Coupling Multiscale Phenomena In Alkaline Electrolyzer Stack Simulation Using Reduced Order Models

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Abstract

Porous three-dimensional electrodes are promising for use in alkaline electrolyzer due to their high surface area. Nickel foams, specifically, serve a dual purpose as both a current collector and an active working electrode, enhancing current density and boosting hydrogen production[1]. Modeling these electrodes can help identify key microstructural parameters—such as porosity, tortuosity, and pore size—that are essential for optimizing electrochemical performance.

Here, 7 cell industrial alkaline electrolyzer is modelled using reduced order models (ROM) with the purpose of speeding up calculations by many X. First, Laminar Flow coupled with phase transport is used to simulate fluid and gas dynamics on cell scale. This multi physics CFD model is validated by comparing simulation results to experimentally determined flow fields inside an electrolysis cell with transparent end plates using colored ink injection. Gas/liquid mixture on cell level gives flow rate/pressure drop and outlet gas fraction relationships described by ROMs. The ROMs are an input for the second step: the manifold scale model that uses turbulent flow and phase transport for gas mixture calculations. After this step, we have obtained separate cell and manifold level calculations. In the third step, when full stack level gas/liquid mixture is achieved, thru combining cell and manifold results, then on top of it the electrochemistry can be applied. Electrode activities, ohmic losses and currents are calculated for the full stack. This allows to estimate voltage losses and parasitic currents in the stack and in turn to optimize manifold dimensions and KOH feed channels in cell frames.

In addition, we demonstrate how to numerically evaluate homogeneity of the flow field inside the cell. Here KOH flow rates and applied current via gas production rates are systematically varied and the optimal cell operating values are suggested by applying the residence time analysis approach and comparison of the flow field components.

The combination of CFD simulations and flow experiments is a powerful tool for stack and cell design optimization. The strategy of using ROMs and solving the model in three steps, makes it feasible to bridge from micro to macro scale phenomena in one model and deliver actionable results with reasonable calculation times, which would not otherwise have been possible. With faster calculation times, it's possible to run parametric studies helping to propose optimal stack operating conditions and shows that Ni foam porous transport electrodes can be a good candidate for improving the performance of alkaline electrolysers.

Reference

F. Rocha. et al. Effect of pore size and electrolyte flow rate on the bubble removal efficiency of 3D pure Ni foam electrodes during alkaline water electrolysis, Journal of Environmental Chemical Engineering, vol. 10, no. 3, p. 107648, Jun. 2022, doi: 10.1016/j.jece.2022.107648.