A Standardized Approach to Electrochemical System Design and Optimization

by
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Technical Summary

To reach net zero emissions, many industries are currently undergoing a period of decarbonization, including the commodity chemicals industry. Commodity chemical production accounts for a significant amount of global greenhouse gas emissions, and reduction of these emissions via electrochemical production of these chemicals has been proposed, but the system design and optimization approach for electrochemical systems is less well defined. In this work, electrochemical system design and optimization is explored through looking at critical materials required as well as two case studies modeling two different electrochemical systems.

First, iridium supply and demand are analyzed to understand if iridium supply can match the demand projected for electrolytic hydrogen produced by proton exchange membrane electrolyzers. Several scenarios are presented that point to the conclusion that significant technological improvements (reduction in iridium loading in anode catalysts and increase in average operating current density) in proton exchange membrane electrolyzers are needed in order to meet hydrogen targets for both 2030 and 2050.

Then, the first of two case studies on electrochemical system design is presented. This first system considers hydrogen production via proton exchange membranes where the electrolyzer is connected to a grid with a variable price of electricity. By defining the current-voltage relationship including overpotentials and utilizing mass and energy balances, a dynamic model is created that can predict hydrogen production as a function of time as well as degradation of the electrolyzer stack as a function of its usage. This model is embedded into an optimization that sizes electrolyzer stack area and hydrogen storage while optimizing operation of the system in order to produce cost-optimal electrolytic hydrogen.

Finally, this approach to modeling electrochemical systems is applied to the production of ethylene via the non-oxidative dehydrogenation of ethane to evaluate process design and techno-economics. This study proposes an electrochemical pathway to producing ethylene as opposed to traditional steam cracking. Three distinct process operating modes are modeled in the thermodynamic limit using Aspen Plus. Results indicate that in this limit operating without any methane recycle as an electrolyzer is the most economical way to operate. The sensitivity analysis in this work shows the levelized cost of ethylene is most sensitive to ethane feed price indicating the need for inexpensive ethane for ethylene produced by electrolysis to be viable.

This work concludes with summarizing the general approach to electrochemical system design and operation in addition to some thoughts on electrochemical process engineering and its place in chemical engineering education.

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