

## **A Development of Multi-Cell Simulation Model of PEM Fuel Cells Considering Temperature and Two-Phase Effects**

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### **ABSTRACT**

A typical control oriented simulation model of a proton exchange membrane fuel cell is a simple extension of unit fuel cell without transport of any physical phenomena. Since the single cell based dynamic model can be used for the design of control logic, intrinsic limitation of single cell based model narrows the degree of freedom in the study of control logic. In this study, a simulation model is developed that simulates cell-to-cell variation of physical phenomena. The model shows temperature variation from cell to cell as well as flooding due to high current operation. The unit cell model includes dynamic response of fuel cell temperature and the flooding inside the cell with multiphase flow model. The simulation parameters of the model are the operating temperatures, various oxygen and vapor concentrations in the gas diffusion media, and liquid water saturation inside the cell. The simulation model is then applied to investigate the cell-to-cell variation of fuel cell stack over various cooling conditions.

### **1. INTRODUCTION**

The worldwide increase in air pollution and power demand brought about an efficient and clean generation of electrical energy. The characteristics of low emissions and very high conversion efficiencies make fuel cells be excellent candidate for the primary power source in the future.

A fuel cell is a device that can directly convert chemical energy to electric and thermal energy. Among different kinds of fuel cells, the proton exchange membrane fuel cell (PEMFC) is very feasible for vehicle and small CHP system. the advantage of a low-operational temperature (20-100 °C), high power density and light weight. PEMFC has gained a lot of attention and is considered as the most promising fuel cell

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technology in the future and a potential alternative power source for vehicle and small size combined heat and power (CHP) generation source. However, substantial technical progresses are still indispensable for the commercialization of the PEMFC. One of the technical challenges of the fuel cell stack for high-power application is the thermal management. Those fuel cells require forced water-cooling systems to cope with high heat rejection. Thermal management of the fuel cell vehicle is more challenging than conventional powertrain cases due to relatively lower operating temperature of the PEMFC. Lower operating temperature requires increased space to package the thermal management system as well as higher performance of the cooling system.

Uneven temperature distribution within the fuel cell is also inevitable in the case of a large active area fuel cell and the temperature distribution could cause a performance penalty. The performance of a PEMFC also depends on the amount of water vapor in the fuel cell. Accordingly, local dehydration or water condensation due to uneven temperature distribution can cause performance degradation. In an ideal situation it is desirable to have all of the cells in a stack to perform uniformly. It has been observed experimentally that usually the cells in a stack do not operate uniformly. Significant variations among the cells may cause long run structural problems and may eventually lead to total failure of the whole system. Possible causes are non-uniform fuel/air flow distribution to individual cells, non-uniform temperature and/or current distribution within the stack. All of these factors are interrelated hence a systematic investigation is necessary to better understand the root causes. Typical PEMFC simulation models only consider single cell or assume that the stack is insulated, so that there is no heat transfer through the surface. And there are only few studies about cell-to-cell variation of fuel cell stack.

In this study, a simulation model is developed to analyze the behavior of fuel cell stack which is modeled as multi-cell stack. The simulation model is composed of electrochemistry model, heat transfer model, gas diffusion model in the gas diffusion layer considering two-phase effect, and mass and energy conservation laws. The simulation model is a multi-cell stack model which has 10 cells module for studying the variation of cell-to-cell performance. This study is focused on the cell-to-cell variation of fuel cell stack associated with the performance of the fuel cell stack associated with humidity of reactants. We investigate the influence of variation on the performance of individual cells connected in series within a stack. In addition to varying the humidity of reactants, this study will address the influence of the operating temperature of the fuel cell stack since the fuel cell can be suffered from the operating temperature.

To improve the fidelity of simulation result, the polarization curve of simulation model is calibrated with experimental result. The dynamic response of single stack under load change was examined with the simulation model.

## **2. MODEL APPROACH**

The multi-cell simulation model is composed of fuel supply, air supply, thermal management, two phase water transfer of gas diffusion layer, and 10-cell stack parts. Since this study is focused on cell-to-cell variation with changes of cooling condition, and operating temperature of the fuel cell stack, calculation of heat transfer through

cell-to-cell and stack to the ambient air is included. The specification of fuel cell stack is presented in Table 1. The fuel and the air are delivered on demand after calculation of stoichiometric flow rate coefficient 1.33 and 2.00 respectively.

### 2.1 Nernst voltage and actual cell voltage

Nernst voltage, which is the reversible cell voltage, can be obtained from

$$V_{Nernst} = -\frac{\Delta g_f^o}{2F} + \frac{RT}{2F} \ln\left(\frac{a_{H_2} a_{O_2}^{1/2}}{a_{H_2O}}\right) \quad (1)$$

The actual cell voltage is reduced by irreversible losses such as reaction loss, activation loss, and ohmic loss. Then the actual cell voltage can be described as

$$V_{FC} = V_{Nern} - J \cdot R(\lambda)_{mem} - \eta \quad (2)$$

In this study, only the cathode over potential is considered, because the anode over potential is negligible compared with the cathode side.

Table 1 Specification of PEMFC stack

Parameters	Value
Fuel cell length	0.15 (m)
Fuel cell width	0.15 (m)
Cell thickness	0.00375 (m)
GDL thickness	0.0005 (m)
Fuel cell temperature	343.15 (K)
Active area	124 (cm <sup>2</sup> )
Total pressure at cathode side	1 (atm)
Total pressure at anode side	1 (atm)

### 2.2 Water transport model

The water transport model is derived from the species conservation with two driving forces, electro-osmotic drag and back diffusion. A net water flow rate coefficient ( $\alpha$ ) is calculated from the water transport model by Eq. (3). First term explains drag force due to electro-osmosis and second term explains back diffusion by concentration difference.

$$\alpha = n_{drag} - \frac{F}{J_{avg}} D_w \frac{\rho_d}{M_m} \frac{\lambda_C - \lambda_A}{t_{mem}} \quad (3)$$

The water contents,  $\lambda_C$  and  $\lambda_A$ , can be expressed in terms of the water activity ( $a_w = x_w p_i / p_{sat}$ ).

### 2.3 Gas diffusion layer with a two-phase effect

The phase of water in a GDL plays a significant role in transport of water and reactants. The GDL model has the consideration of the gas and liquid phase mass transport and the phase changes between liquid water and water vapor. Most of the proposed GDL models neglected the effects of liquid water as assuming that water supplied and generated were vapor phase. But, when liquid water is considered, diffusion characteristics are changed from those in the vapor state.

$$\begin{aligned} \langle D_{m,i} \rangle &= D_{m,i} f(\varepsilon) g(s) \\ &= D_{m,i} \varepsilon \left( \frac{\varepsilon - 0.11}{1 - 0.11} \right)^{0.785} (1 - s)^2 \end{aligned} \quad (4)$$

$$\varepsilon = \frac{V_{pore}}{V_{GDL}}, \quad s = \frac{V_{liquid}}{V_{pore}}, \quad m = O_{2,vap} \quad (5)$$

where  $\langle D_m \rangle$  is the effective diffusivity ( $m^2 s^{-1}$ ),  $D_m$  is the diffusion coefficient ( $m^2 s^{-1}$ ) at a single phase,  $\varepsilon$  is the porosity of the diffusion layer,  $s$  is the liquid water saturation ratio,  $V_{pore}$  is the pore volume of the GDL ( $m^3$ ),  $k$  is the number of each domain in the GDL,  $V_{GDL}$  is the total volume of the GDL ( $m^3$ ), and  $V_{liquid}$  is the volume of the liquid water ( $m^3$ ).

The species conservation equation for oxygen is

$$\frac{d}{dy} \left[ -c M_{O_2} \langle D_{m,O_2} \rangle \frac{dx_{O_2}}{dy} + x_{O_2} M_{O_2} \sum_i \frac{\dot{m}_i}{M_i} \right] = 0 \quad (6)$$

where  $c$  is total mole concentration ( $P/R_g T$ ),  $\dot{m}_i$  is mass flux, and  $M_i$  is molecular weight of species  $i$ . Similarly, the species conservation equation for water vapor is

$$\frac{d}{dy} \left[ -c M_{H_2O} \langle D_{m,H_2O} \rangle \frac{dx_{H_2O}}{dy} + x_{H_2O} M_{H_2O} \sum_i \frac{\dot{m}_i}{M_i} \right] = -\dot{n}_{gl,H_2O} \quad (7)$$

The volumetric condensation rate  $\dot{n}_{gl,H_2O}$  is given by

$$\dot{n}_{gl,H_2O} = M_{H_2O} \gamma \frac{P_{g,H_2O} - P_{H_2O}(T)}{R_g T} \quad (8)$$

The liquid mass conservation equation with a volumetric condensation is

$$\frac{d}{dy} \left[ -\rho_l \frac{K K_{rl}}{\mu_l} \left( \frac{dp_c}{dS} \right) \frac{dS}{dy} \right] = \dot{n}_{gl,H_2O} \quad (9)$$

## 2.4 Heat transfer and energy conservation

Heat production of unit fuel cell by electrochemical reaction is

$$Q_{react} = P_{Nern} - P_{elec} = J_{avg} A_{act} (V_{nern} - V_{FC}) \quad (10)$$

Temperature of fuel cell is varied with load conditions. The energy conservation describes the temperature variation of fuel cell stack over various load conditions

$$\rho c_p V \frac{dT_{FC}}{dt} = Q_{react} - Q_{cool} - Q_{gas} - Q_{conv} - Q_{cond} \quad (11)$$

Heat rejection to the gases is

$$Q_{gas} = \sum \dot{m}_i c_{p,g} (T_{g,o} - T_{g,in}) \quad (12)$$

Heat rejection from fuel cell to coolant is

$$Q_{cool} = \dot{m}_c c_{p,c} (T_{c,o} - T_{c,i}) \quad (13)$$

where  $Q_{cond}$  is the heat transfer due to conduction between the cell and the neighboring cell and  $Q_{conv}$  is the heat transfer due to convection between the surface of 1<sup>st</sup> and 10<sup>th</sup> cell and the ambient air ( $T=298.15K$ ). Fig. 1 shows the heat transfer and energy conservation of the stack.

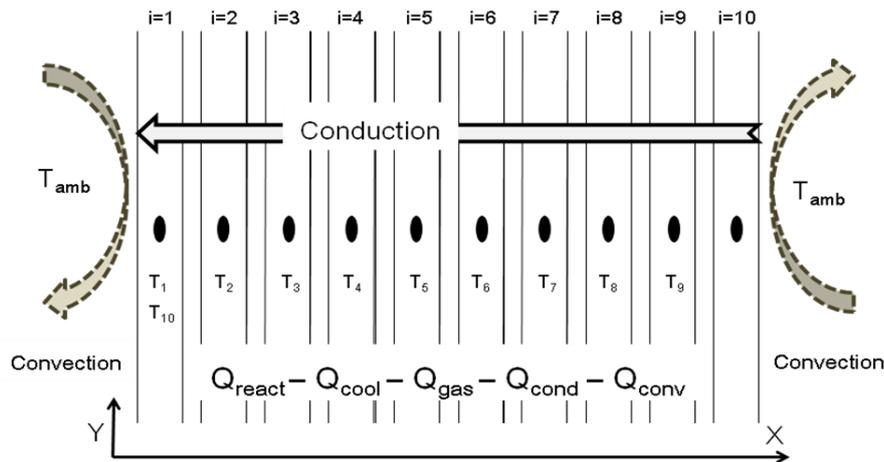


Figure 1 Heat transfer of the multi-cell stack

## 2.5 Solution methodology

Since the processes inside each fuel cell (10 cells) are relatively independent from other cells and are coupled only through the well defined fluxes (i.e. heat, mass), and

the given boundary conditions (temperature, pressure, etc.), it is possible to arrange a stable and time accurate parallel iteration procedure for a coupled solution of cell properties in the stack without excessive communication overhead. The time step, heat flux, and cell temperatures are communicated between neighboring cells in the stack.

Convection heat transfer with the ambient air ( $T=298.15\text{K}$ ) at the cell surface is considered only in the 1st cell and 10th cell and assumed there is no further convection heat transfer. The temperature of each cell is communicated to the adjoining cell. The conduction heat fluxes are then calculated using the received temperature from the neighbor by finite difference method. These fluxes are then shared between cells and are used when calculating the temperature of each cell at the new time level. Because of the relation between the adjoining cells, cell-to-cell variation is showing. Fig. 2 shows the relation between cells.

Fuel and air are humidified 100% in relative humidity according to the saturation temperatures of fuel and air supply parts. While delivering to the each cell, the relative

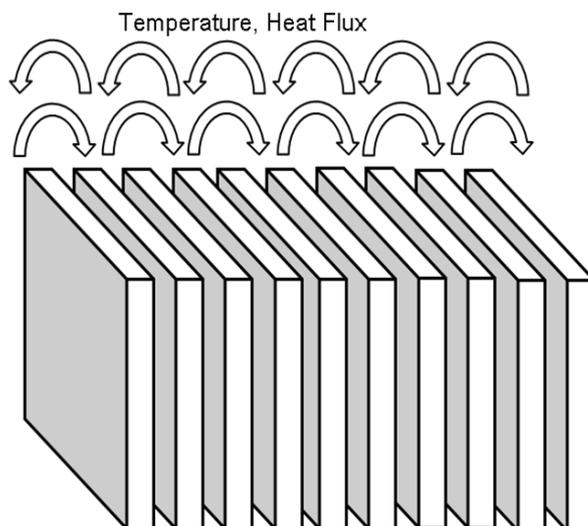


Figure 2 Connection of the cells

humidity can be changed and it affects the performances of each cell. Because of the changes of the relative humidity of gases, the temperatures of each cell are used to calculate the relative humidity of gases again.

Simplifying the calculation of this model several assumption were made. Since the stack has only the cells and has not other components, calculation of energy conservation became simple. The simulation model is developed under Matlab/Simulink® platform and simulation model is shown in Fig. 3.

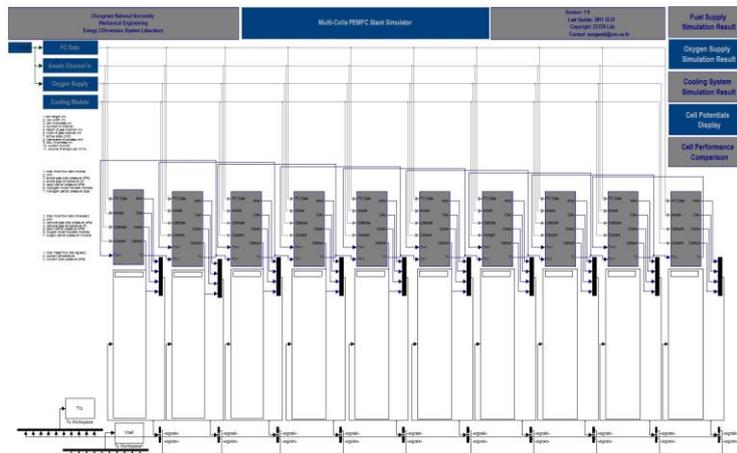


Figure 3 Multi-cell PEMFC stack model

### 3. Results and discussion

Performance of the multi-cell PEMFC stack model was studied by changing cooling condition, humidity of reactants, and operating temperature. For reference, the model was simulated with operating temperature at 343.15K, current density 1A/cm<sup>2</sup>, convection coefficient 5W/m<sup>2</sup>K, reactant gas temperature and coolant temperature 338.15K.

#### 3.1 Calibration of simulation model

Since the polarization curve of stack is available, the potential curve of simulation model is calibrated with experiment which is shown in Fig. 4. In the calibration process, the charge transfer coefficient and activation energy of oxygen reaction rate constant are used to fit the simulation model with experimental result.

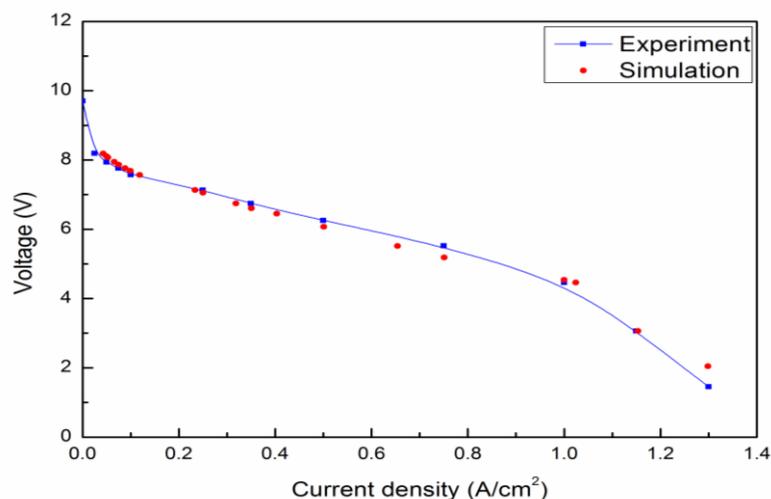


Figure 4 Validation of the model with experiment

### 3.1 Effect of reactants humidity

The reference stack temperature was measured at 5th cell. Coolant is delivered when the stack temperature increases over the set temperature, so that the operating temperature is maintained. As the reference result cell voltages, cell temperatures, and distribution of oxygen and water vapor mole fraction and liquid water saturation and flux are resulted at operating temperature 343.15K and reactants relative humidity 100% with convective heat transfer coefficient 5 W/m<sup>2</sup>K which is shown in Fig. 5 and Fig. 6. The results show voltage and temperature variations. In this steady state, differences of cell temperatures are obtained and compared.

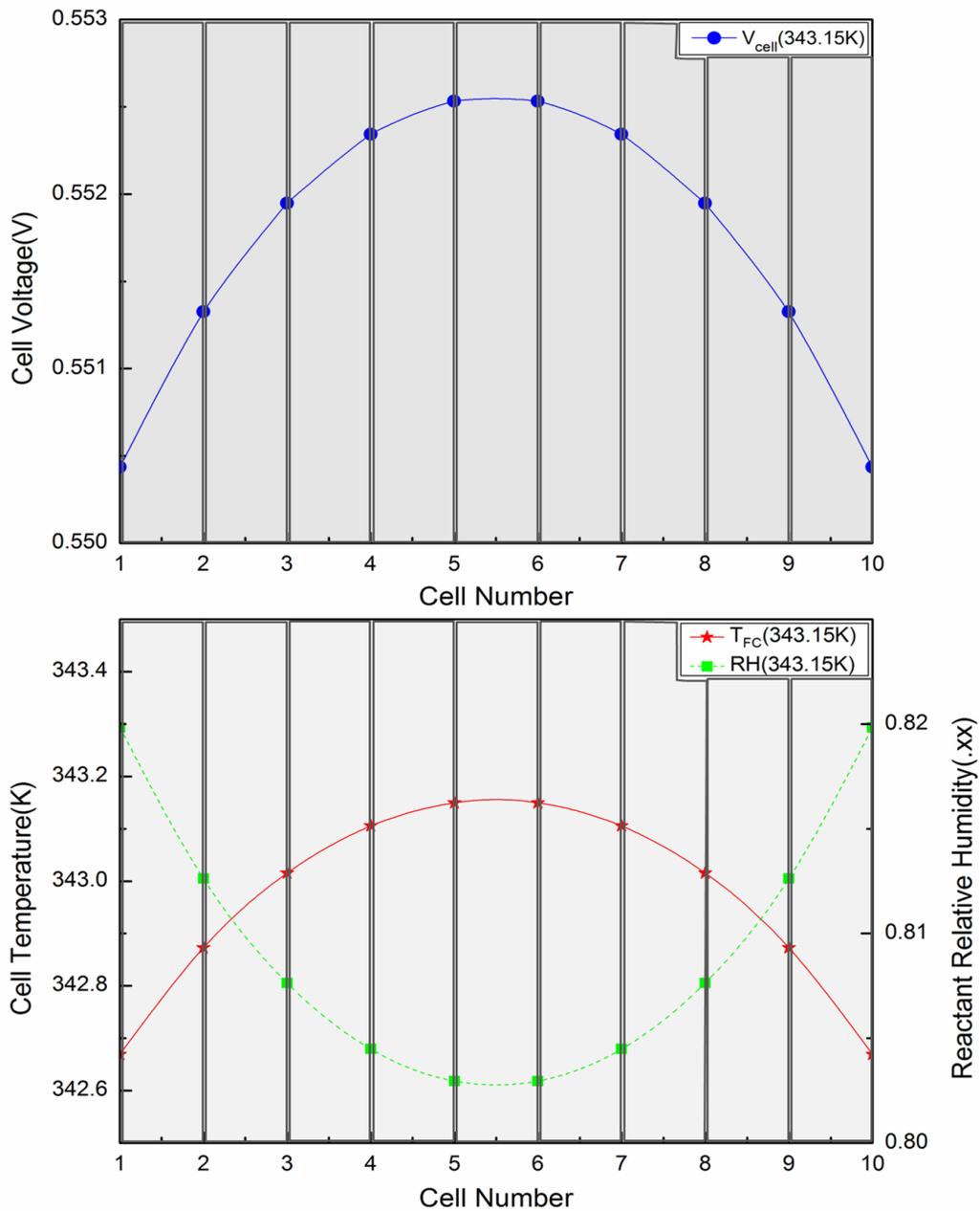


Figure 5 The reference results of simulation

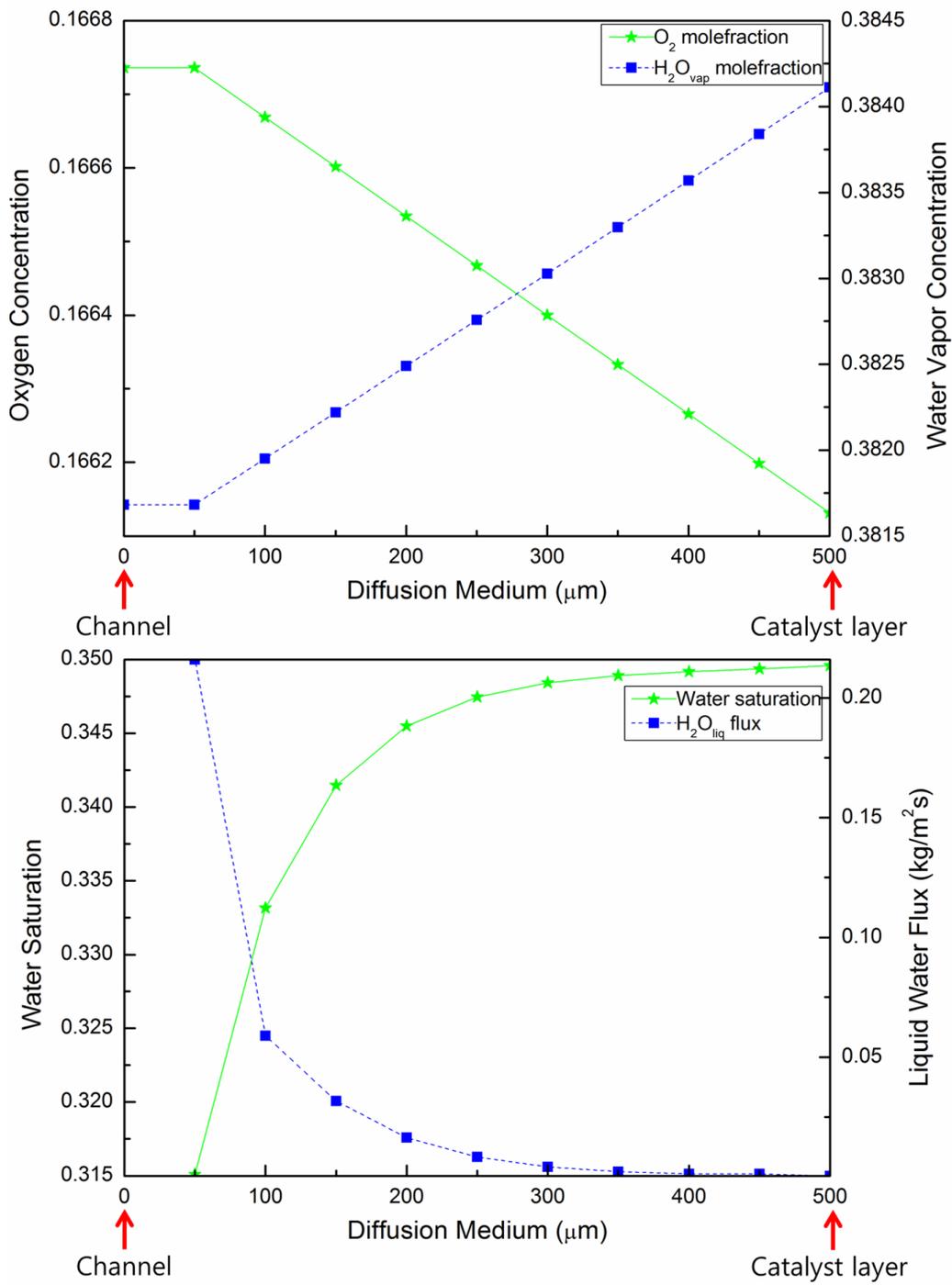


Figure 6 Spatial distribution of oxygen and water vapor mole fraction and liquid water saturation and flux

Relative humidity of reactants was changed from 20 to 100% to study effects of water saturation in gas diffusion layer which is shown in Fig. 7. Even though reactants are supplied with 100% relative humidity to the stack, no significant effect by water saturation, higher cell voltage was obtained.

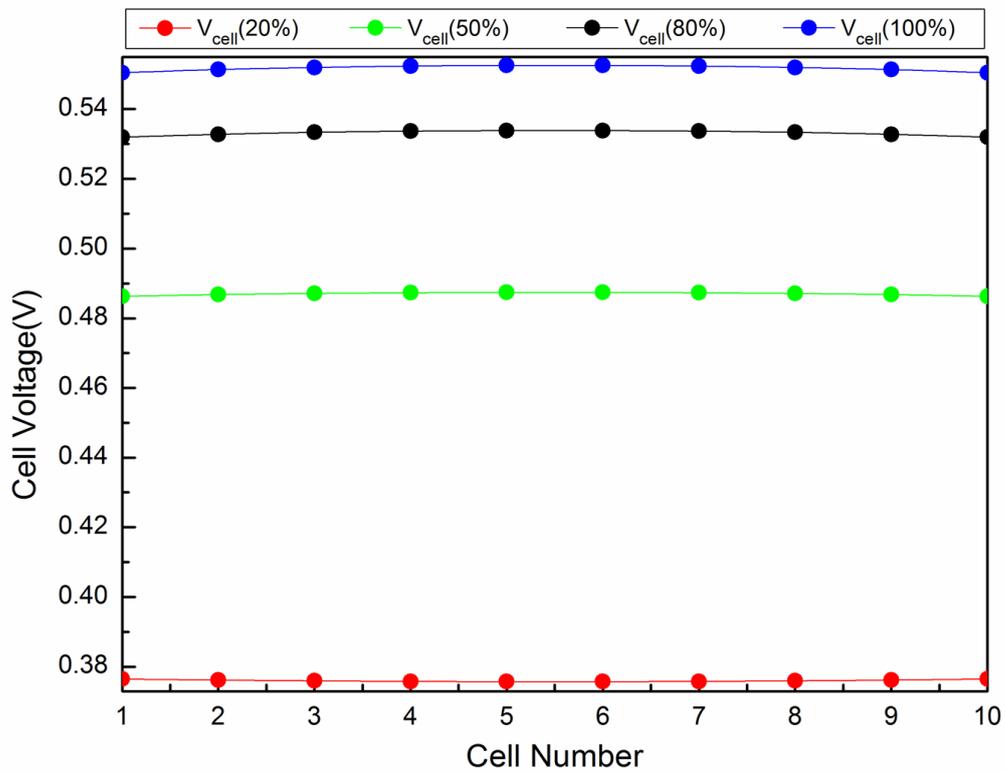
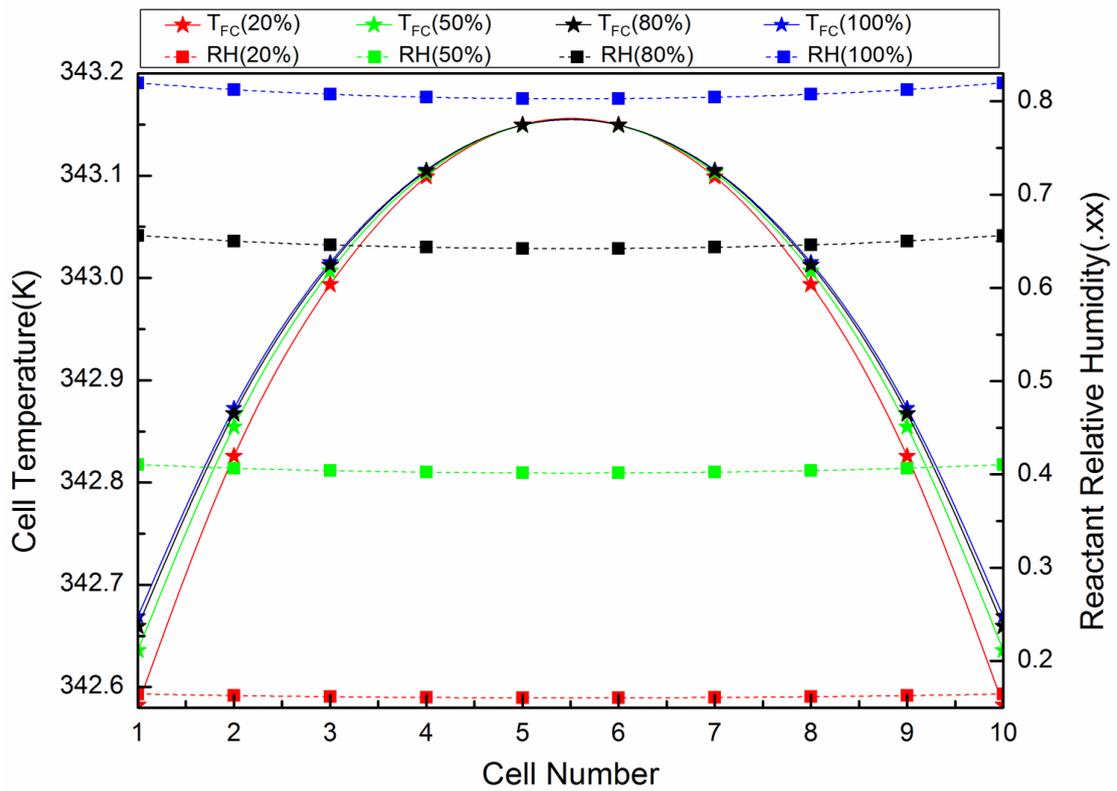


Figure 7 Variation in cell voltage and temperature with different reactants relative humidity

### 3.2 Effect of operating temperature

According to the operating temperature of 5<sup>th</sup> cell, coolant flow rate is decided to keep the operating temperature. While 5<sup>th</sup> cell operating temperature is maintained, comparison of cell voltages and cell temperatures are obtained. The operating temperature varies from 323.15 to 353.15K. The results of simulation are shown in Fig. 8. Changing the stack operating temperature affects cell temperature and voltage variation just little. Along the operation temperature increases variations are increasing slightly. According to the operating temperature of 5<sup>th</sup> cell, reactants relative humidity was set to 100%. So, there is no significant effect by water saturation in gas diffusion layer.

Results of standard deviation about voltage and temperature variation are very small.

## 4. Conclusion

The results of this study indicate that the variations in voltage among cells in a stack can be influenced by cooling condition, reactants relative humidity and operating temperature. Cell-to-cell voltage variations occur partially due to the temperature non-uniformities within a stack of cells which results from naturally occurring symmetry in typical PEMFC stack design. The temperature gradient results in convective and conductive heat transfer among solid–gas and solid–solid components within the stack which helps to mitigate the temperature non-uniformities. Convection through the surfaces of 1<sup>st</sup> and 10<sup>th</sup> cells influences variation, so that performance of the stack is degraded. The results imply that when designing the PEMFC stack system, the end of a stack should have low heat transfer coefficient or be insulated to improve the performance of the PEMFC stack, if not there will be a lot of energy loss.

Even though relative humidity of reactants was changed from 20 to 100% to study effects of water saturation in gas diffusion layer, higher cell voltage was obtained with 100% reactants relative humidity. It is because during the operation of PEMFC, the membrane needs water to conduct hydrogen ion smoothly, so that higher cell voltage is obtained without the affection of water saturation in gas diffusion layer at 100% reactants relative humidity.

This analysis can be extended to more complex multi-channel cells by expanding the heat transfer model in the separator regions and accounting for the geometric ratio of channel to separator-plate thickness.

The present multi-cell model is quite simple in that it accounts only for first order effects. These trends need to be verified in a future work with more refined PEMFC multi-cell stack models.

## Acknowledgement

This research was supported under a Basic Science Research Program through the National Research Foundation of Korea(NRF), Funded by the Ministry of Education, Science and Technology (grant number: NRF-2010-0021304)

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