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Abstract

Model-Based Design and Optimization of Electrochemical Processes for Sustainable Aviation Fuels †

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Aviation accounts for around 12% of all CO_2 emissions from the transport sector, necessitating the use of sustainable aviation fuels. Electrofuels, which are gained from renewable sources, are an attractive option for sustainable aviation fuels. Model-based electrochemical process design and optimization could very well assist in improving the design and operation methods toward better conversion, selectivity, energy conversion, and economics—at a lower cost and time than the experimental approach. Moreover, nowadays, process models are also an indispensable technology for realizing Industry 4.0 and digital twin ideas for process intensification and monitoring. Thus, to design better electrofuel manufacturing processes and create digital process representations, this paper extends our previous work [1] accordingly, i.e., making use of a first-principles model for electroreduction of furfural to furfuryl alcohol and methylfuran, as well as hydrogen evolution. In detail, the Volmer reaction forms adsorbed hydrogen, represented by a Frumkin-type isotherm. The hydrogen evolution is described by the potential-dependent Heyvrosky reaction and the potential-independent Tafel reaction. We critically discuss the simulation results using reference data, and we show the potential application of an AI-assisted process modeling strategy, i.e., predicting an optimal potential profile using the derived first-principles model and a neural network.

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Reference

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