HiTEC Graduate School for energy & climate

Research Project #16

Digital-twin-guided design of CO_2 and bicarbonate electrolyzers through combined computational–experimental workflows (IET-4 & IET-3)

Electrochemical CO_2 conversion in membrane–electrode-assembly (MEA) electrolyzers is a promising approach for sustainable fuel and chemical production. However, current systems still face significant limitations—including carbon losses, mass-transport issues, and narrow operating ranges—that are even more challenging in emerging bicarbonate electrolyzers, which convert CO_2 directly from capture solutions. Increasing evidence indicates that local pH, ion transport, and membrane–electrode coupling are crucial factors affecting carbon efficiency and product selectivity, highlighting the need for a deeper mechanistic understanding. Integrating these systems with a validated digital-twin framework offers a new and powerful solution: by combining imaging, diagnostics, and multiscale modeling, digital twins can deliver continuous feedback, predictive insights, and real-time optimization. This integration has the potential to significantly improve the robustness, efficiency, and industrial viability of next-generation low-temperature CO_2 electrolyzers. [1]

This PhD project aims to develop a validated digital twin for CO_2 and bicarbonate electrolyzers, capable of accurately reproducing local electrochemical conditions—such as potential, pH, and reactant distribution—to optimize system performance. The model will support the development of design rules for advanced MEA components, including membrane selection, gas diffusion electrode architecture, and electrolyte formulations that improve selectivity and CO_2 utilization. Ultimately, this digital framework will provide feedback as well as prognostic and diagnostic insights to guide and interpret experimental behavior. [2,3]

The project will combine experimental and computational approaches from IET-4 and IET-3 into a unified workflow linking electrochemical testing, diagnostics, and multi-scale modeling. This integration will accelerate the design of next-generation electrolyzers and will also provide a transferable modeling framework for other reactive-capture electrochemical systems.

Through model–experiment feedback and optimization, the digital twin will undergo sensitivity analyses and surrogate modeling to identify key performance parameters such as diffusion layer thickness, membrane hydration, and catholyte composition. The optimized model will then guide the design of MEAs and operational strategies that maximize both CO_2 utilization efficiency and product selectivity (targeting over 80%), while also minimizing cell voltage. This approach will lead to improved performance and a deeper mechanistic understanding of CO_2 electrolysis. The specific tasks, organized into physics-based modeling and experimental validation parts, are:

Physics-based modeling (IET-3)

• Develop hierarchical 1D–3D electrochemical multiphysics models for CO_2 and bicarbonate cells, accounting for charge transport, species migration, and water management.

• Incorporate mechanistic sub-models for $CO_2/HCO_3^-/CO_3^{2-}$ equilibria, local CO_2 regeneration, and competing hydrogen evolution.

• Embed all components into a reusable digital-twin framework calibrated using experimental data (EIS, polarization curves, tomography) that provides feedback to the experimental setup.

Experimental validation (IET-4)

• Fabricate and test MEAs for conventional CO_2 and bicarbonate electrolysis, systematically varying membranes (PEM, BPM), electrode structures, and electrolytes suggested by the models.

• Perform in-depth electrochemical characterization (I–V curves, faradaic efficiencies, CO_2 utilization, and impedance analysis) and 3D structure imaging for model validation.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Electrochemical Process Engineering (IET-4), Director: Prof. Dr. Ralf Peters https://www.fz-juelich.de/en/iet/iet-4
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Technologies - Theory and Computation of Energy Materials (IET-3), Director: Prof. Dr. Michael Eikerling https://www.fz-juelich.de/en/iet/iet-3
Specific **requirements**	M.Sc. in (Electro-)Chemistry, Physics, Materials Science, Computational Materials Science or in related disciplines. Experience in numerical simulations would be an advantage.
For **project specific** questions please **contact**	Dr. Joachim Pasel (Head of the Synthetic Fuels Department), IET-4, j.pasel@fz-juelich.de Dr. Thomas Kadyk (Head of the Physical Modeling and Diagnostics division), IET-3, t.kadyk@fz-juelich.de

1. Zhong, Y. *et al.* Electrochemically Integrated Carbon Capture and Utilization. *ACS Materials Lett.* 3952–3973 (2025) doi:10.1021/acsmaterialslett.5c01172.

2. Khiarak, B. N. *et al.* Integrated Carbon Dioxide Capture and Electrochemical Conversion: Chemistry, Electrode and Electrolyzer Design, and Economic Viability. *Advanced Energy Materials* **n/a**, e02564.

3. McLaughlin, D., Bierling, M., Mayerhöfer, B., Schmid, G. & Thiele, S. Digital Twin of a Hierarchical CO2 Electrolyzer Gas Diffusion Electrode. *Advanced Functional Materials* **33**, 2212462 (2023).