Characterization of the Hydrogen Carrier System Based on Aqueous Solutions of Isopropanol and Acetone by Optical and Conventional Techniques

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For the efficient and safe storage and transport of molecular hydrogen (H_2), different types of hydrogen carrier systems are currently discussed. One promising option is the use of hydrogenatable molecules as carriers whose hydrogenated counterparts can reversibly release the bound hydrogen, *e.g.*, in direct fuel cells. For this application, the carrier system based on isopropanol and its dehydrogenated counterpart acetone is discussed. For a stable operation of direct fuel cells, aqueous solutions of isopropanol with a water mole fraction of around 0.96 are used. To optimize the design of such direct fuel cells, accurate thermophysical properties of system-relevant aqueous solutions are required as a function of composition at temperatures up to about 373 K, but only sparsely available.

The present contribution summarizes experimental investigations on viscosity, surface tension, density, and mixture composition of aqueous solutions of isopropanol and acetone using optical and conventional techniques. With the help of surface light scattering (SLS) allowing simultaneous access to viscosity and surface tension, capillary viscometry (CV), and vibrating-tube densimetry, isopropanol, acetone, and their binary and ternary mixtures with water of technically relevant concentrations were characterized between (273 and 403) K. By adding isopropanol and/or acetone to water, a significant increase in viscosity as well as decrease in surface tension and density was observed. To evaluate the liquid-phase composition of mixtures studied by SLS and CV, Raman spectroscopy was employed. In the required calibration procedure using binary mixtures of isopropanol with acetone or water of known composition from (293 to 313) K, the calibration factors were found to be independent of temperature. Further SLS experiments for an aqueous solution with an isopropanol mole fraction of 0.04 showed that dissolved H_2 at saturation pressures up to 7.5 MPa causes no change in viscosity and only a small decrease in interfacial tension.