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Molecular simulation investigation of the miscibility and structure of binary mixtures containing methanol and ethanol mixed with heptane, hexane, and cyclohexane.[1] ABDALLA OBEIDAT, Jordan University of Science and Technology — Transport properties of methanol and ethanol mixed with heptane, hexane and cyclohexane at 300K have been investigated using molecular dynamics simulations with the aid of the OPLS-AA force field. Calculations were performed at the isothermal and isobaric (NPT) ensemble. Estimation of the diffusion coefficients, velocity autocorrelation functions (VACF), density profile, and radial distribution functions have been predicted for six different mixtures. Self- and Maxwell-Stefan diffusion coefficients, as well as the surface tension of methanol, ethanol, and their hydrocarbons binary mixture are determined using equilibrium molecular dynamics and the Green-Kubo formalism. The transport properties of the fluids are calculated over a fixed temperature at 1-atmosphere and compared to experimental and simulation data from the literature. Our results are helpful to understand the relationship between microscopic structures of fluid and its transport properties in dissolving process between alcohols with hydrocarbons. This work not only provides a reliable simulation method for transport properties of an organic compound, but also provides the prediction data for designing and development of physical processes.

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