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3D simulation of membrane electrode assembly with hydrophilic treated GDL

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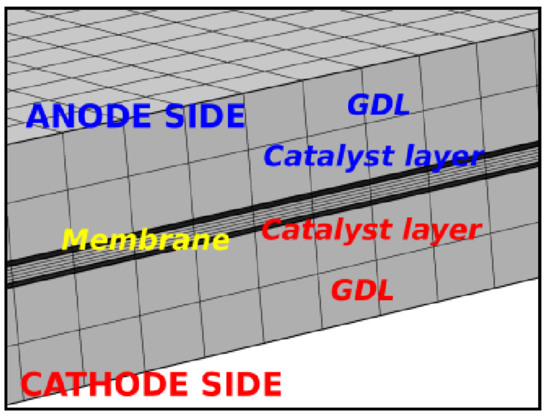
Abstract

We present a three-dimensional numerical model of a PEM fuel cell. Here, we focus on the membrane electrode assembly of the novel thermoneutral fuel cell design. An integral feature of the new design is the hydrophilic treatment of the gas diffusion layer which divides the GDL into the hydrophilic and the hydrophobic regions. The model consists of the Van Genuchten based two-phase flow of the liquid and the gaseous water, the transports of the hydrogen and the oxygen, the temperature field, as well as the electrochemistry described by the electron and proton potentials. Preliminary results show that the model trends are in agreement with the experimentally observed behavior.



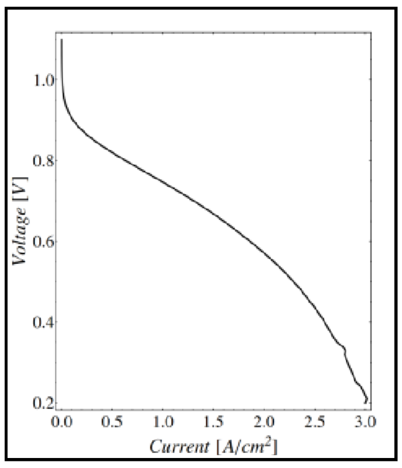


Fig. 1: A detail of the 3D mesh with depicted membrane-electrode-assembly layers (left) and a current-voltage curve (right), where the pressure of inlet gasses is 1.8 bar, the inlet gases are pure hydrogen and pure oxygen, and 100% humidification of inlet gasses is assumed.

Introduction

The fuel cell research conducted in the Capacity Area-A2 aims to develop a novel concept of a thermo-neutral fuel cell operation. Here, the cooling is done by the evaporation of the water that we additionally introduce into the fuel cell and also by the evaporation of the water that is produced during the fuel cell operation. An integral component of the thermo-neutral fuel cell is the GDL with special hydrophilic treatment. This creates regions with different water transport properties, i.e. the hydrophilic and hydrophobic regions, within the porous material. In this setting it is essential that we thoroughly understand the transport of the liquid water and the gases, the heat creation and the heat transport, as well as the phase change processes in the fuel cell's porous materials.

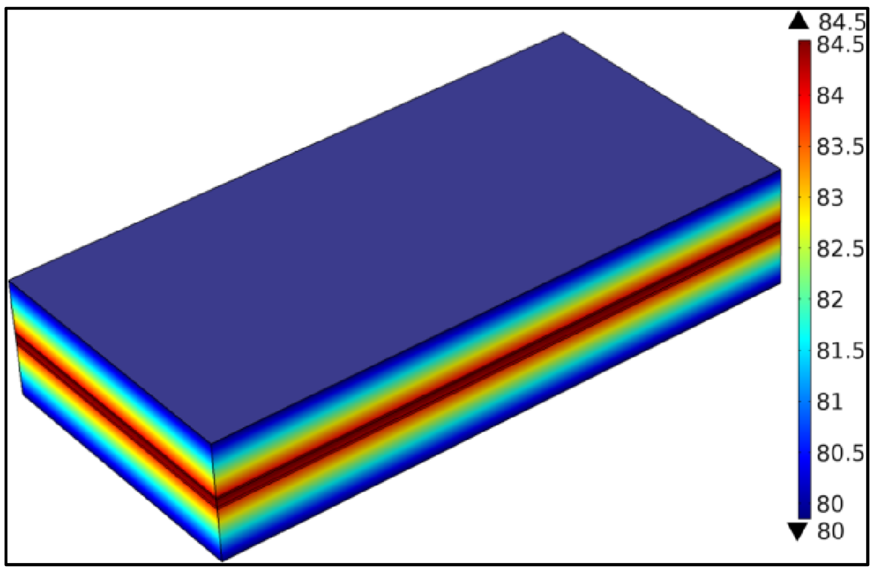


Fig. 2: The distribution of the temperature field [˚C] in an isolated section of membrane electrode assebly at 0.2 V. The temperature is the highest in the middle where the chemical reactions and ion transport take place. In the current stage of the model the temperature field is not yet coupled to the two-phase flow. Therefore, there is no in-plane variation of the temperature.

Model features

- We focus on the membrane electrode assembly which consists of (see Fig.1 left) the cathode side GDL and the MPL, the cathode side catalyst layer, the membrane, the anode side CL and the anode side GDL with MPL.
- The following physical and electrochemical fields are included: the temperature, the electron potential, the proton potential, the dissolved water, the water vapor, the liquid water, the oxygen, and the hydrogen.
- The physical and electrochemical fields are coupled through the sink and the source terms as well as through the transport parameters.
- The two phase flow is based on the Van Genuchten model (e.g. [1]).
- Due to the hydrophilic treatment we further divide the GDL into the hydrophilic and the hydrophobic regions. These regions and the MPL have different values of the Van Genuchten model parameters.
- The Dirichlet/Neuman boundary conditions are set at the boundaries between the MEA's layers.

Results

- We used the COMSOL Multiphysics (see [2]) to build the model.
- In Fig. 1 right we present the current versus the voltage curve obtained with the present model.
- In Fig. 2 we present the distribution of the temperature field in an isolated section of the membrane electrode assembly at 0.2 V.
- In Fig. 3 we focus our attention to the anode side GDL and we present the liquid water saturation distribution.

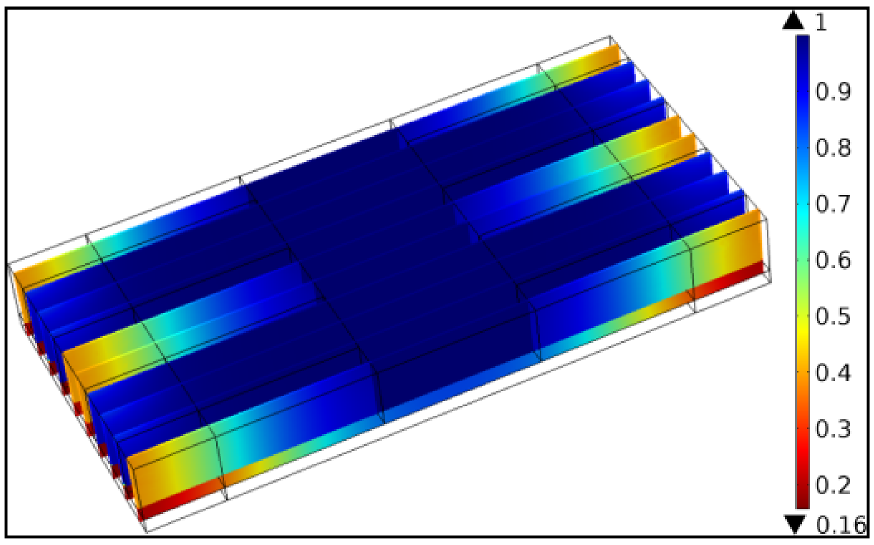


Fig. 3: The liquid water saturation distribution in the hydrophilic treated GDL. The water is accumulated in the hydrophilic regions while the hydrophobic parts of the GDL and the microporous region (bellow) repel the water. Note that the water on the anode side is not produced via chemical reaction but it is introduced as a cooling agent at the GDL boundary.

Conclusion

We presented the current stage of a two-phase three-dimensional numerical model of a PEM fuel cell. The preliminary results show that the model can represent the experimentally observed trends with respect to the electrochemistry and also with respect to the liquid water distribution within the hydrophilic and the hydrophobic porous materials. Further improvements of the model and the model input parameters are ongoing and they include: to finish the coupling between all the included fields, to systematically investigate the different options for boundary conditions related to the liquid water and to include more accurate values for the parameters that describe the liquid water transport.

Acknowledgements

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