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Simulation of Multiphase Transport Phenomena in PEMFC Involving Water Phase Change

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Proton exchange membrane fuel cells (PEMFCs) are energy units that convert the chemical energy of hydrogen-oxygen reaction into electrical energy. Since the conversion process is direct, PEMFCs are considered highly efficient and also zero-emission because of water being the only product of reaction. Due to this, PEMFCs have become a prime choice for the future low power requirements especially for vehicular and mobile systems.

The candidacy of PEMFC has yet to be proven as some of the old time hurdles still persist and need to be corrected in near future. Water management is one of the old timers that still need a deep insight. Nafion™ is one of the commercially available membrane materials and the working is highly water dependant (the details can found in Larminie and Dicks (2003) [3]). Higher water content gives higher proton conduction but this advantage is not a standalone effect as higher water content may block the active sites in the catalyst layer (CL) and gas passages in the porous transport layer (PTL). Since a PEMFC is a multi-disciplinary device with many phenomena working in line, in order to understand the water management and to arrive at a conclusive point for the working point of PEMFC, all the transport mechanisms need to be simulated simultaneously.

In this study, a repeating section of cathode side with interdigitated flow field has been chosen for simulations. The interdigitated flow field has an added advantage to prevent water flooding, Nguyen (1996) [4], in PEMFCs. The reasons for selecting only the cathode side are;

1. Oxygen reduction reactions occurring at the cathode have slow kinetics and determine the overall reaction rate.
2. Water is produced at the cathode side due to electro-chemical reactions.
3. Water is used as a proton carrier in the membrane and each proton drags (electro-osmotic drag) from one to five water molecules, Zawodzinski *et al.* (1993) [8] and Ren and Shimshon (2001)[5], further aiding the flooding of cathode.

Due to the reasons explained above, cathode of PEMFC is critical in determining the overall performance and deep understanding is required for optimization if PEMFCs are to be used as alternate energy sources in near future.

As stated earlier, due to coupling of physical phenomena in PEMFC, the equations employed in this study are mass continuity and momentum, two-phase flow, two-phase temperature and two-phase current. Previously, a good number of PEMFC models have been proposed by many authors looking at different details e.g., effects of catalyst structural parameters by Sun *et al.* (2005) [6] and detailed transport mechanism and parametric optimization of fuel cell design by Yu *et al.* (2009) [7], but, both models lacked in completeness as the former model was single phase flow and the later one is isothermal model. In present study all the details of working of cathode have been modeled so that an effective conclusion can be drawn for optimal performance of PEMFC. The model equations developed for this study were solved simultaneously and iteratively. The equations were discretized using a finite volume method (FVM) and implemented as user defined functions in commercial CFD code. The solution was considered to be convergent when the relative error in all parameters was equal to or less than 10^{-6}. More discussion on the governing equations, boundary conditions and sources terms can be referred to Khan (2009) [2].

Figure 1 shows the concentration level of liquid water in the fuel cell cathode side for the two current densities. The concentration level of liquid water at the inlet and the outlet of the domain is zero because;

1. Both inlet and outlet are considered as infinite sink for liquid water.
2. At the inlet, the partial pressure of water vapor is less than saturation pressure for condensation.

The concentration of the liquid water increases gradually in the porous transport layer by reason of more and more electro-chemical reactions which in turn increases the partial pressure of vapors for condensation and also there is influx of water at membrane/catalyst interface. The concentration for a specific current density is highest in the center of catalyst layer and this is because of the selected boundary condition types for liquid water. By comparing the saturation levels for different operating conditions i.e., current densities, the saturation level of PEMFC operating at higher current density is more as compared to low current density. This difference in saturation level is due to more electro-chemical reactions occurring and higher proton migrations.

The important parameter related to water presence (both liquid and vapor) in PEMFC is the membrane phase conductivity i.e., proton conduction of the supporting material to complete the electro-chemical reactions at the cathode. In this work, the potential difference between catalyst/membrane interface and the local potential in the catalyst layer has been considered as the driving force for proton immigration. The governing relation for the water activity incorporating both states of water is provided by He *et al.* (2009) [1] in which water activity is the product of relative humidity of gas phase and the liquid water saturation. Comparing the trends given in Figure 2, it can be observed that higher conductivity is offered for higher current density because of excess production of water, while at lower operating levels and because of less water production (rate of electro-chemical reactions is small), the conductivity is quite small and demanding the need of external provision of water to the domain. In this study the inlet humidity of 50% has been used to simulate the scenario. The power density for the fuel cell is also a function of operating currents. As the current density is increased, the power density also increases until the mass limitation effects are too much to cause a sharp decrease in the power density as can be seen in Figure 4.

Trends of higher membrane conductivity and maximum power density (Figure 4) at higher current densities suggest PEMFC operation at higher current densities. But as can be seen in Figure 3, potential wasted in deriving the electro-chemical reactions at higher current also increases depicting higher losses and also the liquid water effect (saturation) becomes more prominent as shown in Figure 4 where the present model curves deviates from the results produced by Sun *et al.* (2005) [6] which is a single phase model.

On the basis of above discussion, it can be concluded that although maximum power and membrane phase conductivity occur at higher current densities, it's not feasible to operate PEMFC at those levels because of increase in losses and water saturation effects. The only adverse effect by operating the PEMFC at lower currents is the dryness of membrane that can be effectively tackled by humidifying the inlet supply.

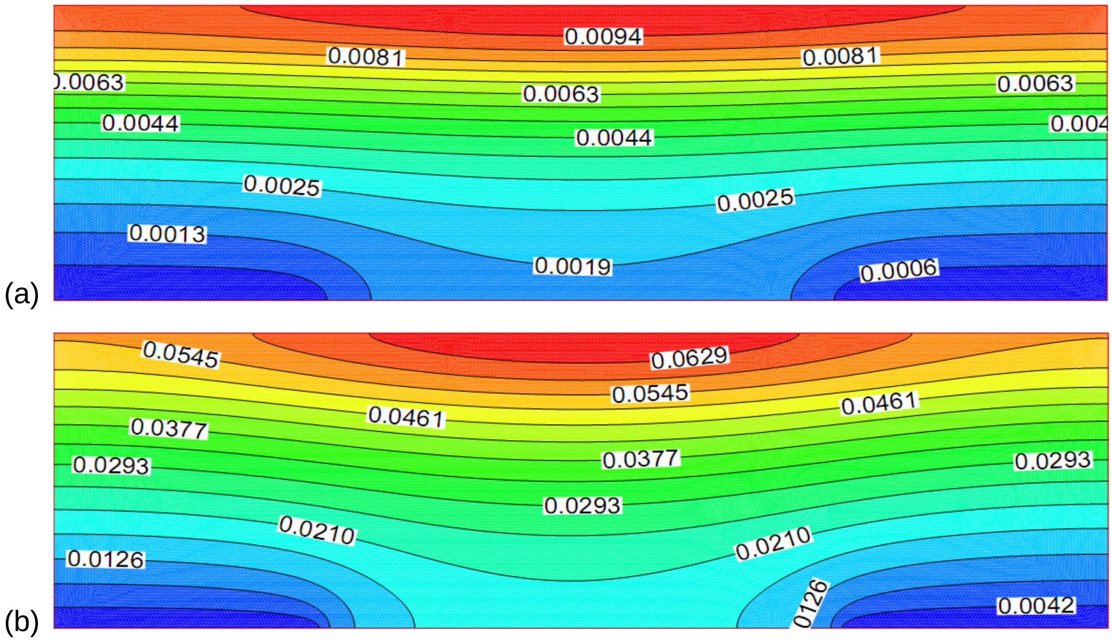

Figure 1: Liquid water saturation at (a) 0.2 and (b) 0.8 A/cm^2.

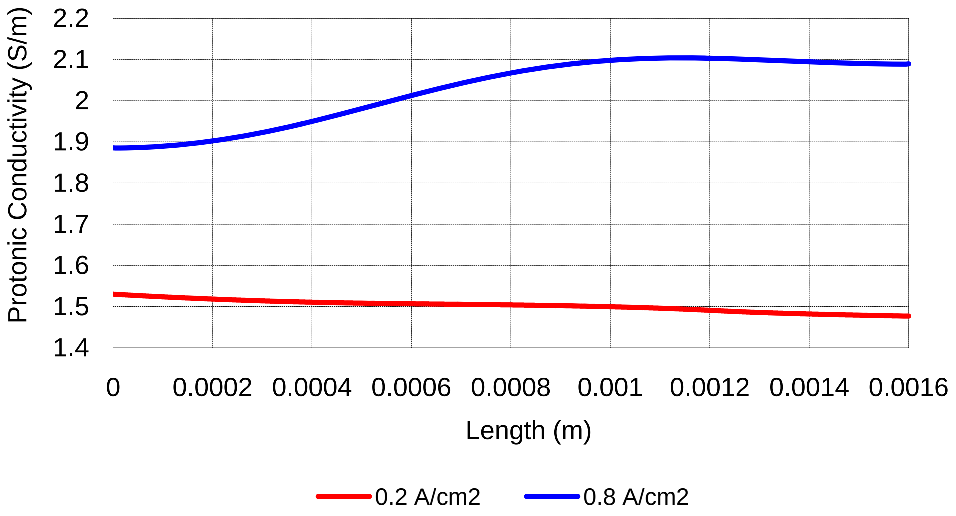

Figure 2: Membrane phase conductivity at CL/PTL interface for different current densities.

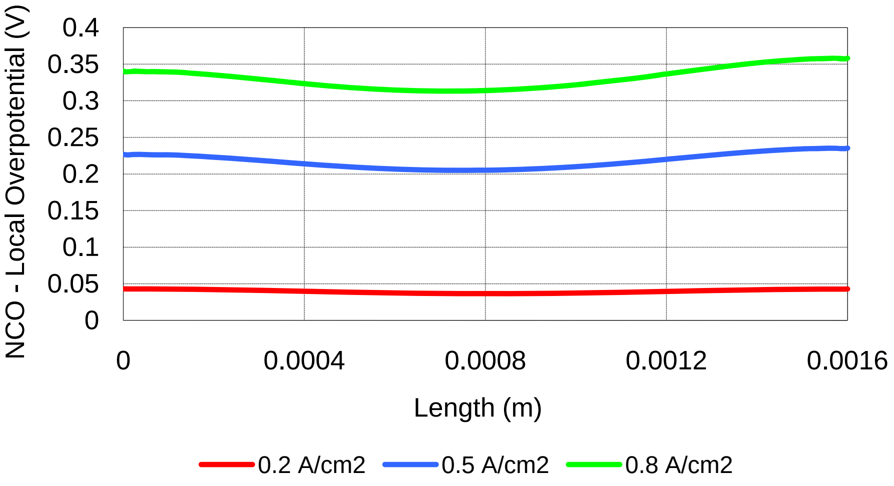

Figure 3: **Driving voltage for electro- chemical reactions at CL/PTL interface.**

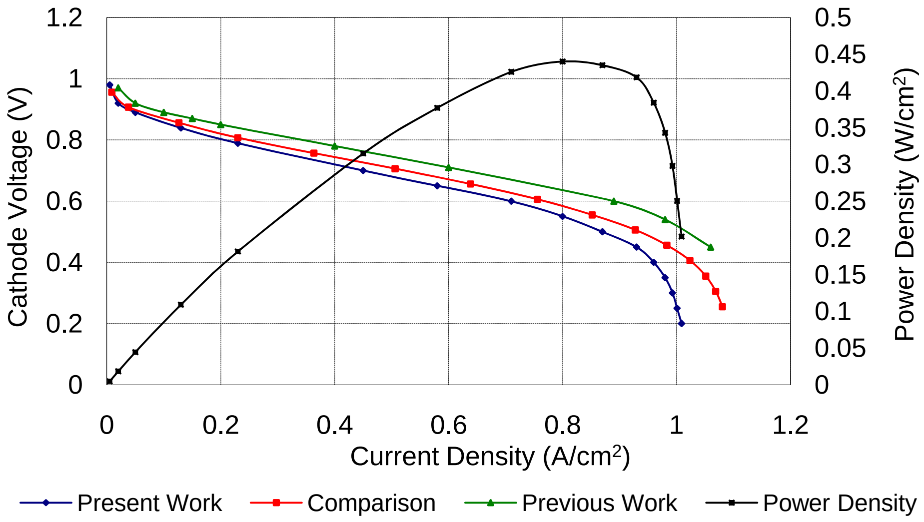

Figure 4: **Polarization curve for PEMFC.**

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