



Dynamic modelling of aquatic exposure and pelagic food chain transfer of cyclic volatile methyl siloxanes in the Inner Oslofjord



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ABSTRACT

The marine fate and pelagic food chain transfer of three cyclic volatile methyl siloxanes (cVMS: D4, D5 and D6) was explored in the Inner Oslofjord, Norway, using two dynamic models (the Oslofjord POP Model and the aquatic component of ACC-HUMAN). Predicted concentrations of D4, D5, and D6 in the water column were all less than current analytical detection limits, as was the predicted concentration of D4 in sediment (in agreement with measured data). The concentrations predicted for D5 and D6 in sediment were also in broad agreement with measured concentrations from the Inner Oslofjord. Volatilisation was predicted to be the most important loss mechanism for D5 and D6, whereas hydrolysis was predicted to dominate for D4. Concentrations of all three compounds in sediment are controlled by burial below the active mixed sediment layer. The marine food web model in ACC-HUMAN predicted “trophic dilution” of lipid-normalised cVMS concentrations between zooplankton and herring (*Culpea harengus*) and between herring and cod (*Gadus morhua*), principally due to a combination of in-fish metabolism and reduced gut absorption efficiency (as a consequence of high K_{ow}). Predicted D5 concentrations in herring and cod agree well with measured data from the inner fjord, particularly when measured concentrations in zooplankton were used to set the initial dissolved-phase aqueous concentrations. Predicted concentrations of D4 and D6 in fish were over- and under-estimated by the model – possibly due to extrapolation of the metabolism rate constant from D5.

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1. Introduction

Cyclic volatile methyl siloxanes (cVMS) are used in a wide range of personal care products (e.g. Horii and Kannan, 2008). Recently, concerns have been raised about their environmental profile (e.g. Brooke et al., 2008a,b,c), particularly their potential for environmental persistence and bioaccumulation. They are relatively long lived in water because they are not biodegradable, although they do undergo acid- and base-catalysed hydrolysis with estimated half lives ranging from a few hours to a few 100 d, depending on the compound, pH and temperature (e.g. Brooke et al., 2008a,b,c). cVMS compounds have very high air: water partition coefficients and they tend to partition to the atmosphere (Whelan et al., 2004; Price et al., 2010) where they can potentially be transported over long distances (McLachlan et al., 2010). Once airborne, they are unlikely to re-partition appreciably to surface media (Wania, 2006) and are broken down primarily by reaction with OH radicals to silanols, which are more water-soluble (Whelan et al., 2004) and are eventu-

ally mineralised to SiO₂, CO₂ and water. A fraction of the chemicals used in personal care products will be transferred to waste water. In waste water treatment plants (WWTPs), cVMS compounds are likely to sorb significantly to sludge solids and to partition to the atmosphere, owing to their unusual combination of hydrophobicity and volatility. However, a small fraction of the influent load will be emitted to surface waters in treated effluent (Sparham et al., 2008; Price et al., 2010). The fate of cVMS compounds in freshwater environments has been discussed by Whelan et al. (2009, 2010) and by Price et al. (2010). However, to date, there has been little consideration of the fate of these chemicals in marine systems.

Whilst they are very hydrophobic, with reasonably high aquatic bioconcentration factors, cVMS compounds have been shown to metabolise in fish (Domoradzki et al., 2006) and are excreted by air-breathing organisms via the lungs, owing to their high volatility. Their behaviour in aquatic food webs is, therefore, potentially complex. Of particular interest is the debate about the propensity of cVMS materials to biomagnify. Powell et al. (2009) have reported that lipid-normalised cVMS concentrations in aquatic organisms sampled from Lake Pepin (Minnesota, USA), a freshwater lake on the Mississippi River, decreased with increasing trophic level (assigned using stable isotope analysis).

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There is a need to improve our understanding of how these materials behave in order to evaluate any environmental risks posed by their use. The objective of this work was to explore the environmental behaviour of three cVMS compounds: (octamethylcyclotetrasiloxane (D4), decamethylcyclopentasiloxane (D5) and dodecamethylcyclohexasiloxane (D6)) in the Inner Oslofjord (Norway) using a bespoke dynamic (time explicit) non-equilibrium multimedia fate and transport model. We also investigate the fate of these compounds in the pelagic food web using a dynamic food web model, in order to evaluate their potential for trophic transfer.

2. Exposure model

We employed the dynamic fugacity-based Oslofjord POP Model (OPM: Breivik et al., 2003, 2004) which was developed from the steady-state QWASI model (Mackay et al., 1983a,b) specifically for representing processes in the Inner Oslofjord (surface area approximately 191 km²: Ruud, 1968). It considers a number of different interconnected aquatic compartments representing the two

main basins of the inner fjord (Vestfjorden and Bunnefjorden: Fig. 1). Each basin is represented by three compartments (each of which, in turn, is composed of water and sediment) which are shown schematically in Fig. 1 with the following mean depth ranges: W1 and W4 (0–20 m); W2 and W5 (20–50 m); W3 and W6 (≥ 50 m). However, it is recognised that there are parts of the deepest compartments which greatly exceed 50 m. The Bunnefjorden has a maximum depth of ca 164 m and the Vestfjorden has a maximum depth of ca 160 m. Water fluxes between freshwater and the coast and between the marine compartments (Fig. 1b) were derived by NIVA, the Norwegian Institute for Water Research (Bjerkeng, 1994). Sediment transfer and organic carbon dynamics were constructed for the inner fjord by Breivik et al. (2003). Salient model parameters are reproduced in the Supplementary Information (Table S1). It should be noted that in the model runs presented in this report no ice cover was assumed. Whilst sea ice does form in the coastal areas of the Inner Oslofjord, most of the sea area usually remains ice free.

Degradation rates in water are expressed in the OPM as bulk half lives. However, hydrolysis (the only aquatic degradation

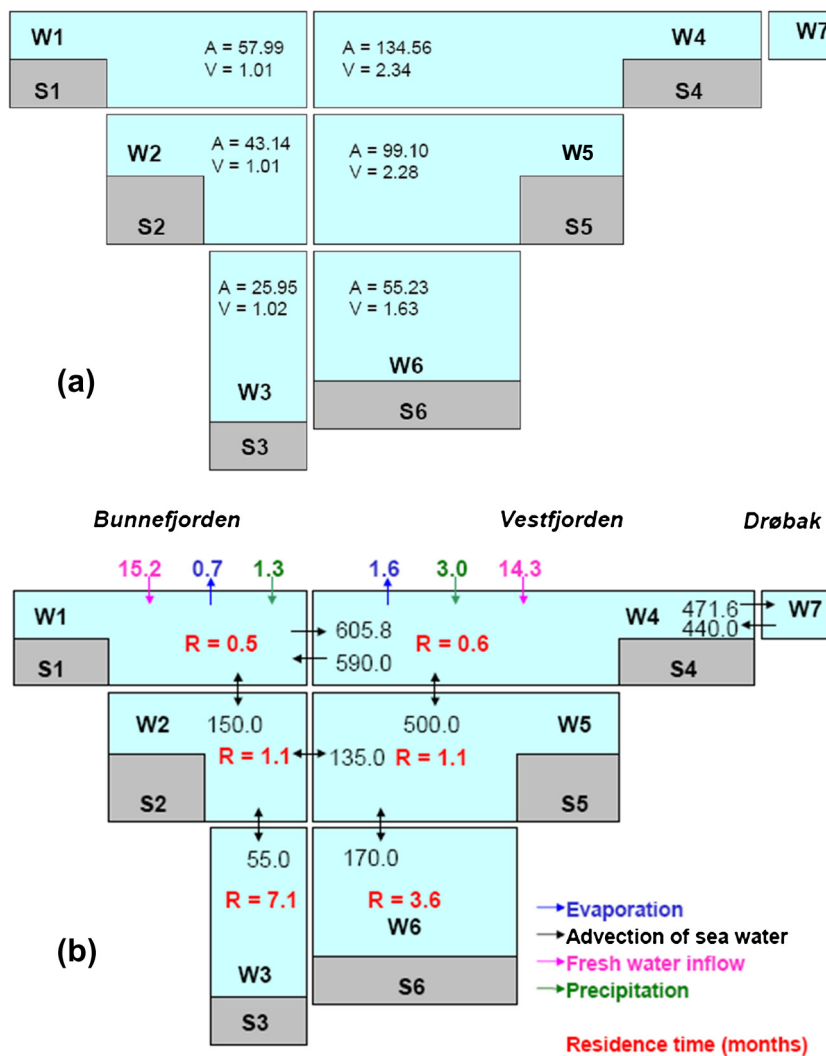


Fig. 1. Schematic representation of the inner Oslofjord in the OPM (from Breivik et al., 2003) showing (a) the area and volume of each compartment and (b) the long term average water balance. A is the surface area of each water compartment in km². V is volume in km³. W1, W2 and W3 are in the Bunnefjorden. W4, W5 and W6 are in the Vestfjorden. W7 represents the outer fjord. S represents the sediment associated with each water compartment. R is the mean residence time of each compartment (months). Water flux estimations are in m³ s⁻¹.

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