eiz Energie-Innovationszentrum Cottbus

b-tu Brandenburgische Technische Universität Cottbus - Senftenberg

MASTER / BACHELOR THESIS or STUDY PROJECT

Chair of Numerical Fluid and Gas Dynamics · Scientific Computing Lab, Energy Innovation Center (EIZ)
Brandenburg University of Technology (BTU), Cottbus, Germany

Multiphysics modeling of electrochemically reacting flows for application to electrolysis

Synopsis – Electrolysis is perhaps the most promising Power-to-X (PtX) application that could help compensate for the volatility of renewable energy sources. Large-scale application of electrolysis is currently prevented by its low efficiency, which is partly due to multiphase flow physics [1]. The situation may be improved by a better understanding of the physical processes with the aid of numerical simulation. This is challenging because of the coupling of electrochemical and hydrodynamical processes, turbulent transfer, multiphase properties (gas bubbles), details of the electrode surface (roughness, porosity), and electrochemical reactions [2]. In this student project, we strive to contribute to a better understanding by subsequently developing numerical models for electrolysis applications. First, multipurpose commercial software (like ANSYS Fluent) or open-source software (like OpenFOAM) will be utilized to obtain benchmark results based on Reynolds-averaged Navier–Stokes (RANS) modeling. After that, we strive to improve the numerical fidelity by utilizing novel stochastic approaches, such as ODTLES [3] or AME [4], which are based on the one-dimensional turbulence (ODT) model [5] that may also be used as standalone tool.

[1] Zeradjanin *et al.* (2021) *Current Opinion in Electrochemistry* **30**:100797 — [2] Zarghami, Deen & Vreman (2020) *Chem. Eng. Sci.* **227**:115926 — [3] Gonzalez-Juez, Schmidt & Kerstein (2011) *Phys. Fluids* **23**:125102 — [4] Kerstein (2022) *Fluids* **7**(2):76 — [5] Kerstein (1999) *J. Fluid Mech.* **392**:277

Modes

- **a) Master / Bachelor Thesis (1 semester):** Simulations with open-source or commercial software
- **b) Study Project (2 semesters):** Same as a), but with more model development
- **c) Study Project and Master Thesis (3 semesters):** Same as b), but with ODT is optional

Tasks

- Review of relevant literature and theoretical foundations
- Visualization, post-processing, and analysis of simulation data
- Comparison with relevant reference data
- Own numerical simulations with commercial, open-source, or in-house software

Desired skills

- Solid knowledge of fluid mechanics, boundary layers, electrolysis, or related topics
- Affinity to programming (preferably Python, Matlab, C/C++, or Fortran)
- Scientific attitude (curiosity, self-motivation, and critical reasoning)
- Experience with data analysis, numerical simulation, or multiphysics modeling is an asset

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