Research Project #13

AI-Enhanced Hierarchical Modeling of Water Electrolysis Cells (IET-3, IET-1 & IET-4)

Electrochemical devices such as electrolyzers, fuel cells, and batteries are central to the transition to renewable energy. Accurate modeling and simulation of these systems requires a comprehensive understanding of the complex physical processes involved and their interactions. Within these devices, multiple phenomena occur simultaneously across different length and time scales and within distinct functional layers, including multi-step electrochemical/chemical reactions, multi-phase transport in porous media, heat and mass transfer, and electrical potential distributions.

Recent advances in macro-homogeneous modeling have enabled coupled simulations of these processes, capturing multi-phase flow, electrochemical/chemical kinetics, and transport phenomena. However, many of these models rely on coarse approximations, empirical sub-models, or simplified representations of key phenomena due to the high computational cost of fully resolved simulations, from atomistic modeling through molecular dynamics to upper-scale modeling. As a result, these simulations often fail to capture the true coupled behavior of the mechanisms in the system, limiting both predictive accuracy and mechanistic understanding.

The primary objective of this PhD project is to integrate artificial intelligence (AI) models directly into macro-homogeneous simulations of electrolysis cells. Instead of resolving computationally expensive sub-scale phenomena within each iteration of the solution process, AI models will capture these behaviors with high fidelity, significantly reducing computational cost while retaining detailed accuracy. Applications include modeling complex multi-step reaction kinetics on electrode surfaces and/or multi-phase transport through porous structures. The AI models will be trained on sub-scale numerical simulations, atomistic/molecular dynamics modeling results, geometry-resolved simulations, and experimental datasets—including computed tomography (CT) or focused ion beam scanning electron microscopy (FIB-SEM) of electrode structures and cell performance measurements. These AI-enhanced models will be embedded within the macro-homogeneous Computational Fluid Dynamics (CFD) framework o*penFuelCell2*, enabling improved prediction of local properties and phenomena under various operating conditions. This approach will support the optimization of cell geometry, functional layer thicknesses, and material properties to maximize electrochemical performance and efficiency.

While the applicability of AI models has been demonstrated for individual physical phenomena[2], the transfer to multiphysical simulations, including those relevant for electrolysis cells, is still pending. The potential gain in computational speed provided by these models would unlock entirely new simulation capabilities and provide deeper insights into the underlying system behavior.

The dissertation research will be conducted in close collaboration with the Institute for Electrochemical Process Engineering (IET-4), and the Institute for Fundamental Electrochemistry (IET-1), providing access to high-quality experimental data and advanced characterization techniques. The AI–simulation interface will be fully integrated into the ongoing development of the open-source simulation framework o*penFuelCell2*, ensuring that the resulting methods are transferable and widely applicable to the broader electrochemical devices community. The specific tasks include:

Physics-based modeling and AI integration

- Develop AI surrogate models on sub-scale resolved simulations, atomistic models, molecular dynamics, and experimental data to improve the fidelity of coarse-grid models.
- Utilize experimental and simulation datasets, including CT/FIB-SEM-resolved electrode microstructures and cell performance measurements, to calibrate and validate the AI–physics models.
- Adapt hierarchical macro-homogeneous models for water electrolyzers, capturing coupled transport, electrochemical kinetics, and/or multi-phase flow processes.

- Implement AI–physics coupling interface with the o*penFuelCell2* framework to predict local electrochemical conditions and optimize cell performance.
- Conduct sensitivity analyses and surrogate modeling to identify key parameters that govern the overall performance of the electrolisys cell

Location of the HITEC Fellow	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
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Director: Prof. Dr. Rüdiger- A. Eichel https://www.fz-juelich.de/en/iet/iet-1 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
Specific **requirements**	M.Sc. in (Electro-)Chemistry, Physics, Materials Science, Computational Science or in related disciplines. Experience in numerical simulations is essential. Prior experience with OpenFOAM would be an advantage. Proficiency in C++ and in Python or comparable programming languages is expected.
For **project specific** questions please **contact**	Dr. Thomas Kadyk (Head of the Physical Modeling and Diagnostics division), IET-3, t.kadyk@fz-juelich.de

[1] S. Zhang, S. Hess, H. Marschall, U. Reimer, S. Beale, W. Lehnert, openFuelCell2: A new computational tool for fuel cells electrolyzers, and other electrochemical devices and processes, Comput. Phys. Commun. 298 (2024) 109092.

[2] D. Froning, E. Hoppe,M. Müller, R. Peters, Flow characteristics of sintered titanium-based porous transport layers using machine learning. Discover Mechanical Engineering, 4(1), 2 (2025).