Transport Diffusion of a Series of Benzene + Acetone + Alcohol Mixtures Predicted by Equilibrium Molecular Dynamics and Measured by Taylor Dispersion

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Liquids appearing in nature and industrial applications are essentially multicomponent. However, only data on binary diffusion coefficients are relatively abundant because higher order mixtures are significantly more complex. Two different approaches are commonly used to describe multicomponent diffusion in liquids, i.e. Fick's law and the Maxwell-Stefan theory, which both contain different sets of diffusion coefficients. Fick diffusion coefficients are accessible by experiment, but the presence of cross coefficients aggravates the interpretation and data processing in experimental work for multicomponent mixtures. Predictive approaches mostly rely on multicomponent extensions of the Darken ratio to yield Maxwell-Stefan diffusion coefficients, although this approach is only valid for ideal mixtures. In this context, molecular modeling and simulation offers a promising route for predicting transport diffusion coefficients and for understanding the underlying phenomena on a microscopic basis. Equilibrium molecular dynamics simulations and the Green-Kubo formalism can be used to predict Onsager and Maxwell-Stefan diffusion coefficients. Subsequently, the thermodynamic factor has to be used to transform these data to Fick diffusion coefficients. The present study reports diffusion coefficients of ternary mixtures of benzene + acetone + three different alcohols, i.e. methanol, ethanol and 2-propanol, which were investigated on the microscopic scale by molecular dynamics simulation and are compared to results measured by Taylor dispersion experiments. The objective is to investigate a series of ternary mixtures under the perspective of finding common features. Moreover, the relations between multicomponent diffusion coefficients and the binary diffusion coefficients of the subsystems are examined.