Modeling and simulation of an alkaline water electrolyzer

S. Hess[1]*, S. Renz[1], S. Zhang[1], S. B. Beale[1], W. Lehnert[1,2]

[1]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research (IEK)
[2]Modeling in Electrochemical Process Engineering,
RWTH Aachen University, D-52056 Aachen, Germany
*s.hess@fz-juelich.de

Detailed 3-D models of electrochemical components may be used to identify local behavior and characteristics that would be either very difficult, or not possible at all to measure in experiments. The information gained from such numerical simulations is an indispensable tool in the ongoing research and development of electrochemical devices, and can thus make a significant contribution to the optimization process. In this study, a comprehensive cell model was implemented in the object-oriented open-source package OpenFOAM® [1]. The model is able to consider single-phase and/or two-phase flows occurring in fuel/electrolysis cells with electrochemical reactions, mass and heat transfer. It is based on the continuum assumption, and employs the finite volume method.

A detailed calculation of a 3-D alkaline water electrolysis cell is presented and validated on the basis of in-house gathered experimental data. The two main objectives of the present work are the prediction of local differences in the concentration of the potassium hydroxide and the formation of the produced gases, which significantly influence the behavior and performance of the cell. The typical structure of the 'zero-gap' cell considered in the present study can be seen in Fig. 1. The simulations of the two-phase flow on the cathode and anode sides are based on the Eulerian-Eulerian approach, whereby the mutual mass transport, momentum exchange and heat transfer between the gas and liquid phases, is described together with local specie concentrations. The physically different regions are coupled with each other, by means of appropriate mapping functions. The electrochemical reactions are characterized by the Butler-Volmer equation that are presumed to take place on electrodes of finite thickness, i.e., within a defined volume (CCL, ACL, see Fig. 1). In addition, the properties within the different porous layers, such as tortuosities and permeabilities, are all assumed to be isotropic at this point. This is the first CFD code developed and used for an anisothermal 3-D alkaline electrolysis cell describing the gaseous and liquid phases as two individual and interacting phases based on an open-source platform. The simulations were performed on the HPC hardware of JARA, under grant JARA0070.

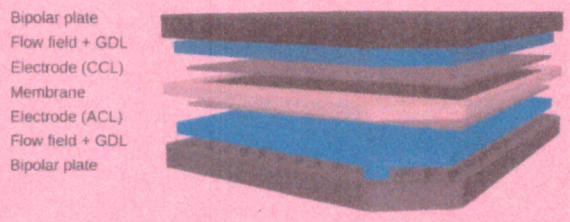

Fig. 1: Cell geometry and the different components

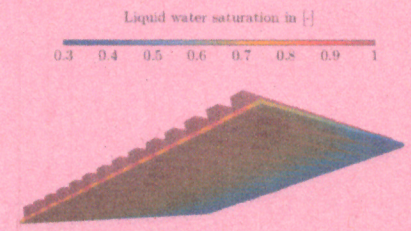

Fig. 2: Liquid water saturation at the anode side

Keywords: Finite volume method, Alkaline electrolyzer, Two-phase flow, Numerical simulation

1. Zhang S. et al., Polymer electrolyte fuel cell modeling - A comparison of two models with different levels of complexity, Int. J. Hydrog. Energy, https://doi.org/10.1016/j.ijhydene.2020.05.060