Binary Diffusion Coefficients of Mixtures of n-Alkanes or 1-Alcohols with Dissolved Gases at Infinite Dilution

Wenchang Wu [S], Tobias Klein, Michael H. Rausch, Thomas M. Koller, Cédric Giraudet [C] and Andreas P. Fröba
Institute of Advanced Optical Technologies - Thermophysical Properties (AOT-TP), Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Erlangen, Bavaria, Germany
cedric.cg.giraudet@fau.de

Knowledge on the mutual diffusivities of gases dissolved in liquids is of increasing interest for the optimization of processes such as the Fischer-Tropsch synthesis. Here, mass transfer is often the rate limiting step compared to, e.g., chemical reactions and/or heat transfer. In a related research project, the benefits of experimental and modeling methods are combined to get a better understanding on how molecular diffusion is affected by the characteristics of the mixture components, which contributes to the development of reliable predictions. In the present contribution, dynamic light scattering (DLS) experiments and molecular dynamics (MD) simulations were performed at macroscopic thermodynamic equilibrium. Binary mixtures of n-alkanes or 1-alcohols with dissolved hydrogen, helium, nitrogen, or carbon monoxide were studied at temperatures between 258 and 423 K and at gas mole fractions below 5 %. With DLS, the relaxation behavior of microscopic equilibrium fluctuations is analyzed to determine simultaneously mass and thermal diffusivities in an absolute way. The present measurements document that even for gas concentrations of 0.3 %, reliable binary diffusion coefficients with typical expanded uncertainties smaller than 5 % can be obtained. The influence of the Lewis number on the resolution of temperature and concentration hydrodynamic modes is discussed. The DLS results serve as a database for MD simulations. Here, thermophysical properties are computed by investigating the dynamics of molecules interacting with each other. Based on suitable models for the mixture components, the self-diffusion coefficient of the gas was determined with expanded uncertainties of about 10 %. In agreement with theory, mutual diffusivities and self-diffusivities were found to be equal. The broad range of mass diffusivities of the studied gas-liquid systems covering about two orders of magnitude allows for developing structure-property relationships. Here, effects of the molecular weight and polarity of solutes and solvents are discussed.