DEVELOPMENT OF A NEW FRAMEWORK FOR THE SIMULATION OF FUEL CELLS, ELECTROLYZER AND OTHER ELECTROCHEMICAL DEVICES

SHIDONG ZHANG[1], STEFFEN HESS[1], HOLGER MARSCHALL[2], UWE REIMER[1], STEVEN BEALE[1,3], WERNER LEHNERT[1,4]

[1]*Institute of Energy and Climate Research, IEK, Forschungszentrum Jülich, 52425 Jülich, Germany, s.hess@fz-juelich.de, s.zhang@fz-juelich.de*

[2]*Department of Mathematics, Computational Multiphase Flow, Technical University of Darmstadt, Germany, holger.marschall@tu-darmstadt.de*

[3]*Department of Mechanical and Materials Engineering, Queen's University, Kingston ON K7L 3N6 Canada, s.beale@fz-juelich.de*

[4]*Modeling in Electrochemical Process Engineering, RWTH Aachen University, Aachen, 52056, Germany*

Keywords: *Computational fluid dynamics, Finite volume method, Multiphase flow, Fuel cells, Electrolyzer, Multi-region*

Fuel cells and electrolyzers have received a great amount of attention over the last several years, due to the efficient and clean conversion of chemical energy directly into electricity and vice versa. A huge number of detailed experiments have been conducted over the last decades trying to understand the mechanism inside of those running cells and their systems. However, detailed experimental investigations are expensive and challenging providing the number of operating conditions and designs. An alternative and by now a common way to conduct these studies is provided by computational analysis. Especially with the steadily increasing high-performance computing resources, the limitations of numerical simulations have substantially decreased.

A modern and versatile C++ library named *openFuelCell2* has been implemented within the open-source platform OpenFOAM [1], [2]. The solver which main structure and some of it's classes base on the *openFuelCell* libraries [3] allows for detailed and large-scale parallel calculations of fuel cells and electrolyzers. It keeps track of the major transport phenomena, including the (two-phase) fluid flow and their interactions via an Eulerian-Eulerian approach, electrochemical reactions, species and charge transfer and heat and mass transfer in the different functional regions inside a cell. In comparison to the recently published PEM fuel cell code based on the unsaturated flow theory by Weber et al. [4] this framework attempts to capture especially more details of the two-phase flow and is also applicable to other cell types, like (PEM) electrolyzers and/or solid oxide fuel cells/ electrolyzers. The goal is to publish the code, make it freely accessible and incorporate new updates over time [5].

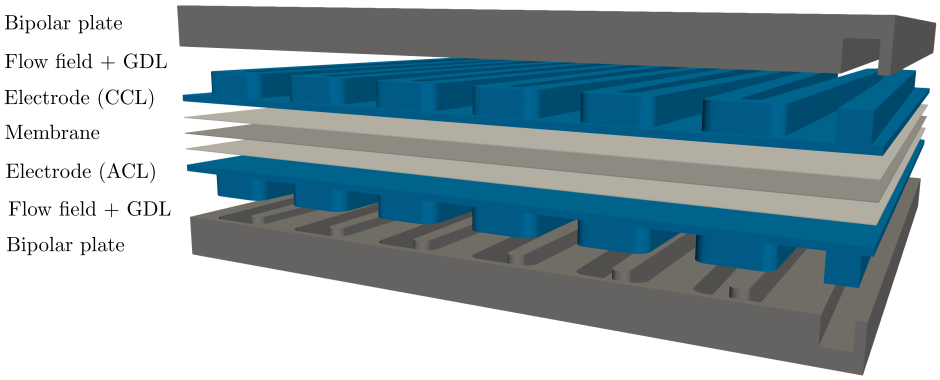

Figure 1: In-house developed polymer water electrolyzer cell design. Depicted are the different components of this cell.

In this particular work the methodology of this code is presented and applied for the simulation of a polymer water electrolyzer cell based on an in-house cell design, see Fig. 1, used for various experimental setups by researchers of the IEK-14 in the Forschungszentrum Jülich. The results are compared to available experimental data.

Acknowledgments

This work is partially supported and funded by AI Data Analytics and Scalable Simulations (AIDAS). Calculations were performed on the HPC hardware of JARA, under grant JARA0070.

References

[1] S. Zhang, U. Reimer, S. B. Beale, W. Lehnert, and Stolten, "Modeling polymer electrolyte fuel cells: A high precision analysis," *Applied Energy*, vol. 233–234, pp. 1094–1103, 2019.

[2] S. Zhang, S. B. Beale, Y. Shi, H. Janßen, U. Reimer, and W. Lehnert, "Development of an Open-Source Solver for Polymer Electrolyte Fuel Cells," *ECS Transactions*, vol. 98, no. 9, p. 317, 2020-09-08.

[3] S. B. Beale, H.-W. Choi, J. G. Pharoah, H. K. Roth, H. Jasak, and D. H. Jeon, "Open-source computational model of a solid oxide fuel cell," *Computer Physics Communications*, vol. 200, pp. 15 – 26, 2016.

[4] N. Weber, "Open-source computational model for polymer electrolyte fuel cells," *OpenFOAM® Journal 3*, p. 26–48, 2023.

[5] S. Zhang, S. Hess, Marschall.H, U. Reimer, S. Beale, and W. Lehnert, "openfuelcell2: A new computational tool for fuel cells, electrolyzers, and other electrochemical devices and processes," *Computer Physics Communications, to be submitted*, 2023.