

AMAZING

Additive Manufacturing for Zero-emission Innovative Green Chemistry

Public Summary

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The goal of the AMAZING project was to develop proton conducting membranes to enhance the non-oxidative dehydrogenation of alkanes to alkenes, which are essential building blocks for the chemical industry. The AMAZING project consists of a German part focusing on the manufacturing of the membranes and the Dutch part on the fundamentals of proton transport through these materials, dehydrogenation catalysis, process design and technical evaluation and mechanical strength studies. This public summary deals with the Dutch part of the project.

The membrane material of choice was lanthanum tungstate (LWO), a mixed proton/electron conductor. The phase composition of LWO derivatives was investigated. A link between oxygen vacancies respectively electron charge compensation while doping and the necessary (single-phase) composition for optimal hydrogen permeation is established. Additionally, a model was developed to derive transport properties of these materials under reducing conditions. Mobility and self-diffusion coefficients of charge carriers, as well as the equilibrium constant of hydrogenation and defect concentrations in the bulk, were derived from total conductivity measurements. These properties are essential for the subsequent modelling of permeation fluxes through the membrane and evaluation of the membrane performance under relevant process conditions. The results show, among other things, that water splitting on the permeate side has a substantial impact on the apparent hydrogen permeation measured in conventional permeation experiments.

The technological and techno-economic feasibility of catalytic membrane-assisted alkane dehydrogenation were investigated using reaction mechanism and process simulation studies. On the catalyst scale, the alkane dehydrogenation rate over a PtSn/ZnAl₂O₄ catalyst was inhibited by high olefin and high hydrogen concentrations, and by repulsive interactions between adsorbed species. Co-feeding steam enhanced product desorption and thereby increased reaction rates, but also structurally modified the Sn content. Pt is therefore preferred to PtSn as catalyst active phase in membrane reactors. Moreover, systems in which Pt was deposited on promising mixed proton-electron conducting (MPEC) and proton pump membranes were considerably less active and less stable than Pt/ZnAl₂O₄. A packed bed membrane reactor containing Pt/ZnAl₂O₄ catalyst particles is therefore preferred to a catalyst-functionalized membrane configuration. On a process scale, MPEC membranes were unsuited for integration with high temperature alkane dehydrogenation, due to a restricted driving force for permeation. On the contrary, the usage of proton pump membranes could be an attractive industrial alternative to traditional olefin production pathways, as its capital investment and energy input are 20-30% lower. Nevertheless, fully renewable electricity needs to be utilized to substantially reduce the carbon footprint. Moreover, electrifying conventional alkane cracking technologies could potentially lead to a similar improvement in carbon footprint as industrial implementation of proton pump membranes. However, it should be noted that the technological feasibility of electrified crackers and electrified proton pump systems still needs to be confirmed.

The manufacturing process of the green hydrogen-generating ceramic membranes was studied from a mechanical point of view. Making these membranes is a challenge, since they are made of new chemical compositions, and they are not uniform, containing pores of different sizes and in different quantities. Due to these features, they often deform and crack during manufacturing. In this project, the manufacturing process was modelled via finite element methods. The virtual reconstruction of the process allowed access to information that is experimentally unavailable: the evolution of the membranes' structure, porosity and internal stresses throughout their manufacturing. Strategies to minimize the manufacturing issues are then identified, both in terms of structure optimization and manufacturing processes. Additionally, an ultra-efficient numerical code is implemented, to enable the path towards a digital twin of the membranes' manufacturing.

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