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Transfer mechanism of water, methanol and ethanol by pervaporation as pure substances in zeolites DD3R

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The study of diffusion through nanoporous ceramic membranes is relevant for the improvement of separation techniques in industry. The zeolite Decadodecasil 3R (DD3R) is a pure silica material with a pore window size that allows molecular size exclusion, selective for water permeation and for its separation from other substances of larger molecular size. In this work experimental data for the diffusion of pure substances (water, methanol and ethanol) by pervaporation through a zeolite DD3R membrane, supported on alumina, were modeled in order to identify the mechanism governing the mass transfer in the membrane. For the three substances under study, different mechanisms of mass transport in porous media were analyzed at different conditions of temperature and pressure. The mass transfer model proposed was surface diffusion, modeled by the Maxwell-Stefan equations, with possible contribution either in parallel or in series flow by Knudsen or capillary condensation diffusion. The adsorption and the Maxwell-Stefan diffusivity parameters are given in the literature. The mass transport through the support layers is known to be given as a combination of Knudsen and viscous flow. It was found that the pervaporation of water in the DD3R zeolite membrane corresponds to a surface diffusion mechanism, in a parallel combination with capillary condensation diffusion through about a 5% of the membrane area. Methanol molecular transport is due to Knudsen diffusion in combination with surface diffusion in series. The last takes place in about 55% of the length of de DD3R layer, due to the pressure profile in the layer. Ethanol permeation can be described exclusively by surface diffusion due to its molecular size which implies a strong interaction with the pore surface.

***Keywords**:* DD3R Zeolite; Knudsen diffusion; Maxwell-*Stefan model e*quations; Pervaporation.