Numerical Investigation of Dynamic Wetting in Coated Gas Diffusion Electrodes for CO_2 Conversion

TECHNISCHE UNIVERSITÄT DARMSTADT

Masterthesis

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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 stability of this interface is critical for process efficiency and can be enhanced by employing structured, micro-porous metal gauzes as electrodes. To investigate the dynamic wetting process of such metal gauze electrodes, numerical multiphase simulations offer valuable insights. Previous studies on uncoated, idealized geometries have identified initial pathways for improving interface stability, but do not capture the complex coating structures that are typically applied to enhance electrochemical performance.

This thesis aims to investigate the dynamic wetting behaviour of coated electrode structures using numerical simulations in OpenFOAM. The influence of different surface coatings, gauze geometries, and wetting properties on interface formation and stability will be analysed. To this end, provided CT scan data of differently coated gauzes will be processed into computational domains and numerical meshes for efficient simulations.

Your Tasks

1. Develop a solid understanding of the Cahn-Hilliard-Navier-Stokes equations for phase-field modelling of multiphase flows and dynamic wetting.
2. Implement the simulations in OpenFOAM and evaluate approaches for efficient geometry and mesh generation based on provided CT scans of coated gauze electrodes.
3. Perform transient simulations on our local servers and, where necessary, on the Lichtenberg cluster.
4. Systematically investigate the influence of different surface coatings, gauze geometries, and wetting properties, and compare your results with reference cases of uncoated, smooth surfaces.

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 and fluid mechanics.
- Initial experience with numerical simulations is an advantage.

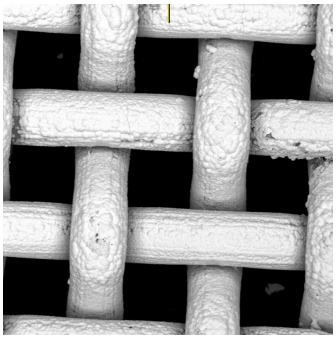
What We Offer

- 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.

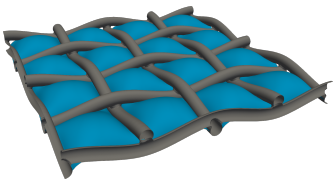
Nano- and Microfluidics

Federal Ministry of Research, Technology and Space

Coated metal electrode



Simulation without coating



Key Facts

- Multiphase simulation
- OpenFOAM
- Industrial application

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Got interested?
Please send me an e-mail!

For more information and other topics see `www.nmf.tu-darmstadt.de` or send us an e-mail!