Environmental Science & Technology Letters

Letter

pubs.acs.org/journal/estlcu

# Assessing the Aquatic Risks of the Cyclic Volatile Methyl Siloxane D4

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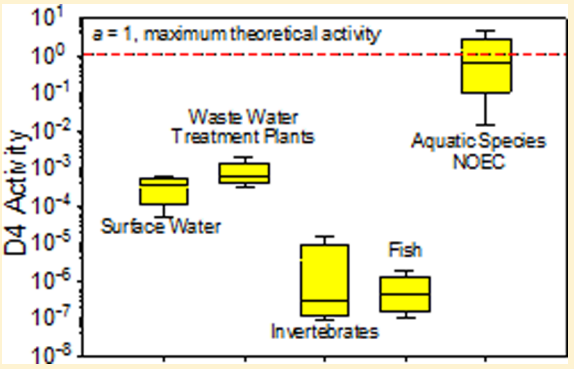
**ABSTRACT:** Assessing the ecological risks of the widely used cyclic volatile methyl siloxane D4 (octamethylcyclotetrasiloxane, CAS Registry Number 556-67-2) to aquatic systems is difficult because of its high volatility and low water solubility, but the potential for long distance atmospheric transport and persistence in the sediments has placed D4 under intense regulatory scrutiny. This paper explores the difficulties inherent in determining the toxicity of D4 to aquatic species and reveals the increased sensitivity of aquatic species tested within artificially closed systems compared to that of similar tests conducted in open systems that allow natural volatilization to occur. The concepts of narcosis mode of action and chemical activity explain the apparent lack of toxicity of D4 to aquatic species under environmentally realistic conditions. Discharge levels for the past 30 years during which D4 has been in use have produced field-measured concentrations that pose negligible risk to aquatic organisms.




## INTRODUCTION

The cyclic volatile methyl siloxane (cVMS) D4 (octamethylcyclotetrasiloxane, CAS Registry Number 556-67-2) has been used widely for nearly 30 years in electronics, textiles, and personal care products, and as an intermediate in the production of silicone polymers with a wide range of uses; registered tonnage use for D4 is 100000−1000000 t/year in Europe alone.[1] It, along with related cVMSs decamethylcyclopentasiloxane (D5, CAS Registry Number 541-02-6) and dodecamethylcyclohexasiloxane (D6, CAS Registry Number 540-97-6), is discharged through water treatment facilities into receiving waters during both manufacturing and product use. Consequently, D4 has been under intense regulatory scrutiny, in a U.K. national assessment,[2] a Dutch national assessment,[3] and an assessment by Canada for classification as a persistent, bioaccumulative, and toxic (PBT) substance.[4] It currently is under review by the European Union for classification as a PBT chemical[5] with subsequent restrictions in use due to perceived risks to aquatic ecosystems.[1] However, assessing the ecological risks of discharges of D4 to aquatic systems is difficult.

As with other chemicals in its class, D4 is highly volatile (vapor pressure of 132 Pa at 25 °C) and has a low water solubility (56.2 μg/L),[2] which presents challenges when standard aquatic toxicity tests are attempted. Additionally, D4 readily sorbs to carbon, thus reducing its bioavailability to aquatic species and increasing its level of binding to sediments. These properties are similar to those of other sparingly soluble substances; even the apparently simple comparison of measured or modeled water concentrations with toxicity thresholds derived from laboratory tests has a high degree of associated uncertainty.[6] These same properties raise concern about the potential for the chemical to cause harm to the environment because of its long distance atmospheric transport and persistence in the sediments. Similarly, the high octanol−water partition coefficient of D4 (log $K_{ow}$ = 6.49 at 25 °C) raises concerns about biomagnification in the aquatic food web with possible but unpredictable effects on high-trophic level consumers.[1]

While many of the existing data on aquatic toxicity are well-known,[5] several studies have not been previously published, and the limitations and uncertainties in the use of the data to predict risk of D4 to aquatic species have not been adequately addressed. This paper explores the difficulties inherent in testing toxicity to species that live in the water column (hereafter termed "aquatic species") of a volatile, super-hydrophic (log $K_{ow} \geq 7$) chemical[7] such as D4 and examines D4 water concentrations measured in representative water bodies to determine if laboratory test conditions are reflective of real-world conditions. The narcosis mode of action of D4[8] explains its low toxicity to aquatic species, and chemical activity[9] can be used to convert laboratory test results and environmental measurements to similar units to demonstrate a lack of environmental risk from water-only exposures. The result is a clearly described, science-based assessment of potential risks to aquatic species exposed to measured environmental concentrations of D4.

**Received:** September 4, 2016
**Accepted:** September 19, 2016

DOI: 10.1021/acs.estlett.6b00341
Environ. Sci. Technol. Lett. XXXX, XXX, XXX−XXX

## Table 1. Aquatic Toxicity Studies with D4

| organism | test | functional solubility ($\mu$g/L)[a] | water characteristics | results ($\mu$g/L) | comments | ref |
|---|---|---|---|---|---|---|
| fish | | | | | | |
| rainbow trout *Oncorhynchus mykiss* | EPA OTS 797.1400, fish acute, flow-through, sealed system, no headspace | 22 | 28−36 mg/L total hardness (as CaCO), 18−24 mg/L total alkalinity (as CaCO), pH 6.8−7.2, specific conductivity of 100−130 $\mu$mhos/cm, total organic carbon content of 0.32−0.95 mg/L | 96 h $LC_{50}$ > 22; 14 day $LC_{50}$ = 10 [8.5−13 95% confidence interval (CI)]; 14 day LOEC = 6.9; 14 day NOEC = 4.4 | no effects at 96 h up to functional solubility, mortality observed at 14 days | 10 |
| | OECD 204, fish prolonged acute toxicity (14 days), flow-through, open system | 29 | test concentrations of 1.9, 3.4, 6.8, 13, and 29 $\mu$g/L | 14 day $LC_{50}$ = 17 (14−21 95% CI); 14 day NOEC = 6.8; 14 day LOEC = 13 | mortality observed at 14 days | 11 |
| | EPA 797.1600, early life stage, sealed system, no headspace | 22 | 28−36 mg/L total hardness (as CaCO), 18−24 mg/L total alkalinity (as CaCO), pH 6.8−7.2, specific conductivity of 100−130 $\mu$mhos/cm, total organic carbon content of 0.32−0.95 mg/L | 93 day NOEC > 4.4 | no effects on embryos, hatch rate, or larval survival at any concentration tested | 10 |
| | prolonged acute toxicity, juvenile survival of a 1 g fish of 18 days, flow-through, sealed system, with headspace | 23 | pH 6.1−7.10, temp of 10.0−12.2 °C, single-test concentration of 23 $\mu$g/L | 18 day NOEC < 23 (80% mortality) | mortality observed at days 5−18 | 12 |
| | prolonged acute toxicity, juvenile survival of a 5 g fish of 18 days, flow-through, sealed system, with headspace | 31 | pH 6.3−6.6, temp of 10.2−11.9 °C, single-test concentration of 31 $\mu$g/L | 18 day NOEC > 31 | no effects at functional solubility | 12 |
| fathead minnow *Pimephales promelas* | EPA 797.1520, prolonged toxicity test and BCF study of 29 daus, flow through, sealed system, no headspace | − | 29−32 mg/L total hardness (as CaCO), 21−25 mg/L total alkalinity, conductivity of 130−140 $\mu$mhos/cm, pH 7.0−7.7 | 28 day NOEC > 0.26 | no effects (mortality, behavior, condition) observed after a 28 day exposure and a 14 day depuration | 13 |
| sheepshead minnow *Cypri nodon variegatus* | EPA OTS 797.1400, fish prolonged acute toxicity (14 days), flow-through, sealed system, no headspace | 6.3 | 20 ppt salinity, pH 7.9−8.1 | 96 h $LC_{50}$ > 6.3; 14 day $LC_{50}$ > 6.3; 14 day NOEC > 6.3 | no effects at functional solubility | 10 |
| invertebrates | | | | | | |
| water flea *Daphnia magna* | EPA OTS 797.1300, invertebrate acute, flow- through, sealed system, no headspace | 15 | 160−180 mg/L total hardness (as CaCO), conductivity of 400−600 $\mu$mhos/cm, pH 7.0 | 48 h $EC_{50}$ > 15; 48 h NOEC > 15 | no effects at functional solubility | 10 |
| | EPA OTS 797.1330, daphnid chronic, flow-through, sealed system, no headspace | 15 | − | 21 day NOEC = 7.9; 21 day LOEC = 15; $LC_{50}$ > 15 (survival); 21 day NOEC < 15 (reproduction) | survival reduced at the solubility limit, no effect on reproduction | 10 |
| mysid shrimp *Americamysis bahia* | EPA OTS 797.1930, mysid acute, flow-through, sealed system, no headspace | 9.1 | 20 ppt salinity, pH 7.9−8.1 | 96 h $LC_{50}$ > 9.1; 96 h NOEC > 9.1 | no effects at functional solubility | 10 |
| algae | | | | | | |
| green alga *Pseudokirchnerella subcapitata* (previously *Se lenastrum capriconutum*) | EPA OTS 797.1050, algal toxicity limit test, sealed, no headspace | 22 (reduced to 3.3 at 96 h) | Marine Biological Laboratory medium (MBL) conductivity from 270 (start) to 360 (end) $\mu$mhos/cm, from pH 7.6 (start) to pH 10.0 (end) | 72 h NOEC < 22 (growth rate); 96 h NOEC < 22 (cell density) | cell density not reduced at functional solubility | 14 |

[a]Functional water solubility is defined as the maximal achievable solubility of D4 under the specific conditions and dilution water quality for a particular study.



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DOI: 10.1021/acs.estlett.6b00341

## MATERIALS AND METHODS

Most of the aquatic toxicity tests for D4 were conducted from the 1970s to early 1990s and included tests of three species of freshwater fish,[10−13] one saltwater fish,[10] two invertebrates,[10] and one algal species[14] (Table 1). A suite of studies conducted by Sousa et al.[10] used nonstandard exposure systems and techniques to force the chemical into solution, because of the high volatility, low water solubility, and superhydrophobicity of D4. These systems included use of stock solutions at concentrations higher than the theoretical water solubility limit to maximize the dissolved concentration of D4, renewal of the stock solution every 24−48 h, and maintaining the entire system (i.e., dilutors, tubes, and exposure chambers) with no exposure to air (i.e., no air−water interface). These techniques were later recommended in OECD guidelines for aquatic toxicity testing of difficult substances.[15] Sousa et al.[10] also used a flow-through toxicant delivery system to minimize chemical sorption to surfaces of the test apparatus. This approach achieved a functional water solubility of 6.3 μg/L (hard water) to 22 μg/L (softwater) in freshwater and 6.3 and 9.1 μg/L in 20 and 30 ppt saltwater, respectively (Table 1); these concentrations are below the maximal solubility of 56.2 μg/L measured in pure laboratory water. Functional water solubility is defined herein as the maximal achievable solubility of D4 under the specific conditions and dilution water quality for a particular study. An algal growth study[14] was conducted in a static, closed system with no headspace. An inadvertent consequence was a reduction in the overall rate of growth of the algae in both the control and treated flasks due to a decreased level of oxygen.[15]

For all acute and chronic (long-term) toxicity tests conducted within these closed systems (Table 1), reduced survival occurred only in adult rainbow trout (*Onorhynchus mykiss*) after exposure for 14 days at ≥6.9 μg/L D4,[10,11] but no mortality occurred in early life stage trout exposed for 93 days to 4.4 μg/L D4 (maximal concentration tested).[10] Toxicity tests with rainbow trout conducted in open systems that allowed volatilization to occur showed mortality at 23 μg/L after exposure of a 1 g fish for 18 days, but no mortality occurred in 5 g fish exposed for 18 days to 31 μg/L D4.[12] No effects (e.g., mortality, behavior, or body condition) were observed in fathead minnow (*Pimephales promelas*)[13] or the saltwater sheepshead minnow (*Cyprinodon variegatus*)[10] exposed up to functional solubility limits in prolonged toxicity tests. Water fleas (*Daphnia magna*) within a closed system experienced reduced survival after exposure for 21 days to the maximal concentration tested (15 μg/L), but reproduction was not affected.[10] Their survival (77%) was only slightly below the allowable 80% survival rate for controls. Saltwater mysid shrimp (*Americamysis bahia*) were not affected at the functional solubility of D4.[10] The cell density of freshwater green algae (*Pseudokirchneriella subcapitata*) was not reduced at concentrations of up to 22 μg/L when compared to that of control vessels with a similarly reduced headspace.[14]

## RESULTS AND DISCUSSION

It is not surprising that D4 has no toxicity or a low level of toxicity in most aquatic species. Like most hydrophobic chemicals, D4 acts via a narcosis mode of action, which requires the accumulation of the chemical in the tissues to achieve a critical (toxic) body burden.[8] As with other cVMS chemicals, D4 is slow to build up in aquatic organisms, particularly during toxicity tests in which the test specimens are not fed. This primarily is due to high metabolism and excretion rates, so much longer test durations are needed to reach the "critical body burden" (CBB) required to cause nonpolar narcosis.[7] Mackay et al.[7] calculated that, on the basis of its physical properties, the time predicted for D4 to reach the CBB needed to cause a 50% effect in rainbow trout is roughly 25 days. The authors concluded that for hydrophobic chemicals such as D4, conventional aquatic toxicity tests with exposure from water respiration for 96 h to 14 days often will fail to reach a toxic end point, especially if there is appreciable biotransformation of the substance. For example, a test with adult rainbow trout exposed to D4 in an open, flow-through system showed no toxicity after 14 days, at concentrations of up to 51.7 μg/L, the natural functional solubility of the chemical.[11] Although the early life stage rainbow trout study conducted by Sousa et al.[10] lasted 93 days, the rapid growth of the larval fish likely resulted in growth dilution such that critical body residues were not achieved even at the functional water solubility concentration. Thus, the occurrence of mortality in adult rainbow trout after exposure for only 14 days is surprising. It may be that forcing the chemical into solution with no headspace for volatilization to occur created some emulsive characteristics that affected the gill surfaces, resulting in a physical effect rather than chemical-induced narcosis.[16]

Assuming the results of the 14 day rainbow trout study in a closed system by Sousa et al.[10] are representative of what would occur in the natural environment begs the question of whether environmental concentrations ever reach such a level. Water samples have been collected from, and D4 levels measured in, freshwater and marine sites in Tokyo Bay,[17] many Scandinavian countries,[18] and receiving water downstream of municipal and industrial wastewater treatment plants in Canada.[19] Figure 1 presents the D4 concentrations of these waters in a cumulative probability distribution[20] and compares these concentrations to the D4 rainbow trout $LC_{10}$ concentration for survival of 7 μg/L [95% confidence interval (CI) of 4−12 μg/L] (the lowest reported fish $LC_{10}$) and the *Daphnia* $LC_{10}$ for control-adjusted survival of 12 μg/L (95% CI of 7−56.2 μg/L).[10] Although the authors calculated $LC_{50}$ concentrations (see Table 1), the $LC_{10}$ values were calculated from the data presented and

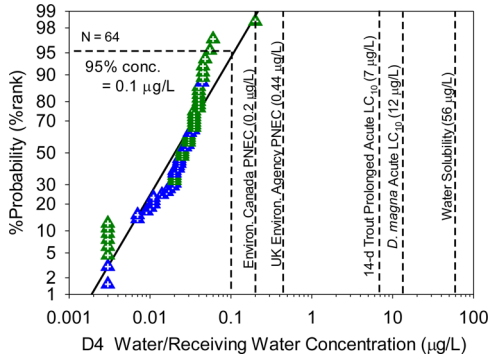


**Figure 1.** D4 water concentration distribution from different locations in Japan,[17] Europe,[18] and North America[19] vs rainbow trout $LC_{10}$ and *D. magna* concentrations,[10] and regulatory PNEC values.[4,21] Green symbols represent data for nondetectable D4 residues assumed to be present at 50% of the D4 minimal detectable level (MDL); blue symbols represent measured D4 concentrations in water.



DOI: 10.1021/acs.estlett.6b00341
Environ. Sci. Technol. Lett. XXXX, XXX, XXX−XXX

used in the figure as conservative hazard estimates for comparison with environmental concentrations. Because selection of an "$x$" in the $LC_x/EC_x$ used in a risk assessment is a matter of policy, not science, the figure also includes the predicted no effect concentrations (PNECs) of 0.2 $\mu$g/L used by Environment Canada[4] and 0.44 $\mu$g/L used by the United Kingdom as the competent authority for the European Union[21] for regulatory assessments of D4; these values are the rainbow trout $LC_{50}$ and NOEC divided by uncertainty factors of 50 and 10, respectively, to account for interspecies and lab-to-field extrapolations. The calculated 95th percentile D4 water concentration is 0.1 $\mu$g/L ($N$ = 64), or 2 times lower than either of the ecotoxicology trigger values and >40 times lower than measured $LC_{10}$ values. These data indicate a lack of overlap between measured environmental concentrations of D4 in the water column and the toxicity threshold values for aquatic species, indicating a lack of risk in aquatic systems. This approach is a highly conservative risk estimate, as it is based on tests conducted in artificially closed systems to reduce volatilization and increase the extent of chemical saturation. In addition, a majority (33 of 64 samples) of the water residue data in Figure 1 are samples with no detectable D4 and are set at 50% of the limit of detection as a conservative estimate.

The conclusion that D4 is nontoxic to water column organisms up to its limits of functional water solubility is further substantiated by addressing the "activity" (or fugacity) of the chemical. The use of activity to describe the degree of saturation achieved by a compound in a given medium is particularly useful for substances that display a narcosis mode of action in aquatic organisms, such as D4,[8] as chemical activities may provide valuable estimates of the proximity of measured concentrations to potentially toxic levels.[9] Chemical activities are easy to calculate and allow the comparison of concentration data in various matrices with differing units. Chemical activities are simply the ratio of a concentration and its solubility, adjusted for salinity, amount of particulate matter, and carbon content.[22] Activities of concentrations in biota are the ratio of the lipid-based concentration and the apparent solubility of the chemical in lipid, which is approximated by the compound's octanol–water coefficient ($K_{ow}$) and its aqueous solubility value. This allows expression of all data to range from 0 to 1, resulting in easy comparison of biota and environmental matrices. An analysis of the chemical activity of D4 in aquatic systems and aquatic organisms is presented in Figure 2. The NOEC values for aquatic organisms exposed to D4 (Table 1) were calculated as the aqueous concentration divided by the functional solubility for each test, resulting in NOEC D4 activities of 0.02–1.0, with a mean value of 0.52. Chemical activities for field-collected fish and invertebrates are approximately $10^{-7}$ to $10^{-6}$, based on tissue concentrations in biota collected simultaneously with the water sampling referenced above. The measured chemical activities of D4 in the water samples presented in Figure 1, adjusted for site-specific salinity and organic carbon, are approximately $10^{-5}$ to $10^{-3}$, far lower than the NOEC values. Overall, these data show that chemical activities of D4 in biota cannot reach values that are associated with nonpolar narcosis (i.e., toxicity) and that discharge levels for the past ~30 years have produced field-measured concentrations that pose negligible risk to aquatic organisms.

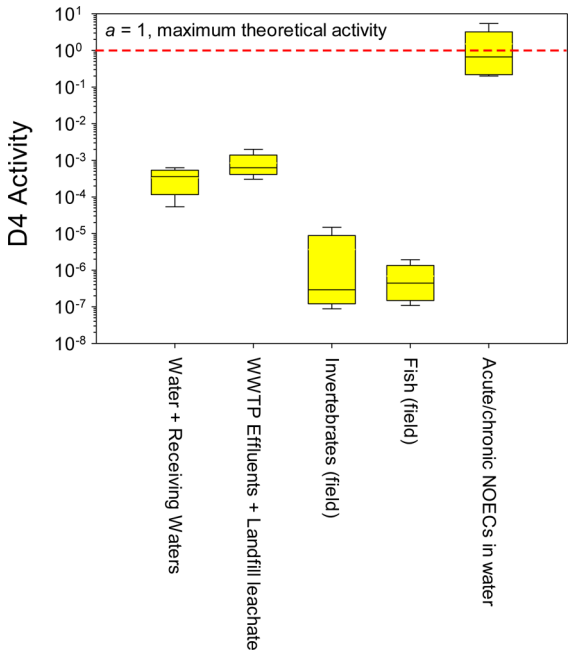


**Figure 2.** D4 activities (unitless) in surface water and receiving waters, wastewater treatment plant effluents, invertebrates, and fish from different locations in Japan,[17] Europe,[18] and North America[19] in relation to the maximal activity [$a$ = 1 (red line)] and chronic no-observed effect concentrations (NOECs) with aquatic organisms (see Table 1). Median concentrations are shown by the black horizontal bar; the yellow boxes show upper and lower quartile concentrations, and the whiskers represent minimal and maximal values.

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### Notes

The authors declare the following competing financial interest(s): Although the work was funded by the American Chemistry Council, Silicones, Environmental, Health, and Safety Center and one author is employed by a manufacturer of the chemical, neither of the authors has a financial interest in the production or sale of the chemical. Employment is not dependent upon the preparation of the paper nor the conclusions reached in the analysis.

## ACKNOWLEDGMENTS

This work was supported by funding from the American Chemistry Council, Silicones, Environmental, Health, and Safety Center under Contract 6971.

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DOI: 10.1021/acs.estlett.6b00341
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DOI: 10.1021/acs.estlett.6b00341
*Environ. Sci. Technol. Lett.* XXXX, XXX, XXX−XXX