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Predicting mass fluxes in the pervaporation process using Maxwell-Stefan diffusion coefficients

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Abstract

In the past decades, it has been proven that pervaporation is an effective and energy-efficient membrane process for the separation of liquids that are difficult to separate in classical processes. The demand for new process applications has increased the need for mass transfer simulation methods, considering the interactions between the system components and the influence of process parameters on the permeation fluxes and at the same time requiring as few experiments as possible.

The aim of the study was to find out whether the calculation of mass fluxes of multicomponent fluids based on the system of generalized Maxwell-Stefan equations (GMSE), using Maxwell-Stefan (M-S) diffusion coefficients, performed according to the method recently proposed by A. Kubaczka [Prediction of Maxwell–Stefan diffusion coefficients in polymer - multicomponent fluid systems, Journal of Membrane Science, 470 (2014) 389-398] could meet these expectations. For this purpose, computational experiments were conducted where the predicted molar fluxes, concerning pervaporative dehydration of ethanol and isopropanol with a poly(vinyl alcohol) (PVA) membrane, were compared with the experimental results. Free volume parameters, necessary for determining the self-diffusion coefficients, were estimated according to J.S. Vrentas and Ch.M. Vrentas' method [Predictive Methods for Self-Diffusion and Mutual Diffusion Coefficients in Polymer-Solvent Systems, Eur. Polym. J. 34 (1998) 797-803] using the PRODE database correlations for viscosity and density of the components of the analyzed systems.

Moreover, the study examined the importance and influence of the controversial parameter ξ_{jp}, being the ratio of the molar volume of the solvent jumping unit to the molar volume of the polymer jumping unit, on the achieved permeation fluxes. The correlations derived from the experimental data necessary for their correlation are also given.

The equilibrium concentrations in PVA were calculated by using the modified UNIFAC-FV method.

The results obtained from the computational experiments have confirmed that the proposed method provides accurate predictions of mass fluxes in pervaporation systems.

Keywords

Pervaporation; Diffusion in polymer; Multicomponent mass transfer; Free volume; Maxwell-Stefan

Nomenclature

$[B]$ - matrix function of inverted binary diffusivities, the elements of which are defined by Eq. (4) [s/m^2]

C - total concentration in the system [kmol/m^3]

D_i - self-diffusion coefficient of component i [m^2/s]

D_{0i} -pro-exponential factor (m^2/s)

E^* -activation energy (kJ/kmol)

$Đ_{ik}$ - Maxwell-Stefan diffusion coefficient for pair i-k[m^2/s]

$Đ_{ij}^{o}$ - infinite dilution diffusivity for component i present in trace amounts in component j [m^2/s]

J - molar diffusion flux relative to the molar average velocity [kmol/m^{2}s]

K_{1j}/γ -free volume parameter of component j [m3/(kg K)]