Dynamic Process Simulation and Kinetic Modeling of Hydrogenation and Dehydrogenation Reactions in LOHC Reactor Systems

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As the demand for safer and more efficient ways to store and release hydrogen grows, Liquid Organic Hydrogen Carrier (LOHC) systems are receiving increasing attention. These systems work by chemically binding hydrogen to an organic carrier, allowing it to be stored and later released when needed. A key example is the reversible reaction between dibenzyl toluene (DBT) and its hydrogenated form, perhydro dibenzyl toluene (DBTH), which has become especially interesting for use in heavy transport applications.

This study presents the development and simulation of a dynamic reactor model for the hydrogenation and dehydrogenation of dibenzyl toluene (DBT). The model is based on a series of experimental runs conducted at different operating temperatures, during which the concentrations of the liquid-phase components were tracked over time to capture the system's dynamic behaviour. These experimental insights were then used to construct a dynamic model capable of replicating the reaction environment, effectively creating a digital twin of the reactor system.

The proposed dynamic model enhances the conventional steady-state approach by incorporating time-dependent mass balance equations within a process simulation environment (Aspen Plus). This allows for the analysis of transient behaviours such as start-up dynamics, changes in feed rate, and the system's response to external disturbances, alongside the integration of a basic control strategy. Model validation was performed by comparing simulation results with corresponding experimental data, showing strong agreement in the predicted molar compositions. Additionally, a sensitivity analysis was carried out to assess the influence of critical parameters, such as catalyst amount and operating temperature, on conversion performance and dynamic reactor behaviour. These findings support the optimization of reactor design by highlighting the most impactful factors.

The simulation model includes not only the dynamic reactor, which is constituted by a cartridge containing the pelletized catalyst, but also the storage tanks, the heat exchangers networks and the purification equipment, providing a general overview of the process design and the equipment required.

The modeling work, carried out under the NACHIP project, confirms the applicability of computational tools for simulating complex LOHC processes and contributes to the development of a reliable framework for designing modular reactors aimed at both mobile and stationary hydrogen applications.

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