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Mechanism of Concentration Dependence of Water Diffusivity in Polyacrylate Gels. SRIRAMVIGNESH MANI, FARDIN KHABAZ, RAJESH KHARE, Texas Tech University — Membrane based separation processes offer an energy efficient alternative to traditional distillation based separation processes. In this work, we focus on the molecular mechanisms underlying the process of separation of dilute ethanol-water mixture using polyacrylate gels as pervaporation membranes. The diffusivities of the components in swollen gels exhibit concentration dependence. We have used molecular dynamics (MD) simulations to study the correlation between the dynamics of solvent (water and ethanol) molecules, polymer dynamics and solvent structure in the swollen gel systems as a function of solvent concentration. Three different polyacrylate gels were studied: (1) poly n-butyl acrylate (PBA), (2) copolymer of butyl acrylate and 2-hydroxyethyl acrylate P(BA50-HEA50), and (3) poly 2-hydroxyethyl acrylate (PHEA). Simulation results show that solvent concentration has a significant effect on local structure of the solvent molecules and chain dynamics; these factors (local structure and chain dynamics), in turn, affect the diffusivity of these molecules. At low concentration, solvent molecules are well dispersed in the gel matrix and form hydrogen bonds with the polymer. Solvent mobility is correlated with polymer mobility in this configuration and consequently water and ethanol molecules exhibit slower dynamics, this effect is especially significant in PHEA gel. At high solvent concentration, water molecules form large clusters in the system accompanied by enhancement in mobility of both the gel network and the solvent molecules.

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