SHERLOHCK

SUSTAINABLE AND COST-EFFICIENT CATALYST FOR HYDROGEN AND ENERGY STORAGE APPLICATIONS BASED ON LIQUID ORGANIC HYDROGEN CARRIERS: ECONOMIC VIABILITY FOR MARKET UPTAKE

Project ID	101007223
PRR 2024	Pillar 2 – H_2 storage and distribution
Call topic	FCH-02-1-2020: Catalyst development for improved economic viability of LOHC technology
Project total cost	EUR 2 563 322.50
Clean H_2 JU max. contribution	EUR 2 563 322.50
Project period	1.1.2021–30.6.2024
Coordinator	Commissariat à l'Énergie Atomique et aux Énergies Alternatives, France
Beneficiaries	Evonik Operations GmbH, Friedrich-Alexander-Universität Erlangen-Nürnberg, Hydrogenious LOHC Technologies GmbH, Kuwait Petroleum Research & Technology BV, Noordwes-Universiteit, Universidad del País Vasco / Euskal Herriko Unibertsitatea

https://sherlohck.eu/

PROJECT AND GENERAL OBJECTIVES

Liquid organic hydrogen carriers are attractive owing to their ability to safely store large amounts of hydrogen (up to 7 wt% or 2 300 kWh/t) for a long time and to release pure hydrogen on demand. The project targets the development of (i) highly active and selective catalysts with partial/total substitution of platinum group metals (PGMs); (ii) a novel catalytic system architecture, with components ranging from the catalyst to the heat exchanger, to minimise internal heat loss and to increase the space–time yield; and (iii) novel catalyst testing, system validation and demonstration through the demonstration unit (> 10 kW, > 200 h).

PROGRESS AND MAIN ACHIEVEMENTS

Requirements have been defined for the hydrogenation and dehydrogenation catalyst, the type and quality of liquid organic hydrogen carriers, hydrogen quality, the testing routine and energy consumption; these are compatible with all the objectives of the project. This initial work has laid the foundation for the whole project. Benzyltoluene was chosen as the reference molecule, and Pt-based catalysts from Clariant were selected as the catalysts' benchmark.

The design of a catalyst through density functional theory predictive analysis has reduced the use of PGM catalysts. Calculations were applied to the dehydrogenation of methylcyclohexane (to toluene) as a reference molecule, as benzyltoluene was too complex for the calculation. The overall dehydrogenation energies calculated for the various alloys considered showed that alloys such as Co, Co_3Pt, SnPt, Sn_3Pt_2, Sn_2Pt and Sn_4Pt could be potential low-Pt-based catalytic materials. Catalyst materials have been synthesised and tested on a laboratory scale with a standardised test protocol. Some Pt-X (X = Fe, Zn, Co or Cu) catalysts supported by alumina outperform the benchmark catalyst in terms of activity. Pt-Co, with a cobalt content of 0.5 wt%, achieved almost the same dehydrogenation activity and selectivity as catalysts with 1 wt% Pt but with half the amount of this noble metal. PGM-free catalysts have very low activity. Furthermore, through experiments with model substances simulating by-product formation, it was possible to gain better insights into the dehydrogenation reaction and catalyst deactivation. Promising results were initially obtained for the first catalyst reactivation by oxidative regeneration with synthetic air procedures executed in batch operations.

In parallel, to explore the advantages of structured heat-exchanger reactors combined with improved catalysts, models were constructed and simulations were performed to support the choice of possible reactor geometries, in particular to define suitable heat-conductive reactor structures. The results indicated that, for both reactions, foam structure, catalyst activity, mass and operating conditions are first-order parameters. 3D monolith structures were prepared to integrate catalyst materials, and a long-term testing campaign was launched, which ran up to June 2024.

FUTURE STEPS AND PLANS

- Sherlohck has integrated the catalyst into the thermally conductive support structure.
- Long-term testing in continuous operation (> 200 h) was ongoing until June 2024.
- Testing of the resistance of catalysts to different poisons is ongoing.
- The modelling of the reaction kinetics for the design of new reactors has started for the dehydrogenation reaction.

PROJECT TARGETS

Target source	Parameter	Unit	Target	Achieved to date by the project	Target achieved?	SOA result achieved to date (by others)	Year for reported SOA result
Project's own objectives	Catalyst selectivity	%	99.8	99.4	⚙	Around 100	2022
	Degree of conversion	%	90	88	⚙	Around 100	2022
	Catalyst productivity in dehydrogenation	gH2 / g catalyst / min	3	0.85	✓	0.85	2022

Clean Hydrogen Partnership
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