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Towards Improved Design of Industrial-Scale Alkaline Water Electrolysers Through Multiphase Flow Simulations

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Extended Abstract

The role of green hydrogen in the energy transition has already been recognised by the scientific community and the International Energy Agency (IEA) [1] through the years as it offers a way to store and deliver usable and clean energy. Nowadays, the two most mature technologies to produce green hydrogen are alkaline and proton exchange membrane (PEM) water electrolysis. From an economic perspective, integrating the strengths of both technologies appears promising, as it combines high production rates per electrode area with cost-effective materials. Recent experimental studies in our group have shown that it is possible to significantly improve the performance of alkaline water electrolysers (AWE) by incorporating 3-D porous electrodes (such as porous nickel foams or 3-D printed triply periodic minimal surface – TPMS – geometries) in a zero-gap cell configuration with forced electrolyte flow [2-4].

Some efforts have been made to apply the same methodology (i.e. zero-gap cell with knitted mesh-type spacer and forced flow) to industrial-scale electrolysers. Unfortunately, it is still difficult to reach similar performance as with the lab-scale setup due to a non-optimal distribution of the electrolyte flow in the anodic and cathodic half-cells. In first intention, single-phase Computational Fluid Dynamics (CFD) simulations were used to quantify flow uniformity and flow recirculation in water electrolysis cells [5]. Pressure drop calculations were performed explicitly on isolated 3-D porous structures to extract representative parameters that were then used at the larger scale to take the structures implicitly into account (based on the Darcy-Forchheimer approximation). Different cell geometries were compared and this methodology showed that the use of foams as porous transport layer (PTL) instead of state-of-the-art knitted mesh-type spacers allows to increase the effective cell volume covered by the electrolyte and at the same time lower the risk of flow recirculation within the cell.

The objective of this work is to extend the analysis by considering the second phase (hydrogen) in the simulations, using the commercial software Ansys-Fluent. To describe the two-phase hydrodynamics within the electrolysis cell, a mixture model formulation for incompressible flow is used, following the work of van der Does et al. [6]. Within this model, each phase is treated as an interpenetrating continuum and the continuity and momentum equations for the gas-liquid mixture are solved by weight-averaging velocity, density and viscosity based on the gas fraction. Gas is introduced inside the domain by imposing a certain gas flux (based on Faraday's law) at the electrode surface. This allows to study the effect of various parameters such as current density, flow rate, inlet/outlet configuration and PTL choice on the performance of the cell. The goal here is to find the optimal geometry that prevents gas accumulation while still distributing the electrolyte homogeneously along the electrode area.

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