Modelling of Transport and Reaction Processes in Gas Diffusion Electrodes for CO_2 Conversion

TECHNISCHE UNIVERSITÄT DARMSTADT

Masterthesis

April 28, 2026

Nano- and Microfluidics

Federal Ministry of Research, Technology and Space

Background

Decarbonizing the chemical industry and utilizing CO_2 as a feedstock are key challenges on the path toward climate neutrality. In the BMFTR-funded project *disruptive*GDE, we tackle both these issues through the development of innovative gas diffusion electrodes (GDEs) for the conversion of CO_2 into valuable chemical products.
In a GDE, a gaseous reactant and a liquid electrolyte interact within a porous structure, forming a gas-liquid interface. The gaseous reactant dissolves into the liquid electrolyte and is transported toward the electrode surface, where electrochemical reactions occur. A detailed understanding of the coupled transport processes and reaction kinetics is essential for optimizing diffusion pathways, electrode architectures, and ultimately reaction conversion and selectivity.

This thesis aims to investigate the transport processes in the electrolyte and the reaction kinetics at the electrode surface using numerical simulations in OpenFOAM. The influence of different electrode structures, reaction kinetics, species concentrations, and electrolyte properties will be systematically analysed with respect to concentration profiles, conversion rates, and reaction selectivity. In addition, the influence of a superimposed convective flow on transport and reaction behaviour will be examined.

Your Tasks

1. Develop a solid understanding of the reaction-convection-diffusion equations governing the transport processes in the liquid electrolyte, as well as of the provided chemical reaction network.
2. Implement the simulations in OpenFOAM.
3. Perform stationary and, where required, transient simulations on our local servers and the Lichtenberg cluster.
4. Systematically investigate the influence of different electrode structures, reaction kinetics, species concentrations, and electrolyte properties on concentration profiles, conversion rates, and reaction selectivity.
5. Examine the effect of a superimposed convective flow on transport and reaction behaviour under selected conditions.

A theoretical analysis and interpretation of the simulation results may be included as an extension. – Your individual ideas and interests are very important to us!

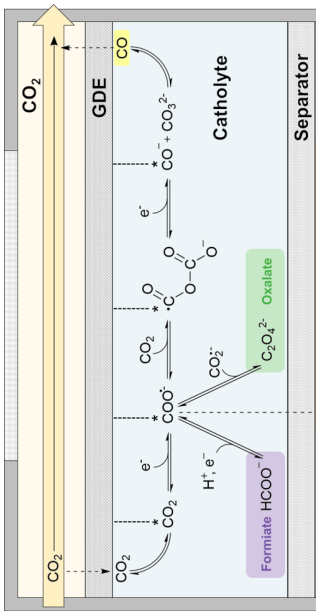
What You Bring

- Interest in working on a current research topic with strong relevance to industrial applications.
- Solid understanding of mathematics, fluid mechanics, and transport processes.
- Initial experience with numerical simulations is an advantage.

What We Offer

- Detailed training and ongoing assistance the whole time.
- Integration into an interdisciplinary research project with regular meetings.
- Systematic support for the development and realization of your own ideas.
- Gain in-depth experience with OpenFOAM. – One of the leading finite-volume frameworks in academia and industry.

Reaction network



Key Facts

- Multiphysics modelling
- OpenFOAM
- Industrial application

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