



Evaporation of decamethylcyclpentasiloxane (D5) from selected cosmetic products: Implications for consumer exposure modeling



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ABSTRACT

Consumer exposure to leave-on cosmetics and personal care products (C&PCPs) ingredients of low or moderate volatility is often assumed to occur primarily via dermal absorption. In reality they may volatilize from skin and represent a significant source for inhalation exposure. Often, evaporation rates of pure substances from inert surfaces are used as a surrogate for evaporation from more complex product matrices. Also the influence of partitioning to skin is neglected and the resulting inaccuracies are not known. In this paper we describe a novel approach for measuring chemical evaporation rates from C&PCPs under realistic consumer exposure conditions. Series of experiments were carried out in a custom-made ventilated chamber fitted with a vapor trap to study the disposition of a volatile cosmetic ingredient, decamethylcyclpentasiloxane (D5), after its topical application on either aluminum foil or porcine skin in vitro. Single doses were applied neat and in commercial deodorant and face cream formulations at normal room (23 °C) and skin temperature (32 °C). The condition-specific evaporation rates were determined as the chemical mass loss per unit surface area at different time intervals over 1–1.25 h post-dose. Product weight loss was monitored gravimetrically and the residual D5 concentrations were analyzed with GC/FID. The release of D5 from exposed surfaces of aluminum occurred very fast with mean rates of 0.029 mg cm⁻² min⁻¹ and 0.060 mg cm⁻² min⁻¹ at 23 °C and 32 °C, respectively. Statistical analysis of experimental data confirmed a significant effect of cosmetic formulations on the evaporation of D5 with the largest effect (2-fold decrease of the evaporation rate) observed for the neat face cream pair at 32 °C. The developed approach explicitly considers the initial penetration and evaporation of a substance from the *Stratum Corneum* and has the potential for application in dermal exposure modeling, product emission tests and the formulation of C&PCPs.

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1. Introduction

Evaluation of the risk induced by chemical exposure due to the use of consumer products requires the assessment of chemical intake via multiple routes. In the case of leave-on cosmetics and personal care products (C&PCPs) intended for daily contact with the skin, dermal absorption of their ingredients is intuitively assumed to be the dominant exposure route. However, after topical application a volatile ingredient in C&PCPs may evaporate into the surrounding air, so that a smaller amount enters the body via the dermal route (Boman and Maibach, 2000), but more is available for inhalation (Girman et al., 1987; Kemmlein et al., 2003; Wang et al., 2009; Xu and Little, 2006). Meanwhile, the released vapor may deposit on the skin and become available

for secondary dermal uptake (Weschler and Nazaroff, 2013). Understanding the emission of volatile substances from consumer products is therefore essential for predicting and mitigating residential air concentrations, as well as for accurate quantification of exposure via different routes. Furthermore, knowledge about the evaporation kinetics of a chemical is needed for environmental fate modeling (Hodgson et al., 2003; Maddalena et al., 2011; Montemayor et al., 2013).

The transport of substances after application or deposition on the skin is governed by two processes: first, by the evaporation from the skin and, second, by the diffusion into the upper layer of the epidermis, the *Stratum Corneum* (SC). During the initial phase the evaporation of a pure compound occurs from a liquid film formed on the skin surface. In this phase, the key factors impacting the evaporation rate are the ambient air temperature and the velocity of the air over the skin surface (Gmehling et al., 1989; Wang et al., 2011). However, after complete evaporation of the substance in the liquid film, the remainder in the SC may diffuse back and evaporate as well. In this phase, the balance between the evaporation and diffusion through the skin into the systemic circulation is largely influenced by its partitioning into the SC intercellular lipids and by protein binding, thus determining the residence time of a substance in the skin (Miselinicky et al., 1988; Yagi et al., 1998).

Abbreviations: BP, biphenyl; C&PCPs, cosmetics and personal care products; D5, decamethylcyclpentasiloxane; GC/FID, gas chromatography with flame ionization detector; HBSS, Hank's Balanced Salt Solution; HEPES, 4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid; M4Q, tetrakis (trimethylsiloxy)-silane; PBPK model, Physiologically Based Pharmacokinetic model; SC, *Stratum Corneum*; SPE, solid phase extraction; THF, tetrahydrofuran; VOCs, volatile organic compounds.

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For a worst-case assessment of inhalation exposure only (e.g. for comparison to lung-related toxicological endpoints) it can be assumed that the rate of evaporation in the initial phase represents the upper bound compared to the evaporation from skin itself. However, if the goal is to achieve a more realistic exposure estimate, it is important to account for the temporal sink effect of the SC. Such a system can be described more accurately by using two distinct rate constants describing the evaporation of the substance from the liquid film and from the SC. While for many substances both evaporation rates can confidently be predicted with e.g. QSARs incorporated in the IH SkinPerm model (Tibaldi et al., 2013), highly lipophilic compounds with $\log K_{ow} > 6.0$ lie outside the model's applicability domain and the development of other reliable (experimental) methods would be beneficial.

The disposition of volatile organic compounds (VOCs) after dermal application has been studied in the past (Gilpin et al., 2009; Kasting et al., 2007; Pendlington et al., 2008). Acknowledging the fact that consumer products designed for topical applications are usually complex and often non-aqueous systems containing multiple ingredients, researchers attempted to investigate the influence of the formulation on dermal absorption (Reifenrath and Robinson, 1982; Saiyasombati and Kasting, 2003) and evaporation (Nihl et al., 2009; Vuilleumier et al., 1995) for a range of VOCs. Several studies were also conducted for decamethylcyclopentasiloxane (D5) (Jovanovic et al., 2008; Koini et al., 1999; Reddy et al., 2007; Wang et al., 2011), a highly lipophilic ($\log K_{ow} = 8.0$) and volatile ($P = 33$ Pa at 25 °C) compound that is incorporated into a variety of C&PCPs as a carrier solvent and emollient (Dudzina et al., 2014; Horii and Kannan, 2008; Wang et al., 2009). However, despite the fact that the respective experiments were all designed to mimic realistic application of C&PCPs, their results vary largely, indicating the need of more consistent research.

This paper presents a novel approach for measuring evaporation rate constants of C&PCP ingredients in a controlled environment, using D5 as a worked example. Both the neat substance and two commercial C&PCP formulations (i.e. deodorant/antiperspirant and moisturizing face cream) were applied to aluminum foil in order to investigate the effect of the product matrix on substance evaporation. To accurately estimate the rate constants from liquid film and SC, finite doses of neat D5 were applied on the aluminum and full-thickness porcine skin *in vitro*, respectively. Special care was taken to ensure a good recovery by minimizing the sink effect in the test chamber (Salthammer, 2004). The experimental results were evaluated in the context of a multi-route consumer exposure assessment by estimating the worst-case and realistic inhalation exposures to D5 after normal use of C&PCPs.

2. Material and methods

2.1. Experiments

2.1.1. Chemicals

Decamethylcyclopentasiloxane (D5; purity >97%), tetrakis (trimethylsiloxy)-silane (M4Q; purity 97%) and biphenyl (BP; purity 99%) were purchased from Sigma Aldrich Germany Ltd. Organic solvents *n*-hexadecane (purity >99.8%; Sigma Aldrich Germany Ltd), *n*-hexane (purity 96%; Scharlab S.L. Spain), methanol (purity ≥99%; Sigma Aldrich Germany Ltd), anhydrous tetrahydrofuran (THF; purity 99%; Acros Belgium), and dichloromethane (DCM; purity >98%;

stabilized; Sigma Aldrich Germany Ltd.) were all of reagent grade. Individual stock solutions of analytes (D5, M4Q and BP) in *n*-hexane as well as their standard mixtures were freshly prepared weekly and stored in air-tight glassware at 4 °C. Deodorant and face cream formulations (Section 1 in the Supplementary Information (SI)) were purchased from a retail store in Utrecht, the Netherlands in 2012 and analyzed for D5 content using the method described in Dudzina et al. (2014). The measured mean concentrations were 426 ± 23 mg/g and 249 ± 11 mg/g for deodorant and face cream, respectively.

2.1.2. Evaporation rates measured gravimetrically

For a comparison with earlier evaporation studies (Koini et al., 1999; Reddy et al., 2007) evaporation rates of pure D5 were measured gravimetrically under similar experimental conditions (see Table 1). Hence, 80 μ L and 350 μ L of neat substance were applied with a micropipette on Petri dishes (diameter = 7.5 cm) covered with filter paper (Schleicher & Schuell AG, Switzerland) of the same diameter and placed on analytical scales (Mettler Toledo, Germany; model AT460 Delta Range, $\sigma = 0.1$ mg/1 mg) in a draft free environment. The ambient air temperature fluctuated between 22.8 °C and 23.5 °C. Every five minutes within half an hour the sample weight was recorded. Additional experiments with aluminum foil were conducted to investigate the retention properties of the filter paper.

2.1.3. Evaporation rates determined from the experiments in the ventilated chamber

Evaporation of D5 was studied in a custom-designed chamber (Fig. 1) under atmospheric pressure. The evaporation vessel was a standard, three-neck glass flask of 250 mL volume. A pure nitrogen flow of 1 L/h continuously flushed the system through perforated polypropylene tube to maintain typical indoor air exchange rate of 4 times/h (Bremmer et al., 2006a; United States Environmental Protection Agency (US EPA), 2011). The gas outlet orifice was positioned 4 cm above the sample surface. A solid phase extraction (SPE) cartridge containing 80 mg of Isolute ENV+ sorbent (hydroxylated polystyrene-divinylbenzene copolymer, purchased from Biotage AB, Uppsala, Sweden) was installed to capture the emitted D5 vapor outflow. Prior to the actual experiments SPE cartridges underwent efficacy testing, showing on average 98% trapping efficiency. More details on the experimental setup are provided in Section 2.1 of the SI.

The evaporation rate of neat D5 from a liquid film on the exposed surface was determined using round aluminum cups of diameter $d = 1.7$ cm that were placed in the center of the evaporation vessel on a glass vial (see Fig. 1). The borders of the cups were ~3 mm in height. Before each experiment the mass of the empty aluminum cup was recorded to allow for the gravimetric determination of the D5 mass loss. Formulated D5 was applied with a spatula to the outer side of the bottom-up cups and spread to cover the entire surface using a flat bottom of a clean glass vial. The substance's volatilization from SC was examined using full-thickness porcine skin. Tissue preparation and handling was carried out whenever possible in accordance with the technical guidance on testing of chemicals' skin absorption *in vitro* (Organisation for Economic Co-operation and Development (OECD), 2004). Skin sections of the outer region of the pig's ears obtained from two female and one male 6–7 months-old pigs were depilated and cut post mortem using an ethanol-sterilized scalpel. Subcutaneous fat was

Table 1
Evaporation rates of pure D5 determined in various gravimetric experiments.

Study	Surface	Amount-to-surface ratio, mg/cm ²	Air flow	Ambient temperature	Evaporation rate, mg cm ⁻² min ⁻¹
(1) Reddy et al. (2007)	Filter paper on Petri dish	7.59	Draft-free	22 °C	0.071 ± 0.027
(2) Koini et al. (1999)	Filter paper on Petri dish	1.62	Draft-free	25 °C	0.016
This study, replication of (1)	Filter paper on Petri dish	7.56	Draft-free	23 °C	0.010 ± 0.002
This study, replication of (2)	Filter paper on Petri dish	1.73	Draft-free	23 °C	0.012 ± 0.004
Additional study	Aluminum circle on Petri dish	7.56	Draft-free	23 °C	0.013 ± 0.002

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