

Direct Isopropanol Fuel Cell (DIP AFC) coupled to a transfer hydrogenation reaction

Couplage d'une pile à combustible à isopropanol direct à un procédé d'hydrogénation par transfert

Level : PhD

Profile of the candidate : Master or equivalent degree in process or chemical engineering, physical chemistry or catalysis. Experience in electrochemistry/electrocatalysis.

Team(s) : CARE (Caractérisation et Remédiation des polluants dans l'air et l'eau)

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Keyword(s) : fuel cell, electrochemistry, hydrogen storage

Scientific context : Whereas it is well established that hydrogen is a key energy vector, its storage and transportation are still a subject of research, because of safety and capacity issues. Stored by hydrogenation in Liquid Organic Hydrogen Carriers (LOHC), its transport becomes safe and the storage capacity exceeds that of liquid or compressed hydrogen at 700 bars. On request, H₂ can be restored in molecular form by catalytic dehydrogenation, highly endothermic, to power a fuel cell. An innovative process consists in carrying out, from the hydrogen-rich LOHC, a transfer hydrogenation of the acetone/isopropanol couple feeding a direct isopropanol fuel cell (DIP AFC, for energy production), as shown in Figure 1. The principle has been proposed in a very recent publication [1]. Many barriers remain to be overcome in this coupled process, such as the choice of LOHC, the catalysts, the type of fuel cell membrane, the operating conditions, the reactor and energy integration, etc.

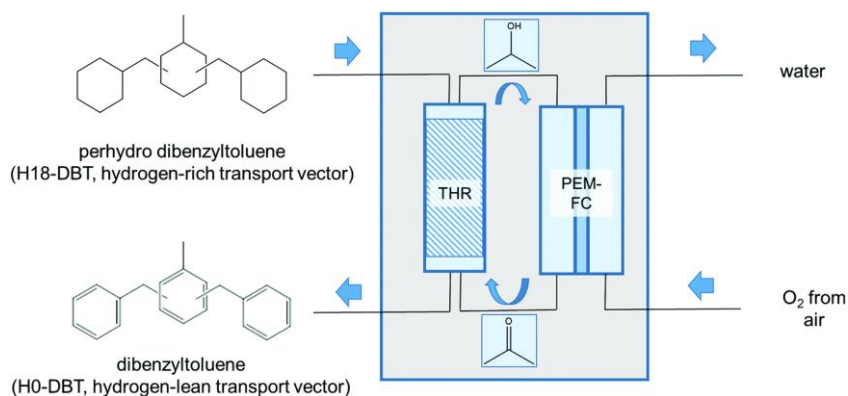


Figure 1: Transfer hydrogenation coupled to DLFC, from [1]

Missions :

The work will be focused on the isopropanol fuel cell for energy production. The main challenge in fuel cell development remains the reduction of the use of Pt as electro-catalyst for the anodic reaction (in this case, the isopropanol electro-oxidation to acetone, $\text{C}_3\text{H}_8\text{O} + \text{H}_2\text{O} \rightarrow 2 \text{H}^+ + \text{C}_3\text{H}_6\text{O} + 2 \text{e}^-$), which is identified as the rate determining step for the fuel cell operation. In this part, the task will be to synthesize new materials for isopropanol electro-oxidation, either by the partial substitution of Pt (in acid media) with several non-noble metals (including Ni, Sn and Bi), or by the partial substitution of Ni (in alkaline media) with Fe and Co. Then, the performance of the anodic materials will be evaluated for direct isopropanol fuel cells. Polymeric membranes in a high temperature range (up to 200°C in acid media, and up to 120°C in alkaline media) will be used as electrolyte. Working in this temperature range will allow for a perfect thermal integration with the catalytic dehydrogenation reactor. The kinetic studies will be coupled with a thorough electrochemical characterization together with high-resolution product analysis. The idea is, for the first time, to find the most efficient electrode material (with the lowest amount possible of Pt) showing high electrochemical performance in fuel cell operation, together with high selectivity for isopropanol oxidation to acetone. In addition, advanced in situ spectroscopic characterization techniques (FTIR) coupled with potentiostatic measurements will be performed to thoroughly understand (at a molecular level) the electrochemical processes taking place during fuel cell operation. At the end of the PhD work, we will try to couple the transfer hydrogenation of acetone with the direct isopropanol fuel cell.

Reference :

[1] Sievi, G.; Geburtig, D.; Skeledzic, T.; Bösmann, A.; Preuster, P.; Brummel, O.; Waidhas, F.; Montero, M. A.; Khanipour, P.; Katsounaros, I.; Libuda, J.; Mayrhofer, K. J. J. & Wasserscheid, P. Towards an Efficient Liquid Organic Hydrogen Carrier Fuel Cell Concept *Energy & Environmental Science*, 2019, 12, 2305-2314

Application: Please send CV, motivation letter, copy of M1 and M2 grades, one or two recommendation letters including contact information **until May 20th, 2020.**