Viscosity and Interfacial Tension of Long-Chained Alkanes, Alcohols, and their Mixtures with Dissolved Gases

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Systems based on long linear and branched alkanes and alcohols with dissolved gases are of interest in many areas of chemical and energy engineering, like the synthesis and utilization of fuels or the storage of hydrogen in liquid organic hydrogen carriers. For an efficient process design, reliable information on the transport and equilibrium properties of such systems is required. Especially the viscosity, which governs, e.g., heat, mass, and momentum transfer, and the interfacial tension, which might influence gas-absorption and wetting of surfaces, are important properties.

The present contribution aims to develop a fundamental understanding of the influence of gases dissolved in long linear and branched alkanes and alcohols on the liquid viscosity and interfacial tension. Here, a systematic variation of the chain length, branching, and hydroxylation of the solvent molecules as well as of the molecular characteristics of the dissolved gases, including their dipole moment and molecular mass and size, was performed. Surface light scattering (SLS) experiments, analyzing microscopic surface fluctuations at macroscopic thermodynamic equilibrium, are used to measure the viscosity and interfacial tension close to saturation conditions at temperatures between (298 and 573) K and mole fractions of the dissolved gas below 0.2 with typical expanded uncertainties of 2.5%. The experiments are complemented by and combined with EMD simulations, which are able to access the viscosity and interfacial tension by studying statistical fluctuations on a nanometer scale. The results from SLS are used as a reference for the validation of the EMD simulations, where a major challenge was the identification and development of a reliable force field (FF) applicable up to 573 K. The results from this work are further used for the test and development of models, which allow the prediction of the viscosity and interfacial tension of systems that have not been studied experimentally so far.