Modeling and Simulation of a PEM Fuel Cell Humidification System

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Abstract—Maintaining proper fuel cell membrane humidification is a key challenge in achieving optimal fuel cell performance. For automotive applications, the load and environment conditions are constantly changing. Therefore, the membrane humidity needs to be properly controlled during transient. A humidifier system using water vapor exchange membrane is modeled and analyzed in this paper. The 4-state humidifier model is integrated with a fuel cell stack. Feedback and feed-forward control algorithms are developed so that the fuel cell maintains its highest membrane water content under a wide range of operation conditions without flooding.

I. INTRODUCTION

Polymer electrolyte membrane fuel cells (PEMFC) have drawn much attention in recent years. They offer a highly efficient and environmentally friendly option for energy conversion [1]. They are actively studied for commercial stationary power generation, residential applications and transportation technologies, especially in ground vehicle applications. PEMFCs commonly employ hydrated Nafion films or other hydrated perfluorinated ionomeric materials as the electrolyte membrane [2]. These membranes need to be properly hydrated in order to achieve maximum performance and extended life. Partial dehydration of the membrane decreases the protonic conductivity and lead to increased resistive loss, decreased net power, and local hot spots that may dramatically reduce the life of the membrane. On the other hand, if excessive water is present in the membrane and/or the gas diffusion layer, a situation that generally referred as flooding, the fuel cell performance will also be adversely affected due to the water blockage of the flow channels, porous electrodes and backing layers [2]. Therefore, water management was recognized as a critical issue for PEMFCs' performance. In addition, PEMFCs for automotive applications operate in a dynamic environment, where the power required from the fuel cells is constantly changing because of the road conditions and the drivers' behavior. The membrane humidity has to be controlled during transient.

There were many papers in the literature discussing the

fuel cell water management issues. A number of experimental studies were conducted to understand the water transport phenomena and to characterize the factors that affect the membrane water content [3-6]. Innovative channel designs have been proposed to better maintain the humidity [7, 8]. A number of mathematic models have been developed to optimize the fuel cell design to maintain high humidity [2, 9-14]. In addition, several types of humidifiers have been designed and analyzed to enhance the stack humidity [15-18]. All of these works aimed to maintain proper membrane water content for improved performance. However, the main purpose of these works is either to understand the system or to size the components. Few dynamic models that are suitable for control purposes exist. Furthermore, the component and channel sizing analysis results in a design optimized around one stack current value, or the average of the whole fuel cell current range. This type of steady state analysis enables the fuel cell to achieve its peak performance when it operates around the points where the design is optimized. It does guarantee a good performance, however, under other operation conditions or during transients.

Previous research has found that the membrane humidity is a function of water diffusion coefficient, electro-osmotic drag coefficient, water sorption isotherms, membrane conductivity and thickness [3, 12, 13, 19]. The membrane humidity is also affected by the fuel cell current, the temperature rise inside the fuel cell, and the inlet gas humidity condition [2, 9, 12, 20, 21]. When the fuel cell is running, the fuel cell current and steady-state temperature are determined by the stack power and the operation of auxiliary devices (e.g., cooling system). In addition, stack temperature significantly influences the efficiency of the membrane and thus should be tightly regulated. The most feasible parameter that can be used to control the membrane humidity is the inlet gas relative humidity, which can be manipulated through an inlet gas humidifier.

This paper is focused on the development of a dynamic humidifier model, and the application of which for fuel cell humidity control. The model presented in this paper captures the fluid flow dynamics, water exchange through the membrane, and the temperature dynamics of the humidifier. Unlike conventional humidifier analysis that assumes steady state condition, this model includes the time varying aspect of gas flow, temperature, pressure and gaseous and membrane RH. Simulations of the humidifier

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are conducted to predict the behavior of the humidifier under transient conditions, especially when there is a sudden change in air flow, corresponding to variation of fuel cell stack current. A feedback control algorithm is developed to reject the effect of the disturbance. The humidifier model is subsequently integrated with a fuel cell system model. A feed-forward control algorithm is developed to compensate the current variation. Simulation results of the integrated humidifier and fuel cell system show that a properly controlled humidifier could help the fuel cell to achieve the best membrane humidity with minimum flooding.

II. ANALYSIS OF HUMIDIFICATION SYSTEM

There exist several humidification mechanisms for PEMFC applications. A simple method that has been widely adopted involves using a spray nozzle to atomize coolant water that leaves the power production section of the stack. The droplets are sprayed uniformly onto a cloth or wire mesh substrate. As the inlet air passes through these wet surfaces, it becomes more humid. If the air is not preheated, however, the amount of water absorbed is inlet temperature dependent. Due to the fact that the air temperature decreases as the water droplet vaporizes into the air, the effectiveness of subsequent layers decreases. Therefore, the RH drops as the air enters the fuel cell stack and reaches the stack operating temperature. Another simple technique commonly used for smaller stacks is to bubble the reactant gas streams through heated bottles of water. Again, the RH achieved is temperature dependent. Furthermore, a considerable pressure drop across the humidifier is common, which requires higher inlet pressure. Therefore, this technique may not be suitable for low pressure fuel cells. In addition, both of the above humidifiers are burdens in the fuel cell system with respect to weight, complexity, cost and parasitic loss [18]. Their existence lowers the overall vehicle efficiency. This is especially a big concern for ground transportation applications. In the effort to overcome the above shortages, An "Enthalpy Wheel" concept was developed [22]. It reuses the fuel cell exhaust gas to humidify the dry inlet gas. Another humidification mechanism also recycles the exhaust energy is the membrane humidification. This humidification method was studied in several previous works [16-18].

This paper will use fuel cell cooling water to humidify and increase the temperature of the dry gas. In this approach, water diffuses from one side of the membrane to the other side, where the gases flow in parallel to the wet membrane. The water transfer is predominately determined by the water and gases flow rates (convective driving force), membrane pressure differential (diffusive driving force), membrane thickness, and the fluid temperatures. A humidifier cell is shown in Fig. 1. There are three channels in each humidifier unit: the humidification channel marked with 'A', a heat transfer channel marked with 'B', and a water channel marked with 'C', where the fuel cell cooling water passes through. The dry inlet gas can be directed to go through either channel 'A' or channel 'B'. When the inlet gas passes through channel 'A', both heat and water vapor exchanges with channel 'C' will occur. On the contrary, when the gas passes through channel 'B', only heat exchange will happen. Depending on the position of the sliding plate, the gas will be directed to go through either channel 'A' to be humidified, or channel 'B' to be heated only.



Based on the size and load of a fuel cell stack, the size and number of humidifier units can be calculated. Assuming there are N humidifier units, the number of units designated as type 'A' can be any number between 0 and N, depending on the desired relative humidity of the exiting air. For example, if the desired humidifier outlet air relative humidity is 100%, the sliding plates are moved so that all the gas goes through the 'A' channels. Similarly, if the desired relative humidity is 0%, all the 'A' channels will be closed. In general, the number of channel 'A' will be $0 \le n \le N$, and is calculated based on the fuel cell stack current, the desired relative humidity and the inlet air relative humidity and temperature. It should be noted that the authority of the humidifier in reducing humidity is limited (or non-existent, if heat exchange effect is ignores). For example, when the inlet air has a non-zero relative humidity, we will not be able to get 0% relative humidity at the outlet even through no channel 'A' is used.

III. CONTROL VOLUMES DEFINITION AND MODELING ASSUMPTIONS

To derive the governing thermodynamic equations, we first need to define the control volumes of the humidifier system. For the humidifier design presented above, two control volumes are defined as shown in Fig. 2. Control Volume 1 includes either Channel 'A' or Channel 'B'. Control Volume 2 includes Channel 'C'. For Control Volume 1, the dry gas inlet mass flow rate, pressure, temperature, and relative humidity (RH) are denoted as $M_{I,in}$, $P_{I,in}$, $T_{I,in}$, and $\Phi_{I,in}$, respectively. The gas outlet mass flow rate, pressure, temperature, and RH are denoted as

 $M_{1,out}$, $P_{1,out}$, $T_{1,out}$, and $\Phi_{1,out}$, respectively. If Control Volume 1 includes Channel 'A', both vapor transfer $M_{v,tr}$ and heat transfer Q_1 occur. If Control Volume 1 includes Channel 'B', only heat transfer Q_1 occurs. For Control Volume 2, the water inlet mass flow rate, pressure, and temperature are denoted as $M_{2,in}$, $P_{2,in}$, and $T_{2,in}$, respectively. The water outlet mass flow rate, pressure, and temperature are denoted as $M_{2,out}$, $P_{2,out}$, and $T_{2,out}$, respectively.



The model assumptions are: 1) The flows in both control volumes are fully developed laminar flows; 2) All gases follow the ideal gas law; 3) The humidifier units are well insulated from its surroundings thus heat transfer only occurs across the membrane, between channel 'A' and 'C' or 'B' and 'C' (which are assumed to have the same heat conductivity); 4) The kinetic and potential energies of the gas molecules are neglected; 5) No external work is done to the system; 6) The flow specific heats are constant; 7) The overall convection heat transfer coefficient is constant; 8) The membrane water transfer is a function of water concentration and temperature gradients; 9) The nominal fuel cell cooling water temperature is assumed to be 80°C; 10) Water is incompressible; 11) The following inlet gas properties are the inputs to the dynamic system: $M_{1,in}$, $P_{1,in}$, $T_{1,in}, \Phi_{1,in}, P_{2,in}, P_{2,out}, \text{ and } T_{2,in}$.

IV. HUMIDIFIER MODELING

Apply the 1st law of thermodynamics to Control Volume 1, the energy equation is [23]

$$\begin{split} \mathbf{m}_{a,1} \, u_{a,1} + \mathbf{m}_{v,1} \, u_{v,1} + \mathbf{m}_{a,1} \, u_{a,1} + \mathbf{m}_{v,1} \, u_{v,1} = \mathcal{Q}_1 + \mathbf{m}_{a,in} \, h_{a,in} \\ + \, \mathbf{m}_{v,in} \, h_{v,in} + \mathbf{m}_{v,tr} \, h_{mem} - \mathbf{m}_{a,out} \, h_{a,out} - \mathbf{m}_{v,out} \, h_{v,out} \\ u_{k1,1} = \int C v_{k1} \, \mathbf{T}_{1,out} \qquad h_{k1,k2} = \int C p_{k1} \, \mathbf{T}_{1,k2} \qquad h_{v,tr} = \int C p_v \, \mathbf{T}_{mem} \end{split}$$
(1)

where Cv_a , Cv_v , Cp_a , Cp_v are the specific heats of the air and vapor. Subscript kI = a or v, represents air or vapor, Irepresents Control Volume 1, tr represents membrane transfer, k2=in or *out*, representing inlet and outlet, respectively. It is also assumed that T_{mem} equals $T_{2,in}$. Apply the 1st law of thermodynamics to Control Volume 2, the energy equation is

$$m_{w,2}Cp_w T_{2,out} = -Q_1 + m_{2,in} h_{w,in} - m_{2,out} h_{w,out} - m_{v,tr} h_{mem}$$
(2)

where $h_{w,k2} = \int Cp_w \dot{T}_{2,k2}$. Cp_w is the specific heat of water. Subscript *w* represents water, and *2* represents Control Volume 2. $\dot{m}_{a,1}$ and $\dot{m}_{v,1}$ are calculated from the mass continuity equation as

$$m_{1,k2} = m_{a,k2} + m_{v,k2}$$
 (5)

$$\omega_{1,k2} = \frac{M_v}{M_{air}} \frac{P_{v,k2}}{P_{a,k2}}$$
(6)

$$\mathbf{\hat{m}}_{a,k2} = \frac{1}{1 + \omega_{1,k2}} \mathbf{\hat{m}}_{k2,1}$$
 (7)

Assuming the flow restriction between the humidifier outlet and the fuel cell inlet is described by a nozzle equation, $\dot{m}_{1,out}$ can be calculated from

$$P_{1,out} = Cr_1 \sqrt{P_{1,out} - P_{fc,in}}$$
 (8)

where $P_{fc,in}$ is the fuel cell inlet pressure, and Cr_1 is a constant which changes with orifice size and the gas density and can be obtained through experiments. $\dot{m}_{w,2}$ can be calculated as

$$m_{w,2} = m_{2,in} - m_{v,tr} - m_{2,out}$$
 (9)

A vapor mass transfer $\dot{m}_{v,tr}$ occurs between the two control volumes and is calculated from [14, 20]

•

$$m_{v,tr} = D_w \frac{C_2 - C_1}{t_m} M_v A \quad D_w = D_\lambda e^{(2416(\frac{1}{303} - \frac{1}{T_w}))}$$
 (10)

where D_w is the membrane coefficient of diffusion. c_2 and c_1 are water concentrations in Control Volume 2 and Control Volume 1, and are defined in Eq. (12). t_m is the membrane thickness. T_w is the membrane temperature in Kelvin, M_v is the vapor molar mass. A is the mass transfer area (i.e., the membrane area). The coefficient D_λ is determined empirically and has a piecewise-linear form [14, 20]

$$D_{\lambda} = \begin{cases} 10^{-6} & \lambda < 2\\ 10^{-6}(1+2(\lambda-2)) & 2 \le \lambda \le 3\\ 10^{-6}(3-1.67(\lambda-3)) & 3 < \lambda < 4.5\\ 1.25*10^{-6} & \lambda \ge 4.5 \end{cases}$$
(11)

The water concentrations in the water channel and the gas channel are

$$C_{k3} = \frac{\rho_{m,dry}}{M_{m,dry}} \lambda_{k3} \tag{12}$$

where $\rho_{m,dry}$ is the membrane dry density and $M_{m,dry}$ is the membrane dry equivalent weight. The subscript k3 is either 1 or 2, which represent Control Volume 1 and 2. Water content λ_1 and λ_2 are calculated from [14, 20]

$$\lambda_{1} = (0.043 + 17.81a_{1} - 39.85a_{1}^{2} + 36.0a_{1}^{3}) \quad a_{1} = \frac{P_{\nu,1}}{P_{sat,1}}$$

$$\lambda_{2} = 14$$
(13)

where $P_{v,1}$ is the vapor partial pressure of Control Volume 1. $P_{sat,1}$ is the saturation pressure of Control Volume 1, and is determined by [14, 20]

$$\log_{10}(P_{sat,1}) = 2.95 \cdot 10^{-2} T_{a,out} - 9.18 \cdot 10^{-5} T_{a,out}^{2} + 1.44 \cdot 10^{-7} T_{a,out}^{2} - 2.18$$
(14)

The vapor partial pressure of Control Volume 1 is obtained from the ideal gas law.

$$P_{v,1}V_{c1} = R_v T_1 m_{v,1}$$

$$P_{a,1}V_{c1} = R_a T_1 m_{a,1}$$

$$P_{1,k2} = P_{v,k2} + P_{a,k2}$$
(15-17)

where R_a and R_v are the air and vapor gas constant, V_{cl} is the volume of Control Volume 1, $P_{a,1} = P_{a,out}$, $P_{v,1} = P_{v,out}$.

The heat transfer rate between the two control volumes can be calculated as [24]

$$\hat{Q}_1 = h A \Delta T_{2/1} \eta_0 \tag{18}$$

where A is the heat transfer area, η_0 is the heat transfer

efficiency, \bar{h} is the heat transfer coefficient defined as

$$\bar{h} = \frac{kN_{uD}}{D_h}$$
(19)

where k is the membrane thermal conductivity, N_{uD} is Nusselt number and D_h is the channel hydraulic diameter. $\Delta T_{2/l}$ is the temperature difference between the water and the gas. For counter flow,

$$\Delta T_{2/1} = \frac{(T_{w,in} - T_{g,out}) - (T_{w,out} - T_{g,in})}{\ln((T_{w,in} - T_{g,out})/(T_{w,out} - T_{g,in}))}$$
(20)

and	the		external			disturbances		include:
<i>w</i> =	$\begin{bmatrix} \bullet \\ m_{1,in} \end{bmatrix}$	$T_{1,in}$	$P_{1,in}$	$\Phi_{1,in}$	$P_{2,in}$	$P_{2,out}$	$T_{2,in} \int_{0}^{T}$	

V. SIMULATION RESULTS AND ANALYSIS

Simulations are performed with the assumption that all the air goes through 'A' channels. The results of changing the inlet air condition are shown in Fig. 3 and Fig. 4. Fig. 3 shows that when there is a step increase in the airflow rate, in order to compensate the air flow increase, the membrane vapor transfer rate and the heat transfer rate both increase with some transient fluctuations. This transient effect adds more water to the inlet, and may cause flooding in the fuel cell. Fig. 4 shows that when there is a step decrease of the inlet air temperature, the heat transfer rate increases and the membrane vapor transfer rate decreases. The decrease and the transient fluctuations may cause the fuel cell to become dehydrated. These issues need to be addressed to maintain fuel cell performance and life.



Fig. 3: System responses under step increase of the inlet airflow rate



Fig. 4: System responses under step decrease of the inlet air temperature

A simple proportional feedback control strategy is used here to control 'n', the number of humidifying cells, and the results are shown in Fig. 5 and Fig. 6. Fig. 5 shows that the large transient deviation in vapor transfer rate is eliminated by the feedback control strategy. Fig. 6 confirms that the temperature disturbance does not affect the output variable under the feedback control.



Fig. 5: System response with and without feed back control under step increase of the inlet airflow rate



Fig. 6: System response with and without feed back control under step decrease of the inlet temperature

VI. HUMIDIFIER AND FUEL CELL INTEGRATION

The humidifier model is integrated with the dynamic fuel cell model developed in [12], which was based on the Ford P2000 experimental vehicle. The fuel cell membrane water content is described by the following equation [14, 20]

$$\lambda_m = \begin{cases} 0.043 + 17.81a_m - 39.85a_m^2 + 36.0a_m^3 & 0 < a_m \le 1\\ 14 + 1.4(a_m - 1) & 1 < a_m \le 3 \end{cases}$$
(21)

where $a_m = \frac{a_{ca} + a_{an}}{2}$, a_{ca} and a_{an} are cathode and anode

RH respectively. Since the membrane water content is a function of the RH of the anode and cathode gases, their relationship is studied. Fig. 7 shows that there is a significant improvement in membrane water content if cathode is amply humidified. The improvement is small if anode inlet gas is also completely humidified. In addition, it is known that anode humidifier is not easy to implement because change in hydrogen temperature creates large variation in RH. Therefore, this paper is focused on adding a humidifier at the fuel cell cathode inlet. Fig. 8 shows the result of the fuel cell with 100% RH at the cathode inlet, under varying fuel cell stack current. The fuel cell membrane water content increases from 10A to 60A, then decreases after 60A despite the fact more water is generated at the cathode. This is caused by decreasing anode RH after 60A, due to proton osmotic drag. From Eq. (21), one can see that the membrane water content is proportional to the anode and cathode RH. When the anode RH decreased, the membrane water content reduces accordingly. Another observation is that the cathode flooding is increased after 60A. This is mainly due to the

fact more water is generated at cathode at higher stack current, while the cathode inlet gas is (improperly) maintained at 100% RH. Obviously, proper control of the RH of cathode inlet gas is necessary to prevent flooding.



Fig. 7: Membrane water content under 4 inlet humidification conditions



Fig. 8: Membrane water content, anode and cathode RH and water liquid collected at anode and cathode under 100% cathode inlet RH

An optimization search is conducted to find the desired cathode inlet gas RH to maintain high fuel cell membrane water content with minimum flooding. The result is shown in Fig. 9. Since more water is generated when current increases, the fuel cell requires less water from its inlet gas. The desired cathode inlet gas RH will be the desired output of the humidifier.



Fig. 9: Desired cathode inlet air RH vs. PEMFC current

Based on this result, a feed-forward control map is developed and implemented in the integrated system. The integrated system block diagram is shown in Fig. 10. The simulation result of this integrated system is shown in Fig. 11, which reveals that a properly controlled cathode inlet RH will maintain the highest fuel cell membrane water content with minimum flooding.



Fig. 11: Fuel cell membrane water content and flooding condition under controlled and non-controlled cathode inlet air RH

VII. CONCLUSIONS

A membrane humidifier for automotive fuel cell systems is modeled and analyzed in this paper based on basic thermodynamic laws. This lumped model describes the transient behavior of the humidification phenomena and captures the time varying aspect of the flow rate, temperature, pressure and relative humidity. The humidifier model is subsequently integrated with a fuel cell model. By controlling the number of humidification cell units, we can actively control the fuel cell inlet air to maintain proper membrane humidification for the fuel cell stack. A simple proportional feedback control algorithm is developed to regulate the inlet air relative humidity. The humidifier simulation results show that the feed back control algorithm works well under many uncertainties, such as inlet air flow rate change and the inlet air temperature variation. A feed forward algorithm is developed to compensate the fuel cell current change. Simulation results on the integrated humidifier and fuel cell system show that the fuel cell membrane water content is humidified with minimum flooding.

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