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Modeling and Experimental study of LOHC systems based on toluene mixtures

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Hydrogen is one of the most promising energy carriers on the path toward a decarbonized future, due to its high energy density and clean combustion product. However, the efficient and safe storage of hydrogen remains a major technological challenge. Conventional storage methods are technologically complex, energy-intensive, and costly. A promising solution to overcome these disadvantages is the reversible binding of hydrogen to organic liquids, which enables chemically stable and safe storage (at atmospheric pressure and ambient temperature), while also allowing transportation via tankers, trucks, and pipelines.
In recent years, the applicability of various mono- and polycyclic aromatic compounds (e.g., toluene, n-ethylcarbazole, n-propylcarbazole, dibenzyl-toluene) and noble metal/oxide-supported and transition metal/oxide-supported catalysts has been investigated in LOHC systems. Among the carriers, toluene has been identified as the most suitable based on process parameters, and achievable conversions, while noble metal-based catalysts have proven to be the most favorable in terms of stability and selectivity.
The aim of the research work was to study and model the hydrogenation of toluene–methylcyclohexane mixtures, to analyze the effects of feedstock composition and process parameters, and to determine the optimal process conditions. A kinetic model was fitted to the experimental data, which served as the basis for constructing the reactor model for both hydrogenation and dehydrogenation. In both cases, the models showed a good fit to the experimental results.

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