Mathematical Polymer-Electrolyte-Membrane Fuel Cell Model

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Abstract: A non-isothermal model of a low temperature polymer electrolyte membrane fuel cell is presented. The model is based on conservation equations coupled with physical, electrochemical and empirical expressions. The model focuses on the implemented electrical subsystem. Thermal and mass balance are coupled to allow for a self-humidifying procedure. The simulation results are compared with experimental data. The model can be used to optimize the thermal and flow-field layout

Introduction
Polymer-electrolyte-membrane fuel cells (PEMFCs) are expected to play an important role in tomorrow’s energy conversion devices. During the past few decades, researchers have focused on cell optimization, layout and design in order to be more competitive. In this context, mathematical modeling is an indispensable tool which helps predict the behavior of a functioning self-humidified cell. Although complex, the models tend to be more beneficial as they offer tremendous possibilities to arrive at reasonable conclusions while designing fuel cells.

Basics – What is a fuel cell?
Electrons and protons reach the cathode side through a bipolar plate, external load and proton conducting membrane respectively. In the meantime, water either in vapor or liquid phase is produced depending on the local operating conditions. Besides, heat is produced due to strong exothermic reaction when electrical power is drawn using the external load.

About fuel cell modeling
Fuel cell modeling is solving for all conservation equations coupled with electrochemical, empirical equations and material parameters. Conservation laws are generally represented by the following general partial differential equation:

\[ \frac{\partial}{\partial x} \left( \rho \frac{\partial \Phi}{\partial x} \right) = 0 \]

Where \( \Phi \) is the dependent variable of interest. Once the conservation laws are solved, the remaining boundary conditions are applied to the solution domain. The boundary conditions can be divided into: initial and/or boundary conditions, initial conditions, boundary conditions, and numerical methods.

**Numerical methods**
Computational fluid dynamics (CFD) is used to solve for this model. The meshing (Fig. 1) is a two-dimensional, steady-state conditions model (SIM) using a finite element method (FEM). The resulting mesh consists of 5,406 triangular elements with a two local refinements as can be seen in Fig. 2. The element mesh consisted of 56.85 degrees of freedom. As for the cell layout, a channel-to-land ratio of 1/1 was used for the flow-field design. The active area was 0.005 [m²].

Model validation against experimental investigations
To validate the model set-up, the simulations are compared to a life test investigation. All experimental investigations were run at ZBT facility in 201, D-47057 Duisburg, Deutschland. As for the cell channel a channel-to-land ratio of 1/1 was used for the flow-field design. The active area was 0.005 [m²].

Using the computational domain in Fig. 2, data from experimental studies are delivered for the remaining species, mechanical properties and material parameters. Conservation laws are delivered as the remaining conservation laws.

**Energy conservation**

\[ \text{Energy conservation:} \]

\[ \frac{\partial}{\partial x} \left( \rho \frac{\partial \Phi}{\partial x} \right) = 0 \]

**Initial and boundary conditions**

**Initial and boundary conditions**

**Initial solver settings (if necessary – update**

**Data postprocessing**

Fig. 3. Sequentially solution procedure

A grid independence test is carried out and showed there is no notable difference in quantities behavior. For the standard case (single phase calculations), the solution time was around 3,600 seconds on a Windows PC platform (1GBRAM) to obtain a convergence within 70 iteration steps. Solving for two-phase flow (see Fig. 7), dramatically increase the complexity of the equation system and 279 iterations are needed for a converged solution. In order to get more stability into the highly nonlinear equation system, non-ideal constraints are used for the membrane water transport equation and for pore saturation calculations.

Simulating the electrical subsystem
The following plots do show various quantities related to the electrical subsystem. Conservation of charge needs to be solved for electrical and ion phase potential.

Fig. 4. Solid and ionic phase potential

Fig. 5. Reaction layer current density

Fig. 6. Electrical and ionic current density distribution

Model validation against experimental investigations

Operating conditions
Gases are fed at room temperature with a relative humidity of 15% (dry) and 45% (up) respectively. To maintain self-humidification, the cell runs at a voltage of 0.65 [V]. The operating temperature is maintained at a temperature of 33.15°C. Fig. 5, shows the comparison of the polarization curves. The low current density results from the low cell voltage level and operating conditions and is projected for such life test investigations. Now, back diffusion of water in the membrane of the cell overcome the electro-osmosic drag resulting in a net water flux from cathode to anode.

**Hydrodynamics**

**Local mesh refinement**

**Focusing the electrical subsystem**

**Volumetric anode and cathode current density**

\[ j_a = \rho_a \left( \frac{\partial \Phi}{\partial x} \right) \]

**Experimental**

**Initial solver settings (if necessary – update**

**Data postprocessing**

Fig. 8. Center for Fuel Cell Technology (Zentrum für Brennstoffzellentechnik (ZBT) gGmbH) in Duisburg/Germany

Fig. 9. Typical fuel cell test stand at ZBT

Fig. 10. Simulation of the life time operating condition (Relative humidity and temperature distribution over the computational domain)

**Conclusions**

A two-dimensional, non-isothermal PEMFC model is presented and validated. The electrolyte subsystem is integrated in the fuel cell for the CFD study. It delivers fundamental data for solving remaining conservation laws.

**Phase potential and local current density distribution**

**Operating conditions**

**Data postprocessing**

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