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Research on One Dimensional Dynamic Model in Water Transportation of PEM Fuel Cell

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Abstract

Water balance has a significant impact on the overall fuel cell system performance. Proper water management should provide an adequate membrane hydration and avoidance of water flooding in the catalyst layer and gas diffusion layer. Considering the important of advanced water management in PEM fuel cell, this study proposes a simple one dimensional water transportation model of PEM fuel cell for use in a dynamic condition. The model has been created by assumption that the output is the water liquid saturation difference. The liquid saturation change is the total difference between the additional water and the removal water on the system. The water addition is obtained from fuel cell reaction and the electro osmotic drag. The water removal is obtained from capillary transport and evaporation process. The result shows that the capillary water transport of low temperature fuel cell is high because the evaporation rate is low.

Keywords : PEM fuel cell, Modelling, Water management, Water balance

Nomenclature

n_d : Electro osmotic drag coefficient
ρ : Density, [kg·cm^{-3}]
M_r : Relative molecular mass, [kg·mol^{-1}]
κ : Permeability, [m^2]
s : Liquid saturation level, [-]
ε : Porosity
μ : Dynamic viscosity, [m^2·s^{-1}]
T : Temperature, [℃]
δ : Thickness, [m]
λ : Latent heat, [kJ·kg^{-1}]
h : Heat transfer coefficient, [W·m^{-2}·K^{-1}]
I : Current density, [A·m^{-2}]
A : Cross section area, [m^2]
F : Faraday constant, [C·mol^{-1}]
ϕ : Humidity ratio, [g·kg^{-1}]
m : Mass, [kg]
γ : Specific volume, [m^3·kg^{-1}]
V : Volume, [m^3]
Q : Flow rate, [m^3·s^{-1}]

1. Introduction

In this work, the governing physics of water transport in both hydrophilic and hydrophobic diffusion media are described along with an

one-dimensional analytical solutions of related transport processes. It is found that liquid water transport across the gas diffusion layer (GDL) is controlled by capillary forces resulting from the gradient in phase saturation [1]. The water transportation of the membrane electrode assembly (MEA) is depended on the fuel cell current. In a hybrid fuel cell system for vehicle, the current is controlled constantly. But if the power demand of vehicle is lower than the power generated from the fuel cell, then the energy is taken from the battery. Hence, the dynamic water management system is important in this case. The good dynamic water management system requires the water transportation model to predict how much water that would be added and removed from the fuel cell system. Therefore an one-dimensional analytical solution for water transport is needed to keep up with the water behavior in the balance condition.

2. Modelling method

A water transportation equation in PEM fuel cell is governed by the following phenomena: generation of water at the cathode due to the oxygen reduction reaction (ORR), molecular diffusion (MD) of water across the membrane, electro-osmotic drag (EOD) of water from anode to cathode, and convective removal of water to the gas channel as sketched in Fig. 1.

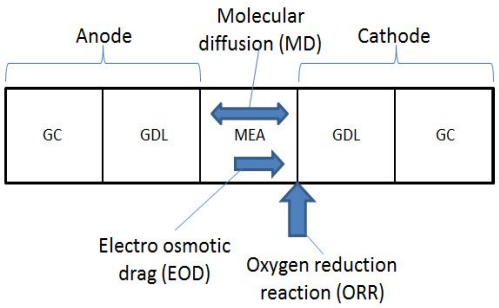

Figure 1. One dimensional control volume

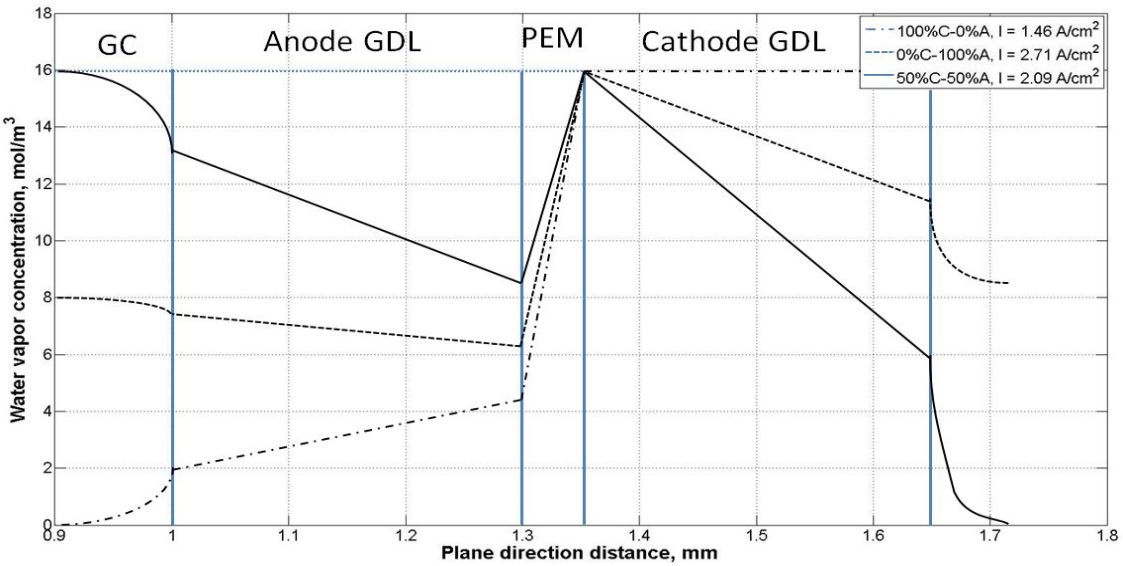

Figure 2. Water concentration variation at various important locations

The convective mass-transfer coefficient at the channel-GDL interface is calculated by using the analogy between the heat transfer and mass transfer. The Sherwood number and the mass-transfer coefficient are independent of air velocity in the channel and can be calculated as:

$$Sh_D = N_D \frac{Sc}{\mathrm{Pr}} \tag{1}$$

$$h_m \frac{Sh_D D^{H_2O}}{D_h} \tag{2}$$

The water concentrations at the threshold current density at various interfaces across the membrane electrode assembly for different humidity levels is shown in Fig. 2. In this figure, the maximum water concentration is located in the cathode catalyst layer (CCL). The water transported by molecular diffusion is relatively small compared to EOD and ORR. hence, the water generation rate in the CCL can be simplified and expressed as the total water production rate from ORR and the water that is dragged from the anode side as shown in Eq. (3) [2-4].

$$\dot{m}_{rct} = M_r (c_d + 1) \frac{IA}{2F} \tag{3}$$

Based on ASHRAE standard formula calculating the air properties [5], the water addition from the input humid air can be derived from the relationship between the humidity and the volumetric flow rate as given in Eq. (4).

$$\dot{m}_{air} = \frac{\phi Q}{\gamma} \tag{4}$$

Pasaogullari et al. [1] have studied the steady state water transportation in GDL of PEM fuel cell. In their works, the governing physics of water transport in both hydrophilic and hydrophobic diffusion media is described along with the one-dimensional analytical solutions of related transport processes. Also, it was found that the capillary transport is the dominant transport process for removing water from flooded GDLs.

$$\kappa_{rl} = s^3 ; \kappa_{rg} = (1-s)^3 \tag{5}$$

Where, s is the liquid saturation level. On the other hand, the capillary pressure between two phases is expressed as

$$p_c = \sigma \cos(\theta_c) \left(\frac{\varepsilon_{GDL}}{\kappa} \right)^{0.5} J(s) \tag{6}$$

Above equation $J(s)$ is the Leverette function and is given by the following relation:

$$J(s) = \begin{cases} \theta_c < 90^o, \\ 1.417(1-s) - 2.120(1-s)^2 + 1.263(1-s)^3 \\ \theta_c > 90^o, \\ 1.417s - 2.120s^2 + 1.263s^3 \end{cases} \tag{7}$$

The mass flow rate of water transported by capillarity pressure driven given by:

$$\dot{m}_{cap} = \frac{\kappa_{rl}}{\mu} \kappa \left[\nabla p_c + (p_l - p_c) g \right] \tag{8}$$

Due to very small dimensional geometry of PEM fuel cell, the gravity effect can be neglected. By substituting Eq. (6) and Eq. (8) and then it results Eq. (9).

$$\dot{m}_{cap} = -\frac{s^3}{\mu}\kappa\sigma\cos(\theta_c)\left(\frac{\varepsilon}{\kappa}\right)^{0.5}\nabla J(s) \quad (9)$$

The Laverette function for hydrophobic media is given by Eq. (10).

$$J(s) = 1.417s - 2.120s^2 + 1.26s^3 \quad (10)$$

By combining Eq. (9) and Eq. (10) it yields Eq. (11).

$$\dot{m}_{cap} = -\frac{\sigma\cos(\theta_c)(\varepsilon\kappa)^{0.5}}{\mu} \times s^3(1.417 - 4.240s + 3.789s^2)\nabla^2 \quad (11)$$

Considering the one-dimensional transport of liquid water only through plane direction, the Eq. (11) reduces to an ordinary differential equation, which can solve analytically as given by Eq. (12).

$$s^3(1.417 - 4.240s + 3.789s^2)\frac{ds}{dx} = \dot{m}_{cap}\frac{\mu}{\sigma\cos(\theta_c)(\varepsilon\kappa)^{0.5}} \quad (12)$$

Fig. 2 shows the linear gradient of the liquid saturation ratio along the GDL therefore the gradient of the saturation level along GDL is given by Eq. (13).

$$\frac{ds}{dx} = \frac{s_{CCL}}{\delta_{GDL}} \quad (13)$$

Mass flow rate of the water transported by capillarity process is given by Eq. (14).

$$\dot{m}_{cap} = s^4(1.417 - 4.240s + 3.789s^2) \times \frac{\sigma\cos(\theta_c)(\varepsilon\kappa)^{0.5}}{\mu\delta_{GDL}} \quad (14)$$

In general, the evaporation rate can be calculated by Eq. (15).

$$\dot{m}_{evap} = \frac{h(4s+2)(V_p)^{2/3}|T_{liq} - T_{air}|}{\lambda} \quad (15)$$

The water liquid saturation level (s) is the flooding or drying indicator and it can be defined as the volume fraction of the total void space of porous medium occupied by the liquid phase as shown in Eq. (16). And then the liquid saturation change is calculated using Eq. (17).

$$s = \frac{V_{liq}}{V_{tot}} \quad (16)$$

$$\Delta s = \frac{\dot{m}_{rct} + \dot{m}_{air} - \dot{m}_{sat} - \dot{m}_{cap} - \dot{m}_{evap}}{\rho V_p} \quad (17)$$

3. Simulation results and discussions

The liquid transport of the water inside the GDL is affected by temperature. When the temperature is high, the balance between water addition and water removal is not reached. Fig. 3 and Fig. 4 respectively show the capillary liquid water transport and the evaporation rate in the different temperature condition of the high PEM fuel cell power demand of 10kW. The capillary water transport of low temperature fuel cell is higher because the evaporation rate became low. Hence, fuel cell with 40°C air temperature and

23.5 g/kg humidity has stopped after 300 seconds operation because the pore of the GDL blocked with the liquid phase of water.

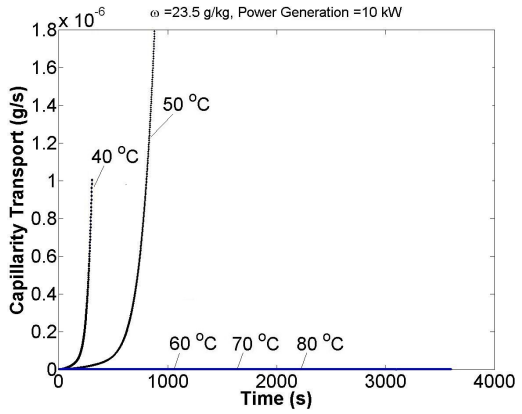

Figure 3. Capillary transport in GDL

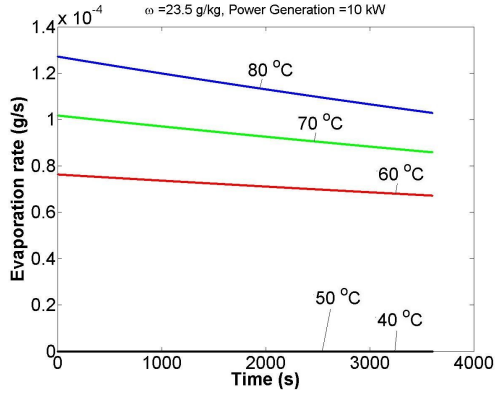

Figure 4. Evaporation rate in GDL

In PEM fuel cell with humid input air operation, the temperature is important. Fig. 5 shows that the flooding is happened at the low temperature of PEM fuel cell under stationary power demand 10kW. The unbalanced water between water addition and the water removal is happened at low temperatures. In this case, the water production is high as much as the electrical power production proportionally, but the water liquid removal by evaporation rate is low.

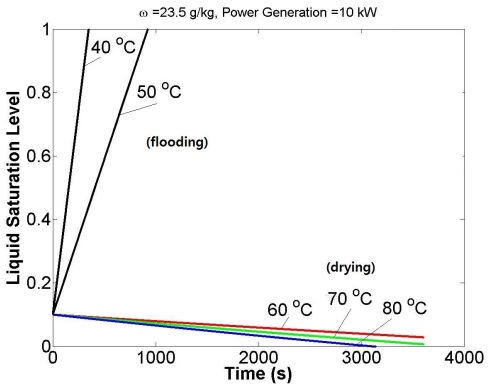

Figure 5. Liquid saturation level

4. Conclusions

The model has created with the liquid saturation difference becomes the output. The liquid saturation change is the total difference between the additional water and the removal water on the system. The water addition is obtained from fuel cell reaction and the EOD. The water removal is obtained from the capillary transport and the evaporation process.

The liquid water in the CCL produced when the water vapor is beyond the saturated and condensed. When the liquid water removal is lower than the liquid water addition, water can be accumulated into the pore of CCL and also at cathode GDL. Thus, the rate of liquid water accumulation is a vector that has a plus value when the addition rate of liquid water is higher than the removal rate of liquid water. As a result, when the water accumulation rate has a plus value and remained for long time, this will produce a flooding.

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