기체확산층 두께에 따른 **PEMFC**의 성능분석과 **SIMULATION**

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EFFECT OF THE GAS DIFFUSION LAYER THICKNESS OF THE PEM FUEL CELLS AND THE APPLICATION OF SIMULATION

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INTRODUCTION

Proton exchange membrane fuel cell (PEMFC) engines can potentially replace the internal combustion engine for transportation because they are clean, quiet, energy efficient, modular, and capable of quick start-up. Since a PEMFC simultaneously involves electrochemical reactions, current distribution, hydrodynamics, multicomponent transport, and heat transfer, a comprehensive mathematical model is needed to gain a fundamental understanding of the interacting electrochemical and transport phenomena and to provide a computer-aided tool for design and optimization of future fuel cell engines.

The diffusion layer in a PEMFC consists of a thin layer of carbon black mixed with polytetrafluoroethylene (PTFE) that is coated onto a sheet of macro-porous carbon backing cloth. This diffusion layer provides a physical micro-porous support for the catalyst layer while allowing gas transport to and from the catalyst layer. Although the diffusion layer is a seemingly minor component in a fuel cell, it has been shown that altering the composition of the diffusion layer can lead to substantial improvements in the performance of the cell. The improvements reported relate to the thickness of the layer, and the porosity of the layer.

The diffusion layer was prepared by screen-printing that could make it very thin. The effect of diffusion layer thickness was attributed to a decrease in the electrical resistance of the gas diffusion electrode as the diffusion layer thickness was increased. A thinner diffusion layer will improve gas diffusion properties by providing a shorter path for gas diffusion. However, if the diffusion layer is made too thin, some other factors become pertinent. The reason for lower cell performances at low diffusion layer loadings is high electronic resistance in the electrode, since the electronic contact area between the catalyst and diffusion layers is thought to become too small at low diffusion layer loadings.

The goals of this work are to find the optimum thickness of the gas diffusion layer and analyze the variables related to the electrode by simulation.

EXPERIMENTAL

Electrodes were prepared by the following process, which included several pretreatment procedures. The first step was to deposit a diffusion layer on the carbon cloth substrate. Carbon powder (Vulcan XC-72, Cabot Co.), PTFE (60 wt.%, Aldrich) and isopropyl alcohol (IPA) were mechanically mixed

in a supersonic mixer. The carbon and PTFE loadings were maintained at a fixed ratio of 10:3. The viscous mixture was screen-printed on to the wet-proofed carbon cloth and then dried for one day. Screen-printing method has an advantage of getting diffusion layer thickness thinner, which makes it possible to control the diffusion layer loading. Then a thin catalyst layer was prepared by spraying method. That is, 0.4 mg cm^{-2} Pt, 20 wt. % on Vulcan XC-72 (Electrochem Inc.), 0.6 mg cm^{-2} Nafion solution (5 wt.%, Aldrich) and IPA were mixed and sprayed on to the diffusion layer. Nafion[®]115 membranes were pretreated with H_2O_2 and H_2SO_4 to remove organic and mineral impurities, respectively. Next, the membranes were rinsed several times with hot distilled water. MEAs were fabricated by hot pressing at 120 ℃ and 3 metric ton for 3 min.

MODEL DEVELOPMENT

In this paragraph, a description of the mathematical model developed for the solid polymer electrolyte fuel cell is presented. The following equations are governing equations.

Continuity : $\frac{\partial (\varepsilon \rho)}{\partial t} + \nabla \cdot (\rho u) = 0$ Momentum conservation : \vec{v})+ $\nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F}$ ∂ $\frac{\partial}{\partial y}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{r}) + \rho \vec{g} + \vec{F}$ *t* $(\rho \nu)$ + $\nabla \cdot (\rho \nu \nu) = -\nabla p + \nabla \cdot (\tau) + \rho$ Darcy's law : $\nabla p = -\frac{\mu}{\alpha} \vec{v}$ Energy conservation : $\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i(\rho E + p)) = \frac{\partial}{\partial x_i}(k_{\text{eff}} \frac{\partial T}{\partial x_i} - \sum_j h_j J_j + u_j(\tau_{ij})_{\text{eff}}) + S_h$ ∂ ∂ $\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i(\rho E + p)) = \frac{\partial}{\partial x_i}(k_{eff} \frac{\partial T}{\partial x_i} - \sum_i h_j J_j + u_j(\tau_{ij})_{eff})$ Species conservation : $\frac{\partial}{\partial t}(\epsilon \rho C^k) + \nabla \cdot (\gamma \rho u C^k) = \nabla \cdot (\rho_l D_{l, \epsilon \theta}^k \nabla C_l^k + \rho_g D_{g, \epsilon \theta}^k \nabla C_g^k) - \nabla \cdot [(C_l^k - C_g^k)j_l] + m^k$ *t* $+\nabla \cdot (\gamma p u C^k) = \nabla \cdot (\rho_i D_{i \text{ eff}}^k \nabla C_i^k + \rho_{\sigma} D_{\sigma \text{ eff}}^k \nabla C_{\sigma}^k) - \nabla \cdot [(C_i^k - C_{\sigma}^k)_{j_i}] + m$ $\frac{\partial}{\partial t}(\varepsilon \rho C^k) + \nabla \cdot (\gamma \rho u C^k) = \nabla \cdot (\rho_i D^k_{i,\text{eff}} \nabla C^k_i + \rho_g D^k_{g,\text{eff}} \nabla C^k_g) - \nabla \cdot [(C^k_i - C^k_g)]$

FLUENT (version 6.0) is used to solve the coupled governing equations. The data relevant to varying thickness of gas diffusion layer were obtained by using this tool. Figure 1 shows the system of channel and electrode in this experiment. And simulation conditions are followed.

Inlet velocity : 2.14 $\frac{m}{s}$ Inlet temperature : 353 K Cell temperature : 348 K Electrode porosity : 0.51, 0.57, 0.61

Figure 1. Three-dimensional schematic diagram of flow channel

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RESULT AND DISCUSSION

Figure 2. Influence of diffusion layer thickness on fuel cell performance (porosity 0.57)

Cell potential-current density plots for cells of varying thickness and porosity are shown in Figure 2, 3, respectively.

As shown in Figure 2, the effect of diffusion layer thickness was attributed to a decrease in the electrical resistance of the gas diffusion electrode as the diffusion layer thickness was increased.

As can be noted in Figure 3, the effect of diffusion layer porosity has a significant effect on cell performance, especially at high current densities. The increase in performance was attributed to high porosity being better able to remove water from the cell, resulting in a reduction in cathode flooding.

Figure 4, 5, and 6 are concentration distributions according to the thickness of the diffusion layer.

These show the concentration drops between the inlet and outlet channels. And the effect of diffusion layer thickness according the decrease of the concentration $O₂$ was shown as the diffusion layer thickness was increased.

Figure 4. Contour of concentration of O_2 (0.20 mm)

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Figure 5. Contour of concentration of O_2 (0.35 mm) Figure 6. Contour of concentration of O_2 (0.50 mm)

CONCLUSION

In this work, simulation of fluid in channel and gas diffusion layer was developed to investigate the effects of electrode variables: gas diffusion layer thickness, porosity and distribution of pore. The results show that the application of simulation enables to design the flow channel and the structure of the electrode effectively.

ACKNOWLEDGEMENTS

This work was supported by Korea Research Foundation Grant. (KRF-2001-A1008-2001-005-E00030)

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