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MODEL PARAMETER ESTIMATION BY TRACKING SIMULATOR FOR THE INNOVATION OF PLANT OPERATION

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Abstract: This paper proposes a new application of the tracking simulator relevant to future plant operation. The tracking simulation technique will enable matching of physical and virtual worlds. The simulator receives sensor data from the plant and the model parameters in the simulator are constantly adjusted to match the actual plant behavior. Model parameter estimation is one application of the tracking simulator. Here, the tracking simulator showed good simulation accuracy with model parameters to estimate the functions of its related variables. A fuel cell simulator was used for model parameter estimation in this study.

Keywords: Modeling and Simulation, Parameter Estimation, PEM Fuel Cell, Real-time Systems, Process Monitoring, Fault Diagnosis

1. INTRODUCTION

There are many issues and problems surrounding plant at present. Especially, we focus on the issues related to plant operation. Today's plant operations are more complicated because they are engaged in high-level production of multiple products with highly rigorous specifications. At the same time, plant operation must conserve energy and require the minimum number of operators. Therefore, plant operators must monitor a much wider area in the plant. It is virtually impossible for a human operator to grasp all process data and information in the plant. On the other hand, recent developments in information technology with advances in computer technology have facilitated plant automation. However, plant operators are therefore less attuned to the actual operation and begin to lose the sense of "manufacturing touch" because there are fewer opportunities for manual operations. Another major problem facing the operator is having too many alarm signals in the control system. In the operational room of the plant, the operator may be subject to data flooding.

We proposed an online tracking simulator, which should impact plants operation over the next ten years.(Nakaya and Ootani, 2005) The tracking simulator can make the virtual world run parallel with the actual plant. The model parameters are adjusted to match measured data from the plant in the tracking simulator. As a result, the tracking simulator can simulate the target accurately.

If the simulator can make the virtual world run in parallel with the real word, the simulator can provide entirely new applications. We expect in following novel applications in plant operation.

(1) Visualization of data that cannot be actually measured, such as inside devices where sensors cannot be installed and temperature distribution within a reactor.

(2) Prediction of plant behavior in future by making the computer run faster than reality.

(3) Optimization toward optimal conditions for plant operations.

(4) Normal maintenance and diagnosis of abnormal conditions by monitoring the trends in model parameters.

There are additional novel applications for utilizing the plant model, including plant design and operator training. It is necessary to construct an accurate simulation model to realize these applications. Figure 1 shows that deciding the initial parameters, tracking simulation, and data reconciliation techniques are useful for obtaining a good simulation model. Here, we explain how the parameters are estimated in the fuel cell simulation model as an example of a plant.

2. TRACKIG SIMULATION TECHNIQUE

The most important element in our research is to ensure that the virtual world on the computer agrees with the actual world—this is called the tracking simulation technique. The tracking simulator receives the actual temperature, pressure, and flow rate data directly from the plant. The model parameters in the simulator are constantly adjusted to gradually match the actual plant behavior. Therefore, the tracking simulator permits the virtual world to run in parallel with the actual world.

For example, in simulating the temperature of the reactor, the heat transfer coefficient is chosen as the tracking parameter and adjusted to match that the reactor
temperature. In our research, the change method of the tracking parameter is as follows:

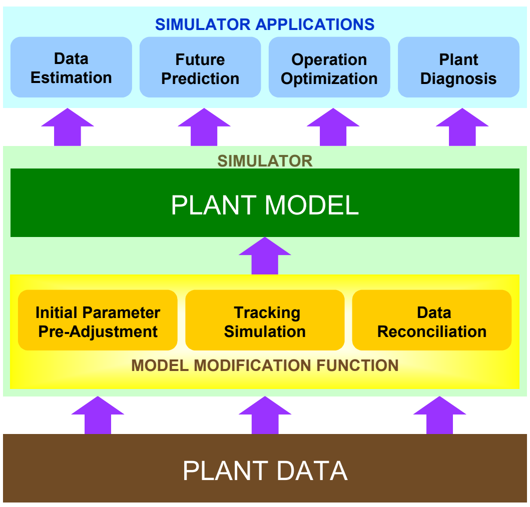

Fig. 1. Modification method for accurate model and tracking simulator applications

$$\begin{cases} \Lambda(t) = \Lambda(t-1) + \Delta\Lambda \\ \Delta\Lambda = K_p e \\ e = e^{Measured} - e^{Simulation} \end{cases} \qquad (1)$$

Where, Λ is a tracking parameter, Kp is gain parameter for the adjustment, $e^{Measured}$ is sensor-measured data, and $e^{Simulation}$ is calculation result by the simulator.
We also simulated the reactor's temperature by changing the reaction velocity as a tracking parameter and reported that multiple tracking simulations were performed at same time in the methane steam reforming system.(Nakabayashi, 2006)

3. RECENT WORK

We reported our application of tracking simulation to the fuel cell in determining the driving condition.(Kawaguchi, 2005) In the fuel cell, moisture control is very difficult. Attention must be paid to moisture in the cell because a high moisture level would markedly reduce the power generation performance. As the load current is drawn from the fuel cell, water molecules are both produced in the cathode and dragged from the anode to the cathode by the hydrogen ions. As the concentration of water in the cathode increases, the concentration gradient causes water to diffuse from the cathode to the anode. The conventional fuel cell simulator could not accurately simulate experimental data with changing water content.

In Fig. 2, the parameters of the conventional simulator were set at a relative humidity of 61% but the calculation results of high humidity did not match the measured data. The tracking simulation was performed at a relative humidity of 83% for model parameter estimation. Using this parameter, the

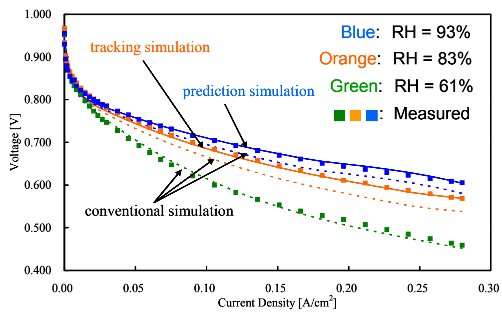

Fig. 2. Simulation result of prediction under high humidity driving condition by tracking simulation

predicted result matched the measured data well at a relative humidity of 93%. These results indicated that the prediction simulation by the tracking simulator was useful for determining driving conditions.

4. PEMFC EXPERIMENTAL APPARATUS

We studied the tracking simulator with the fuel cell power generation system in our laboratory. The tracking simulator was connected to this experimental system. Figure 3 shows the experimental test bench of the fuel cell generation system and a schematic diagram of the Polymer Electrolyte Membrane Fuel Cell (PEMFC) experimental apparatus is shown in Fig. 4. Both H2 and AIR gas were supplied from gas cylinders, and then passed through a humidifier before entering the fuel cell to keep the membrane hydrated. The fuel cell temperature also plays an essential role in keeping the membrane well hydrated, and this was controlled by circulating coolant water. Finally, exhaust gas from fuel cell was cooled to separate the water and gas. The electrical load was connected to the fuel cell to measure the polarization curve, which represents the major characteristics of the PEMFC. The fuel cell employed for the experiment had power output of 25 W with an active fuel cell area of 132 cm2.

5. PRE-ADJUSTMENT SIMULATION PARAMETERS

Determination of the initial simulation model parameters is an important issue. It is very important to adjust the initial values of the parameters in the tracking simulator. Therefore, it is important to set the initial simulation parameters to gain as precise as possible agreement between the simulator and the target. The output voltage of the fuel cell can be written as (J.T.Pukrushpan, 2004)

$$V = E - \eta_{act} - \eta_{ohm} - \eta_{con} \qquad (2)$$

where E is the "Nernst Voltage," ηact is the activation overvoltage, ηohm is the ohmic loss, and ηcon is the concentration loss. The typical polarization curve of the fuel cell is shown in Fig. 5. At the low current region, the activation loss dominates the output voltage and at the middle current region the ohmic loss contributes to total voltage loss. Although the concentration loss may contribute at the high current region, we omitted the concentration loss ηcon in this case for simplicity.
It is difficult to fit the measured polarization curve at the low and middle current regions at the same time to make rough estimates, and it is easier to estimate each parameter step by step. Therefore, we first adjusted the model parameter of the activation loss

Fig. 3. PEMFC test bench

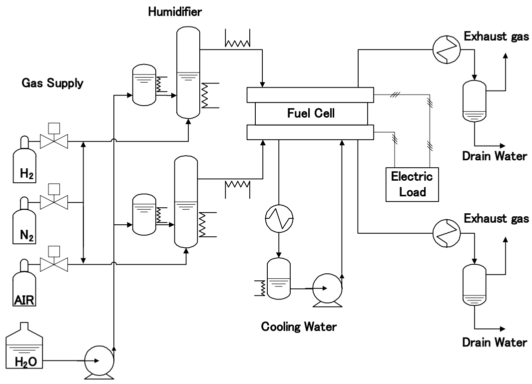

Fig. 4. Schematic diagram of PEMFC experimental apparatus

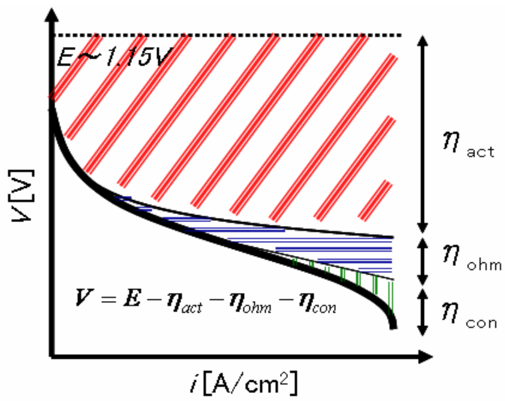

Fig.5. The polarization curve of PEMFC

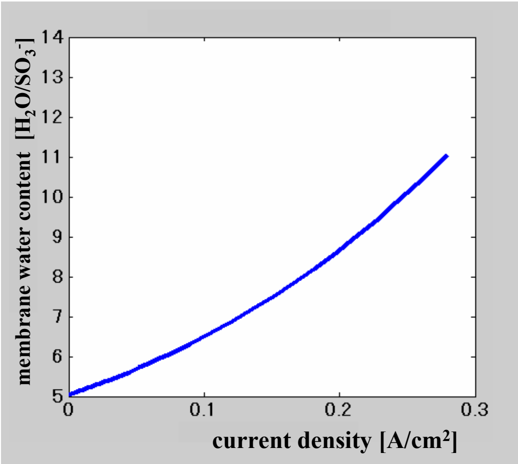

Fig.6. The relation between current density and the membrane water content

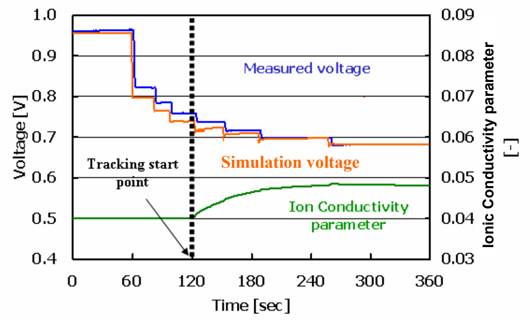

Fig. 8. Tracking simulation result

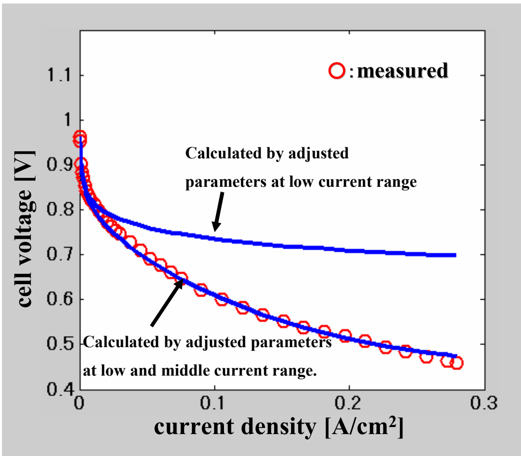

Fig.7. Simulation result using estimated parameters in pre-adjustment

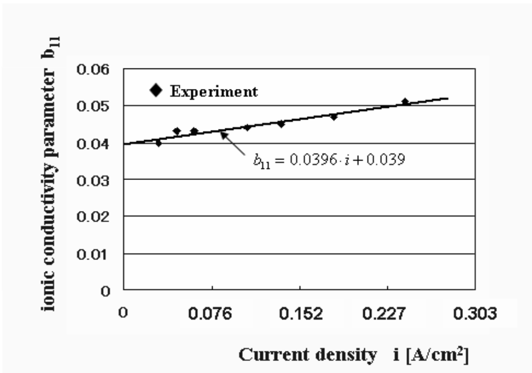

Fig. 9 Approximation of ionic conductivity parameter

model then we adjusted the ohmic loss model parameters.

At the low current region (below 0.01 A/cm2) the activation loss is used to model the output voltage of the fuel cell. The activation loss arises from the need to activate the electrochemical reaction. The relation between the activation overvoltage ηact and the current density i is described by the Tafel equation as:

$$\eta_{act} = A \ln\left(\frac{i}{i_{ex}}\right) \tag{3}$$

where A is a constant and iex is the exchange current density, which is also a constant. We first applied logarithmic to the experimental data measured under driving conditions and estimated A and iex from the gradient and the intercept of the straight line, respectively. Then, we finally estimated the parameters using nonlinear regression ("lsqcurvefit" in the MATLAB optimization toolbox).

In the middle current range (over 0.05 A/cm2), where both the activation loss and the ohmic loss are dominant, the ohmic loss arises from the resistance to transfer of protons in the polymer membrane. The voltage drop that corresponds to the ohmic loss is proportional to the current density

$$\eta_{ohm} = \frac{t_m}{\sigma_m} i \tag{4}$$

where tm is the thickness of the membrane and the membrane conductivity σm is a function of membrane water content λm and fuel cell temperature Tfc.

$$\sigma_m = (b_{11}\lambda_m - b_{12}) \exp\left[350\left(\frac{1}{303} - \frac{1}{T_{fc}}\right)\right] \tag{5}$$

The relation between current density and membrane water content is shown in Fig. 6 considering the electro-osmotic drag and the diffusion of water in the membrane. Using this relation, the experimental data were fit to the relation between the membrane conductivity σm and the membrane water content λm. We estimated b11 and b12 according to the linear section between ionic conductivity σm and water content λm. Fig. 7 shows the fitting result, which was calculated using adjusted parameters. The result matched the experimental data.

6. PARAMETER ESTIMATION BY TRACKING SIMULATOR

After pre-adjustment of the model parameters in the fuel cell simulator, we drove a fuel cell under arbitrary driving conditions and then performed tracking simulation for parameter estimation. The output voltage data of the fuel cell were input into the tracking simulator directly and we adjusted the parameter b11, which is related to ionic conductivity in the polymer membrane. Figure 8 shows the results of tracking simulation. At time 0 s, calculated output voltage matched the measured data because the initial simulation parameters had been tuned sufficiently. However, as the load current was increased in steps over time, the simulation results deviated far from the measured data. The tracking simulator was started at time 120 s. After the tracking simulator was done, the tracking parameters were adjusted and the simulation result approached the measured data. Finally, the simulation results agreed with the measured data. When the water content of the polymer membrane is high, ionic conductivity rises. Therefore, ion conductivity as a tracking parameter is strongly related to the current. The parameter of the ionic conductivity should be a function of the current of the fuel cell. From the tracking simulation results, ionic conductivity was a function of the current density. In Fig. 9, the ionic conductivity from the tracking simulator was plotted as the function of the current density. It is possible to approximate the ionic conductivity with the mathematical formula as the function of the current density.

Figure 10(a) shows the results of conventional tracking simulation, while Fig.10(b) shows the simulation results using the mathematical formula between the ionic conductivity and the current density. In Fig. 10(a), the simulator did not express the transient state because the tracking parameter could not be adjusted fast enough in the case of a sudden current change. The overshoot of the output voltage wave form can be seen in Fig. 10(a). As shown in Fig. 10(b), the transient state was simulated exactly because of the approximation formula for the ionic conductivity. We propose that one useful

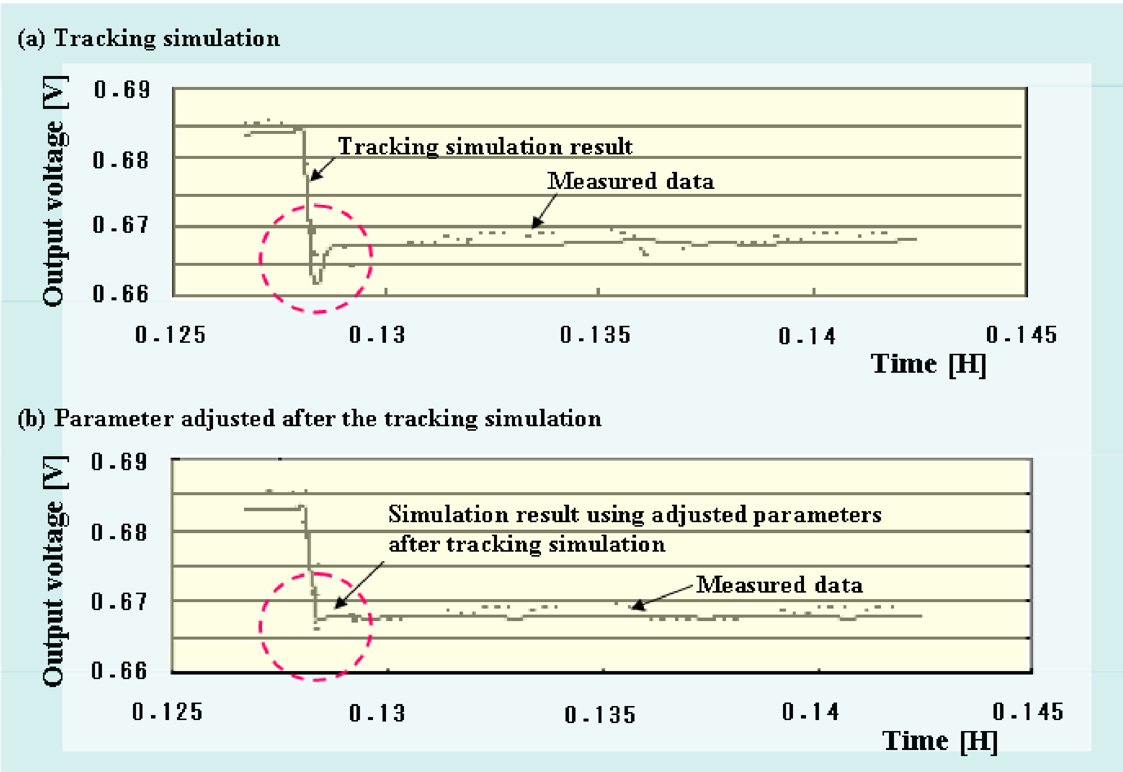

Fig. 10. Conventional tracking simulation result and simulation result using approximation formula

application of the tracking simulator is to decide the simulation parameters.

7. CONCLUSION

Using the tracking simulator is useful to estimate the model parameters where actual measurements cannot be taken. The tracking simulator provides a good simulation with model parameters to estimate the functions of its related variables. In this study, it was shown that the ionic conductivity that is strongly dependent on the driving condition of a fuel cell could be approximated as a function of load current by the tracking simulator. It was possible to estimate parameters that fluctuate with the operational status and time. Estimation of parameters that are impractical to measure is one of applications of the tracking simulator. In addition, the tracking simulator will provide an accurate plant model the parameters of which can be adjusted by the tracking simulation technique. With monitoring of the changes in the model parameters, an accurate plant model will be applicable to plant fault detection and diagnosis.

One of our final goals is to apply the tracking simulator to fault detection and abnormal diagnosis of the plant utilizing a precise plant model.

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