THREE-DIMENSIONAL, MULTI-PHASE MODEL OF THE GAS DIFFUSION ELECTRODES IN A PEM FUEL CELL

Torsten Berning and Ned Djilali
Institute for Integrated Energy Systems
University of Victoria, Canada

In order to further improve the performance of a PEM Fuel Cell numerous computational models have been devised in the past to shed insight in the various transport phenomena that occur during fuel cell operation. These models have become more increasingly more sophisticated, moving from one- and two-dimensional, single phase models [1-3] towards two- and three-dimensional, multi-phase models [4-6]. A three-dimensional, two-phase model of a PEM fuel cell, however, has not been presented, yet. This paper describes the numerical model that has been developed at the University of Victoria during recent years. Employing the methods of computational fluid dynamics, and building on a 3D single-phase model [7] we have implemented a multi-phase model into the commercial software code CFX 4. Altogether, the model accounts for multi-phase, multi-component transport in porous media with electrochemical reactions and heat transfer. Transport of liquid water is described via Darcy's law and a capillary pressure in conjunction with the Leverett's equation to describe the capillary pressure function . Both anode and cathode are included. A binary gas mixture of hydrogen and water vapour is considered at the anode and humidified air at the cathode. Figure 1 shows the distribution of the liquid water saturation in both gas diffusion electrodes. Under the conditions investigated, there is a significant amount of liquid water not only in the cathode side but at the anode side as well. This is due to the fact that when fully saturated hydrogen enters the cell, the consumption of the reactants lead to an oversaturation, since the molar fraction of water vapour increases. This leads to condensation inside the GDEs. The condensation water is dragged along with the gas phase towards the catalyst layer, and can only leave the cell via the build-up of a capillary pressure gradient, which drives the water out of the cell. Figure 2 shows the development of the average liquid water saturation in the gas diffusion layers with current density. Overall, the saturation levels are of the same order as those reported by Wang *et al.* [4]. The drop-off of the liquid water saturation in the cathode at a high current density can be explained by the higher fraction of the total current being generated under the channel area [7], which reduces the diffusion path of the water out of the cell. At the same time, the rate of evaporation increases, as is shown in Figure 3. The direction of phase change inside the GDE is governed by the relative humidity. Three different underlying mechanisms of phase change have been identified: i.) an increase in temperature due to the electrochemcial reaction leads to an increase in the saturation pressure, causing evaporation in the presence of liquid water; ii.) the pressure drop inside the GDE (Darcy's law) leads to a decrease in the partial pressure of water vapour and causes evaporation as well; iii.) the consumption of reactants leads to an increase in the molar fraction of water vapour, which causes condensation. The second effect is strongly controlled by the properties of the GDE, especially the hydraulic permeability. A high permeability leads to a reduced pressure drop and causes less evaporation.

References:

[1] T. E. Springer , T. A. Zawodzinski and S. Gottesfeld: *J. Electrochem. Soc.*, Vol. 138, No. 8, 1991.
[2] D. M. Bernardi and M. W. Verbrugge, *J. Electrochem. Soc.*, Vol. 139, No. 9, 1992.
[3] T. V. Nguyen and R. E. White, *J. Electrochem. Soc.*, Vol. 140, No. 8, 1993.
[4] Z. H. Wang , C. Y. Wang and K. S. Chen, *J. Power Sources*, Vol. 94, 40-50, 2001.
[5] D. Natarajan and T.V.Nguyen, *J. Electrochem. Soc.*, Vol. 148, No. 12, 2001.
[6] S. Dutta, S. Shimpalee and J.W Van Zee, *J. Applied Electrochem.*, Vol. 30, 135-146, 2000.
[7] T. Berning, D. Lu and N. Djilali, *J. Power Sources*, Vol. 45, No. 11, 2002.

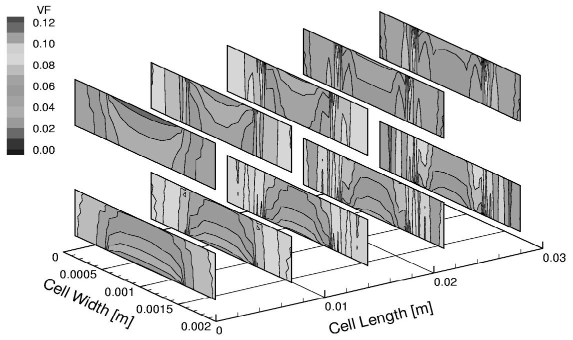

Fig. 1: Liquid water saturation inside the cathodic (lower) and anodic (upper) GDE. The channel interface area lies between between 0.5 mm and 1.5 mm.

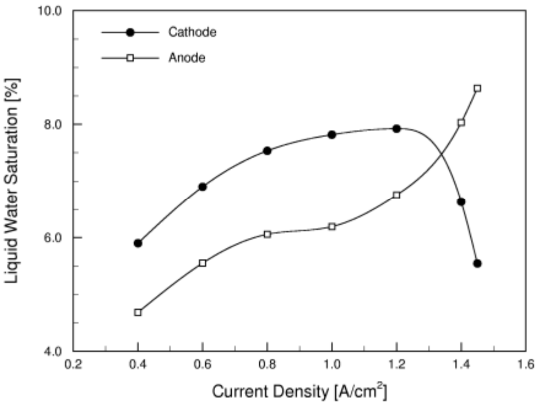

Fig. 2: Average liquid water saturation in the gas diffusion electrodes. The limiting current density is 1.5 A/cm^2, and is governed by the oxygen diffusion limitation.

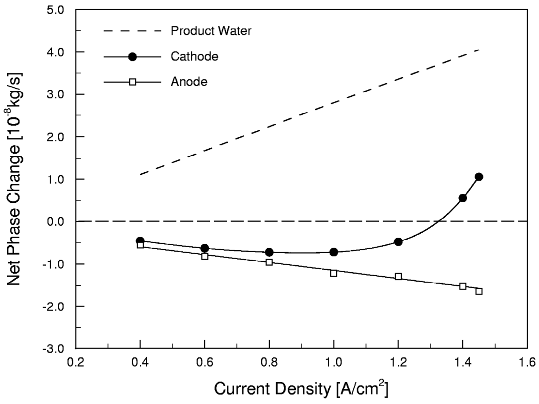

Fig. 3: Overall amount of phase change in the gas diffusion electrodes. The zero line indicates that, on average, the same amount of water vapour leaves the cell as enters, whereas positive values indicate that, overall, product water evaporates.