A Simulation of Polymer Electrolyte Fuel Cells with Co-flow / Counter-flow Pattern under Dry Condition

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Introduction

Polymer Electrolyte Fuel Cells (PEFCs) posses various virtues and are expected to be standard in the next generation. However, great progress still remains to be made for its realistic use in the society. For instance, there are factors such as material, structure, and operating condition that are necessary to be optimized. To cope with these issues, experimental effort is indispensable, but there are also problems proper to experiments: numerous experiments must be performed to gain insights, and it is difficult to measure the PEFC when it is under operation.

Due to such situation, computational approach is attracting much interest and research is performed eagerly in this direction [1]. Among numbers of expectations directed toward computer simulation, one is to extract knowledge about operation under extreme conditions that are difficult to perform in laboratory experiments.

In this work, a simulation of a PEFC under dry condition, which is a representative case difficult to perform an actual operation, is attempted. Experimental results are reproduced quantitatively by fitting a few parameters included in the model.

Simulated system

An operation under dry condition, which is reported in ref [2], has been selected for simulation. The shape and size of the PEFC, the pattern of the flow field, and the direction of the injection of the fuel gas are shown in a schematic diagram of Fig.1.The experiment is performed for two flow patterns: the co-flow (left) and the counterflow (right). The thickness of the MEA (0.05mm), the gas diffusion layer (0.4mm), and the width and the depth of the flow field (1mm, respectively) are also shown in the same figure. The aim of the simulation is to clarify the effect of the pattern of the flow field, i.e., the difference between the co-flow pattern and the counter-flow pattern.

Operational conditions are shown in Tab.1. Both the anode gas (hydrogen) and the cathode gas (air) are injected without humidity. The stoichiometric ratio is 1.25. Gas pressure and temperature are 0.2MPa and 350K, respectively. Operation was performed in the region of current density($0 \sim 1.0$ A/cm²).

Models

In our calculation, water and proton transport in the membrane is modeled according to the model proposed by Nguyen and White [3]. Calculational results were quantitatively fitted to the experimental results by choosing the water diffusion coefficient and the electric conductivity as fitting parameters. Electrochemical reactions are assumed to follow the Butler-Volmer equation. The flow field is modeled as follows. In the flow channel, the flow field is subject to the one-dimensional advection-diffusion equation. The pressure drop is assumed to be of the laminar pipe flow. In the gas diffusion layer, the flow field is subject to the three-dimensional advection-diffusion equation. The pressure drop is assumed to follow the Darcy's law.

Results and discussions

The calculational result of current-voltage characteristic is shown in Fig.3. The relative humidity of the gas is varied in the region $0 \sim 5\%$. From this, one can see that the experimental result is quantitatively reproduced for both cases of the co-flow pattern and the counter-flow pattern. This was achieved by fitting two parameters, the water diffusion coefficient in the membrane and the drag coefficient. In the co-flow case, the cell voltage drastically changed as the relative humidity of the gas varied. This instability, which is also seen in the experimental result, can be traced to the extreme exhaustion of humidity in the upstream. On the other hand, the cell voltage was relatively stable in the counter-flow case, which also agrees with experiment. This feature can be explained by the homogeneity of vapor activity, which is realized in the counter-flow case.

The potential applicability of computer simulation for extreme operational conditions such as dry condition was shown in this study. By comparing calculation with experiment, improvement of the model and the acquisition of data will further be proceeded. These efforts are aimed to contribute to the design of PEFCs.



Fig1. Schematic diagram of the fuel cell flow field.

	Anode gas	Cathode gas
Com ponents	hydrogen	A ir
Relative hum idity	D ry (0%)	
Stoichiom etric Ratio	1.25	
Pressure	0.2M Pa	
Temperature	350K	
Current density	$0 \sim 1.0 \text{ A} / \text{cm}^2$	

Tab1. Operation condition



Fig.2 Comparison of Polarization Curves between Experiment and Calculation

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