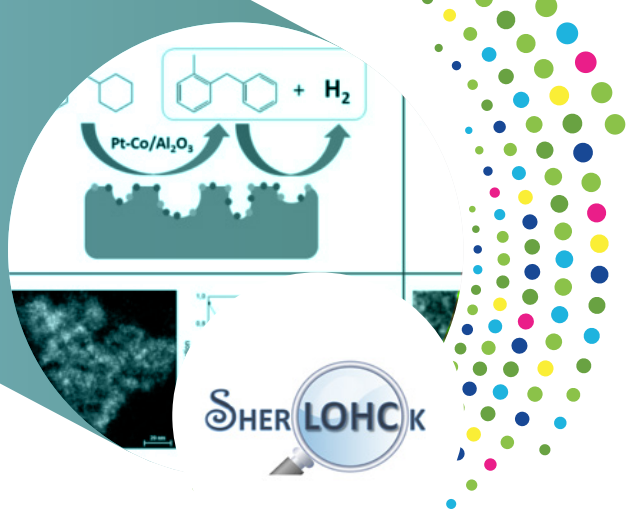
SHERLOHCK

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
PRD 2023:	Panel 2 – H2 storage and distribution
Call topic:	FCH-02-1-2020: Catalyst development for improved economic viability of LOHC technology
Project total costs:	EUR 2 563 322.50
Clean H_2 JU max. contribution:	EUR 2 563 322.50
Project period:	1.1.2021–31.12.2023
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 OBJECTIVES

Liquid organic hydrogen carriers (LOHCs) are attractive due 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, including the catalyst and the heat exchanger, to minimise the internal heat loss and to increase the space–time yield; and (iii) novel catalyst testing, system validation and demonstration in the demonstration unit (> 10 kW, > 200 hours).

PROGRESS AND MAIN ACHIEVEMENTS

Requirements in line with the objectives of the project have been defined for the hydrogenation and dehydrogenation catalysts; liquid organic hydrogen carrier type and quality; hydrogen quality; testing routine; and energy consumption. This initial work has enabled the foundations to be laid for the whole project. Benzyltoluene was chosen as the reference molecule, and Pt-based catalysts from Clariant were selected as catalysts' benchmark.

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

In parallel, to explore the advantages of structured heat exchanger reactors combined with improved catalysts, models and simulations were used to support the choice of possible reactor geometries, in particular to define suitable heat-conductive reactor structures. The results indicate that, for both reactions, foam structure, catalyst activity, mass and operating conditions are first-order parameters. Initial three-dimensional monolith structures have been prepared to integrate catalyst materials.

A communication and dissemination plan was developed at the beginning of the project. The communication activities carried out involve:

- the project website;
- diffusion of activities on LinkedIn (https://www.linkedin.com/in/sherlohck/?originalSubdomain=es) and Twitter, now known as X (https://twitter.com/SherlohckProj);
- participation in promotional events (conferences, workshops);
- distribution of newsletters and press releases.

The project has standardised the test protocol.

FUTURE STEPS AND PLANS

- SherLOHCk will integrate the catalyst into the thermal conductive support. The design of the first conductive support is ongoing.
- Long-term testing in continuous operation (> 200 hours) has not started yet.
- Testing of the resistance of catalysts to different poisons has not started yet.
- The modelling of the reaction kinetics for the design of new reactors has started for the dehydrogenation reaction.

QUANTITATIVE TARGETS AND STATUS

Target source	Parameter	Unit	Target	Achieved to date by the project	Target achieved?	SoA result achieved to date (by others)	Year of SoA target
Project's own objectives	Catalyst productivity in dehydrogenation	g of H_2/g of catalyst/min	3	5.3	✓	0.85	2022
	Degree of conversion	%	90	74	⚙	~ 100	
	Catalyst selectivity	%	99.8	99.04	⚙	~ 100	

Clean Hydrogen Partnership
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