Flooding Prediction in Polymer Electrolyte Fuel Cells

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A comprehensive, multi-physics, two-phase model has been developed to simulate the polymer electrolyte fuel cells (PEFC). The developed model accounts simultaneously for electro-chemical kinetics and multi-component, multi-phase transport of species. A whole cell is considered, including all components of PEFC: flow channels, gas diffusion layers and catalyst layers for both electrodes, and the polymer electrolyte membrane. Model equations formulated in a single domain were built from the multiphase mixture model (i.e. M^2 model) for porous media; therefore the model does not require interfacial boundary conditions between the components of the cell.

A unique treatment of water transport through the membrane, which includes the various modes such as electro-osmotic drag and diffusion of water molecules, is included in the model; therefore it is able to provide comprehensive water management study, which is essential for PEFC operation in order to achieve high performance. In PEFC operation, the polymer electrolyte membrane must be kept hydrated in order to exhibit high proton conductivity. On the other hand, water is produced at cathode catalyst layer due to oxygen reduction reaction (ORR) and condenses when it exceeds the saturation concentration in the gas phase. Liquid water then covers part of the active reaction surface and blocks the pores of gas diffusion layer for oxygen transport to reaction sites, thereby reducing the cell performance.

The developed model is solved by a commercially available CFD software, Fluent, which is customized with User Defined Functions (UDF). In this study, emphasis is placed on understanding the nature of vapor condensation and flooding phenomena in PEFC and their effect on performance. Two-phase transport phenomena and electrochemical kinetics in PEFC are discussed in detail, and the effects of humidification of inlet streams and surface characteristics of gas diffusion layers on performance are investigated. The model is validated with available experimental data with reasonable agreement.

It is found that capillary transport is the dominant transport mode in the two-phase region. Calculated current density for a serpentine flow field PEFC is given in Figure 1. Since oxygen concentration is higher, the maximum current density is seen near the inlet of gas channel. Therefore, the maximum amount of liquid water is generated near the inlet. This is where the maximum liquid saturation in gas diffusion electrodes is seen, as shown in Figure 2. Effect of two-phase transport on membrane hydration is also investigated. Figure 3 shows the water content of the membrane under two-phase conditions.

Moreover, the effect of the surface characteristics (i.e. surface tension and contact angle) on the liquid saturation distribution and flooding is discussed in detail.

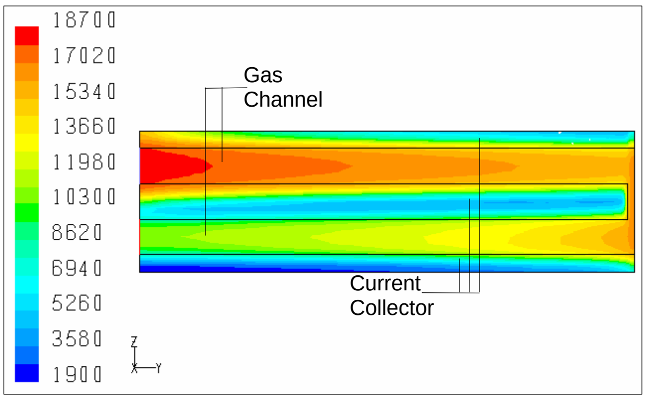

Figure 1 Local Current Density [A/m^2] of the serpentine flow field PEFC operating at 0.4 V

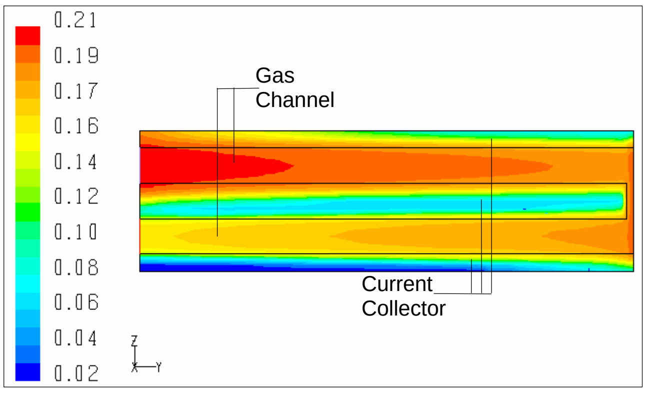

Figure 2 Liquid Phase Saturation at Cathode Catalyst Layer and Cathode Gas Diffusion Electrode Interface (Cell Voltage = 0.4 V, Average Current Density= 1.19 A/cm^2)

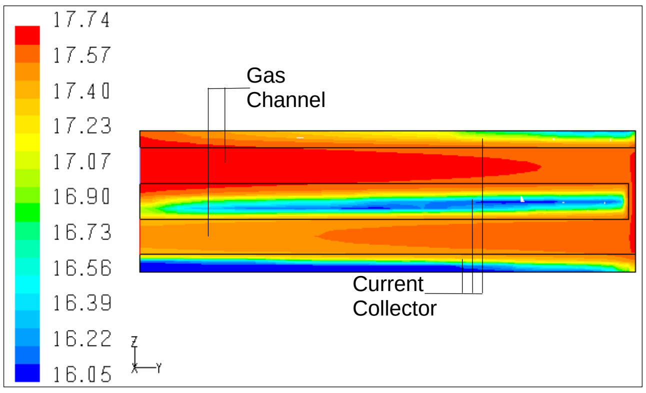

Figure 3 Water Content of Membrane (l) at Cathode Catalyst Layer and Membrane Interface (Cell Voltage = 0.4 V, Average Current Density= 1.19 A/cm^2)

REFERENCE

[1] Z.H. Wang, C.Y. Wang and K.S. Chen, *J. Power Sources* **94**, 40 (2001),
[2] S. Um, C.Y. Wang and K.S. Chen, *J. Electrochem. Soc.* **147**, 4485 (2000),
[3] T.E Springer, T.A. Zawodzinski, S. Gottesfeld, *J. Electrochem Soc.* **138**, 2334 (1991),

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