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Numerical Study of Bubble-Induced Overpotentials in Flow-based Water electrolyzers

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Extended Abstract

The transition to a sustainable energy system requires viable technologies for large-scale production, storage, and utilization of green fuels such as renewable hydrogen. Water electrolysis presents a promising approach using renewable energy to generate hydrogen in a carbon-neutral manner. Conventional water electrolyzers that utilize membranes or separators face challenges such as high costs and complexity, which have hindered cost-effective hydrogen production from this technology. Flow-based electrolyzers (FBEs) provide a distinct opportunity to overcome these barriers through innovative cell architectures that eliminate membranes, which are the main source of degradation [1]. By relying on fluidic flows for product gas separation, FBEs can significantly simplify cell fabrication and reduce balance-of-plant costs [2]. The main objective of this study is to numerically investigate the effect of bubble flow on the efficiency and product purity in FBEs. Furthermore, the effect of surfactants on the production separation and overpotentials are investigated.

An FBE consists of two electrodes and a flowing liquid electrolyte between the electrodes. In these electrolyzers, bubble nucleation and growth reduce the active electrode area, while bubbles flowing between electrodes increase ohmic resistance, both leading to overpotentials. This research quantifies these bubble-induced overpotentials in FBEs through 3D numerical simulations using the Aphros multiphase flow solver [3]. The simulations model bubble nucleation, coalescence, and flow in an FBE configuration. The geometry of the electrolyzer is based on [4], with an interelectrode distance of 1 mm, electrode height of 1 mm, and electrode length of 10 mm. The electrolyte used is 1 M sulfuric acid with a resistivity of 0.0385 Ohm.m. The simulations are carried out at a current density of 450 mA/cm^2 and two different flow rates of 300 ml/min and 1200 ml/min [5].

At a lower flow rate of 300 ml/min, bubble overpotential exhibits higher fluctuations due to pronounced bubble accumulation and coalescence. The overpotential is significantly higher (23.25 mV) at 300 ml/min, indicating a larger energy penalty associated with bubble nucleation and coalescence. Conversely, a higher flow rate of 1200 ml/min results in a substantially lower overpotential of 9.61 mV, suggesting increased electrolyte flow effectively mitigates bubbles' adverse effects. Furthermore, at 300 ml/min, higher bubble volume fraction in the interelectrode area leads to increased coalescence and larger bubbles. At this flow rate, the bubble distribution is wider and closer to the centerline, indicating a higher gas cross-over tendency. In contrast, the higher 1200 ml/min flow rate results in more separated gas streams, reducing gas cross-over.

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