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3차원 CFD 시뮬레이션을 활용한 고분자전해질 연료전지 스택의 매니폴드 크기 최적화

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Optimal Sizing of the Manifolds in a PEM Fuel Cell Stack using Three-Dimensional CFD Simulations

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Abstract >> Polymer electrolyte membrane (PEM) fuel cell stacks are constructed by stacking several to hundreds of unit cells depending on their power outputs required. Fuel and oxidant are distributed to each cell of a stack through so-called manifolds during its operation. In designing a stack, if the manifold sizes are too small, the fuel and oxidant would be maldistributed among the cells. On the contrary, the volume of the stack would be too large if the manifolds are oversized. In this study, we present a three-dimensional computational fluid dynamics (CFD) model with a geometrically simplified flow-field to optimize the size of the manifolds of a stack. The flow-field of the stack was simplified as a straight channel filled with porous media to reduce the number of computational meshes required for CFD simulations. Using the CFD model, we determined the size of the oxidant manifold of a 30 kW-class PEM fuel cell stack that comprises 99 cells. The stack with the optimal manifold size showed a quite uniform distribution of the cell voltages across the entire cells.

Key words : Fuel cell(연료전지), Manifold(매니폴드), Computational fluid dynamics(전산유체역학), Stack design (스택 설계), Optimization(최적화)

Nomenclature

n : normal direction
p : pressure, Pa
S_m : momentum source
u : superficial velocity, m/s
x : Cartesian coordinates, m
α : gas permeability cofficient, $Pa \cdot s^2/m^2$
β : gas permeability cofficient, $Pa \cdot s/m$
ΔP : pressure drop, Pa
ρ : gas density, kg/m^3
Φ : physical variables
τ : stress tensor components

Subscripts

i : Cartesian coordinate index

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j : Cartesian coordinate index
0 : inlet condition

1. Introduction

Polymer electrolyte membrane (PEM) fuel cell stacks are constructed by stacking several to hundreds of unit cells depending on their power outputs required. PEM fuel cells for mobile applications, such as cars, forklifts, or boats, consume hydrogen and air as a fuel and an oxidant, respectively. The fuel and oxidant are distributed to each cell of a PEM fuel cell stack through so-called *manifolds*[1] as shown in Fig. 1. Typically, PEM fuel cell stacks are designed to be made up of 6 manifolds in them: two manifolds for each stream (fuel, oxidant, and coolant). During operations of the stack, distributions of the fuel and oxidant should be balanced among the cells both to achieve the maximum performance of a stack and to prolong the durability. The fuel and oxidant can be uniformly distributed among the cells by performing an optimal design of the manifolds. If the manifold sizes are too small, the fuel and oxidant would be unevenly distributed among the cells. On the contrary, the volume of a stack would be too large if the manifolds are oversized. Several studies have been performed on flow distributions in the manifolds using various approaches[2-7] such as simplified momentum balances, pressure correlations, and computational fluid dynamics (CFD) simulations. The size of a manifold can be optimally determined from CFD simulation results, since fluid dynamics of the reactant gases in a manifold are strongly related to their distributions to the fuel cells.

In general, the CFD analysis even for a single fuel

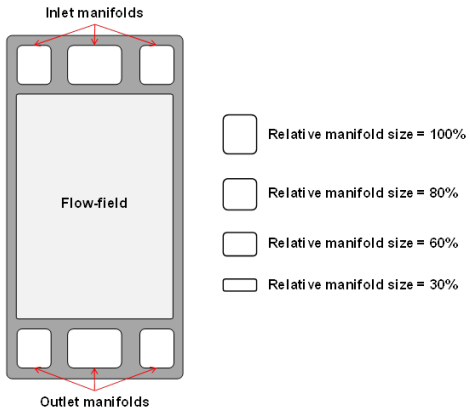

Fig. 1 Schematic of a bipolar-plate with fuel, oxidant, and coolant manifolds and the relative sizes of the oxidant manifolds used in CFD simulations

cell demands a large amount of computational cost even using a state-of-the-art parallel computing machine because we have to generate hundreds of thousands of meshes (also called grids or cells) to tens of millions to solve a system of partial differential equations in reasonable accuracy. This mainly arises from geometrical complexity of the flow-fields of a bipolar plate which is one of the main components along with membrane electrode assembly (MEA) constructing a single fuel cell. Considering a stack which may comprise several to hundreds of cells, we must generate several millions of meshes to hundreds of millions if we preserve the same geometrical complexity as used for the single cell. Needless to say, the CFD analysis with this tremendous number of meshes demands an exhaustive computational cost and sometimes is unrealistic to get the convergence solutions. Therefore, it is necessary to downsize the number of meshes enormously by employing a simplification method of the stack without sacrificing the reliability of the simulation results.

In this study, we present a geometrical simplification

method for the flow-fields to reduce the number of meshes required for CFD simulations of the manifolds of a PEM fuel cell stack. To validate the simplification method, the simulation results obtained from the simplified model are compared with those from the full model. Then, we optimize the manifold sizes of a 30 kW-class stack using a three-dimensional CFD model along with simplified geometry for the flow-fields.

2. Model Description

A geometrical simplification method for the flow-fields of a stack is employed to reduce the number of meshes for the three-dimensional CFD analysis. Because the major concern is not the flow-fields but the manifolds in predicting fluid patterns inside the manifolds, the flow-fields can be geometrically simplified under the assumption that the fluid patterns can be preserved inside the manifolds if an appropriate approximation is made for the flow-fields. In this study, a simple approximation based on Darcy's law[8] is used for the flow-field of each cell which is simplified as a straight channel filled with a porous media through which the pressure drop is expressed as a function of the gas velocity as follows:

$$\Delta p = \alpha |u|^2 + \beta |u| \quad (1)$$

where Δp denotes the pressure drop through a channel (Pa), u is the superficial gas velocity through a channel (m/s), and α (Pa·s^2/m^2) and β (Pa·s/m) are the gas permeability coefficients. The pressure drop through the straight channel must be equivalent to that through the original flow-field. Consequently, the total number of meshes generated on the stack can be largely reduced up to one hundredth of that generated on the original flow-field because it is not necessary to generate the meshes on the flow-field region.

A commercial CFD code STAR-CD[9] was used to solve the following partial differential equations governing fluid dynamics in the stack after combining the porous media model described in Eq. (1) into the differential equations:

Continuity equation:

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (2)$$

Momentum equation:

$$\frac{\partial}{\partial x_i}(\rho u_i u_j - \tau_{ij}) = \frac{\partial p}{\partial x_j} + s_m \quad (3)$$

where x_i denotes Cartesian coordinate (i=1, 2, and 3), u_i is the absolute fluid velocity component in direction x_i, p is the pressure, ρ is the density, τ_{ij} is the stress tensor components, and s_m is the momentum source. Additional equations describing the turbulent model can be found in the technical manual[8] of STAR-CD. In this study, the standard k-ε model for the turbulence was chosen from various turbulent models. The boundary conditions of the governing equations are $\Phi = \Phi_0$ at the inlet of the stack and $\partial\Phi/\partial n = 0$ at the outlet, where n represents normal direction to the outlet and Φ is physical variables such as velocity, pressure, etc.

3. Model Validation

We have to first find the gas permeability coefficients α and β in Eq. (1). The pressure drops through the

flow-field of a single cell was measured while changing the superficial linear velocity of the oxidant entering the cell. Based on the measured pressure drops, the coefficients α and β were found to be 0.1172 $Pa{\cdot}s^2/m^2$ and 0.3051 Pa·s/m, respectively, by performing a least square fitting of the measured pressure drops with the calculated ones. Fig. 2 shows the final fitting results of the pressure drops with respect to the linear velocity. As shown in the figure, the fitting equation well predicts the measured pressure drops.

The CFD model described in the previous section was validated through comparing CFD simulation results. Three-dimensional CFD simulations were performed for a 50-cell stack the flow-field of which was modeled both as geometrically simplified straight channels (called simplified model) and as the original shape without simplification (called full model). Fig. 3 shows the full and simplified models for the CFD simulations. The number of cells required for generating 3-dimensional meshes on the full model was 1,682,424. However, it was reduced by about one fourth for the simplified model owing to the simplified geometry of the flow-field. Consequently, the CPU time required for obtaining convergence solutions was considerably reduced by nearly one seventh as summarized in Table 1.

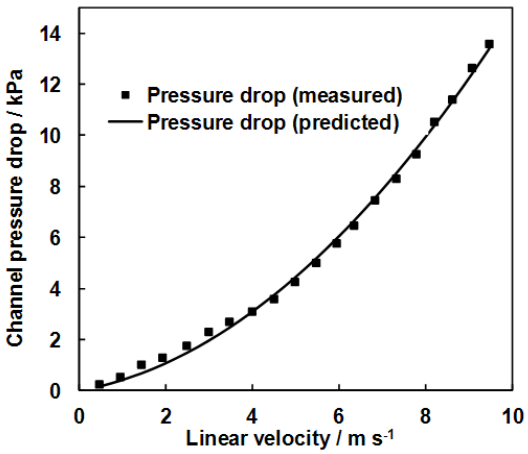

Fig. 2 Comparison of the measured and predicted pressure drops through a single cell

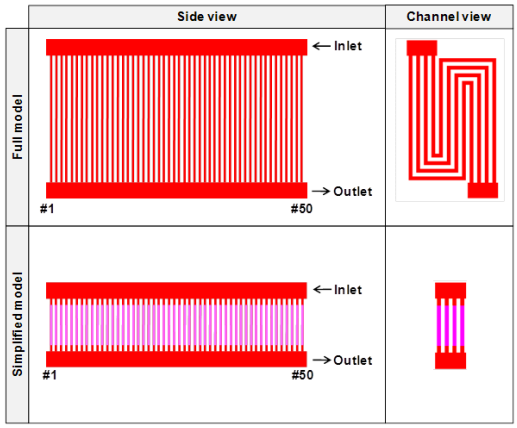

Fig. 3 Full and simplified models for a 50-cell stack the flow-field of which was modeled as geometrically simplified straight channels in the simplified model

Table 1 Comparison of the number of meshes and CPU time between the full and simplified models

Model	Number of cells	CPU time (s)
Full model	1,682,424	2,361.6
Simplified model	396,024	354.6

Simulation results from the simplified model were compared with those from the full model. Fig. 4 illustrates comparison of the distributions of velocity magnitudes inside the oxidant manifolds between the full and simplified models. As can be seen in the figure, the distributions of velocity magnitudes predicted from the two models are very similar to each other. Fig. 5 compares the mass flow deviation profile along the cell number obtained from the simplified model with that from the full model. As shown in the figure, the profile from the simplified model is in good agreement with that from the simplified model within an error range of 1%. Therefore, the three-dimensional CFD model integrated with a simplified

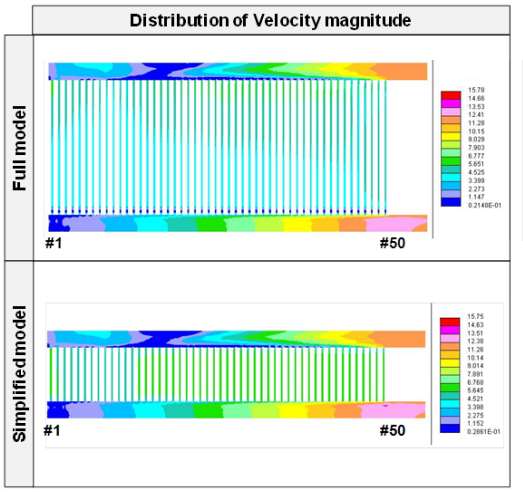

Fig. 4 Comparison of the distributions of velocity magnitudes inside the oxidant manifolds between the full and simplified models

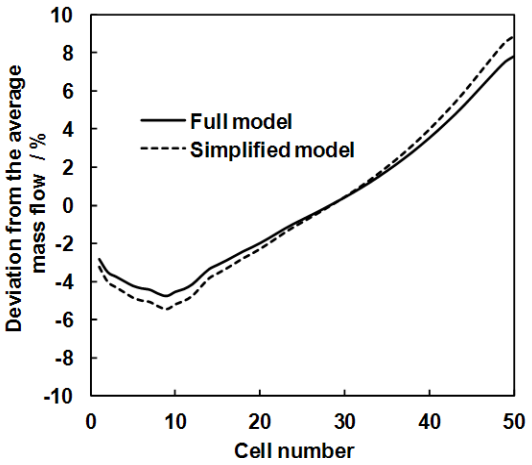

Fig. 5 Comparison of the mass flow deviation profiles along the cell number obtained from the full and simplified models

geometry for the flow-fields well predicts fluid patterns inside the manifolds of the stack.

4. Results and Discussion

The sizes of the oxidant manifold of a 30 kW-class stack were determined using the three-dimensional CFD model integrated with a simplified geometry for the flow-field. The stack comprises 99 cells and has an active area of 295 cm^2 to generate a maximum power of 30 kW at an average cell voltage of 0.65 V. The oxidant flow-field of the stack was simplified as a straight channel filled with porous media. Then, the following four different sizes of the oxidant manifold were designed as shown in Fig. 1 to find an approximate size to the optimum: the relative size of the oxidant manifold = 100% (8.8 cm^2), 80%, 60%, and 30%. Finally, four different CFD models were prepared each of which has the same geometry as one another except for the shape and size of the oxidant manifold. The number of meshes required for the four CFD models ranged from 1,494,462 to 1,559,038 depending on the relative size of the manifold. For each size of the manifold, several CFD simulations were carried out with the three different simulation conditions: 1) stoichiometry 1.0 and current density 0.7 A/cm^2 at 0.65 V, 2) stoichiometry 1.5 and current density 0.7 A/cm^2 at 0.65 V, and 3) stoichiometry 3.0 and current density 0.7 A/cm^2 at 0.65V.

Fig. 6 shows a simulation result that plots the mass-flow deviations from the average mass-flow entering each cell when the oxidant stoichiometry was set at 1.5. The distribution of the air among the cells in the stack is more balanced as the mass-flow deviations for the entire cells approach zero. As shown in the figure, the mass-flow deviations along the cell number are much less than 1.0% for the manifold sizes of 100%, 80%, and 60%. However, when the manifold size was further reduced to 30%, large deviations of the mass-flow rates were observed especially around the entrance of the oxidant manifold. Fig. 7 plots the maximum deviation of the mass flow as a function of the relative size of the oxidant

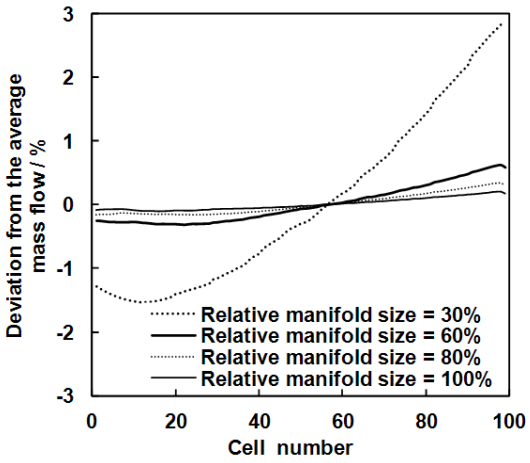

Fig. 6 Mass-flow deviations from the average mass-flow entering each cell for the relative manifold size of 30%, 60%, 80%, and 100% when the oxidant stoichiometry was set at 1.5

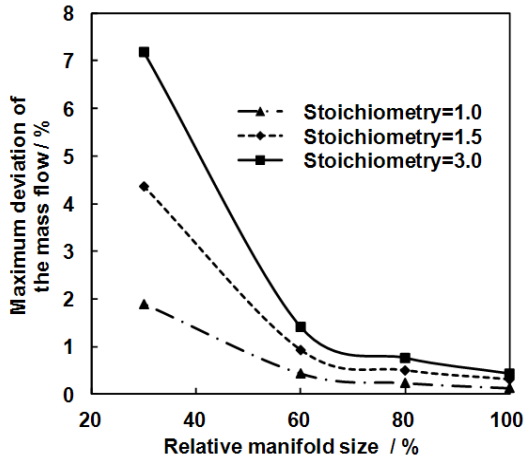

Fig. 7 Maximum deviation of the mass flow as a function of the relative size of the oxidant manifold for the oxidant stoichiometries of 1.0, 1.5, and 3.0

manifold for the oxidant stoichiometries of 1.0, 1.5, and 3.0. As shown in the figure, the maximum deviations from the average mass flow rate are drastically increased for all the three stoichiometries (1.0, 1.5, and 3.0) when the relative manifold size was reduced to less than 60%. The maximum deviations reached 4.5% and 7.3% for the stoichiometries of 1.5 and 3.0, respectively, when the relative manifold size

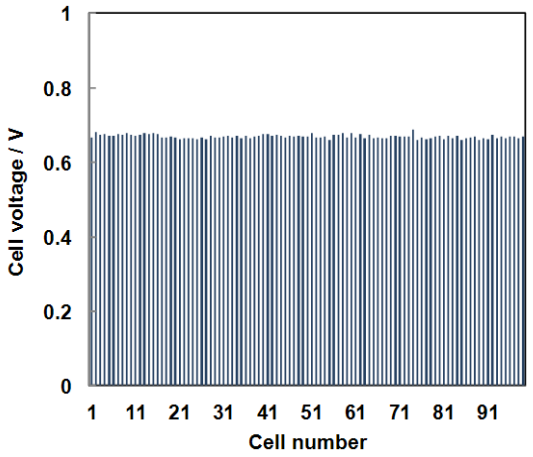

Fig. 8 Cell voltage distributions measured for the 99-cell stack

was reduced to 30%. These deviations are quite large, causing a significant performance difference among the cells in the stack when the oxidant manifold size is too small. Considering a safety margin, in this study, the size of the oxidant manifold was determined to be 70% that corresponds to 5.3 cm^2 in its size.

The manifold size found from the simulations was reflected in designing a 30 kW-class PEM fuel cell stack. Fig. 8 shows the cell voltage distributions measured for the 99-cell stack. As shown in the figure, the cell voltage distribution is quite uniform across the entire cells: the standard deviation of the cell voltages is 0.0053 V. Therefore, we can conclude that the size of the oxidant manifold was optimally determined using the proposed CFD model.

5. Conclusions

A three-dimensional CFD model with a geometrically simplified flow-field was employed to optimize the size of the manifolds of a PEM fuel cell stack. In this model, the flow-field of the stack was simplified as a straight channel filled with porous media. The CFD

model was validated using numerical validation methods.

Using the CFD model, we determined the size of the oxidant manifold of a 30 kW-class PEM fuel cell stack comprising 99 cells. The stack with the optimal manifold size showed quite uniform distribution of the cell voltages across the entire cells. Therefore, it is expected that the geometrical simplification method can be effectively applied to design the manifolds of PEM fuel cell stacks.

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