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Determination of the sorption and desorption kinetics of perfume raw materials in the liquid phase with vesicular dispersion: Application of SIFT-MS

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HIGHLIGHTS

- ▸ Dynamic behavior of perfume raw materials (PRMs) and surfactants is studied.
- ▸ Coumarin, hexyl acetate and octanal are used as PRM.
- ▸ Diethyl ester dimethyl ammonium chloride (DEEDMAC) is used as surfactant.
- ▸ Selected ion flow tube mass spectrometry (SIFT-MS) is used as measuring technique.
- ▸ Sorption and desorption coefficients are determined for PRM.

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ABSTRACT

Perfume raw materials such as coumarin, hexyl acetate and octanal are used in domestic fabric softeners together with cationic quaternary ammonium surfactants during the last rinsing step of a wash cycle. Selected ion flow tube mass spectrometry (SIFT-MS) is used to analyze the gas phase concentration of these perfume raw materials in an experiment, mimicking this rinsing step when fabric softeners are applied together with a vesicular diethyl ester dimethyl ammonium chloride (DEEDMAC) dispersion in a bubble column. A continuous stirred tank reactor (CSTR) model is proposed to obtain sorption and desorption kinetics for the mass transfer between the liquid phase and the vesicular dispersion from experimental gas phase concentration data. Sorption coefficients of $(4.8 \pm 0.3)\ 10^{-3}$, $(9.4 \pm 0.1)\ 10^{-3}$ and $(4.0 \pm 0.1)\ 10^{-3}\ s^{-1}$ are obtained for coumarin, hexyl acetate and octanal. Desorption coefficients for these components are respectively reported as $(5.4 \pm 0.6)\ 10^{-5}$, $(1.8 \pm 0.1)\ 10^{-5}$ and $(3.5 \pm 0.2)\ 10^{-5}\ s^{-1}$. From an engineering point of view, SIFT-MS is considered to be a promising experimental technique to evaluate the dynamic behavior, i.e., the sorption and desorption kinetics, of molecules in a vesicular dispersion using the proposed CSTR model.

1. Introduction

Vesicles consist of one or multiple surfactant bilayer shells surrounding an aqueous core. Because of the amphiphilic character of the vesicle bilayer, they have been used as delivery systems for solutes of low water solubility. In medicine, examples of lipophilic and amphiphilic drugs loaded into vesicles are porphyrins, amphotericin B, minoxidil, peptides and anthracyclines [1]. In cosmetics, vesicles are of interest for their resemblance to the lipid barrier of the skin and they are mainly intended for the delivery of encapsulated active ingredients. Since the surfactants are well hydrated, they can also be the active ingredients themselves that reduce dryness of the skin, which is the primary cause of its aging [1]. In general, the rules for topical drug applications and delivery of other compounds are less stringent than the ones for parenteral administration. Hence, vesicles have also great potential in dermatology [2,3]. In the agro-food industry, an example can be found in cheese fermentation processes in which encapsulated enzymes may shorten the fermentation time by 30–50% and improve the quality of the product by spatial and temporal release of the enzymes as well as their protection against chemical degradation [4,5]. Next to cosmetic and agro food applications, there is a large number of studies of the interaction between DNA and different cationic surfactant systems, lipid vesicles and liposomes, because of its

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