Key Thermophysical Properties of the Methylcyclohexane/Toluene System as Liquid Organic Hydrogen Carrier

Elisabeth González-Cortés[1], Alejandro Moreau[1], Xavier Paredes[1], Fredy Vélez[1] and M. Carmen Martín[2, S, C]

[1]*University of Valladolid, Valladolid, Spain*
[2]*Research Institute on Bioeconomy, University of Valladolid, Valladolid, Spain*
mcarmen.martin@uva.es

Liquid organic hydrogen carriers (LOCHs) are liquids or low-melting solids that can be reversibly hydrogenated and dehydrogenated at elevated temperatures in the presence of catalyst and the initial structure of the LOHC compound remains the same after the rechargeable hydrogen is released. Their compatibility with existing fuel infrastructure and their capability to store hydrogen without losses even in the long-term or when transported overseas under standard conditions are some of the advantages of these compounds. Candidate vehicular LOHCs need to meet stringent conditions including (i) an acceptable toxicity profile to ensure safety in accidental release such as in automobile collisions, (ii) thermal stability against undesired decomposition pathways, (iii) good biodegradability, (iv) ability to liberate H_2 of sufficient purity for the intended application and return the dehydrogenated product in sufficient purity for multiple recycling, (v) good kinetics for reversible H_2 release, catalyzed as necessary, (vi) cheap manufacture on a global scale, (vii) low melting point, and (viii) good gravimetric and volumetric capacity [1].

The hydrogenation/dehydrogenation reactions can be tuned by controlling various parameters, such as the catalyst, the reactor and reaction conditions. Therefore, thermophysical characterization through density, heat capacity and viscosity and their modelling are needed at different conditions to improve the reliability of designing, developing, optimizing, and deploying these hydrogen storage processes.

Using accurate experimental techniques available in our laboratory, such as a vibrating-tube densimeter, a flow calorimeter, or a falling-body viscometer, the determination of density, heat capacity, or viscosity is performed in wide temperature and pressure ranges. The results for the system methylcyclohexane/toluene will be presented in this work.

Acknowledgments

This work is funded by Spanish State Research Agency project number PID2021-125749OB-I00 and ERDF and Junta de Castilla y León project number CLU-2019-04.

References

1. Askko-Saksa P.T. et al. Liquid organic hydrogen carriers for transportation and storing of renewable energy-Review and discussion. J. Power Sources 396, 803–823 (2018).