

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
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Project total cost	EUR 2 563 322.50
Clean H ₂ JU max. contribution	EUR 2 563 322.50
Project period	01-01-2021 - 30-06-2024
Coordinator Beneficiary	COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES, FR
Beneficiaries	KUWAIT PETROLEUM RESEARCH and TECHNOLOGY BV, HYDROGENIOUS LOHC TECHNOLOGIES GMBH, NOORDWES-UNIVERSITEIT, UNIVERSIDAD DEL PAIS VASCO/ EUSKAL HERRIKO UNIBERTSITATEA, EVONIK OPERATIONS GMBH, FRIEDRICH-ALEXANDER-UNIVERSITAET ERLANGEN-NUERNBERG

<http://sherlohck.eu>

PROJECT AND GENERAL OBJECTIVES

Liquid organic hydrogen carriers are attractive due to their ability to safely store large amounts of hydrogen (up to 7 % wt or 2 300 KWh/ton) for a long time and to release pure hydrogen on demand. SHERLOHCK targets the development of (i) highly active and selective catalysts with partial/total substitution of platinum group metals (PGM), (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 hours).

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, testing routine, and energy consumption, to ensure compatibility with the project objectives. This initial work has laid the foundation for SHERLOHCK.
- Benzyltoluene was chosen as the reference molecule and Pt-based catalysts from Clariant were selected as the catalysts' benchmark.
- The catalyst design through density functional theory predictive analysis has reduced the use of PGM catalysts. Calculations were made for the dehydrogenation of methylcyclohexane (to toluene) as a reference molecule instead of benzyltoluene which was too complex for the calculation. The overall dehydrogenation energies calculated for the various considered alloys showed that Co, Co₃Pt, SnPt, Sn₃Pt₂, Sn₂Pt, and Sn₄Pt could be potentially low Pt-based catalytic materials.
- Catalyst materials have been synthesised and tested on a lab scale with a standardised test protocol. 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 catalysts with 1 wt.% Pt but with

half the amount of this noble metal. PGM-free catalysts show very low activity.

- Experiments with model substances simulating by-product formation provided better insights into the dehydrogenation reaction and catalyst deactivation.
- Promising results have been obtained for the first catalyst reactivation procedures by oxidative regeneration with synthetic air executed in batch operation.
- Models and simulations were performed on structured heat-exchangers reactors combined with improved catalysts, in order to support the choice of possible reactor geometries, in particular, to define suitable heat conductive reactor structures. These results indicate that for both reactions, foam structure, catalyst activity, mass, and operating conditions are first-order parameters.
- 3D monolith structures have been prepared to integrate catalysts materials.
- A long-term test campaign has been launched and ran until June 2024.
- The communication activities carried out are integrated with the Project website (<https://sherlohck.eu/>), diffusion of activities on two social platforms: LinkedIn (<https://www.linkedin.com/in/sherlohck/originalSubdomain-es>) and 'X' (<https://x.com/SherlohckProj>) and participation to promotional events (conferences, workshops, newsletters, and press releases).

FUTURE STEPS AND PLANS

- SherLOHCK has integrated the catalyst into the thermal conductive support structure.
- Long-term testing in continuous operation (> 200 hours) was ongoing until June 2024.
- Testing of the resistance of catalysts to different poisons was 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	⚙️	~100	2022
	Degree of conversion	%	90	88	⚙️	~100	2022
	Catalyst productivity in dehydrogenation	g H ₂ / g catalyst/ min	3	5.3	✓	0.85	2022