Hierarchical Modeling of Polymer Electrolyte Membrane Fuel Cells

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Abstract

Introduction
In the energy hungry modern world, the need to replace the fossil fuel based systems with sustainable and clean energy technologies is enormous. The leading replacement candidate in the transport applications as well as in stationary applications are the hydrogen fuelled polymer electrolyte membrane fuel cells (PEMFC). In PEMFCs the chemical energy of hydrogen and oxygen is transformed into electricity, whereas the only by-product is pure water.

The research and development of PEMFC systems is an ongoing process with an increasing demand for accurate numerical models. The two main obstacles when modeling the PEMFCs are: (I) the large area to thickness ratio of PEMFCs which makes a 3D analysis of the whole cell computationally very expensive (impossible) and (II) numerous coupled physical and electrochemical processes and solution variables which make the model very complex and numerically unstable.

In order to tackle the first obstacle (I) we divided our model into a combination of two separated 2D regions, which are connected by the 1D regions. The 2D regions capture all the significant in-plane phenomena, while the connecting 1D regions model the through-plane processes in the membrane electrode assembly (MEA). We tackle the second obstacle (II) by carefully choosing which processes/fields are included in the model and what type of parametrization is used.

Use of COMSOL Multiphysics®
A schematic representation of the MEA geometry is shown in Figure 1. Our current model (Model 1) includes the following seven physical fields: temperature (regions 1-5), electron potential (regions 1,2,4,5), proton potential (regions 2-4), dissolved water (regions 2-4), water vapor (regions 1,2,4,5), oxygen (regions 4,5) and hydrogen (regions 1,2).

The model was implemented in COMSOL Multiphysics® by defining the geometry, including seven General Form PDEs and by prescribing appropriate Dirichlet/Neuman boundary conditions (at boundaries 1-6). We then further developed Model 1 by adding new fields and by increasing the complexity by using different descriptions (parametrizations) of the fields. Model 2 represents an extension of Model 1, where we are adding one new General Form PDE to describe the capillary diffusion of liquid water (regions 1,2,4,5) and coupling it to the existing

model framework.

Results
With Model 1 we have performed an extensive parametric analysis. In Figure 2 we plot the current-voltage curves for different boundary temperatures and also the influence on results if one feeds the fuel cell with air or with pure oxygen.

Conclusion
The research and development of PEMFC numerical models is of great importance for the energy sustainable future. Our experience shows that COMSOL Multiphysics® is a perfect testing ground for MEA model development. One can easily change the model and see the influence of a particular field/parameter on the results, which is a good guidance to what is important and which effects can be neglected in the model. We also use the COMSOL Multiphysics® results as a reference point for our in-house software, which is later used to perform 2D+1D simulations on complex gas distribution flow-fields.

Figures used in the abstract

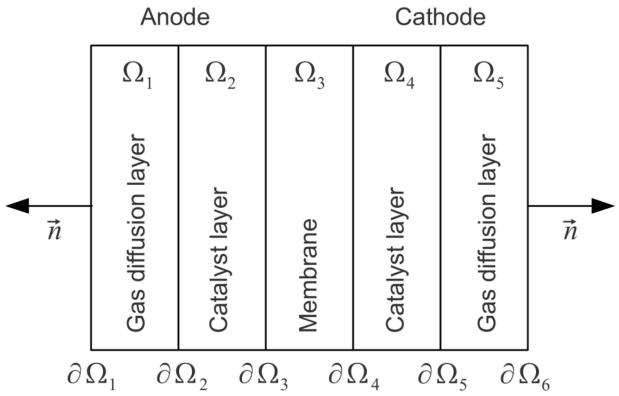

Figure 1: MEA geometry

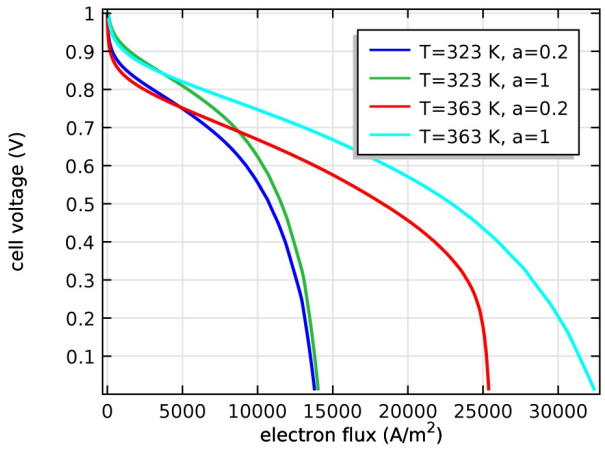

Figure 2: Current versus voltage curves