (OECD 2004), after which the resulting suspension was tested. No effects were observed at the highest loading after 4 days.

The acute effects of untreated SAS to daphnia (*D. magna*) were also examined in two studies. In the first study, test solutions were prepared by stirring excess loadings (1000 and 10 000 mg/L) for 20 hours, and the resulting suspensions were tested. After 24 hours of exposure, 7.5% and 2.5% of the daphnia were immobile at the loading rate of 1000 and 10 000 mg/L, respectively. However, the observed effects were not dose-dependant, and the presence of particles on the appendages of immobile animals was observed. Therefore, it is likely that the effects on mobility were caused by a physical hampering of the animals (OECD 2004). In a second study, three test solutions were prepared using three methods:

- 1) Excess loading of 1000 and 10 000 mg/L stirred for 20 hours,
- 2) Excess loading of 1000 and 10 000 mg/L stirred for 20 hours and filtered on perlon wool, and
- 3) Excess loading of 1000 and 10 000 mg/L stirred for 20 hours and filtered through a microfiber-glass filter (1.75 μm and 1.2 μm successively).

Using the first method, 5% and 25% of daphnia were immobile after 24 hours exposure to 1000 and 10,000 mg/L, respectively. With the second method, 10% and 22.5% of daphnia were immobile after 24 hours exposure to 1000 and 10 000 mg/L, respectively. Finally, with the third method, no significant immobilization was observed. Therefore, it is suspected that the immobility observed could be attributed to physical effects (OECD 2004).

Based on the experimental data, both surface-treated SAS and untreated SAS present low toxicity to aquatic organisms.

In summary, a range of analogues for the major component of OMSSA, the surface-treated SAS and the untreated SAS, exhibited low toxicity to zebra fish and daphnids. Some daphnid immobilization was observed following exposure to an unfiltered suspension of untreated SAS, however these effects were most likely resulted from the physical hampering of the organisms due to the high concentrations of large diameter particles in the test substance. Therefore, the experimental evidence available for the suitable analogue substances to the major component of OMSSA, the treated SAS component, indicated that this substance is not expected to cause acute harm to aquatic organisms at low exposure concentrations.

B - In Other Environmental Compartments

The rat as the animal model can be used as a surrogate to wild terrestrial organisms. Toxicity via inhalation of the surface-treated SAS (CAS RN 68611-44-9), an analogue of OMSSA, to rats was described in a High Production Volume Assessment Report prepared by NOTOX (2002). Since mammalian studies are typically described in the context of human health, the details pertaining to the results from the exposure of rats are described in the Health Effects Assessment section of this screening assessment. With respect to the substance OMSSA, conclusions drawn from the rat inhalation studies in the context of human health are considered applicable to terrestrial organisms.

Ecological Exposure Assessment

No data concerning concentrations of OMSSA in water in Canada have been identified; therefore, environmental concentrations are estimated from available information, including estimated substance quantities, release rates, and size of receiving water bodies.

A – Industrial Release

The aquatic exposure of OMSSA is expected if the substance is released from industrial use to a wastewater treatment plant and the treatment plant discharges its effluent to a receiving water body. The concentration of the substance in the receiving water near the discharge point of the wastewater treatment plant is used as the predicted environmental concentration (PEC) in evaluating the aquatic risk of the substance. It can be calculated using the equation

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

where

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

A site-specific exposure analysis was conducted for the aquatic compartment at a single industrial site where OMSSA was reformulated into adhesives and sealants (Environment Canada 2010c). In 2006, the imported quantity of OMSSA was just under 100 000 kg. The selection of this site is, therefore, expected to represent a realistic worst-case release scenario across Canada based on a general assumption that the quantity released is proportional to the quantity consumed or produced.

In this site-specific exposure analysis, the site includes one facility, a wastewater treatment plant and one receiving water body. The PEC in the receiving water was estimated based on the concentration in the wastewater treatment effluent and a dilution factor of 10 provided by the receiving water. The concentration in the wastewater treatment effluent can be based on either estimated or reported data. Due to the lack of reported data, this concentration was estimated based on a fraction of the substance lost from the facility to a local municipal wastewater treatment plant, a wastewater treatment plant removal rate and its effluent flow. The loss fraction was conservatively estimated as 1.1% resulting from the chemical container handling operations and the industrial processes relevant to the facilities under consideration. It should be noted that this range is expected to represent the upper bound of the losses to wastewater and the release from an actual facility is expected to be at any level below this upper bound. The removal rate by a local wastewater treatment plant was estimated to be 95.2% (ASTreat Model 2006). The effluent flow of a local wastewater treatment plant is proportional to the population served and was nearly 300 000 m³ per day for the site considered.

Based on the above assumptions, the PEC for the surface treated SAS component of OMSSA is estimated to be 4.9×10^{-5} mg L for the industrial user of OMSSA. An assumption for the frequency of release was also used in the estimation which is 365 days/year for larger sized facilities. Since only one user was considered in this site-specific analysis along with certain upper-bounding assumptions, the PEC value obtained is considered to represent the level of exposure under a realistic worst-case release scenario in the receiving water near the point of the discharge from the wastewater treatment plant at an industrial site in Canada.

B – Commercial Release

OMSSA is found in commercial products that are not available to the general public; however the use of these products tends to be dispersive. Therefore, OMSSA can be released to water as the commercial products containing this substance are used.

Mega Flush, Environment Canada's spreadsheet tool, was employed to estimate the substance concentration in multiple water bodies that receive wastewater treatment plant effluents to which commercial products containing OMSSA may have been released (Environment Canada 2009). The spreadsheet tool provides these estimates for approximately 1000 release sites across Canada based on realistic assumptions.

The realistic assumptions include:

- loss to sewer at 2.7–2.8%
- wastewater treatment plant removal rate estimated at 0.0 % in case of no treatment,
- 46.9% for primary only treatment and 95.2% for primary-secondary combined treatment,
- number of annual release days at 365 days/year, and
- receiving water dilution factor in the range of 1 to 10.

The PEC of the surface treated SAS component of OMSSA in the receiving water bodies was estimated to be in the range of 2.3×10^{-7} to 1.8×10^{-3} mg/L, based on the different water bodies considered. The estimate is based on approximately 100 000 kg/year for the quantity of the substance used by consumers. The equation and inputs used to calculate the PEC are described in Environment Canada (2010d).

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 CEPA 1999. Lines of evidence considered include a comparison of conservative exposure estimates with available ecotoxicity data, as well as information on persistence, bioaccumulation, sources and fate of the substance.

OMSSA is expected to be persistent in air, water, soil and sediment. It is expected to have a low bioaccumulation potential based on the evaluation of its major component, the surface treated SAS.

The moderate importation volumes of OMSSA at a single site in Canada, a large amount of which is exported, indicate that the most significant releases to the aquatic environment will occur primarily at this industrial site. The releases to the Canadian environment are primarily to water and to a limited extent air. Once released to air, the majority of OMSSA will deposit to water and soil based on the relatively high density and low vapour pressure of the treated SAS component (>90%) of OMSSA. In addition, occupational health and safety practices have limited the amount of respirable particles less than or equal to $10 \mu\text{m}$ (i.e. PM_{10}) released to air. Therefore, fugitive emissions from the single site in Canada would likely not pose any risk to air-breathing mammals.

Based on its hydrophobicity and large size, along with experimental toxicity data ($\text{EL}_{50} > 10\,000$ mg/L) for the most suitable analogue data (i.e. CAS RN 68611-44-9), the surface treated SAS component of OMSSA has a low potential for harm to aquatic organisms.

When OMSSA is released into a water body, it partitions into suspended particulate matter and to bottom sediments, where sediment-dwelling organisms would be exposed to the substance. However, no environmental monitoring data specific to sediment-dwelling organisms are available for this substance. Moreover, the toxicity of particulate substances such as OMSSA to the benthic community cannot be extrapolated based on the equilibrium approach using the aquatic compartment. For particles, the relationships governing the substance characteristics such as toxicity and behaviour in the aquatic compartment may not hold in the sediment compartment. Therefore, the toxicity of OMSSA to sediment-dwelling organisms cannot be presently addressed with certainty due to lack of data and unsuitability of extrapolation from the aquatic compartment for this type of a substance. However, toxicity of OMSSA to benthic organisms is not expected to be high.

In summary, consideration of the conservative predicted environmental concentrations of OMSSA associated with its releases into the environment as a result of industrial and commercial activities, with the low toxicity of the surface treated SAS component of OMSSA indicates that this substance is unlikely to cause ecological harm in Canada.

Uncertainties in Evaluation of Ecological Risk

Uncertainties in this risk assessment exist due to a lack of data on physical and chemical properties specific to the treated SAS component of OMSSA (e.g. solubility in water). However, read-across approaches and close analogue data were used to fill critical data gaps within an acceptable margin of error.

In addition, the surface-treated SAS component of OMSSA may be present in this substance with varying particle sizes and levels of surface treatment both of which would lead to variability in the environmental fate and hazard of the substance depending on the material tested. Based on the information submitted by industry (Environment Canada 2010a) it was assumed that the surface-treated SAS component of OMSSA relevant to the Canadian environment was present as either coarser agglomerates $\leq 10 \mu\text{m}$ or finer aggregates ($\ll 10 \mu\text{m}$ but $> 10 \text{nm}$) with a negligible amount of any discrete primary particles (average primary particle size of 10nm); that the level of surface treatment was 3.5–4.5 wt%, rather than the calculated range of 1–3% that was indicated by authors as uncertain; and that the material was primarily hydrophobic (i.e. insoluble in water: water solubility $< 0.001 \text{mg/L}$). Analogues with similar characteristics were chosen for hazard assessment determinations in this assessment; however, there is still some uncertainty due to the variation in particle size and level and type of surface treatment which could not be avoided.

The experimental concentrations for analogues of the surface-treated SAS component of OMSSA associated with toxicity to aquatic organisms have an additional source of uncertainty in that these concentrations exceed the solubility of the chemical in water (either experimental or predicted). Despite this, the available data indicate that the surface-treated SAS component of OMSSA is not highly hazardous to aquatic organisms.

OMSSA is known as a UVCB (Unknown or Variable composition, Complex reaction product or Biological material), and it cannot be represented by a single, discrete chemical structure. Therefore, for the purpose of analogue comparison, an approach using “representative components” that allows for conservative estimates was employed. Given that more than one representative structure may be derived for the same UVCB, it is recognized that structure-related uncertainties exist for this substance.

Although there is the possibility that other consumer/commercial products containing OMSSA may be imported into Canada in addition to those reported as a result of industry surveys conducted pursuant to section 71 of CEPA 1999, no information is available on the quantity of such imports. It is anticipated that the life cycle stages and proportional losses resulting from use of these other products would not be significantly different from

those considered and estimated above. However, the actual mass of the substance lost from each of the life cycle stages may be higher than the estimates provided above, if such information was available for consideration.

Potential to Cause Harm to Human Health

Exposure Assessment

Environmental Media

Empirical data on concentrations of OMSSA in environmental media in Canada or elsewhere were not identified. OMSSA is not expected to be found in food or beverages. ChemCAN, a Canada-specific environmental exposure model, was used to estimate concentrations of OMSSA in various environmental media (ChemCAN 2003).

This model is a level III fugacity model that is used to estimate average concentrations in various media to estimate general population exposures from the environment. ChemCAN differs from the point-source models used in the ecological assessment section of the document.

Based on the information submitted in response to a notice published under section 71 of CEPA 1999, the total quantity in commerce was reported to range from 10,000 kg to 100,000 kg in 2006 (Environment Canada 2010a). The loss percentages predicted by the Mass Flow Tool (see Table 3) applied to the upper value of the range (100,000 kg) of OMSSA in Canadian commerce in 2006 were used to derive conservative upper-bounding daily intakes of OMSSA for the general population in Canada. This resulted in a total upper-bounding estimate of exposure from environmental media of less than a nanogram per kg-bw (kilogram of body weight) per day. Accordingly, the potential for exposure of the general population to OMSSA through environmental media in Canada is expected to be negligible.

Consumer Products

There were no reports under section 71 on the use of OMSSA in consumer products in Canada (Environment Canada 2010a). OMSSA is only used in industrial settings in Canada (Environment Canada 2010a). Therefore, exposure to the general public from consumer products is not expected.

Health Effects Assessment

OMSSA has not been classified for human health effects by any national or international agencies. No empirical data associated with OMSSA were identified in the open literature and quantitative or qualitative structure-activity relationship ((Q)SAR) models

could not be used to predict the potential toxicity of OMSSA since they are not considered appropriate to predict the toxicity of UVCBs. Therefore, the analogue of OMSSA, Silane, dichlorodimethyl-, reaction products with silica (CAS RN 68611-44-9), was considered in the assessment of potential health effects of OMSSA. It is associated with the largest hazard database among all analogues identified in Table 2b.

The toxicity of the surface-treated SAS has been tested in experimental animals via different routes and for various durations of exposure. These data are briefly summarized below.

In a 24-month oral feeding study, Wistar rats were administered the surface-treated SAS at a single dose level of 100 mg/kg-bw per day. No treatment-related clinical signs and no carcinogenic effects were observed (NOTOX 2002). In a 6-month oral feeding study, Wistar rats were treated at a single dose level of 500 mg/kg-bw per day. A slight progressive but reversible transformation of the adrenal cortex in females was observed, which was considered to be attributed to chronic stress (IUCLID Data Set 2000; NOTOX 2002). In another oral feeding study (5 to 8 weeks), Wistar rats were treated at 500, 1000, or 2000 mg/kg-bw per day initially, and then doses were gradually increased to 4000, 8000 and 16000 mg/kg-bw per day, respectively. Decreases in body weight and food consumption combined with apathy and decreased grooming activity were observed in the 8000 or 16000 mg/kg-bw per day groups, whereas decreased cytoplasmic glycogen in hepatocytes were observed in the 1000 to 16000 mg/kg-bw per day groups, which may indicate a starving condition of tested animals. At the highest dose level, four animals died. The lowest observed adverse effect level (LOAEL) was determined to be 1000 mg/kg-bw per day (NOTOX 2002).

Exposure to the surface-treated SAS via inhalation was also tested in rats. In a 13-week inhalation study, Wistar rats were exposed at 35 mg/m³. Granuloma-like lesions in the lungs, accumulations of alveolar macrophages, alveolar spaces filled with granular material, debris and polymorphonuclear leucocytes, alveolar bronchiolization, interstitial fibrosis and enlarged mediastinal lymph nodes were observed in the treated animals (NOTOX 2002). In a 2-week inhalation study, Wistar rats were exposed at 0, 31, 87 or 420 mg/m³. A concentration-related decrease in body weight was observed at 87 mg/m³ and higher. The lungs showed similar effects as those observed in the 13-week inhalation study. At the top dose level, the rats showed severe respiratory distress and apathy (NOTOX 2002).

The surface-treated SAS was not mutagenic in the bacterial reverse mutation assays with *Salmonella typhimurium* strains TA98, TA100, TA1537 and TA 1538. It is not mutagenic in *E. coli* WP2 uvrA. The substance also tested negative in an *in vitro* chromosome aberration assay in Chinese hamster ovary (CHO) cells (NOTOX 2002).

Two reproductive/developmental toxicity studies were identified. In a 6-month, 1-generation study combined with fertility and parental toxicity testing, male and female rats were administered the substance at 500mg/kg-bw per day in their food, 8 weeks before mating for the first progeny and 17 weeks before mating for the second progeny.

No treatment-related effects were observed in the parents or in the offspring. No effects on the female/male gonads were observed (NOTOX 2002). In a 2-generation reproductive toxicity study, male and female rats were given 100 mg/kg-bw per day via oral feed for 24 months. No effects on fertility and on offspring were observed (NOTOX 2002).

Characterization of Risk to Human Health

As no empirical health effects data were identified for OMSSA, its analogue, silane, dichlorodimethyl-, reaction products with silica, was considered in the characterization of potential human health effects of OMSSA. The possible health effects associated with exposure to OMSSA are mainly on the respiratory system. Exposure of the general population to OMSSA through environmental media and food is expected to be negligible. General population exposure to OMSSA from use of consumer products is not expected. As exposure to the general population through environmental media in Canada is expected to be negligible, the risk to human health is considered to be low.

Uncertainties in Evaluation of Risk to Human Health

Uncertainty in this environmental exposure estimation of OMSSA is high. This is because no concentrations of OMSSA in environmental media were identified in the literature. Therefore, the known quantity of OMSSA in commerce in Canada for the year 2006 was used to model environmental concentrations. Since the upper value of the range of OMSSA in commerce was used for modeling, it is likely that the modeled results are conservative estimates of environmental exposure. In addition, there is uncertainty due to assumptions used in the model.

Due to the lack of empirical health effects data available for OMSSA, confidence in the health effects database is low.

Conclusion

Based on the information presented in this screening assessment, it is concluded that OMSSA does not meet the criteria in paragraphs 64(a) and (b) of CEPA 1999, as it 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. Additionally, OMSSA meets criteria for persistence, but does not meet the criteria for bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Based on the available information on human health, it is concluded that OMSSA does not meet the criteria in paragraph 64(c) of CEPA 1999, as it 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 OMSSA does not meet any of the criteria under section 64 of CEPA 1999.

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