Advancing Sustainability in Hydrocarbon Production: Breakthroughs in CO_2 Hydrogenation with Iron-Based Catalysts and Comprehensive Life Cycle Assessment of Environmental Impacts

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This study investigates the catalytic activity and environmental impact of Fe-based nano hydrotalcite catalysts, synthesized via ultrasonic-assisted co-precipitation, for Fischer-Tropsch mediated CO_2 hydrogenation (FTS-CO_2). The catalysts evaluated include $Mg_{0.65}Fe_{0.3}Cu_{0.05}$ (Fe30), $Mg_{0.55}Fe_{0.4}Cu_{0.05}$ (Fe40), and $Mg_{0.23}Co_{0.42}Fe_{0.3}Cu_{0.05}$ (Co45), characterized using XRD, ICP-OES, SEM, TEM, BET, and TPR. Co-containing catalysts demonstrated higher catalytic activity and selectivity for heavier hydrocarbons (C7+) at temperatures between 250 and 350°C. Fe30 exhibited approximately 10% higher CO_2 conversion than Fe40 at temperatures below 300°C, primarily producing lighter hydrocarbons. At 300°C, all catalysts achieved a balance between conversion rates and longer-chain hydrocarbon production, reflecting Fischer-Tropsch process goals.

A comprehensive Life Cycle Assessment (LCA) was conducted using SimaPro 9.4 to evaluate the environmental impacts of catalysts production and use. System boundaries encompassed stages from raw material extraction to catalyst preparation and use. The study first assessed the environmental impact of the catalysts' production alone, followed by an evaluation of the entire operational Fischer-Tropsch CO_2 mediated process. Consequently, the functional units were defined as 1 kg of catalyst produced and 1 kg of hydrocarbons produced.

Life cycle inventory (LCI) data were collected from primary sources, such as experimental data from laboratory operations, and secondary sources, such as existing literature and Ecoinvent 3.8 database. Impact assessment methods included Global Warming Potential (IPCC 2013), Cumulative Energy Demand (CED), Acidification Potential, Eutrophication Potential and Human Toxicity Potential (CML-IA).

Results indicated that Co45, despite superior catalytic performance, had higher environmental impacts during production compared to Fe-based catalysts. Fe30, with slightly lower conversion rates, had a more favorable environmental profile due to lower energy and material inputs. The LCA highlighted the trade-offs between catalytic performance and environmental sustainability, emphasizing the need to balance operational efficiency with environmental impact.

This study offers a dual evaluation of Fe-based nano hydrotalcite catalysts, combining experimental performance assessments with detailed LCA. The insights guide future research and optimization to develop sustainable, efficient catalysts for CO_2 hydrogenation, advancing green chemistry and sustainable industrial practices. The findings provide a basis for further exploration to optimize these catalysts, ensuring a balance between high performance and minimal environmental impact.