Abstract

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

Fenila Francis Xavier 1 and René Schenkendorf 2,*

1 Institute of Energy and Process Systems Engineering, TU Braunschweig, Langer Kamp 19b, 38106 Braunschweig, Germany; f.francis-xavier@tu-braunschweig.de
2 Automation & Computer Sciences Department, Harz University of Applied Sciences, Friedrichstr. 57-59, 38855 Wernigerode, Germany
* Correspondence: rschenkendorf@hs-harz.de

Abstract: Aviation accounts for around 12% of all CO2 emissions from the transport sector, necessitating the use of sustainable aviation fuels. Electrofuels, which are gained from renewable sources, are attractive options for sustainable aviation fuels. Model-based electrochemical process design and optimization could very well assist in improved design and operation methods towards 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 makes 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 Heyrovsky reaction and the potential independent Tafel reaction. We critically discuss the simulation results using reference data and show its potential application for an AI-assisted process modeling strategy, i.e., predicting an optimal potential profile using the derived first-principles model and a neural network.

Keywords: process systems engineering; system identification; hybrid modeling; electrochemical synthesis

Citation: Xavier, F.F.; Schenkendorf, R. Model-Based Design and Optimization of Electrochemical Processes for Sustainable Aviation Fuels. Proceedings 2022, 69, x. https://doi.org/10.3390/xxxxx

Academic Editor(s):

Published: date

Publisher’s Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Copyright: © 2022 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (https://creativecommons.org/licenses/by/4.0/).