Phase-Equilibria of Renewable Fuel Blends, Water, and Additives

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Fuels based on renewable feedstocks are essential for achieving the goal of net-zero carbon dioxide emission in the transportation sector. Promising renewable fuel candidates are poly(oxymethylene) dimethyl ethers (OME), which can also contribute to an emission reduction of other pollutants like nitrogen oxides [1], and hydrogenated vegetable oils (HVO) [2]. Both OME and HVO are potential diesel substitutes and could also be used as OME-HVO blends. One crucial drawback of OME and HVO is that they exhibit a liquid-liquid equilibrium (LLE) at low temperatures or if already tiny amounts of water are present [3], which strongly hampers their applicability in combustion engines.

One possible solution is using additives as solubilizers; however, their influence on the LLE of OME-HVO blends has not yet been systematically studied. Modeling the LLE of these blends is further complicated because both OME and HVO are usually present as complex mixtures that can often not be fully elucidated analytically, which is the prerequisite of using classical thermodynamic approaches.

In the present work, the influence of various fuel additives on the LLE in mixtures of OME-HVO blends with water is systematically explored in a simulation study. For characterizing the OME-HVO blends, the novel methodology of NMR Fingerprinting [4] was used, which enables obtaining information on the composition of unknown complex mixtures in an automated way using standard NMR experiments and machine-learning algorithms. The obtained characterizations were subsequently combined with a novel, hybrid (physics-based + machine-learning) version of UNIFAC [5] for predicting the LLE. Multiple promising additives could be identified in the simulations.

References

1. A. Garcia et al., Fuel 275 (2020) 117989.
2. H. Aatola et al., SAE Int. J. Engines 1 (2009) 1251-1262.
3. C. Breitkreutz et al., Fuel 338 (2023) 127337.
4. T. Specht et al., Magn. Reson. Chem. 1 (2023).
5. F. Jirasek et al., Phys. Chem. Chem. Phys. 25 (2023) 1054-1062.
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