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Numerical modeling of patterned porous materials for thermo-neutral fuel cells

Numerical modeling of polymer electrolyte fuel cells (PEFC) allows for a better insight into the complex operation of a fuel cell and it also serves as a tool to systematically optimize the fuel cell components. We present a macrohomogeneous two-phase model for water transport simulation of patterned gas diffusion layers (GDLs) which are an essential component of the thermo-neutral fuel cell. 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 to the experimental ex-situ imbibition results obtained by neutron radiography imaging. The results are in good agreement. In the next phase we will use the computer model to improve the pattern design of the new GDL.

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Introduction

The new GDL design, developed at PSI, is a succession of hydrophobic and hydrophilic regions [1]. It is capable of better removing water from the electrodes towards the flowfield. This design was first characterized experimentally by measuring the local saturation as a function of the capillary pressure applied. Neutron radiography was used as imaging technique (see Fig. 1 left), allowing for quantification of the water thickness.

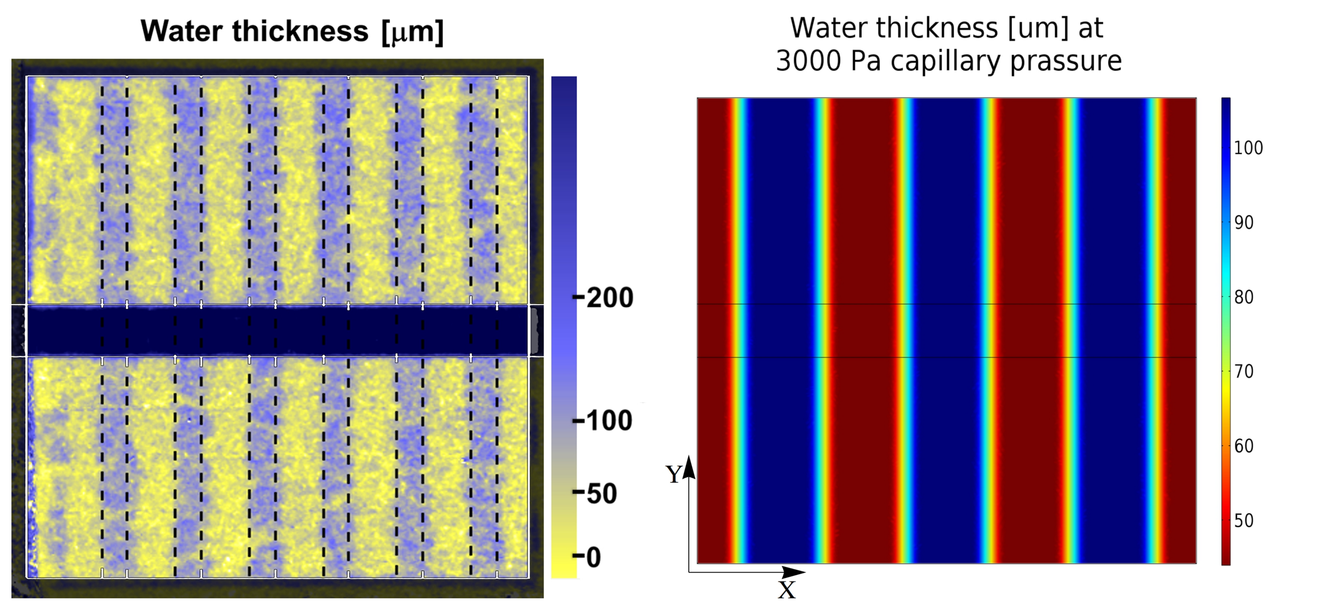

Figure 1: The experimentally (left) and the numerically (right) obtained distribution of the total water thickness in the patterned GDL. A cell with 1x1 cm of active area was used in the experiment while a smaller portion of 4350×4350 μm was considered in the simulation. The water accumulates in the hydrophilic domains. Neutron imaging (left) also captured the water in the injection channel spanning from left to right.

In a second step a coupled macrohomogeneous computer model (see [2]) was built in COMSOL Multiphysics (see [3]) and compared with the ex-situ experimental measurements (see Figs. 1 and 2). Additionally, a simulation of an operating fuel cell has been performed to study the intricate couplings in an operating fuel cell and to examine the patterned GDL effects (see [2] and Fig. 3).

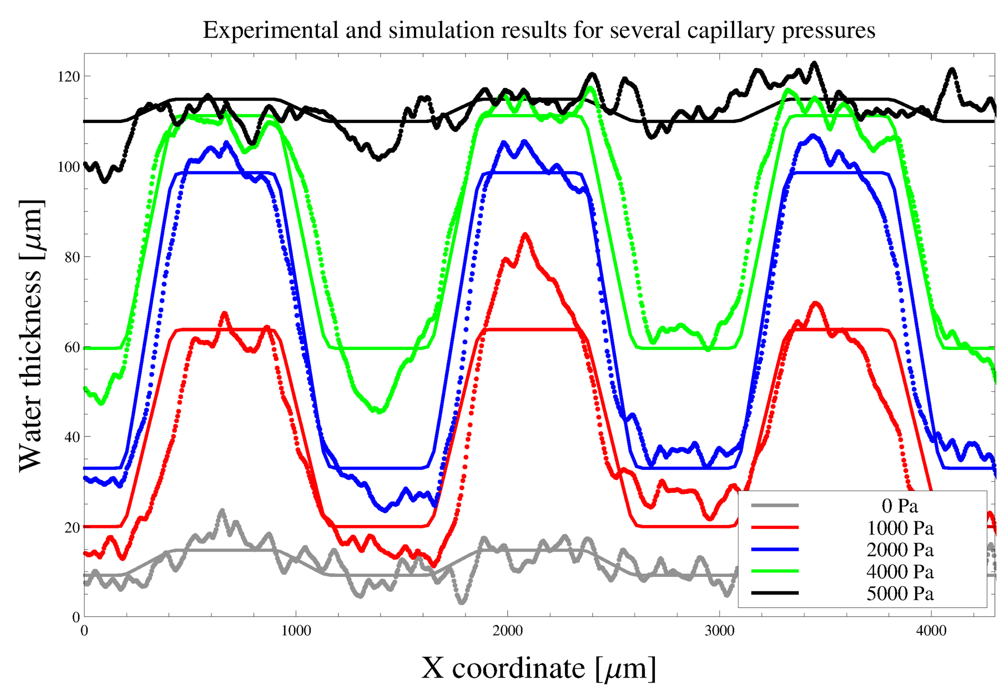

Figure 2: The comparison of the experimental (dotted) and the simulated (full line) water thickness results as a function of position for different applied capillary pressures. The results of the experiment and the simulation are in good agreement. The succession of hydrophobic and hydrophilic regions is clearly seen along the X axis.

Numerical Model and Results

- The simulated fuel cell area (2900×4000 μm) includes two full repetitions of channel/rib and hydrophilic/hydrophobic patterns.
- The GDL's properties vary with the X-position (see Figs. 1 and 2). Three regions are consider: hydrophilic (500 μm), transition (225 μm) and hydrophobic (500 μm) .
- The model consists of: (i) mechanical part representing the assembly procedure, (ii) the two-phase flow with condensation and evaporation, (iii) the convective and diffusive transport of gas species and (iv) the electrochemical part.
- The oxygen diffusion coefficient is modified to take into account the blockage of pores with liquid water.
- At the GDL-CL boundary we assume an electro-chemical interface.

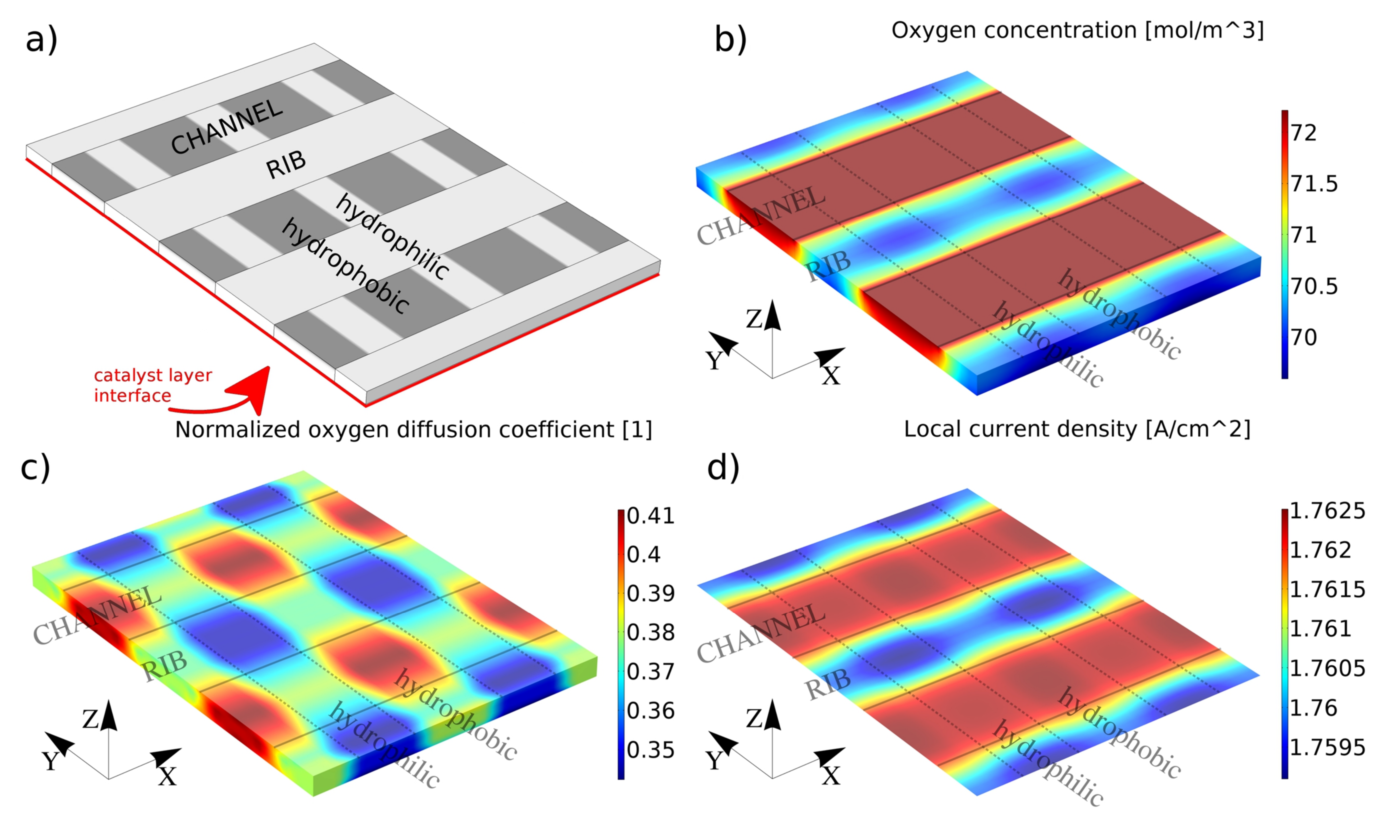

Figure 3: a) the geometry of the FC model consisting of the rib and channel regions which are perpendicular to hydrophilic/hydrophobic pattern, b) the distribution of the oxygen concentration, c) the distribution of the saturation dependent oxygen diffusion coefficient and d) the local current density distribution. Both the rib/channel and the hydrophilic/hydrophobic pattern play a role in the distribution of liquid water, the distribution of gases and the final local current density. As expected we obtain the highest current under the channels in the hydrophobic region and the lowest current under the ribs in the hydrophilic regions, where the liquid water blocks the most pore space.

Expected impact

Further technological innovation and system optimization is needed to facilitate the commercial breakthrough of the PEFCs technology into individual mobility. In this context, accurate models can be used as a tool to optimize towards higher efficiency, energy density and reliability. The presented model will be in the next steps further developed and used to find the optimal GDL pattern design to improve the performance of the thermo-neutral fuel cell. The novel concept of the thermo-neutral fuel cell operation will reduce system complexity and therefore increase the volumetric energy density. The expected reduction in costs will promote market penetration of the clean fuel cell technology into automotive applications.

References

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