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**Effects of polymer hydrophobicity on the diffusivity of water and ethanol in acrylate copolymer gels** FARDIN KHABAZ, SRIRAMVIGNESH MANI, RAJESH KHARE, Texas Tech University — Pervaporation is an energy efficient process for separating dilute alcohol-water mixtures. The efficiency of the pervaporation process is governed by the solubility and diffusivity of the water and alcohol molecules in the polymer. Molecular simulations can be used to provide detailed insights on the dependence of the diffusivity on the molecular structure of the polymer. Polyacrylate systems with varying degree of hydrophobicity are built by changing the relative concentrations of butyl acrylate and 2-hydroxy ethyl acrylate monomers which are hydrophobic and hydrophilic, respectively. In order to create the membrane structure, a random copolymer of these monomers that is cross-linked with pentaerythritol tetracrylate, is obtained using the simulated annealing polymerization technique. The volumetric properties of the systems such as density and glass transition temperature ( $T_g$ ), are compared with the experimental values to validate the model structures. The diffusivity of the water and ethanol molecules inside the membrane is characterized by determining their mean squared displacement (MSD) in systems with varying degree of hydrophobicity and cross-linker concentration. The calculated diffusion coefficients of water and ethanol from simulations will be compared with available experimental diffusion data. The correlation between the diffusivities and the degree of hydrophobicity as well as the molecular packing in these systems will be identified.

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