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HYBRID TANDEM CATALYTIC CONVERSION PROCESS TOWARDS HIGHER OXYGENATE E-FUELS

E-TANDEM - Deliverable report

D2.4 Catalysts and hybrid process for syngas conversion to ether fuels

Publishable summary

The E-TANDEM project develops, and experimentally validates at TRL 4, a process for the direct production of a new higher-oxygenate, diesel-like e-fuel (HOEF). This oxygenated fuel is produced directly from water and CO_2 (as the sole carbon source) using renewable electricity as the only energy input. Process intensification is achieved *via* the tandem integration of catalytic reactions, leveraging *in situ* intermediate processing and "kinetic protection" effects to maximize yields of higher oxygenates. First, a mixture of CO and H_2 (e-syngas produced from CO_2, H_2O, and renewable power) undergoes Fischer-Tropsch (FT) synthesis to yield primarily linear C_{5+} α-olefins, alongside linear paraffins. This step is integrated in a single reactor with the reductive hydroformylation (RHF) of olefins to their corresponding alcohols, lengthening the 1-olefin intermediates by one carbon atom. Prior deliverables of E-TANDEM reported significant milestones, including productivities to higher alcohols ≥ 200 mg g_{metal}^{-1} h^{-1}.

In a particularly preferred realization, the HOEF consists mainly of higher (C_{10+}) aliphatic ethers. As discussed in an earlier report, these compounds exhibit desirable diesel properties for internal-combustion engines: very high cetane numbers (even in excess of 100), adequate flash points, soot suppression, low hygroscopicity compared to alcohols, among others. These higher ethers are obtained by catalytic dehydration of the synthetic higher alcohols.

This report presents lab- and bench-scale results from Task T2.3, "*Catalysts and process for a tandem, direct conversion of syngas to higher ethers*," within WP2, "*Catalysts and Processes for Hybrid Catalytic Conversion of CO_2 and Water to Higher-Oxygenate e-Fuels (HOEF)*." It focuses on the synthesis of higher ethers as major HOEF components and examines the opportunities and limitations of single-pot tandem integration to guide further process intensification.

The results reveal how alcohol chain length and regioisomerism (branched vs. strictly linear) affect dehydration kinetics and selectivity. These factors are critical in the context of the E-TANDEM process, because integrating FT and RHF inevitably produces a complex mixture of higher alcohols (as starting point for ether production) with varying chain lengths (following the Anderson–Schulz–Flory distribution) and both linear and 2-methylated (branched) regioisomers. Additionally, the co-integration of etherification with the syngas-conversion tandem is explored. Based on these findings, a process design is proposed to maximize yields of higher aliphatic ethers.

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Project partners:

#	Partner short name	Partner Full Name
1	CSIC	SPANISH NATIONAL RESEARCH COUNCIL (CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS)
2	MPG	MAX-PLANCK-GESELLSCHAFT ZUR FÖRDERUNG DER WISSENSCHAFTEN EV
3	DTU	TECHNICAL UNIVERSITY OF DENMARK (DANMARKS TEKNISKE UNIVERSITET)
4	OWI	OWI SCIENCE FOR FUELS GMBH
5	UNR	UNIRESEARCH BV
6	T4F	TEC4FUELS GmbH
7	AVL	AVL LIST GMBH
9	UZ	UNIVERSITY OF ZAGREB, FACULTY OF MECHANICAL ENGINEERING AND NAVAL ARCHITECTURE (SVEUCILISTE U ZAGREBU, FAKULTET STROJARSTVA I BRODOGRADNJE)
10	UCT	UNIVERSITY OF CAPE TOWN
11	KAUST	KING ABDULLAH UNIVERSITY OF SCIENCE AND TECHNOLOGY

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