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Dynamic Modeling of the Water Balance in the Cathode Gas Diffusion Layer of Polymer Electrolyte Fuel Cells

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Development of PEMFC for use as a portable devices like mobile phones, computer notebooks, digital cameras, etc and transport devices are receiving more coverage in recent research due to their low cost-per kW, fast start-up, lower operating temperature and zero pollution. The operation in these applications is generally dynamic. So the development of dynamic models is highly important. During fuel cell operation, management of water produced is crucial to enhance PEMFC performance. Generally, water is produced at the cathode/membrane interface due to the electrochemical reactions. Also, due to the humidification of gas at the anode and cathode inlets to supply water to the membrane, condensation takes place in the gas diffusion layer (GDL) preventing the diffusion of gas to the reactive sites. The lack of gas in the reactive sites increases diffusion loss, and leads to a decrease of the cell voltage. So its water-transport characteristics must be studied in order to reduce potential loss, flooding and enhance PEMFC performance.

The continuity equation (or mass conservation) which describes the change of mass concentration of i with respect to time at a fixed point in x direction of porous medium due to the motion of i and chemical reactions producing i is give by the concept mathematical of equation [1,2]:

$$\frac{\varepsilon_0(1-s)}{RT}\frac{\partial P_i}{\partial t}+\frac{\partial N_i}{\partial x}=R_i \tag{1}$$

The quantity $\varepsilon_0(1-s)$ represents the volume occupied by gas species in the porous medium. The source or sink terms R_i is the rate of generation or consumption of species i.

When water is present in the GDL, transport in the porous electrode is induced by capillary force and gas flow-driven shear force. The governing equation for liquid water can be expressed as [1,2]:

$$\varepsilon_0\rho_w\frac{\partial s}{\partial t}+\frac{\partial N_w}{\partial x}=-M_w R_w \tag{2}$$

Where ρ_w, M_w , N_w and R_w are density, molecular weight of liquid water, molar flux of liquid water and the interfacial mass-transfer rate of water between liquid and water vapour respectively.

The electrochemical kinetics is governed by the Voltmer-Butler equation, and since the cathode kinetics is sufficiently slow, it can be expressed by Tafel kinetics, i.e in the form [1,2]:

$$I = (1-s)\, a_c i_0 \frac{P_{cons}^{O_2}}{RT\, C_{ref}^{O_2}} \exp\left(-\frac{\alpha_c F}{RT} \eta_c \right) \tag{3}$$

Where the factor $(1-s)$ represents the reduced surface area due to liquid water that covers the active reaction sites., i_0 the exchange current density, a_c the reactive surface area, $P_{cons}^{O_2}$ the gas pressure of local oxygen, $C_{ref}^{O_2}$ the reference oxygen concentration , η the cathode overpotential and α_c the transfer coefficient for oxygen reduction.

The schematic illustration of capillary pressure P_c and gradient dP_c / ds are represented in fig.1. The capillary pressure is defined as the difference between gas and liquid-phase pressures. It interesting to note that the gradient dP_c / ds is not constant in the range of 0 and 1 of saturation. In order to bring out the variation of dP_c / ds we represented from saturation of liquid water in GDL the graph of capillary pressure P_c and the gradient dP_c / ds fig.2. The absolute valued of capillary pressure is higher at the GDL/membrane interface where saturation is higher than the GDL/ channel interface. It is interesting to note that the gradient of capillary pressure which is responsible for driving force for liquid water flow is confirmed. Furthermore, the gradient dP_c / ds which has most time taken as a constant [3-5] to reduce mathematical difficulty or to take into account the assumption of low saturation is not constant. The main conclusion of these studies is the assumption of gradient dP_c / ds constant should be used for uniform saturation or very low saturation but when saturation can be varied in the range of 0 and 0.8 this assumption can not be used.

In order to study the effect of condensation on the polarisation curve, we allowed condensation in fig.3 at pressure of 325 kPa. This figure shows the polarizations curves of fuel cell for both condensation and without condensation on GDL at 100% of relative humidity. It can be seen in this figure that the dynamic polarization curve without condensation is better than the polarisation curve with condensation before purge. When water vapour condenses in the GDL, liquid water is produced and reduces the volume available for diffusion. The concentration or pressure of reactant decreases at electrochemical reaction sites resulting in low voltage as it can be seeing in fig.3. The increase of liquid water is related to saturation increase which in return increases the activation overpotential due to relation between them.

Fig.4 presents the study state profile of cell voltage with control of condensation phase. The main reason for this decrease in performance is due to the fact that gas pressure at inlet is still constant so that the pressure or the concentration of oxygen decreases with the distance before reaching the DGL/membrane interface and also the liquid water condensed in GDL. The poor concentration of oxygen at the interface and the liquid water condensed reduce the electrochemical reaction rate and also the cell performance.

The model results reinforce some important points such as GDL, condensation effect, evaporation effect on fuel cell behaviour. The condensation of liquid water affects fuel cell performance by reduced the voltage magnitude. The liquid water saturation level accumulates at the interface GDL/membrane is responsible for such situation than that in GDL due to the small thickness of GDL The gradient dP_c / ds depends strongly on the range of saturation. It should not be taken as a constant for large range saturation. The non-linear equation of liquid water should be resolved for dynamical model without assumption of constant gradient dP_c / ds.

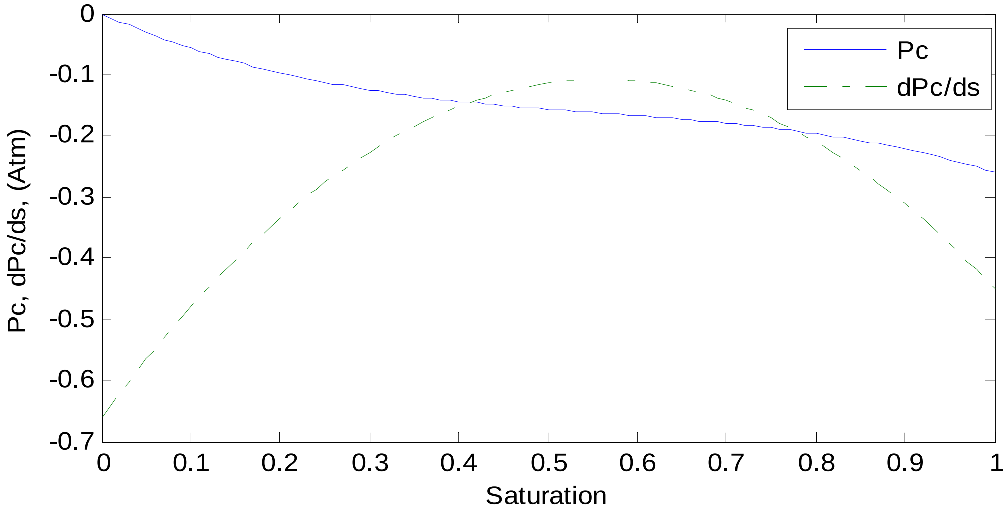

Figure 1: **Graph of Capillary pressure P_c and gradient dP_c / ds.**

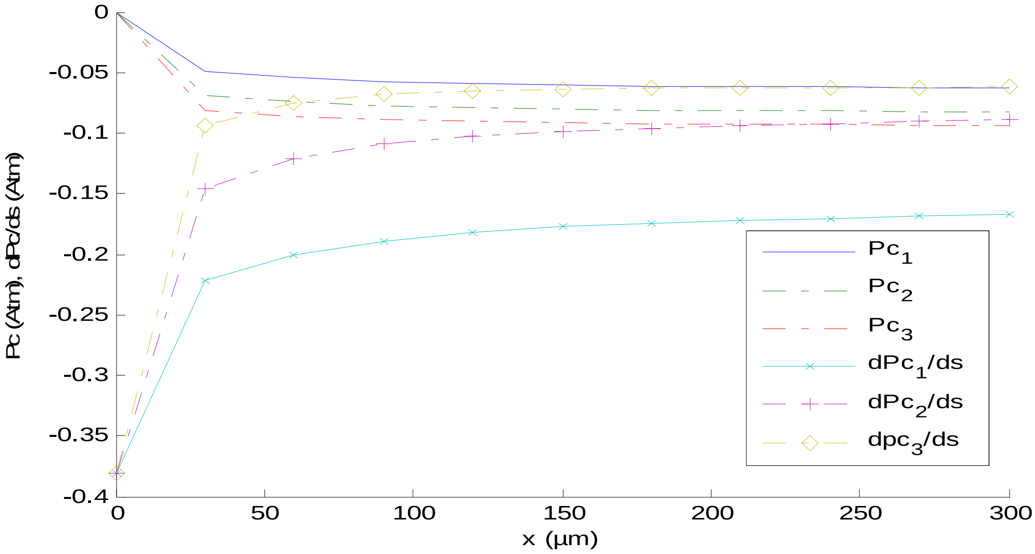

Figure 2: **Schematic representation of P_c and dP_c / ds at (1):60 s,(2):100 s and (3):136 s.**

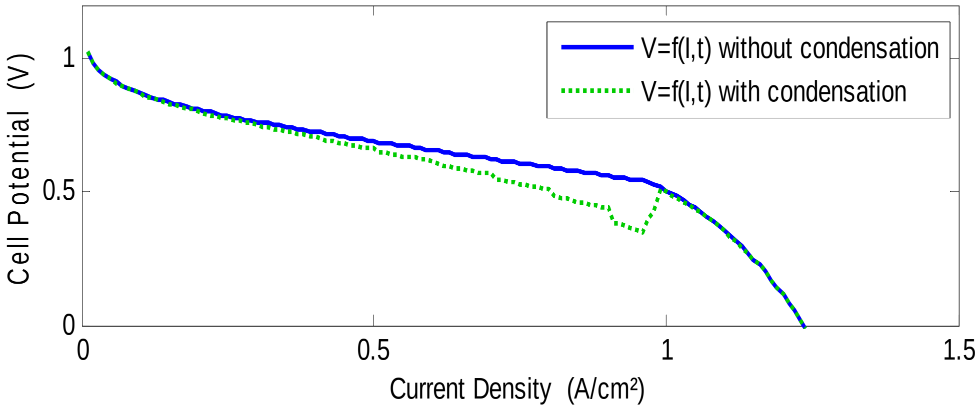

Figure 3: **Effect of condensation on polarization curve of fuel cell at 325 kPa with condensation and without condensation at relative humidity (RH) of 100%.**

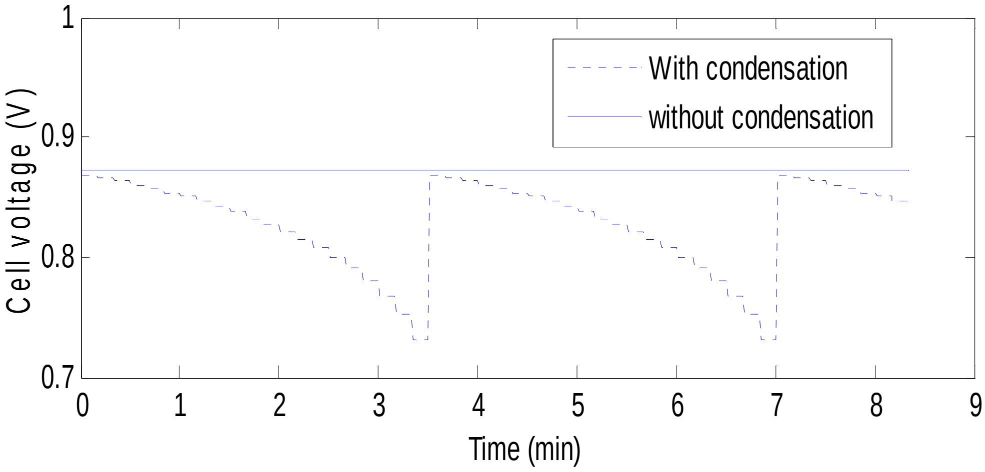

Figure 4: **Steady state profile of cell voltage with condensation phase control (GDL thickness of 300 µm, 0.5A/cm²).**

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