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Contributed Paper

Estimation of Water Content in PEM Fuel Cell

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ABSTRACT

The Polymer electrolyte membrane fuel cell (PEMFC) is a high potential alternative energy to apply for the automotive application due to its advantages such as clean energy source and compact size. To achieve high performance, the amount of water content in PEMFC should be in the suitable range that is adequate to hydrate membrane but not disturb the transportation of the reactant gas. Because of the difficulty to monitor the water content in PEMFC and limitation of the hardware installation, this research proposed the new technique to predict the water content in PEMFC via the state estimation. The concept of extended Luenberger observer is applied to estimate the water content. The membrane water content is calculated from the relation of membrane resistance and the amount of water in each channel is calculated from the mass balance. The simulation results of proposed method compared with that of open-loop observer are presented. From the simulation, the extended Luenberger observer can eliminate the offset while the open-loop observer can not.

Keywords: PEM fuel cell, parameter estimation, state estimation, water management.

1. INTRODUCTION

The energy crisis is continuously a critical problem in many countries due to the rapid depletion of fossil fuel, in which it needs to be addressed. Fuel cell is an alternative energy source that can generate electrical current from electrochemical reaction between oxygen and hydrogen. The most well-known type of the fuel cell development is polymer electrolyte membrane fuel cell (PEMFC) because the size and the operating temperature of PEMFC are suitable to apply for the automotive applications. The effective water management in PEMFC is one of the key issues to ensure high performance and should be addressed. If the membrane is too dry, the proton conductivity decreases due to the lack of water to solvate the proton. In contrast, if the membrane is too wet, the transport rate of reactant decreases because porous passages are blocked by water.

The research works on water monitoring were received many attentions in recent years [1, 2, 4-10]. For example, Mench et al. [7] used the gas chromatography to measure the in situ water vapor distribution in the gas channels of an operating PEMFC. Chen et al. [1] used neutron radiography to observe the water distribution in anode and cathode gas diffusion layers. The other hardware to monitoring the water is the Agilent real-time gas analyzer [2].

Due to the problem about installation and accuracy of hardware sensor, McKay et al. [6] presented the technique to estimate the humidity of electrode by using a lump dynamics model of PEMFC and the measured pressure and temperature of each electrode. Gorgun et al. [4] proposed the on-line estimation of the membrane water content by using the dynamics model of the partial pressure of reactant gas and the voltage model with available measurements of voltage, current, temperature, and total pressure in both electrodes. However, this technique can be applied only for non zero current. The commercial computational fluid dynamics software (CFD) was also used as the alternative technique to study the water transport and distribution in PEMFC [5, 8, 9, 10]. State observers are usually classified as exponential and asymptotic observer. The exponential observer including extended Kalman observer and extended Luerberger observer can control the rate of convergence by adjusting tuning parameters. However, the accuracy of this observer is strongly based on the quality of dynamic models. In contrast, the asymptotic observers do not require the high quality of dynamic model but the convergence rate of estimation strongly depends on operating condition.

This work presents the new technique to estimate quantity of water content in the PEMFC by applying the concept of the extended Luenberger observer due to its simplicity and the developed dynamic models of PEMFC that are not complicate. In the algorithm, the proposed method estimates the unmeasured state variables and then the values of estimated states variables are use to predict membrane water content via the membrane resistance. Amount of water in each channel can be calculated from water balance in each side.

This paper is organized as follow. The mathematical models are formulated and the observer designs are presented briefly in section 2. Section 3 shows and discusses the results from the estimation compared with that of open-loop observer. Finally, the concluding remarks are given in section 4.

Nomenclature

Alphabets

A	Area (m^2)
D_w	Water diffusivity (cm^2/s)
F	Mass flow rate (kg/s)
$\mathfrak{F}$	Faraday's constant (coulomb/mol)
C	Current density (A/cm^2)
M	Molecular weight (kg/kmol)
n	Number of cell
N	Number of mole
p	Partial pressure (bar)
P	Total pressure (bar)
R	Gas constant (J/mol.K)
T	Temperature (K)
Vol	Volume (l)

Greek symbols

ϕ	Relative humidity
λ	Water content
ρ	Density (kg/m^3)

Superscripts and subscripts

a	Anode
av	Average
c	Cathode
i	Inlet
m	Membrane
o	Outlet
sat	Saturation
v	Vapor
w	Water

2. ESTIMATION OF WATER CONTENT IN PEMFC

2.1 Mathematical model

The water content in PEMFC can be estimated by using dynamics model of hydrogen, oxygen, water at anode, water at cathode partial pressure in (1)-(4) and voltage (5).

$$\frac{dp_{H_2,ao}}{dt} = \frac{RT}{Vol_a}\left(\frac{1}{M_{ai}}\frac{p_{H_2,ai}}{P_{ai}}F_{ai} - \frac{1}{M_{ao}}\frac{p_{H_2,ao}}{P_{ao}}F_{ao} - \frac{nC}{2\mathcal{F}}\right) \tag{1}$$

$$\frac{dp_{O_2,co}}{dt} = \frac{RT}{Vol_c}\left(\frac{1}{M_{ci}}\frac{p_{O_2,ci}}{P_{ci}}F_{ci} - \frac{1}{M_{co}}\frac{p_{O_2,co}}{P_{co}}F_{co} - \frac{nC}{4\mathcal{F}}\right) \tag{2}$$

$$\frac{dp_{W,ao}}{dt} = \frac{RT}{Vol_a}\left(\frac{1}{M_{ai}}\frac{p_{W,ai}}{P_{ai}}F_{ai} - \frac{1}{M_{ao}}\frac{p_{W,ao}}{P_{ao}}F_{ao} - \frac{D_W\Delta\phi}{\mu M_W}\right) - \frac{d\phi_{ai}}{dt} \tag{3}$$

$$\frac{dp_{W,co}}{dt} = \frac{RT}{Vol_c}\left(\frac{1}{M_{ci}}\frac{p_{W,ci}}{P_{ci}}F_{ci} - \frac{1}{M_{co}}\frac{p_{W,co}}{P_{co}}F_{co} + \frac{D_W\Delta\phi}{\mu M_W} + \frac{nC}{2\mathcal{F}}\right) - \frac{d\phi_{ci}}{dt} \tag{4}$$

$$\frac{dV}{dt} = \frac{RT}{2\mathcal{F}}\left(\frac{1}{2p^{av}_{H_2}}\frac{dp_{H_2,ao}}{dt} + \frac{1}{4p^{av}_{O_2}}\frac{dp_{O_2,co}}{dt}\right) \tag{5}$$

where M_{ao} and M_{co} are molecular weight of anode outlet, molecular weight of cathode outlet. $\frac{d\phi_{ai}}{dt}$ and $\frac{d\phi_{ci}}{dt}$ are the derivative of the inlet relative humidity at anode and cathode with respect to time. In this work, the anode is fed with fully humidified hydrogen and cathode is fed with dry air implied that the $\frac{d\phi_{ai}}{dt}$ and $\frac{d\phi_{ci}}{dt}$ can neglect. The average partial pressure of hydrogen and oxygen is given by

$$p^{av}_{H_2} = \frac{p_{H_2,ao} + p_{H_2,ai}}{2} \qquad p^{av}_{O_2} = \frac{p_{O_2,co} + p_{O_2,ci}}{2} \tag{6}$$

μ is defined as

$$\mu = \frac{M_m t_m}{n\rho_m M_v A} \tag{7}$$

D_w is water diffusivity calculate from (8)

$$D_w = d_{w1}\phi_m - d_{w0} \tag{8}$$

where $d_{w1} = 0.0026$ and $d_{w0} = 0.00054$, is membrane relative humidity which is the average of humidity between anode and cathode.

$$\phi_m = \frac{(\phi_c + \phi_a)}{2} \tag{9}$$

Relative humidity at each side is defined as

$$\phi_a = \frac{(\phi_{ai} - \phi_{ao})}{2} \qquad \phi_c = \frac{(\phi_{ci} - \phi_{co})}{2} \tag{10}$$

$\Delta\phi$ is the different of relative humidity between anode and cathode

$$\Delta\phi = \phi_c - \phi_a \tag{11}$$

The eqs. (1)-(5) are formulated based on the assumption that activation loss resistance (R_a) and mass transport loss resistance (R_{mass}) are constant and calculated from precondition operation. The membrane resistance (R_m) calculated from (12)

$$R_m = \frac{(E_a - CR_a - CR_{mass} - V)}{C} - r_{load} \tag{12}$$

where E_a is theoretical voltage calculated from Nernst's equation, i is current density, and r_{load} is resistance from external load. Membrane water content (λ_m) is the function of membrane resistance.

$$R_m = \frac{t_m}{A_m(0.00154\lambda_m - 0.00326)} \times \exp\left[1268\left(\frac{1}{T} - \frac{1}{303}\right)\right] \tag{13}$$

where A_m is active area and t_m is membrane thickness. The total water in each channel is computed from overall mass balance as shown in (14)-(15)

$$\frac{dN_{w,a}}{dt} = \left(\frac{P_{sat,ai}F_{ai}}{(P_{ai} - P_{sat,ai})M_{ai}}\right) - \left(\frac{P_{sat,ao}}{P_{ao} - P_{sat,ai}}\right)\left(\frac{F_{ai}}{M_{ai}} - \frac{nC}{2\mathcal{F}}\right) - \frac{D_W\Delta\phi}{\mu M_W} \tag{14}$$

$$\frac{dN_{w,c}}{dt} = \left(\frac{P_{sat,ci}F_{ci}}{(P_{ci} - P_{sat,ci})M_{ci}}\right) - \left(\frac{P_{sat,co}}{P_{co} - P_{sat,ci}}\right)\left(\frac{F_{ci}}{M_{ci}} - \frac{nC}{4\mathcal{F}}\right) + \frac{nC}{2\mathcal{F}} + \frac{D_W\Delta\phi}{\mu M_W} \tag{15}$$

The liquid water accumulated in chambers is given by

$$N_{w,(.),l} = N_{w,(.)} - N_{w,(.),v} \tag{16}$$

where (.) is replaced by *a* for anode and *c* for cathode. The mol of vapor is defined as

$$N_{w,(.),v} = \min\left\{N_{w,(.)}, N^{sat}_{w,(.),v}\right\} \tag{17}$$

where $N^{sat}_{w,(.),v}$ is the maximum of vapor that can exist in channels.

2.2 Estimation via extended Luenberger observer

Consider the general form of nonlinear processes

$$\dot{x} = f(x,u) \tag{18}$$

$$y = h(x) \tag{19}$$

where x, y, and u are a vectors of state variables, measured variables, and manipulate variables, respectively. The Extended Luenberger observer equation in [3] is governed by

$$\dot{\hat{x}} = f(\hat{x},u) + L(e) \tag{20}$$

$$e = y - \hat{y} \tag{21}$$

where L is a vector of tuning parameters that adjusts convergence speed of estimation, called observer gains. In this case, the vector of state variables is

$$x = \left[p_{H_2,ao} \quad p_{O_2,co} \quad p_{W,ao} \quad p_{W,co} \quad V\right]^T \tag{22}$$

and the measured variable is $y=V$. The schematics of membrane water content (λ_m) estimation via open-loop and extended Luenberger observer are shown in Figure 1. This work assumes that the piecewise of disturbance occurring in the voltage monitoring.

3. RESULTS AND DISCUSSION

The application of proposed method is illustrated on the PEMFC 50 cm^2 operate at 353 K with the constant loaded current at 0.4 A/cm^2. The piecewise disturbance, d = 0.05 V, is constantly applied in the voltage monitoring. The fed reactant at the anode, hydrogen, is fully humidified while the fed reactant at the cathode is dry air.

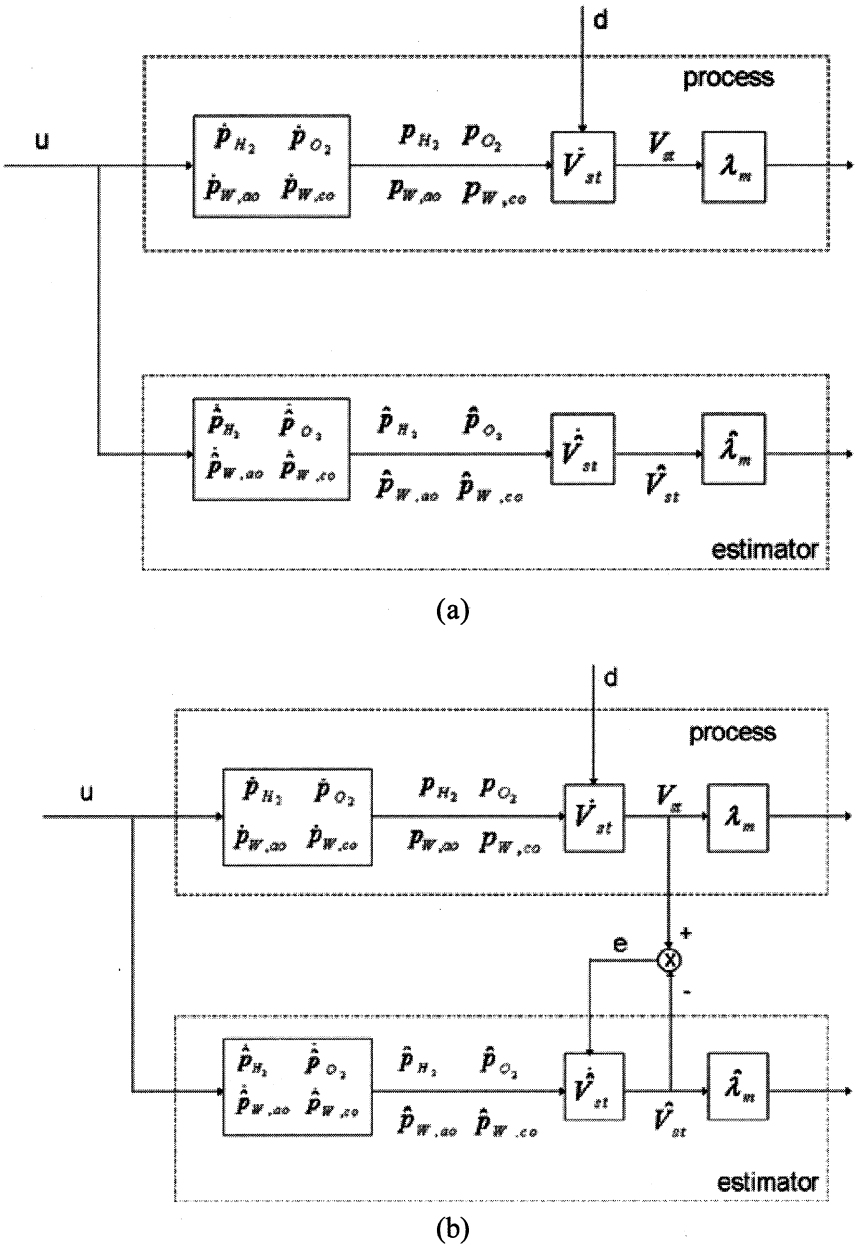

Figure 1. (a) Open-loop observer design, (b) extended Luenberger observer design.

Figure 2, Figure 3 and Figure 4 show the estimated of hydrogen and oxygen partial pressure, the estimated of water partial pressure in cathode and anode and the predicted voltage, respectively. The results show that the prediction of hydrogen, oxygen and water partial pressures from both open-loop and extended Luenberger observer have no offset because the disturbance is not directly affect to the state dynamics. However, the predicted voltage via open-loop observer in Figure 4 shows the offset while the predicted voltage via extended Luenberger observer can eliminate the error.

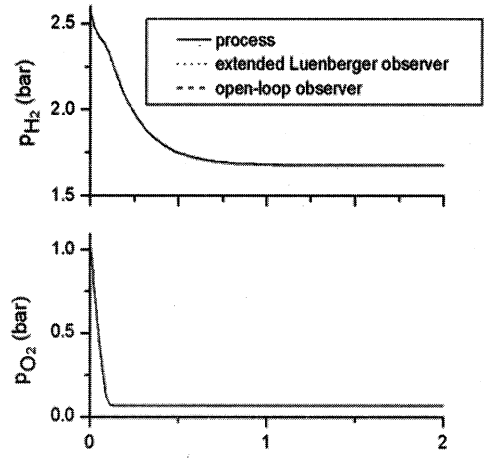

Figure 2. Dynamic responses of hydrogen and oxygen partial pressure.

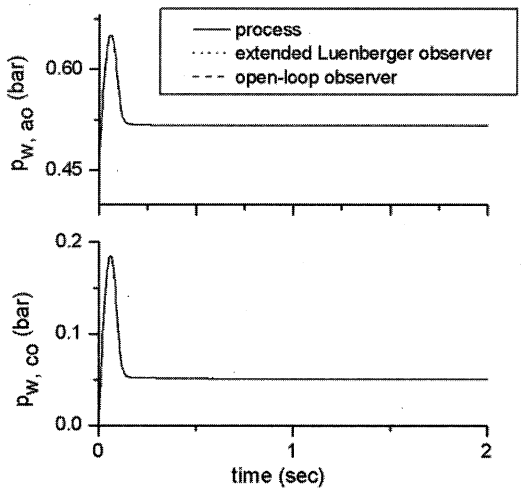

Figure 3. Dynamic responses of water partial pressure.

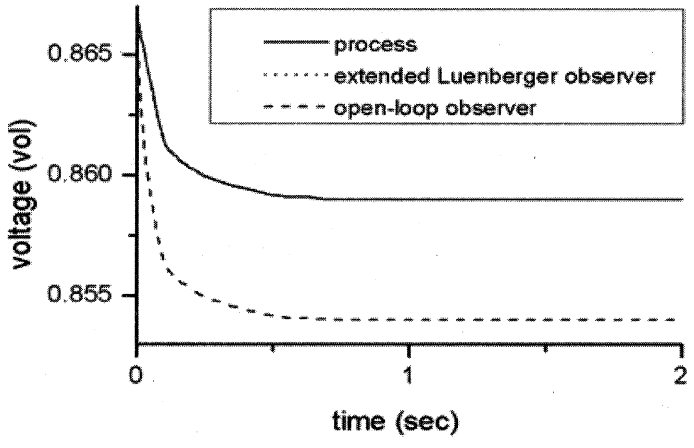

Figure 4. Dynamic responses of voltage.

Figure 5 shows the membrane water content calculated from the relation with voltage as shown in (13). The predicted membrane water content is asymptotically decayed to the actual process value regardless the disturbance. In Figure 6, predicted amount of water accumulate in anode and cathode channels is shown. With the fully humidified hydrogen gas, the figure shows that the cathode will flood after 25 minutes. The water at both sides will condense to liquid phase due to the water partial pressure higher than saturation pressures. The cathode will flood before anode because the electrochemical reaction generates water at only the cathode side. The PEMFC is flooding very quickly due to the constant loaded current that generates the water $1x10^{-4}$ mol/s while volume of channel is $2.8x10^{-3}$l which can hold the liquid water 0.1556 mol. After flooding, PEMFC can not operate anymore because the liquid water disturbs the transportation of reactant gas.

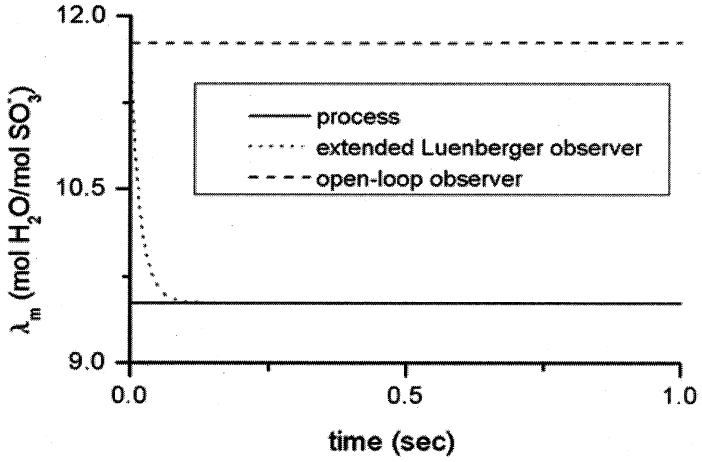

Figure 5. Dynamic responses of membrane water content.

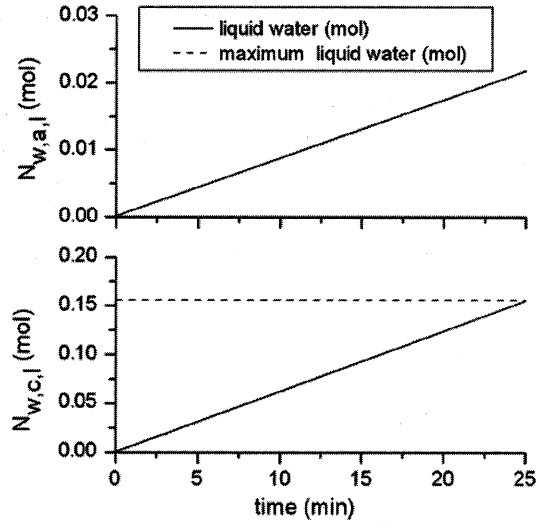

Figure 6. Dynamic responses of liquid water in channels.

4. CONCLUSIONS

In this paper, the new technique to estimate the membrane water content and also the water content in both anode and cathode channels were presented. The simple dynamic models of PEMFC ware used to design the observer. The extended Luenberger observer was demonstrated to give higher accuracy than the prediction via open-loop observer. This technique can be applied for the PEMFC control system.

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REFERENCES

[1] Chen, Y., Peng, H., Hussey, D., Jacobson, D., Tran, D., Baset, T., and Biernacki, M., Water distribution measurement for a PEMFC through neutron radiography, J. Power Sources, 2007; 170: 376-386.

[2] Dong, Q., Kull, J., and Mench, M., Real-time water distribution in a polymer electrolyte fuel cell, J. Power Sources, 2005; 139: 106-114.

[3] Fissore, D., Pisano, R., and Barresi, A., Observer design for the Selective Catalytic Reduction of NO_x in a loop reactor, Chem. Eng. J., 2007; 128: 181-189.

[4] Gorgun, H., Arcak, M., and Barbir, F., An algorithm for estimation of membrane water content in PEM fuel cells, J. Power Sources, 2006; 157: 391-413.

[5] Liu, Z., Mao, Z., Wang, C., Zhuge, W., and Zhang, Y., Numerical simulation of a mini PEMFC stack, J. Power Sources, 2006; 160: 1111-1121.

[6] McKay, D., and Stefanopoulou, A., Parameterization and validation of a lumped parameter diffusion model for fuel cell stack membrane humidity estimation, IEEE Proceedings of 2004 American Control Conference, Boston, Massachusetts, United states, June 30–July 2, 2004; 816-821.

[7] Mench, M., Dong, Q., and Wang, C., In situ water distribution measurements in a polymer electrolyte fuel cell, J. Power Sources, 2003; 127: 90-98.

[8] Shimpalee, S., Greenway, S., Spuckler, D., and Zee, J., Predicting water and current distributions in a commercial-size PEMFC, J. Power Sources, 2004; 135: 79-87.

[9] Um, S., and Wang, C., Computational study of water transport in proton exchange membrane fuel cells, J. Power Sources, 2006; 156: 211-223.

[10] Wang, Y., and Wang, C., Simulation of flow and transport phenomena in a polymer electrolyte fuel cell under low-humidity operation, J. Power Sources, 2005; 147: 148-161.