Thermophysical Properties of Liquid Organic Hydrogen Carriers

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Liquid organic hydrogen carriers (LOHCs) are a promising option for the safe storage and transport of hydrogen with reasonable energy densities. The design and modeling of associated catalytic hydrogenation and dehydrogenation processes as well as the handling of LOHCs require accurate information on their thermophysical properties at process-relevant conditions. For bicyclic hydrocarbon LOHCs being in the focus of this contribution, the availability of such data is limited, especially at high temperatures and in the presence of pressurized hydrogen being dissolved in the liquid phase. A systematic characterization of the thermophysical properties of such LOHC systems like that based on diphenylmethane is challenging since the handled mixtures consist of the unloaded or dehydrogenated component, its fully hydrogenated counterpart, and partially hydrogenated reaction intermediates. This situation is further complicated by the isomerism of polycyclic LOHC systems like benzyltoluene carrying side chains attached to the carbon rings. Furthermore, the combination of individual LOHC systems like diphenylmethane with biphenyl and/or benzophenone is regarded to be of advantage for merging their beneficial characteristics or realizing novel process concepts such as autothermal dehydrogenation. Finally, influences of process-related byproducts such as fluorenes, which also undergo hydrogenation/dehydrogenation cycles, need to be known.

The present contribution summarizes the recent research activities of the institute AOT-TP for characterizing the aforementioned LOHC systems regarding their thermophysical properties such as viscosity, interfacial tension, diffusivities, and density as well as their mixture composition over broad ranges of thermodynamic states by optical and conventional measurement techniques as well as molecular dynamics simulations. The presentation will not only discuss results for pure LOHC components and their mixtures as well as the influences of the degree of hydrogenation, isomerism, process-typical byproducts, and dissolved hydrogen on their properties, but also highlight metrological challenges successfully met on the path to the underlying data.