Design of Metal Gauze Electrodes for the Electrification of the Chemical Industry

Masterthesis

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Background

Decarbonizing the chemical industry is a key challenge on the path to CO_2 neutrality. For this reason, we are working in the BMBF-funded future cluster ETOS on the transformation of the chemical industry towards more climate-friendly electrochemical technologies. One promising approach for this is the use of so-called gas diffusion electrodes (GDEs). These are hierarchically structured metal gauzes at which a liquid and a gaseous reactant meet. However, when using organic electrolytes, a technical concept for the stable positioning of the forming phase boundary is still lacking. Together with partners from academia and industry, we aim to solve this problem by adapting the structure and wetting properties of the metal gauze and controlling the position of the phase boundary via the differential pressure between the gas and liquid phases.

In this work, the wetting of abstract gauze structures is to be investigated using numerical simulation with OpenFOAM. In particular, the influence of different orifice geometries and wetting properties on the forming phase boundary and a possible bubble formation at too high differential pressures shall be investigated.

Your Tasks

- 1. Learn and understand the Cahn-Hilliard-Navier-Stokes equations for modeling of multiphase flows and dynamic wetting.
- 2. Implement the simulations in OpenFOAM.
- Run transient simulations on our servers and, where necessary, the Lichtenberg cluster.
- 4. Systematically vary the orifice geometry and wetting properties to evaluate the effect on phase separation and bubble formation.
- 5. Evaluate the results qualitatively and quantitatively.

In addition to the simulations, a theoretical evaluation of the results is a possible extension. – Your ideas and interests are very important to us!

What You Bring

- Interest in working on a current research topic with a close connection to industry-related applications.
- · Good 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 a interdisciplinary research project with regular meetings.
- Systematic support for the development and realization of your own ideas.
- Become an expert in simulations with OpenFOAM. One of the leading finite-volume codes in science and industry.



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Key Facts

- Multiphase simulation
- OpenFOAM
- Flexible starting date

Got interested? Please send me an e-mail!

Simulated bubble formation at a single orifice and a simple metal gauze:





Lazouski et al., Nature Catal., 2020, 3, 463



