Porous Electrode Optimization For An Integrated Photovoltaic-electrolyser

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Abstract

Photovoltaic-powered electrolysis (PV-EC) though the most mature technology for zero-carbon integrated solar to hydrogen conversion, is still only approaching industrial and commercial relevance, and devices with light absorber area larger than 100 cm2 are quite rare [1,2]. Here, we present simulations of the effects of electrode substrate materials on the performance of a large-area (over 100 cm2 solar absorber area) integrated PV-EC device.

We used Batteries & Fuel Cells Module and CFD Module to construct a multi-physics model of fluid flow, electrochemistry (tertiary current distribution and Butler-Volmer kinetics), and in some simulations also heat transfer to study and optimize the operation of an alkaline EC (1.0M KOH electrolyte). When heat transfer was considered, non-isothermal flow was solved to determine the electrolyte flow and temperature distribution, and this result was used as an input for the electrochemical model.

The heat transfer model was validated using comparisons with thermal camera images of the PV surface taken during outdoor operation and generally showed a good match. The simulations indicated relatively low EC operating temperatures compared to those typical of PEM and alkaline ECs (Figure 1. a), so we focused on low-temperature operation.

We also studied nickel (Ni) foam (NF) and stainless steel (StS) mesh as substrate materials for the electrodes. While both are porous metal structures, they differ from each other also in other aspects than the base material (Figure 2.). Additionally, both materials come in a variety of grades, i.e. pore diameter of foams (or pores per inch, PPI, count) and threads per inch (TPI) count of meshes, and the properties of the different grades differ from each other. We used simulations with parameterized models of Ni foam and StS mesh to study the performance of these materials, relative to each other and the effect of the pore diameter and the TPI count. Generally, at current densities (j) less than about 100 mA/cm2 the higher surface area of the Ni foams yielded better performance than the StS meshes, but with increasing j the transport losses began to favor the StS meshes as a substrate material (Figure 1. b). In both cases the material grade with the highest specific surface area needed the lowest voltage bias to achieve a given j and thus has the best performance.

References
[1] J.H. Kim, D. Hansora, P. Sharma, J.-W. Jang, J.S. Lee, Chem. Soc. Rev. 48 (2019) 1908-1971.
[2] S. Calnan, S. Aschbrenner, F. Bao, E. Kemppainen, I. Dorbandt, R. Schlatmann, Energies 12 (2019) 4176.

Figures used in the abstract

Figure 1 : a) simulated temperature distribution in PV and KOH, b) typical simulated polarization curves of electrocatalysts on NF (solid) and StS mesh (dash) at ca. 25 °C temperature

Figure 2 : Photos (a and b) and SEM images (c and d) of Ni foam (a nd c) and StS mesh (b and d)