

Thermal and Mass Diffusivities of 1-Alcohols Containing Dissolved Gases by Dynamic Light Scattering

M. Kerscher, W. Wu, T. Klein, M. H. Rausch, T. M. Koller, C. Giraudet, and A. P. Fröba

*Institute of Advanced Optical Technologies - Thermophysical Properties (AOT-TP),
Department of Chemical and Biological Engineering (CBI) and Erlangen Graduate School in Advanced
Optical Technologies (SAOT),
Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Germany*
manuel.kerscher@fau.de

Systems based on liquids containing dissolved gases are of interest in many areas of chemical and energy engineering such as separation processes or catalytic reactions. One key property required for the optimum design of corresponding processes is the Fick diffusion coefficient. In a current research project, experimental and theoretical methods are combined to get a fundamental understanding on the influence of the thermodynamic state on the diffusive mass transport in liquids with dissolved gases.

In the present contribution, dynamic light scattering (DLS) experiments were performed at macroscopic thermodynamic equilibrium. Binary mixtures of 1-alcohols with dissolved hydrogen, helium, carbon monoxide, nitrogen and carbon dioxide (CO₂) were studied as a function of temperature and concentration. All 15 binary mixtures were investigated at temperatures between 303 and 423 K and at gas mole fractions below 5%. Binary mixtures consisting of 1-hexanol and CO₂ were studied at CO₂ mole fractions between 0.01 and 0.95 and temperatures from 303 to 353 K. With DLS, the mean lifetime of microscopic fluctuations in temperature and species concentration is analyzed to determine simultaneously thermal and mass diffusivities in an absolute way. The Fick diffusion coefficient could be assessed with typical expanded uncertainties of about 5%. These results serve as reference for the validation of molecular dynamics simulations as well as for developing structure-property relationships. Agreement within combined expanded uncertainties was generally found between the simulated and the experimental Fick diffusion coefficients. Here, effects of the molecular weight and polarity of solutes and solvents as well as the influence of the structural effects at the molecular scale are discussed.