



# Simulated use and wash-off release of decamethylcyclopentasiloxane used in anti-perspirants



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## ABSTRACT

The cyclic volatile methylsiloxane, decamethylcyclopentasiloxane (D<sub>5</sub>) is used in a large variety of personal care products. Based on the physical–chemical properties of D<sub>5</sub>, it is likely that losses due to volatilisation may strongly influence the levels entering the aquatic environment. The aim of this study was to quantify the amount of D<sub>5</sub> in waste wash water, after typical application and use in a range of deodorant and anti-perspirant (AP) products. Results implied significant losses after a 24 h period (>99.9%), and suggest that the use of D<sub>5</sub> in leave-on products, such as deodorants/AP is not likely to contribute a significant down-the-drain emission source. An illustrative example is presented, based on data reporting the use of D<sub>5</sub> in a range of personal care products (both wash-off and leave-on), which suggests that the contribution of D<sub>5</sub> used in wash-off products to the aquatic environment may be considerably more significant. Limitations associated with our understanding of the actual D<sub>5</sub> inclusion levels in the products, the market share of the products containing D<sub>5</sub>, and the variability of consumer habits, are identified as data gaps that need to be addressed in order to better refine down-the-drain emission estimates.

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## 1. Introduction

Cyclic volatile methylsiloxanes (cVMS), which are defined as volatile, low-viscosity silicone fluids consisting of ((CH<sub>3</sub>)<sub>2</sub>SiO)<sub>x</sub> structural units in cyclic configuration, where *x* = 3, 4, 5, 6, etc., are the most widely used type of silicone in personal care products (PCPs) (Reisch, 2011). In a recent Canadian survey it was reported that decamethylcyclopentasiloxane, or D<sub>5</sub>, is the dominant cVMS ingredient in PCPs, with concentrations observed at 680 mg g<sup>-1</sup> in an antiperspirant (AP) product (Wang et al., 2009). Given recent concerns regarding the environmental fate of D<sub>5</sub>, as highlighted by its proposed designation as persistent and bioaccumulative (EC/HC, 2008), assessing the use and potential release to the environment is important for better understanding its environmental safety. Risk assessments performed by both Environment Canada and the UK Environment Agency provide detailed information related to the manufacture and use of D<sub>5</sub> in Canada and the UK/EU, respectively (EC/HC, 2008; Brooke et al., 2009). Based on these risk assessments, the use of D<sub>5</sub> in PCPs, such as skin creams, deodorants/AP, liquid soaps, shampoos and conditioners represent the most important vectors for environmental release (EC/HC, 2008; Brooke et al., 2009).

Predicting the use of PCPs by consumers and potential human exposure to a chemical ingredient has evolved to encompass

increasingly complex exposure scenarios (Boyce and Garry, 2002). Recent activity, for instance, has aimed at developing a thorough understanding of the routes and magnitudes of chemical exposures that consumers might experience as a result of using a wide range of PCPs, information that can then be used to better quantify consumer risks associated with a chemical exposure through the use of PCPs (Hall et al., 2007). Modelling techniques have thus evolved from simple deterministic analyses to more detailed probabilistic analyses that can accommodate statistical distributions of input parameters (Boyce and Garry, 2002; Hall et al., 2007; McNamara et al., 2007; Cowan-Ellsberry and Robison, 2009; Wu et al., 2010).

While the development of improved models for assessing human exposure to chemicals used in PCPs and risk have been rapidly evolving, efforts to combine human exposure information with our understanding of environmental exposure of chemicals used in PCPs has not necessarily developed to the same extent. For instance, the main route of emission into the environment for chemicals used in PCPs is typically via the domestic waste water treatment (WWT) system, with these substances being commonly referred to as “down-the-drain” chemicals. As an initial screen, the predicted environmental concentration (PEC) at the effluent discharge source, for chemicals used in PCPs, is estimated based on their inclusion levels and the domestic per capita consumption of the product and estimated population, adjusted for removal in sewage treatment (Keller et al., 2007). This approach thus assumes 100% of the chemical is discharged down-the-drain, and is based

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on the wide dispersive use EU Technical Guidance Document (TGD) detergent scenario (IC5/UC9). Under this emission scenario, after cleaning of the substrate, the cleaning solution is discharged with the waste water such that 100% of the product ingredients enter the WWT system (EC, 2003).

The assumption that all chemicals used in PCPs will have a similar environmental release, however, fails to consider how the physical–chemical properties of the substance will influence the fraction that will be discharged, and consequently may greatly over-estimate the PEC and therefore environmental exposure. Verdonck et al. (2005), for instance, note that volatility is a critical parameter for the exposure assessment, particularly for highly volatile substances, and further identify that the key parameters influencing an environmental risk assessment, on the exposure side, will be tonnage, release scenario, biodegradability, the octanol–water partition coefficient, and volatility. Consequently, the use of  $D_5$  in a wide variety of PCPs and its unusual physical–chemical properties provide a unique opportunity to assess the potential relationship between consumer use of products containing  $D_5$  and its environmental release. For instance,  $D_5$  is known to be both highly volatile and hydrophobic, two parameters identified as being important in estimating environmental exposure (Verdonck et al., 2005). Thus its use in PCPs, described as either leave-on, such as skin creams, deodorants/AP, and wash-off, such as liquid soaps, shampoos and conditioners, combined with its unique properties may greatly influence the total amounts being discharged down-the-drain. Given that the percent inclusion levels of  $D_5$  in PCPs is reported as highly variable and that dermal absorption potential is estimated to be relatively low (Reddy et al., 2007; Horii and Kannan, 2008; Wang et al., 2009), our ability to quantify how consumers use PCPs containing  $D_5$  in relation to the potential fraction that might be discharged down-the-drain would help reduce uncertainty in the PEC estimate used in an environmental risk assessment.

The primary objective of this study was to quantify the amount of  $D_5$  in waste wash water, after typical application and use of a range of leave-on deodorant/AP products. The products include a range of application matrices (spray, soft-solid, and stick) and application rates were representative of typical EU applications (Hall et al., 2007). Variability and uncertainty regarding application rates and how they influence our understanding with respect to estimating total amounts entering a WWT system is further investigated based on a qualitative evaluation of consumer use of  $D_5$  containing PCPs.

## 2. Methods

The application and wash off studies were carried out by a total of six participants (P1–P6, all male), between 28 July and 28 August, 2009. The deodorant/AP test items (T1–T5) were applied to the axilla with applicator weights (before/after), time of application and participant recorded.

### 2.1. Reagents and chemicals

Decamethylcyclpentasiloxane ( $D_5$ ) standard was purchased from Sigma–Aldrich (>98% w/w purity, Gillingham, UK). The internal standard used in the study was  $^{13}C_5$ -decamethylcyclpentasiloxane ( $^{13}C_5$ - $D_5$ ), synthesised by Moravek Biochemicals (>99% pure, Brea, CA, USA). Acetone was glass distilled grade and purchased from Rathburn Chemicals (Walkerburn, UK). Ultrapure water was obtained from a Milli Q Plus® system (Millipore, Watford, UK).

Aqueous solution preparation for headspace was carried out in a clean air cabinet (Big Neat, Waterlooville, UK) in order to

minimise potential background problems due to  $D_5$  in the air (Kierkegaard and McLachlan, 2010; Sparham et al., 2011). The glassware and caps for the headspace work were obtained from Kinesis Solutions (St. Neots, UK). These comprised 20 mL headspace glass vials (actual volume 21 mL) with 20 mm butyl/PTFE crimp caps. Both the vials and caps were used as received, without any pre-treatment. Shower gel used throughout the study was purchased off the shelf in the supermarket and was observed to contain no residual  $D_5$ .

### 2.2. Amount of test item applied

The following rationale was used for application of test items. Accurate weights of products before and after application were recorded to enable the weight of material applied to be calculated.

#### 2.2.1. Test item 1 (T1) (soft solid)

A leaflet supplied with the product recommended the dose for each underarm to be 2 clicks of the product applicator (assuming the product has been primed i.e. the dial rotated several times to expose product on the surface of the applicator). The amount of product dispensed following these procedures was shown to be equivalent to 0.4 g per axilla, or approximately 0.2 g of  $D_5$ , based on measured inclusion level. In order to ensure a clean surface prior to application, the applicator was primed by wiping a few times on a tissue and the collected material discarded.

#### 2.2.2. Test item 2 (T2) (aerosol)

Data obtained from Hall et al. (2007) for deodorant/AP spray exposure ranged between a P50 value of  $3.153 \text{ g d}^{-1}$  to a P90 value of  $6.095 \text{ g d}^{-1}$ . After homogenisation of the aerosol contents, achieved by shaking the can, a 2 s spray was chosen as a target to deliver approximately 1.7 g of product per axilla (equivalent to 0.12 g  $D_5$ ).

#### 2.2.3. Test item 3 (T3) (stick) – test item 4 (T4) (stick) – test item 5 (T5) (stick)

The figures obtained from Hall et al. (2007) for antiperspirant non-spray exposure ranged between a P50 value of  $0.820 \text{ g d}^{-1}$  and a P90 value of  $1.509 \text{ g d}^{-1}$ . A target application of 0.7 g per axilla was therefore used (equivalent to approximately 0.2 g  $D_5$ ). On each day of application the stick was primed by wiping a few times on a tissue and the collected material discarded. This ensured exposure of a clean surface. The stick was applied to the axilla in a wiping up and down motion (6 wipes total).

### 2.3. Application and wash off of products over 24 h

The test items were applied as described in Section 2.2, above. The product was worn for a period of 24 h without washing. Each participant washed each axilla separately (starting with the left) using 1 mL of shower gel, applied thoroughly to the axilla (time not recorded but allowing thorough contact). The wash water (1 L,  $35 \pm 10 \text{ }^\circ\text{C}$ ), used to thoroughly rinse off the applied shower gel, was collected via a stainless steel funnel in a 1 L Duran placed under the sink (waste pipe disconnected). The volume of water collected was  $1000 \pm 50 \text{ mL}$ . A second wash was carried out in a repeat procedure. The participant was then able to re-apply deodorant/AP to commence another 24 h testing cycle.

To avoid cross-contamination between samples, the sink was flushed with copious amounts of water. Separate sinks were used for the first and second wash samples. To monitor for background levels of  $D_5$  in experiments, sink blank samples were taken by washing 1 mL of shower gel into a 1 L Duran as described above. To assess the potential for  $D_5$  residues on shirts worn by participants, the axilla area of selected shirts worn during the 24 h period

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