



# Benthic invertebrate exposure and chronic toxicity risk analysis for cyclic volatile methylsiloxanes: Comparison of hazard quotient and probabilistic risk assessment approaches



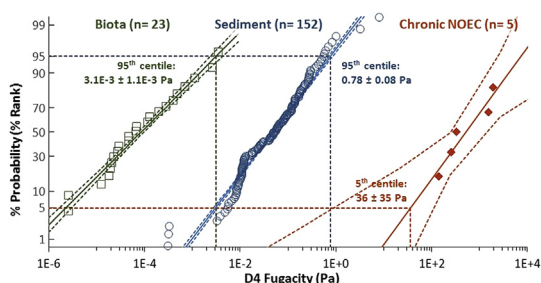
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## HIGHLIGHTS

- Risk to benthic invertebrate organisms assessed for cyclic methylsiloxanes (cVMS).
- Probabilistic risk assessment (PRA) and hazard quotient (HQ) methods compared.
- Used fugacity to allow direct comparison of chemical levels in varying matrices.
- Risk outcomes consistent between HQ and PRA methods.
- No risk predicted for D4 or D5 and negligible risk predicted for D6.

## GRAPHICAL ABSTRACT



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## ABSTRACT

This study utilized probabilistic risk assessment techniques to compare field sediment concentrations of the cyclic volatile methylsiloxane (cVMS) materials octamethylcyclotetrasiloxane (D4, CAS # 556-67-2), decamethylcyclopentasiloxane (D5, CAS # 541-02-6), and dodecamethylcyclohexasiloxane (D6, CAS # 540-97-6) to effect levels for these compounds determined in laboratory chronic toxicity tests with benthic organisms. The concentration data for D4/D5/D6 in sediment were individually sorted and the 95th centile concentrations determined in sediment on an organic carbon (OC) fugacity basis. These concentrations were then compared to interpolated 5th centile benthic sediment no-observed effect concentration (NOEC) fugacity levels, calculated from a distribution of chronic D4/D5/D6 toxicologic assays per OECD guidelines using a variety of standard benthic species. The benthic invertebrate fugacity biota NOEC values were then compared to field-measured invertebrate biota fugacity levels to see if risk assessment evaluations were similar on a field sediment and field biota basis. No overlap was noted for D4 and D5 95th centile sediment and biota fugacity levels and their respective 5th centile benthic organism NOEC values. For D6, there was a small level of overlap at the exposure 95th centile sediment fugacity and the 5th centile benthic organism NOEC fugacity value; the sediment fugacities indicate that a negligible risk (1%) exists for benthic species exposed to D6. In contrast, there was no indication of risk when the field invertebrate exposure 95th centile biota fugacity and the 5th centile benthic organism NOEC fugacity values were compared.

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## 1. Introduction

### 1.1. Chemicals of interest

The cyclic volatile methylsiloxanes (cVMS) are a class of silicone compounds that have an unusual combination of physico-chemical properties that has led to their wide use in consumer (e.g., shampoos, deodorant, cosmetic) and industrial (e.g., polymer production, dry cleaning solvents, industrial cleaning fluids) applications (Hori and Kannan, 2008; Wang et al., 2009). These cVMS materials have relatively low to moderate molecular weights, high vapor pressures (~5–130 Pa at 25 °C), and low water solubility (5–56 µg L<sup>-1</sup>), resulting in high air/water partition coefficients (K<sub>AW</sub>), octanol/water partition coefficients (K<sub>OW</sub>) and soil sorption coefficients (K<sub>OC</sub>). Table 1 presents more detailed information on selected properties of the three cVMS compounds that were investigated in this work: octamethylcyclotetrasiloxane (D4, CAS RN 556-67-2); decamethylcyclopentasiloxane (D5, CAS RN 541-02-6); and dodecamethylcyclohexasiloxane (D6, CAS RN 540-97-6). These siloxanes may be released into the environment, either as a result of their use or from products that they are used to manufacture. Uses that result in release to the environment have raised concerns as to the fate and effects of these substances in aquatic ecosystems for governments in the United States (USEPA, 2014), Canada (Environment Canada, 2008a, 2008b, 2008c; Environment Canada, 2010), the UK (Environment Agency, 2009a, 2009b, 2009c), and the Nordic States (Norden, 2005). Redman et al. (2012) and Mackay et al. (2015a) determined via field and laboratory cVMS body burden data that it is likely that these materials act via a narcosis mode of action. The lipophilic nature of these cVMS materials is apparent from their log K<sub>OW</sub> and K<sub>OC</sub> values (i.e., log K<sub>OW</sub> > 6 and log K<sub>OC</sub> > 4, see Table 1), which indicates that sediment sorption is a likely efficient removal mechanism of these compounds from water; water and sediment field data support this concept (Norden, 2005; NILU, 2007). As a result, the highest exposure to D4, D5, and D6 in aquatic systems is likely via sediment (Mackay et al., 2015b). For this reason, while a risk assessment of pelagic systems with D4 has been performed (Fairbrother and Woodburn, 2016), the current work has focused on benthic invertebrate species and quantifying the potential risk these materials may pose to such organisms. Lastly, a common risk assessment challenge is how to best compare divergent field data collected in concentrations expressed on a mass or lipid basis to toxicity levels typically expressed on the basis of volume or mass. In this work, we propose a fugacity approach as a unit conversion to obtain a common basis for comparing concentrations; using this method, it is possible to assess the probability of risk to benthic organisms using different matrices such as sediment and biota in comparison to standard chronic toxicity benchmarks.

### 1.2. Risk assessment process: point estimate versus probabilistic methods

Natural and anthropogenic materials enter the environment on a regular basis, and it is frequently of interest to estimate the probability or likelihood of adverse effects of a chemical to wildlife organisms. The simplest ecological risk assessment method compares a measure of exposure with some threshold for detrimental effects. On a screening basis, this can be done using the calculation of a 'hazard quotient' (HQ), where a point estimate of the measured or predicted exposure concentration (PEC; e.g., a maximum concentration) is divided by a toxicity reference value. This reference value is generally the threshold level to assess chronic risk, such as a no-observed effect concentration (NOEC), determined from a dose-response relationship in a chronic toxicology study (USEPA, 2015) or a concentration of concern (COC), depending on the extent of data available. The values of COC in hazard assessment are often derived using assessment factors (AFs), which are arbitrary protection factors used to account for uncertainty based on potential differences in inter- and intraspecies variability, laboratory-to-field variability, and extrapolation of acute to chronic effects (USEPA, 2013; USEPA, 2012):

$$HQ = \frac{\text{Exposure concentration}}{AF * NOEC \text{ or } COC} = \frac{PEC}{PNEC} \quad (1)$$

If the measured or predicted exposure concentration exceeds the predicted no effect concentration (PNEC) (i.e., HQ > 1), then the screening level assessment indicates a potential for risk to the receptor. An HQ equal to or greater than unity, however, does not necessarily suggest a likelihood of adverse effects. Because of the inherent conservatism of the HQ methodology, 'exceedances' (i.e., values > 1) must be evaluated on a case-by-case basis, considering such factors as the confidence level of the assessment, statistical variance, the slope of the dose-response curve, and the magnitude of the exceedance. The HQ method represents the initial tier of an assessment, meant only to rebut the presumption of a potential adverse effect. As conservative assumptions apply to both exposure and toxicity endpoints in the HQ assessment, the HQ method is inherently protective in nature, but not predictive as to the level of potential risk. This uncertainty associated with HQ is a significant issue in their application in risk assessment, as the method provides no deterministic quantitation as to the overall level of risk involved.

The term "risk" implies an element of likelihood or probability, which cannot be calculated from point estimates such as an HQ. A tiered risk assessment process has been recommended for ecological application by the US-based National Research Council (NRC, 2009), in which increasingly complex and resource-intensive levels of assessment are conducted. Higher tier methods utilize more probabilistic approaches, which determine the probability of an exposure concentration exceeding some probability of effect or

**Table 1**  
Physico-chemical properties for D4, D5, and D6.

Chemical	Molecular Weight (g mol <sup>-1</sup> )	Water Solubility (23 –25 °C) (mg L <sup>-1</sup> )	Log K <sub>OW</sub> <sup>a</sup>	Log K <sub>OC</sub> <sup>a</sup>	Henry's law constant at 25 °C (Pa m <sup>3</sup> ·mol <sup>-1</sup> ) <sup>a</sup>	OC Sorption Capacity <sup>b</sup> (mg kg-OC <sup>-1</sup> ) or (Pa)	Z <sub>water</sub> (mol Pa <sup>-1</sup> ·m <sup>-3</sup> ) <sup>c</sup>	Z <sub>lipid</sub> (mol Pa <sup>-1</sup> ·m <sup>-3</sup> ) <sup>d</sup>	Z <sub>OC</sub> (mol Pa <sup>-1</sup> ·m <sup>-3</sup> ) <sup>e</sup>
D4	297	0.056	6.49	4.22	1.21E+06	929 or 229	8.24E-07	2.55	0.014
D5	371	0.017	8.03	5.17	3.34E+06	2514 or 153	2.99E-07	32.1	0.044
D6	445	0.0053	9.06	5.81	4.94E+06	3422 or 59	2.02E-07	232.3	0.131

<sup>a</sup> Data from Environment Agency, 2009a; Environment Agency, 2009b; Environment Agency, 2009c for D4, D5, and D6, respectively.

<sup>b</sup> OC Sorption Capacity = Water Solubility \* K<sub>OC</sub> (mg kg-OC<sup>-1</sup>) and Water Solubility \* K<sub>OC</sub> / [Z<sub>OC</sub> \* Molecular Weight] (Pa), from Gobas et al. (2015).

<sup>c</sup> Z<sub>water</sub> = 1 / Henry's Law constant (Pa·m<sup>3</sup>·mol<sup>-1</sup>).

<sup>d</sup> Z<sub>lipid</sub> = K<sub>LW</sub> \* Z<sub>water</sub> ~ K<sub>OW</sub> \* Z<sub>water</sub>.

<sup>e</sup> Z<sub>OC</sub> = K<sub>OC</sub> \* Z<sub>water</sub>.

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