

Modeling and evaluation of CO<sub>2</sub>-based Formic Acid Production Process

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Formic acid receives attention from a candidate for chemical hydrogen storage due to its easily decomposing characteristics to hydrogen and CO<sub>2</sub>. The CO<sub>2</sub>-based formic acid production process, which produces formic acid from CO<sub>2</sub> and hydrogen, is being investigated as a sustainable alternative to the conventional formic acid production process. The aim of formic acid purity is 99 wt. % for the utilization of a hydrogen carrier. Notably, the CO<sub>2</sub> hydrogenation reaction occurs in a trickle bed reactor, which has a high complexity of multiphase reaction. In addition, the thermodynamic data of certain components not found in the database are estimated by the group contribution method and the COSMO-RS package. The modeling of the reactor is conducted by MATLAB, and the CO<sub>2</sub>-based formic acid process is evaluated by techno-economic analysis and CO<sub>2</sub> life cycle assessment based on the mass and energy balance of the simulation results.