

# **An Integrated multistep CO<sub>2</sub>-to-Jet Conversion Process Under mild conditions: Experimental Validation and Modular Process Simulation**

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## **Introduction**

Decarbonizing aviation requires scalable synthetic fuel pathways that bypass biomass limitations while enabling full compatibility with existing infrastructure. Power-to-Liquid (PtL) routes based on CO<sub>2</sub> valorisation are emerging as a promising alternative, but novel current approaches remain constrained by energy inefficiencies, limited TRL in some of the possible reaction such as the electrochemical CO<sub>2</sub> reduction (CO<sub>2</sub>RR), and the lack of experimentally validated intermediates downstream of syngas.

In this work, it is presented recent advances in MEA-based CO<sub>2</sub> electrolyzers, and alcohol-to-jet (ATJ) catalytic systems, integrated into a coherent and experimentally supported PtL chain. Within the framework of 4AirCRAFT project (H2020-LC-SC3-2020-NZE-RES-CC), this research introduces a novel cascade route enabling to convert CO<sub>2</sub> into long chain hydrocarbon (jet-fuel-range) under mild conditions.

## **Methodology**

A PtL test bench was developed, considering two core processes: an electrochemical module and biomimetic reaction module.

The electrochemical module consists of a zero-gap MEA (Membrane Electrode Assembly) CO<sub>2</sub>RR cell employing a ZnAl-LDH electrocatalysts operated at 25 °C. This module is responsible for converting CO<sub>2</sub> into carbon monoxide as the primary

intermediate. A specific test bench containing gas conditioning, and online GC quantification enabled the systematic evaluation of GDL configurations, as well as studies of catalyst loading, sealing materials, and overall cell configuration.

In the case of the biomimetic module a cascade ATJ system was experimentally implemented formed by the alcohol dehydration (using both homogeneous TfOH and functionalized-clay heterogeneous catalysts), and olefin oligomerization (using heterogeneous catalysts). Continuous flow reactor design were also evaluated to ensure process scalability.

Finally, all units were integrated into a steady-state digital twin model in COCO Simulator, allowing comprehensive mass and energy balance evaluation of the full PtL concept.

## **Results**

The CO<sub>2</sub>RR cell achieved high Faradaic Efficiencies (FE) for CO production (> 90%) using earth-abundant catalysts, demonstrating stable operation and identifying the influence of sealing and GDL configuration on performance.

Biomimetic dehydration experiments validated both homogeneous and heterogeneous catalytic routes, with activated clays showing promising selectivity and conversion (> 90%) at 150-180 °C. Oligomerization produced jet-fuel-range oligomers with high conversion (> 90%) and long chain selectivity (up to 88%).

Finally, full-process simulation quantified electrical-to-chemical efficiencies, energy bottlenecks, and evaluate the impact of FE current density, conversion, and operating conditions on system performance.

## **Conclusions**

This work demonstrates one of the first experimentally validated and computationally integrated PtL pathways coupling electrochemical CO<sub>2</sub> conversion, and biomimetic ATJ synthesis working under mild conditions. The electrochemical reduction demonstrates the CO<sub>2</sub> reduction to CO can be achieved using earth abundant catalysts in zero-gap configuration. The biomimetic ATJ module confirmed the possibility to perform alcohol dehydration and subsequent oligomerization under mild operational conditions.

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