Radial diffusion model for fragrance materials: prediction and validation

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March 11, 2021

Abstract

A predictive model based on Fick's second law for radial diffusion is proposed and validated for modeling the diffusion of fragrances. A pure component, two binary systems, and a ternary system were used for validation. The model combines the prediction model to represent the liquid phase non-idealities, using the UNIFAC group contribution method, with the Fickian radial diffusion approach. The experimental headspace concentrations were measured in a diffusion chamber using the solid-phase microextraction (SPME) technique and quantified using gas chromatography with a flame ionization detector (GC-FID). The numerical solutions were obtained along with an analytical model considering constant surface concentration. The odor intensities of the studied systems were calculated using Stevens' power law and the strongest component model, respectively. The numerical simulation presented good adherence to the experimental gas concentration data. The proposed methodology is an efficient and validated tool to assess the radial diffusion of fragrance and volatile systems.

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