INVESTIGATION OF EVAPORATION AND TRANSPORT OF PERFUME INGREDIENTS IN AIR WITH COMPUTER SIMULATION USING COMSOL MULTIPHYSICS AND COSMOtherm

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Nowadays the computer assisted simulation is a well used alternative in studying of transport phenomena for the researchers and industrial specialists. Although the computer assisted simulation is faster than classical experiments, in most cases a control of reliability is necessary.

The evaporation rate of a multi-component system is governed by the rate of diffusion of molecules from the surface. The particle flux at the surface (according to Fick's first law) depends on the diffusion coefficient and the concentration gradient of molecules in the gas phase over the surface. The gas phase concentration is over the liquid phase is determined by the vapor-liquid equilibrium:

$$c_i = \frac{P_i}{RT} = \frac{y_i \cdot P}{RT} = \frac{x_i \cdot \gamma_i \cdot P_i^{\Theta}}{RT}$$

where x_i, γ_i and P_i^{Θ} are the mole fraction, activity coefficient and vapor pressure of component *i,* respectively. However, due to the mass transfer, the liquid phase composition and the activity coefficients of the components and therefore their concentration and concentration gradients in the gas phase are permanently changing during the evaporation.

We investigated these complex processes iterative by computer simulation in MATLAB environment. The activity coefficients of the components in the liquid phase and the vapor-liquid equilibrium were estimated by the COSMOtherm program, which is based on COSMO-RS theory of interacting molecular surface charges computed by quantum chemical methods. The diffusion coefficients of the perfume ingredients were calculated according to the method of Wilke and Lee.

The nonsteady state transport of perfume ingredients in the gas phase were predicted using a dynamic approach, where the external transfer processes are described by the continuity equation

$$\frac{\partial c_i}{\partial t} + \nabla\left(-D\nabla c_i + uc_i\right) = 0$$

solved by the computer program COMSOL Multiphysics.

The simulations for the permanently changing boundary and initial conditions have been resulted in the concentration gradients and concentration profiles of the molecules.