Abstract

Perfumes and fragrances are widely incorporated into our daily lives from the use of scented personal care products to household cleaning supplies. Constructing fragrance mixtures may seem simple enough to do at home by mixing various essential oils and alcohol, without the need to study the scientific background behind it. However, in reality, the formulation of desirable fragrance mixtures is a complex field of scientific study that requires the understanding of chemical engineering and thermodynamic principles. Such knowledge can help synthesize longer lasting scents, predict the fragrance performance of the mixture and its components, and convert them into perceived sensations for the consumers. Each component in the multicomponent mixture has a different physicochemical property, and the interactions that occur within the mixture must be considered. The odorant-odorant interaction, the odorant-matrix interaction, and odorant-substrate interaction may all need to be researched for an optimal quality of fragrance. In this thesis, mathematical models were developed and simulations were performed using COMSOL Multiphysics in order to study the diffusion profiles and odor intensities of binary mixtures. This thesis contributes to the field as a fundamental proof-of-concept that has the potential to be extended to simulate higher component fragrance mixtures and to be a predictive tool that can be used simultaneously with experiments. Three different binary mixtures' headspace and receptor chamber concentration surface profiles, concentration line profiles, and flux profiles were mathematically modeled and simulated. The effects of varying diffusion coefficients and composition of the mixtures were also studied, and the odor intensity model was applied to convert diffusion into perceived sensations.