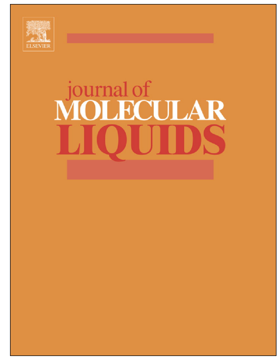

A compositional model based on SAFT-VR and Maxwell-Stefan equations for pervaporative separation of aroma compounds from aqueous solutions

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A compositional model based on SAFT-VR and Maxwell-Stefan equations for pervaporative separation of aroma compounds from aqueous solutions

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Abstract

In this study, the SAFT-VR equation of state combined with the Maxwell-Stefan theory was employed to develop a mass transfer model for the pervaporation process. For this purpose, the SAFT-VR equation of state was used for thermodynamic modeling of the sorption step as one of the main steps of the mass transfer in the pervaporation process and the Maxwell-Stefan theory was applied to describe the transport of permeating compounds through the membrane. The Maxwell-Stefan diffusion coefficients were estimated based on the free volume theory. The model was then validated using the experimental data obtained from the sorption and pervaporative separation of volatile aroma compounds like 3-methyl butanal, isoamyl acetate and n-hexanol from their binary aqueous solutions with the polydimethylsiloxane (PDMS) membrane. The proposed model was successfully able to predict the influence of feed aroma concentration and operating temperature on the aroma and water partial fluxes and aroma separation factors. The predicted partial and total fluxes of 3-methyl butanal, isoamyl acetate and n-hexanol aqueous solutions showed good agreement with the measured fluxes at various feed aroma concentrations and operating temperatures. Therefore, the proposed mass transfer model based on the SAFT-VR and Maxwell-Stefan equations satisfactorily described the mass transport in the hydrophobic pervaporation