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Risk Assessment and Regulation of D5 in Canada

CHARACTERIZATION OF ECOLOGICAL RISKS FROM ENVIRONMENTAL RELEASES OF DECAMETHYLCYCLOPENTASILOXANE (D5)

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Abstract: Decamethylcyclopentasiloxane (D5) is used in personal care products and industrial applications. The authors summarize the risks to the environment from D5 based on multiple lines of evidence and conclude that it presents negligible risk. Laboratory and field studies show that D5 is not toxic to aquatic organisms or benthic invertebrates up to its solubility limit in water or porewater or its sorptive capacity in sediment. Comparison of lipid-normalized internal concentrations with measured concentrations in benthos indicates that field-collected organisms do not achieve toxic levels of D5 in their tissues, suggesting negligible risk. Exposure to D5 resulted in a slight reduction of root biomass in barley at test concentrations 2 orders of magnitude greater than measured D5 levels in biosolids-amended soils and more than twice as high as the maximum calculated sorptive capacity of the soil. No effects were observed in soil invertebrates exposed to similar concentrations, indicating that D5 poses a de minimis risk to the terrestrial environment. High rates of metabolism and elimination of D5 compared with uptake rates from food results in biodilution in the food web rather than biomagnification, culminating in de minimis risk to higher trophic level organisms via the food chain. A fugacity approach substantiates all conclusions that were made on a concentration basis. *Environ Toxicol Chem* 2015;34:2715–2722. © 2015 SETAC

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INTRODUCTION

Decamethylcyclopentasiloxane, commonly known as D5 (CAS no. 541-02-6), has been used in a variety of personal care products over the past 30 yr, including shampoos, conditioners, skin creams, cosmetics, and deodorants. Decamethylcyclopentasiloxane is also used in industrial applications, such as dry cleaning solvents and industrial cleaning fluids [1–3]. Environmental releases of D5 are approximately 90% to air, 9.5% to water, and the remainder to biosolids and soil [4]. However, relatively rapid degradation (half-life = 6.9 d) and the low potential for deposition reduce the importance of the air transport pathway; wastewater effluents and land applications of sludge represent more significant sources of D5 in the environment [4,5]. Decamethylcyclopentasiloxane is a relatively large molecule (molecular wt = 370.77 g/mol) with a high Henry's Law constant (33 atm m^3 mol^{-1}), low water solubility (17 μg/L), a high lipophilicity, and a high organic carbon–water partition coefficient, which promotes transfer of D5 into sediment [4,6–8]. Decamethylcyclopentasiloxane has been detected in naturally exposed aquatic organisms in the environment, especially benthos [3].

Decamethylcyclopentasiloxane has become the subject of considerable scientific and regulatory interest because of its low aqueous solubility, high octanol−water partition coefficient (log K_{ow}) [9], and measured laboratory-based bioconcentration factors ranging between 1120 L/kg and 10 200 ± 3100 L/kg [10]. In Canada, chemicals are classified as "inherently toxic" if effects are observed in chronic studies at concentrations less than 100 μg/L. With an aqueous solubility of 17 μg/L, and thus no ability to test up to 100 μg/L, D5 could be considered "inherently toxic" even if no effects were observed at its aqueous solubility limit. Decamethylcyclopentasiloxane also has been identified as a suspected bioaccumulative chemical in several categorization exercises [10–15] and met the lower-tier regulatory screening criteria for persistence and bioaccumulation potential [15,16]. Environment Canada subsequently identified D5 as a substance requiring a screening assessment as per Section 74 of the Canadian Environmental Protection Act [17]. Information about environmental concentrations and toxicity was made available to a scientific Board of Review convened as per section 333(1) of the Canadian Environmental Protection Act. The Board of Review concluded that "taking into account the intrinsic properties of Siloxane D5 and all of the available scientific information,. . . [s] iloxane D5 does not pose a danger to the environment" [18].

In the present study, we evaluated the toxicity and risk to the environment from D5 and tested the Board of Review's conclusion [18] that D5 does not pose a risk to aquatic or terrestrial environments. Receptors of concern included

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sediment organisms (benthos), fish and water column invertebrates, soil organisms (invertebrates and plants), and higher trophic level species. Responses of representative species in standardized toxicity tests were compared with limits of solubility or sorptive capacity of D5 in various media and to ranges of measured environmental concentrations. Our analysis also used a probabilistic approach to compare distributions of lipid-normalized internal concentrations of D5 in benthic invertebrates derived from toxicity tests with the range of lipid-normalized concentrations of D5 measured in sediment biota collected from the field to examine the probability of field-collected benthos exceeding the toxicity reference values. Bioaccumulation and the biomagnification potential of D5 are described by Gobas et al. [10] and Gobas et al. [19], respectively, on both a chemical concentration and fugacity basis and are discussed in the present study as an additional line of evidence to characterize the potential risks of D5 in higher trophic level species.

METHODS

Toxicity data

We collated data from existing toxicity studies to derive toxicity information for water column organisms, benthic organisms, and soil organisms. Chronic data were preferred because they represent long-term environmental exposures. Such data were available for aquatic organisms and terrestrial invertebrates. Data for terrestrial plants were available only from short-term exposure studies. A dataset on acute and chronic effects of D5 generated following standard test protocols and Good Laboratory Practices [20] is available and has been summarized by Redman et al. [21] for aquatic organisms and the Board of Review [18] for all species tested (Tables 1–3). Although these data have been reviewed by regulatory bodies, not all of the reports have been published in the peer-reviewed scientific literature but are available by request from the Silicones Environmental, Health, and Safety Center, a sector group of the American Chemistry Council.

For sediment organisms, available no-observable-effect concentration (NOEC) data (Table 1) were compiled into a cumulative distribution function, and the 5th centile NOEC concentration (HC_5) was calculated [22]. Multiple tests with the same species were averaged and the geometric mean included in the distribution. Although it is preferable to use adverse effect concentration data from concentration–response functions when critically evaluating toxicity data [23], the standardized toxicity test protocols were designed to generate NOEC values which were used by the Board of Review in their assessment of D5 toxicity and hence are used herein as well. We used solubility limits in water and sorptive capacity for sediments and soils (as calculated by Mackay et al. [4] and shown in Tables 1–3) to bound the maximum exposure concentrations. This was done because concentrations in media above the solubility or sorptive capacity of the chemical are thermodynamically unattainable via partitioning and cannot occur in the environment unless there is a spill. Concentrations in toxicity tests that exceed the solubility or sorptive capacity indicate the presence of neat chemical in the test. Although the presence of neat chemical can act as a stressor, exerting physical effects on test organisms unrelated to direct toxicity, relevant toxicity testing should be performed only up to the saturation concentration in the specific media to associate adverse effects with specific exposure concentrations. Hence, reported chemical concentrations above the solubility or sorptive capacity cannot be used for environmental hazard or risk assessment.

Environmental concentrations

Expected and measured environmental concentrations are detailed in companion papers in this issue and applied to our risk analysis. Specifically, Mackay et al. [4] described the fate and transport of D5 in the environment, including field measurements of sediment concentrations (Figure 4 in Mackay et al. [4]) and exposure concentrations for all media (Table 8 in Mackay et al. [4]). They also calculated solubility limits and sorptive capacities in all matrices (Tables 1 and 3 in Mackay et al. [4]) and described the role of organic carbon in absorption of D5 onto particles.

Risk characterization methods

Decamethylcyclopentasiloxane readily binds to organic matter in water, sediments, and soil [4,6–8], such that the amount of organic carbon present in environmental media is an

Table 1. Summary of decamethylcyclopentasiloxane (D5) sediment toxicity studies

Organism	Duration (d)	Most sensitive endpoint	% OC	μg/g dry weight[a] NOEC	μg/g dry weight[a] Max	μg/g–OC[b] NOEC	μg/g–OC[b] Max	Fugacity (Pa[c]) NOEC	Fugacity (Pa[c]) Max	Reference[d]
Hyalella azteca	28	Survival/growth	4.8	130	120	2708	2500	36	22.7	[50]
Hyalella azteca	28	Survival/growth	0.5	62	12	12 400	2500	163	22.7	[51]
Hyalella azteca	28	Survival/growth	11	641	275	5827	2500	77	22.7	[51]
Mean				278		6978		92		
Chironomus riparius	28	Male development	2.0	69	51	3450	2500	45	22.7	[52]
Chironomus riparius	28	Development rate	3.2	70	82	2188	2500	29	22.7	[53]
Mean				69.5		2.819		37		
Lumbriculus variegatus	28	Survival/reproduction	3.7	1 272	95	34 378	2500	88.2	22.7	[54]
Lumbriculus variegatus	28	BSAF test	5 (nominal)	>336 (highest dose)	122	>6720	2500	n/a	22.7	[55]

[a]Max = sediment-specific maximum sorption capacity = $C_W \times K_{OC} \times f_{OC} \times 0.001$, where C_W is the water solubility of 17 μg/L, K_{OC} is $10^{5.17}$ or 147 911 L/kg, f_{OC} = fraction organic carbon, and 0.001 kg/g is a units correction.
[b]OC = organic carbon. Max = OC-adjusted maximum sediment sorption capacity = $C_W \times K_{OC} \times 0.001$, where C_W is the water solubility of 17 μg/L, K_{OC} is $10^{5.17}$ or 147 911 L/kg and 0.001 kg/g is a units correction.
[c]Pa = Pascals; Max = maximum fugacity in sediment [19].
[d]Contact the corresponding author to obtain study reports (afairbrother@exponent.com).
OC = organic carbon; NOEC = no-observed-effect concentration level.

Table 2. Calculated mean species porewater NOECs for decamethylcyclopentasiloxane from chronic toxicity studies with benthic organisms

	NOEC sediment		NOEC porewater
Species	μg/g dry wt	μg/g OC[a]	μg/L[b]
Hyalella azteca	278	6978	47
Chironomus riparius	69.5	2819	19
Lumbriculus variegatus	1272	34 378	232

[a]$C_{pw} = C_{sed}\text{-OC} \times 1000/K_{OC}$, where, C_{pw} is the pore water concentration, C_{sed}-OC is the NOEC for each species (μg/g-OC), K_{OC} is 147 911 L/kg, and 1000 is a units correction factor (g/kg).
[b]Maximum water solubility for all tests = 17 μg/L.
NOEC = no-bserved-effect concentration level; OC = organic carbon.

important determinant of its bioavailability and potential toxicity and determines the maximum matrix solubility or sorptive capacity [4]. Therefore, exposure data were carbon-normalized for comparison with benthic toxicity information.

Measured D5 concentrations in sediment porewater were not available, but were estimated by Mackay et al. [4] for the standard toxicity test data, using the concept of equilibrium partitioning [24] (Table 2). The maximum concentration in sediment porewater was the maximum aqueous solubility of D5 (17 μg/L) for all test sediments. Table 2 indicates treatment concentrations of D5 in the benthic experiments with *Hyalella azteca* and *Lumbriculus variegatus* exceeded the sorptive capacity of the sediments, because calculated NOECs in porewater were greater than the aqueous solubility of D5.

The risk of D5 to sediment organisms was examined by comparing concentrations in field-collected biota to calculated internal concentrations in benthos corresponding to NOECs. In this context, risk does not imply a probability of achieving adverse effects but merely assesses the likelihood that D5 environmental concentrations are approaching concentrations that are close to, but still below, the toxicity threshold. There are no controlled dose–response studies that directly measured internal concentrations in the organisms that were tested. Internal D5 concentrations were not measured in biota from feeding and metabolism studies. Therefore, for the present risk assessment, we assumed that concentrations in tissues of chronically exposed organisms in the laboratory were at equilibrium with respect to the amount of D5 in their environment, and we calculated internal concentrations associated with no-effect observations by multiplying the laboratory-derived, carbon-normalized NOECs for sediment biota shown in Table 1 by 5.3, the greatest biota sediment accumulation factor (BSAF) for D5 for field-collected benthic invertebrates. Field-derived BSAFs for a site (e.g., Lake Pepin) were calculated by averaging the BSAFs for each colocated sediment and biota sample within the site. The BSAF values for D5 in midge (*Chironomus sp.*) and burrowing mayfly nymphs (*Hexagenia sp.*) in Lake Pepin sediments were 5.3 and 1.1, respectively [25]. The more bioaccumulative BSAF value of 5.3 was used in our risk analysis, and mean no-effect internal concentrations were calculated for the 3 benthic species for which D5 NOEC values exist: *Chironomus riparius*, *H. azteca*, and *L. variegatus*. The resulting D5 no-effect internal concentrations were 1.5×10^4 μg/g lipid, 3.1×10^4 μg/g lipid, and 1.8×10^5 μg/g lipid, respectively. Plotting these values as a log-normal distribution versus their ranked probability (Probability = Rank/[N + 1]) and deriving a linear regression of the log-transformed data (Figure 1) results in an extrapolated 5th centile no-effect internal concentration of 1.7×10^3 μg/g lipid. A similar method was used by Redman et al. [21], who estimated a 5th centile of the no-effect internal concentration of 0.96×10^3 μg/g lipid. Application of the 5th centile calculation method of Stephan et al. [26], written for use in water quality guideline development by the USEPA, results in a 5th centile no-effect internal concentration of 1.75×10^3 μg/g lipid; it appears the proposed D5 5th centile no-effect internal concentration benthic species value of 1.7×10^3 μg/g lipid is a reasonable estimate. Finally, we compared the calculated no-effect internal concentrations to the distribution of measured concentrations of D5 in a wide array of invertebrate species (μg/g lipid) collected from Lake Pepin, Minnesota, USA [25]; Inner and Outer Oslofjord [27] and Lake Mjøsa [28], Norway; Lake Erie, Canada [29]; and Lake Mjøsa and Lake Randsfjorden, Norway [30] (Figure 1).

Because a significant route of release of D5 to the environment (other than to air) is through wastewater discharge, our analysis is focused on the aquatic environment, based on concentrations of D5 in sediment. However, we also conducted a risk analysis for terrestrial plants and soil invertebrates based on concentrations of D5 in soil resulting from the incorporation of biosolids into soils. The available concentration data from soils were collected at unspecified times after application [31,32] and most likely were lower than what would be found immediately after application due to losses of D5 from volatilization and degradation (range: 0.006 mg/g dry wt to 0.221 μg/g dry wt in Canada and 0.031 mg/g dry wt to 0.038 μg/g dry wt in Spain). Therefore, for the purposes of our analysis, we used an estimated initial soil concentration calculated by Mackay et al. [4] of 0.03 mg/g dry weight to 1.6 μg/g dry weight, based on the range of predicted final sludge concentrations and the Canadian biosolid loading rate (considered a high-end estimate of biosolid application [31]).

Another approach for estimating risk is to compare toxicity data and environmental concentrations on the basis of fugacity [33]. The advantage of the fugacity approach is that it expresses NOECs and exposure concentrations from different types of studies (e.g., water and sediment toxicity tests) in

Table 3. Summary of decamethylcyclopentasiloxane soil toxicity studies [36]

			NOEC		
Organism	Exposure duration (d)	Most sensitive endpoint	μg/g dry wt	μg/g–OC[a]	Soil sorptive capacity μg/g OC[a]
Barley (*Hordeum vulgare*)	14	Root dry mass	77	2567	2500
Springtail (*Folsomia candida*)	28	Survival of adults	377	12 567	2500
Earthworm (*Eisenia andrei*)	56	Number of juveniles	507	16 900	2500

[a]Organic carbon concentration in test soils was not reported; therefore, a value of 3% was assumed, which is typical for Organisation for Economic Co-operation and Development artificial soils and the high end of agricultural soils in the United States [4,48].
NOEC = no-observed-effect; OC = organic carbon.

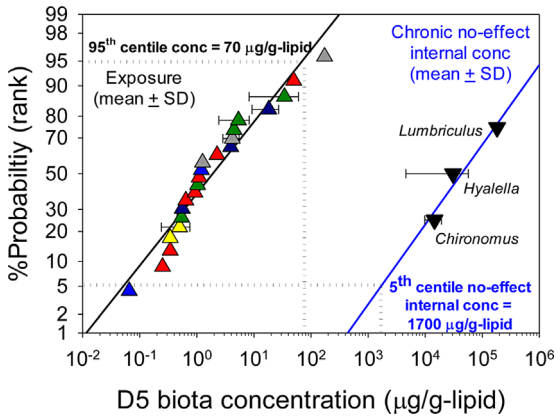

Figure 1. Cumulative probability plot for data on concentrations of decamethylcyclopentasiloxane (D5) in biota (μg/g lipid) measured in field samples compared with chronic benthic invertebrate no-effect internal concentration values for D5 in biota (biota sediment accumulation factor = 5.3, assumed). A linear regression on log-transformed data was used to fit the D5 biota concentration data, with $N = 22$, intercept = –0.29, slope = 1.05, $r^2 = 0.937$. A linear regression on log-transformed data was used to fit the chronic no-effect internal concentration data, with $N = 3$, intercept = –5.41, slope = 1.17, $r^2 = 0.947$. Body concentrations are means and standard deviation (SD) for each organism. Legend: blue = jellyfish; red = plankton/zooplankton; yellow = arthropods; green = bivalves; dark blue = emergent benthic invertebrates; gray = oligochaetes.

common unit terms (i.e., Pa), allowing direct comparisons across all media. This cannot be done when expressing concentrations in water as mass per unit volume and sediment as mass per unit weight, because the units are not directly comparable. A fugacity approach allows comparisons of exposure and response data using a much larger dataset. Gobas et al. [19] used fugacity to compare toxicity thresholds to environmental concentrations and described the potential for D5 to biomagnify in the aquatic and terrestrial food chains. We summarize their findings as a supplement to our characterization of risk to organisms exposed to environmental matrices of water, sediment and soils. Finally, we present all the lines of evidence to support conclusions regarding risks of D5 to aquatic or terrestrial ecosystems [34].

RESULTS AND DISCUSSION

Risk from aqueous exposures

The empirical toxicity data show that exposures of aquatic organisms to D5 in water elicit no adverse effects at concentrations at or below its solubility limit even after reaching steady state exposure. This was demonstrated by 2 *Daphnia magna* bioassays conducted under flow-through conditions (a 48-h acute study [35] and a 21-d full life-cycle test [36]), and 14-d and 45-d studies with rainbow trout (*Oncorhynchus mykiss*) under flow-through conditions [37,38]. To verify that early life stages are not more sensitive to D5, Lee [39] conducted a 60-d early life stage (eggs to juvenile stage) rainbow trout study, and Parrott et al. [40] conducted a similar 28-d study with fathead minnow (*Pimephales promelas*). Both studies showed no statistically significant effects at concentrations of D5 up to its aqueous solubility. It is also noteworthy that no adverse effects were seen in a study in which fish were provided unrealistically high environmental D5 dietary exposures (~500 μg/g food daily) for 35 d [41]. Accurately determining effect concentrations with algae may be difficult because of rapid volatilization of D5 in the static test system [42]. Nonetheless, 2 freshwater green algae (*Pseudokirchneriella subcapitata* and *Scenedesmus subspicatus*) tests in water treated with D5 at the limits of solubility resulted in no observable effects during the first 24 h, indicating no acute response [43]. Based on the currently available aqueous toxicity data, it can be concluded that concentrations of D5 in water up to the solubility limit of 17 μg/L do not appear to be associated with adverse effects in fish or other aquatic organisms. Furthermore, concentrations of D5 in water samples collected from municipal and industrial wastewater treatment plant (WWTP) influent and effluent and ambient water concentrations available from 87 field-collected samples (Figure 3 in Mackay et al. [4]), reveal that the median concentration of D5 in water is 0.06 μg/L, nearly 280-fold less than the water solubility limit. Notably, the 95th centile D5 field water concentration of 7.3 μg/L is more than 2-fold less than the water solubility. The analysis therefore indicates negligible risk to pelagic species. The present study agrees with the conclusion reached by the Siloxane D5 Board of Review [18] that exposure to D5 in water up to the solubility limit of 17 μg/L causes no effects to fish or other aquatic organisms.

Risk from sediment exposure

The NOEC values for D5 in sediment with tested benthic species are shown in Table 1, on an "as measured" dry weight basis, on an organic carbon (OC)-normalized basis, and on a fugacity basis. Chronic, 28-d sediment toxicity assays were conducted with *Hyalella*, *Chironomus*, and *Lumbriculus* species under standard Organisation for Economic Co-operation and Development (OECD) guidelines. The lowest NOECs were similar for both *Hyalella* and *Chironomus*, 62 μg/g dry weight to 70 μg/g dry weight (Table 1). With only 1 exception, all sediment NOECs were at or above the maximum sorptive capacity of D5 in sediment (Table 1), indicating the presence of neat chemical within the sediment. This makes it very unlikely that benthos will be exposed to toxic concentrations in sediments in the field.

Sediment D5 concentrations measured in more than 170 samples collected from 15 locations, reported in the literature, and from industry studies were compiled by Mackay et al. [4]. For the present study, all sediment samples with concentrations less than the method detection limit were considered to contain D5 residues at 50% of the method detection limit, and a 2% OC content was assumed for samples where OC was not reported. The 95th centile concentration of D5 of 55 μg/g OC (Figure 2) is approximately 45 times less than the estimated maximum D5 sorptive capacity in sediment of 2500 μg/g OC (Table 1) and approximately 6 times less than the 5th centile extrapolated threshold toxicity NOEC level of 400 μg/g OC (Figure 2). The only location to exceed the 5th centile chronic NOEC value was a Canadian WWTP sediment lagoon, a location receiving waste from an industrial site producing D5 [30]; this is shown in Figure 2 as a red triangle. Furthermore, when all sediment data were combined into a single cumulative distribution, the probability of elevated sediment concentrations (e.g., 95th centile) exceeding the chronic NOEC from a highly sensitive benthic invertebrate species is less than 1%.

Risk associated with sediment porewater

Using equilibrium-partitioning theory to calculate carbon-adjusted porewater NOECs from sediment NOECs (Table 2) suggests that D5 is exceeding its water solubility limit. However, what this means is that in the toxicity tests, D5 was present in both dissolved and neat form. The presence of neat D5 in the test can be viewed as an experimental artifact that

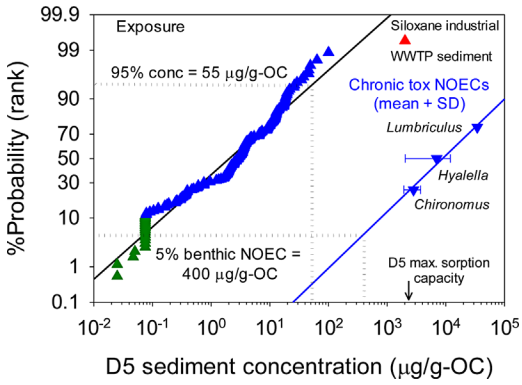

Figure 2. Cumulative probability plot for decamethylcyclopentasiloxane (D5) sediment concentration data (μg/g organic carbon [OC]) measured in field samples, compared with chronic benthic invertebrate no-observed-effect concentration (NOEC) values for D5 in sediment and its maximum sorptive capacity (~2500 μg/g-OC). A linear regression on log-transformed data was used to fit the sediment D5 data, with $N = 174$, intercept = –0.350, slope = 1.14, $r^2 = 0.962$. The red symbol represents sediment data from a siloxane measurement from an industrial WWTP sediment lagoon, and this datum was not used in the linear regression model. The blue symbols indicate detectable residues, whereas the green symbols indicated samples less than the limit of detection that were interpreted as being present at 50% of the limit of detection. A linear regression on log-transformed data was used to fit the chronic NOEC data, with $N = 3$, intercept = –4.77, slope = 1.21, $r^2 = 0.975$. Sample locations include: Lake Pepin, MN, USA; Inner and Outer Oslofjord [25,27], Lake Mjøsa, Norway [27]; Lake Erie, Canada [28]; and lakes Mjosa and Rnadsfjorden, Norway [29]. conc = concentration; WWTP = wastewater treatment plant; tox = toxicity.

normally would not be encountered in the real environment unless there is a spill of D5. This suggests that D5 cannot reach concentrations in sediment that are toxic to benthic organisms via porewater exposure. These calculations also indicate that D5 was present in the sediment of laboratory studies at concentrations that were not at equilibrium with porewater, suggesting there may have been substantial amounts of neat chemical associated with the sediments. This is in agreement with the conclusion reached by the Board of Review [18].

Risks associated with internal no-effect concentrations in sediment organisms

Figure 1 illustrates the internal no-effect concentrations of D5 in predominately sediment biota in relation to concentrations of D5 in field-collected invertebrate species. The invertebrate organisms were collected in Lake Pepin, Minnesota, USA [25]; Inner and Outer Oslofjord, Norway [27]; Lake Erie, Canada [28]; and Lakes Mjøsa and Randsfjorden, Norway [27,29]. The lipid-normalized concentrations of D5 from field-collected biota fit a log-transformed linear regression line with an $R^2 > 93\%$ and resulted in an estimated 95th centile residue of 70 μg/g lipid D5. Given that the 5th centile no-effect internal concentration is 1.7×10^3 μg/g lipid, it is apparent that D5 concentrations in field-collected organisms generally are much smaller than those corresponding with no-effect concentrations in toxicity tests (i.e., 95th centile of 70 μg/g lipid), suggesting that internal concentrations of D5 within field-collected biota are not associated with adverse risks.

Risk to secondary consumers (bioaccumulation)

Gobas et al. [10] and Gobas et al. [19] reviewed in detail the potential for D5 to bioaccumulate or biomagnify in aquatic or terrestrial food webs and concluded that the risk of biomagnification was negligible. Briefly, D5 is a very hydrophobic organic substance (log $K_{OW} = 8.09$) with a low affinity for

Table 4. Lines of evidence in assessing risks of decamethylcyclopentasiloxane to aquatic and terrestrial environments

Line of evidence	Environmental compartment		
	Water column	Sediment	Soil
Toxicity	No toxicity below D5 solubility for rainbow trout, fathead minnow, *Daphnia*, algae	No toxicity below D5 sorptive capacity for studies on *Hyalella*, *Chironomus*, *Lumbriculus*	No toxicity below D5 sorptive capacity for studies on barley, clover, earthworm, springtail
Solubility limits or sorptive capacity	No effects up to solubility limits in water	Effects seen only above porewater solubility limits and maximum sorptive capacity of the sediment	Plant and invertebrate studies show minor effects only at concentrations greater than maximum sorptive capacity of the soil
Bioaccumulation	Metabolism and elimination rates greater than intake rates	BSAF from laboratory and field correspond [10]	Exhalation and metabolism rates greater than intake rates
Internal no-effect concentration	N/A	Concentrations in field-collected organisms less than internal no-effect concentration	N/A
Measured environmental concentrations	Do not exceed water solubility	<1% chance of measured sediment concentrations exceeding 5th centile (NOECs)	Two orders of magnitude less than thresholds of toxicity
Fugacity	N/A	Observed fugacities in the environment are << corresponding with NOECs [19]	Observed fugacities in the environment are << corresponding with NOECs [19]

D5 = decamethylcyclopentasiloxane; BSAF = biota sediment accumulation factor; NOEC = no-observed effect concentration level; N/A = not available.

organic carbon relative to its K_{OW} (organic carbon partition coefficient = 5.17). It is metabolized by many aquatic organisms at a moderate (0.007 d^{-1}) to high (0.04 d^{-1}) rate, as noted in studies with bolus administration of labeled ^{14}C-D5 in trout [43], which, when combined with low assimilation or transfer rates between species (~10% [44]), results in trophic dilution of D5 in aquatic food webs. This occurs despite the fact that the primary route of exposure to D5 for fish is through the diet and not bioconcentration via the water column. The bioaccumulation behavior of D5 resembles that of certain phthalate esters, which, like D5, also are very lipophilic substances that exhibit trophic dilution in food webs [45]. In terrestrial ecosystems, it is likely that the high rate of loss of D5 via exhalation (as a result of its relatively low octanol–air partition coefficient of 4.93) and rapid metabolism ensure that D5 depuration rates exceed dietary uptake rates. As such, biomagnification in terrestrial food webs does not occur. Analysis of tissues from mink captured near Lake Pepin, Minnesota, validates the conclusion of biodilution, with average D5 concentrations in mink fat significantly less than lipid-adjusted D5 residues in fish from Lake Pepin and benthic invertebrates [46]. This is consistent with the fugacity data discussed in *Fugacity approach*.

Fugacity approach

The maximum fugacity of D5 is well characterized at 22.7 Pa (the vapor pressure of D5), corresponding to a sediment sorptive capacity of 2500 μg/g OC [19]. Consequently, concentrations in excess of this value indicate the presence of neat material. Therefore, fugacity-based NOECs greater than 22.7 Pa indicate that the test organism was exposed to the neat material. Any responses observed at fugacities greater than 22.7 Pa most likely result from the physical effects of the oily D5 liquid coating gills and other breathing surfaces and are not a true measure of the inherent toxicity of material found in the environment. The fugacity-based NOEC concentrations for D5 shown in Table 1 for sediment organisms clearly show that with perhaps one exception (i.e., the NOEC for *H. azteca* of 24.5 Pa, which is close to the maximum fugacity of 22.7 Pa), all NOECs exceed 22.7 Pa. This also supports the conclusion that adverse effects will most likely only be observed when neat material is present. In addition, the available data for concentrations of D5 in environmental media and biota were compiled and expressed in terms of fugacities by Gobas et al. [19]. Figure 2 from Gobas et al. [19] illustrates that, with the exception of one observation in an effluent sample from a WWTP of a silicone producer in Germany, all fugacities of D5 in all effluents and in all environmental media for which data are available are less than the maximum D5 fugacity of 22.7 Pa. In most cases, the fugacities are many times less than this maximum.

Risk in terrestrial systems

Plant (*Hordeum vulgare* [barley] and *Trifolium pratense* [red clover]) and soil invertebrate (*Eisenia andrei* [earthworm] and *Folsomia candida* [springtail]) toxicity tests were conducted by Velicogna et al. [47]. Among these species, adverse effects were observed only for barley root biomass, yielding an NOEC of 77 μg/g dry weight; none of the other terrestrial species showed any response at the concentrations tested. A simple comparison with field-measured D5 soil concentrations showed that the maximum reported concentration of D5 in soils (0.221 μg/g dry wt [31]) was nearly 400 times less than the NOEC. Using the estimated maximum soil concentration of D5 based on calculated biosolid loading rates (1.6 μg/g dry wt; see Mackay et al. [4]), the lowest terrestrial NOEC is still more than 50 times greater than the estimated exposure concentrations; these conclusions are all based on soil values that were not carbon-normalized. Assuming soil organic concentrations of 3% (typical for OECD artificial soils used in plant and invertebrate toxicity testing and the high end of agricultural soils in the US [4,48]), carbon-normalized NOECs were compared with carbon-adjusted maximum solubility limits or sorptive capacity for D5. Test concentrations of D5 were much greater than would be possible under field conditions, indicating the presence of large amounts of neat material coating the particles in the test soils. These data are consistent with the conclusion of the Siloxane D5 Board of Review's [18]; that is, there are no significant effects in terrestrial organisms from D5 in biosolids that are incorporated into soil.

CONCLUSION

An analysis of the currently available toxicity data on D5 indicates a lack of effect on survival, growth, and development in several species at all concentrations up to the aqueous solubility or maximum sorptive capacity of D5, and in some cases, even at concentrations above the solubility and maximum sorptive capacity. In essence, this means that based on currently available information, D5 can be expected to cause no effects in the environment in any circumstance with the possible exception of D5 spills. This analysis is consistent with the conclusion of the Siloxane D5 Board of Review [18] that D5 does not pose a danger to either the aquatic or terrestrial environments and that future uses of this substance will not pose a danger to the environment. Although the available toxicity data support a conclusion of no toxicity for D5, the limited number of species tested to date also contributes uncertainty around toxicity threshold values for D5. It is unlikely, however, that other species will be orders of magnitude more sensitive than those tested, which would be necessary for the effects of D5 to be seen at concentrations less than the solubility limits in water or the maximum sorptive capacity in sediment.

The analysis of the toxicity of D5 conducted in the present study and by the Siloxane D5 Board of Review provides some useful insights. First, it demonstrates that a substance that in a first screening appears to be of serious environmental concern due to its high K_{OW} and low aqueous solubility can be innocuous in the environment. This suggests that assessments based on persistence-bioaccumulation-toxicity criteria are not always accurate in identifying substances of environmental concern. Second, the approach taken in Canada to identify substances as having "inherent toxicity" if they exhibit an NOEC less than 0.1 mg/L can misidentify the toxicity of a substance, such as D5, which is not inherently toxic but exhibits a chronic NOEC less than 0.1 mg/L due to its low aqueous solubility. Decamethylcyclopentasiloxane is a neutral hydrophobic organic substance that can be expected to cause nonpolar narcosis at internal concentration in organisms of approximately 2 mmol/kg in the body or at 50 mmol/kg lipid to 100 mmol/kg lipid or 0.3% to 1% in lipid. However, D5 is not able to reach such concentrations as evidenced by the lack of toxicity. The main reason for not achieving toxic threshold values is that D5 is biotransformed by organisms. Fugacity calculations substantiate that biotransformation occurs at multiple steps in the food chain, resulting in trophic dilution, which eliminates the risk of trophic magnification and potential high exposure concentrations to upper-trophic level species such as birds and human subpopulations [49]. Finally, there are now sufficient field measurements of tissue residue concentrations in a range of benthic invertebrate species

to support the conclusion that organisms are not accumulating D5 in the environment to amounts that would result in a measurable adverse response. Together, these multiple lines of evidence (Table 4) bolster the conclusion that D5 does not pose a risk to aquatic or terrestrial environments.

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