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Computer simulation of liquid water saturation in porous media of fuel cells

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Abstract

We present a finite element method model for an analysis of the liquid water saturation in the porous media of the polymer electrolyte membrane fuel cells. Here, we focus on the 2D simulation of the cathode's gas diffusion layer. The model consists of the mechanical part, the two phase flow, the transport of gas species and the electrochemical part. The results of the model are compared with the results obtained by the neutron radiography imaging. The comparison shows a good agreement between the experiment and the simulation.

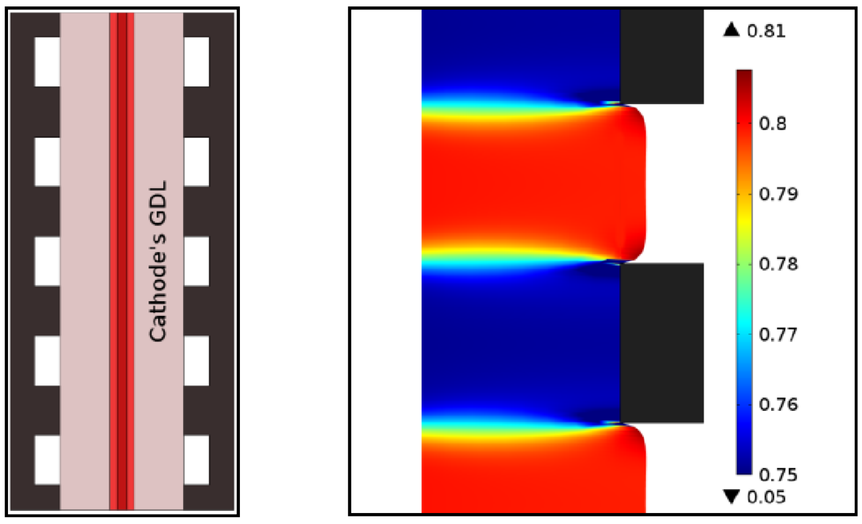

Fig. 1: The cross-section of the differential cell (left) and the distribution of the effective porosity of the cathode's GDL due to 20% mechanical compression (right).

Introduction

The research and the development of PEMFC systems is an ongoing process with an increasing demand for accurate numerical models. One of the main challenges that require further investigation is related to the two phase (liquid and gas) water transport in the porous media of the polymer electrolyte membrane fuel cells. The numerical simulations are essential to thoroughly understand the two phase flow, as well as the phase change processes in the porous materials and on cell level. The neutron radiography captures the behavior of the functioning fuel cell and also serves as the verification of the numerical model.

Both the neutron radiography and the numerical models are essential to analyze and predict the conditions for the thermoneutral operation of the proton exchange membrane fuel cells.

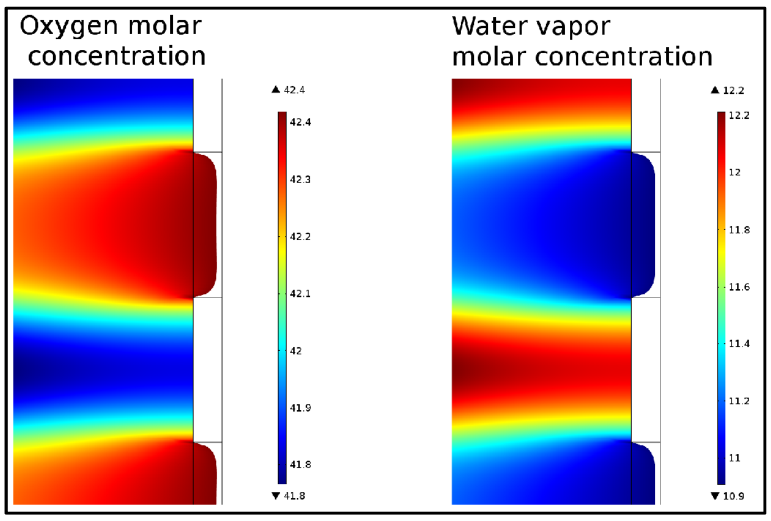

Fig. 2: The distribution of the oxygen concentration (left) and the water vapor concentration (right).

Liquid water saturation model of the cathode's GDL

- We focus on the cathode's gas diffusion layer and model it in 2D.
- When a fuel cell is assembled, the bi-polar plates compress the MEA. We include this effect by using the mechanical part of the model.
- The effective porosity of the GDL ε_{eff} is related to the intrinsic porosity ε and the volumetric strain ε_v obtained by the mechanical model: $\boxed{\varepsilon_{eff} = \frac{\varepsilon + \varepsilon_v}{1 + \varepsilon_v}}$
- The two phase flow is based on the Van Genuchten model (e.g. [1]).
- The transport of oxygen and water vapor considers the diffusion and the convection.
- The volumetric rate of interfacial mass transfer between the liquid phase and the water vapor phase is modeled by using the Hertz-Knudsen-Langmuir condensation equation (see [2]).
- At the boundary between the GDL and the catalyst layer we assume an electro-chemical interface. Here, oxygen is consumed and water vapor is produced. The rates of production are dependent on the local current density.

Results

- We used the COMSOL Multiphysics (see [3]) to build the model.
- We assumed the following fuel cell's operating regime:
  - the pressure of the inlet gas is 2.0 atm,
  - the fuel cell's curent density is 1 A/cm^2,
  - the cathode's inlet gas is composed of 100% oxygen with 100% rel. humidity,
  - the temerature of the fuel cell is 70˚C.
- The effective porosity of the compressed GDL is presented in Fig. 1.
- The distribution of the oxygen and water vapor concentration is shown in Fig. 2.
- In Fig. 3 we compare the results of the model with the results obtained by the neutron radiography imaging.
- The experimentally measured quantity of liquid water present in the GDL is expressed with the water thickness δ. This can be converted to the water saturation fraction s by using the following formula: $\boxed{s = \frac{\delta}{\varepsilon \cdot 10\text{mm}}}$

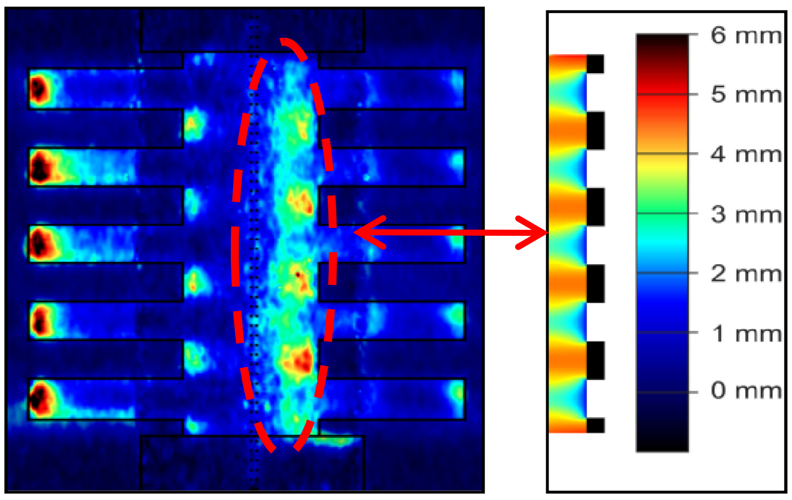

Fig. 3: The quantity of water present (water thickness) in the fuel cell obtained by the high resolution in plane neutron imaging (left) and the simulated water thickness in the cathode's GDL (right).

Conclusion

We presented the numerical liquid water saturation model of the cathode's gas diffusion layer. The model's results predict a lower level of effective porosity under the bi-polar plates' ribs. The concentration of oxygen is greater under the open channels, whereas the concentration of water vapor is greater under the ribs. Both the neutron radiography and the numerical model show the accumulation of liquid water under the ribs. Experimental data and simulation results are in good agreement.

Acknowledgements

The authors gratefully appreciate financial support from The Swiss Commission for Technology and Innovation CTI.

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