NUMERICAL CHARACTERIZATION OF LIQUID WATER EXHAUST CAPABILITIES IN FLOW CHANNELES FOR POLYMER ELECTROLYTE MEMBRANE FUEL CELLS

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Polymer electrolyte membrane fuel cells (PEMFCs) are promising power generation technologies with higher efficiency and clean emission. The water management is currently among challenging issues for improving the performance and durability of PEMFCs. Liquid water produced in PEMFCs should be properly exhausted especially during high current operations. Otherwise, the product water floods the porous electrodes and channels, leading to a degraded performance or an unstable operation. In addition, liquid water in PEMFCs which operate at a cold weather should be thoroughly purged after each operation in order to prevent the mechanical failures due to freezing of residual water. In this study, computational fluid dynamics (CFD) simulations were conducted to study the liquid water transport behaviors in the flow channels having different geometries and surface properties (hydrophilic and hydrophobic). The liquid water exhaust capabilities of the simulated flow channels for PEMFCs were also quantitatively analyzed in the CFD simulations. The results showed that hydrophobic flow channels generally have better liquid water exhaust capabilities than hydrophilic ones. In addition, hydrophobic channels did not show a significant deterioration in the exhaust capability when the flow rate of air was reduced, but hydrophilic channels did show. It was also found that a smaller width is desirable for hydrophobic flow channels while a larger width is desirable for hydrophilic ones. The above results were explained as being due to the different droplet morphologies which develops in hydrophobic and hydrophilic channels.

Keywords: polymer electrolyte membrane fuel cell (PEMFC), flow channel, water transport, contact angle, hydrophilic, hydrophobic, computational fluid dynamics (CFD), volume of fluid (VOF)

1. INTRODUCTION

Continued use of hydrocarbon fuels for heat and power generation has caused global environmental problems such as air pollution, climate change (due to greenhouse gas), etc. In addition, fossil fuels are expected to be limiting resources in the future. The development of alternative energy sources which is free of negative environmental impacts is thus important to solve these problems. Fuel cells which operate with hydrogen are promising power sources for their environmentally friendliness and high efficiency.

Fuel cells produce electricity by direct electrochemical combination of hydrogen and oxygen, and also produce heat and water as by-products. Among many types of fuel cells, the polymer electrolyte membrane fuel cell (PEMFC) is currently one of the most advanced fuel cell technologies near commercialization and its primary application fields include the automotive and residential power generation.

A repeating unit in PEMFCs is composed of a membrane electrode assembly (MEA) for electro-chemical reactions, gas diffusion layers (GDL) for uniform diffusion of fuel and oxidant gases, and bipolar plates for flow distribution and current collection. Water management problem is currently among the technological issues that should be solved to achieve better performance of PEMFCs with higher current density operations.

Water is generated in the cathode by electro-chemical reactions during the operation of PEMFCs. Water is favorable for enhancing the ionic (protonic) conductivity of the polymer membrane, and thus essential for the operation of PEMFCs. However, excessive water present in PEMFCs leads to another problem called as flooding: liquid water limits the reaction rate in catalyst layer, reduces the diffusion rate in GDL, and interferes with the uniform flow distribution in flow channel. This results in the deterioration of the PEMFC performance.

In this paper, computational fluid dynamics (CFD) simulations were carried out to identify the design factors for flow channels having better capability in exhausting liquid water from PEMFCs. The transport behavior of liquid water droplets in hydrophilic or hydrophobic flow channels of PEMFCs was predicted by employing the volume of fluid (VOF) two-phase model. The surface tension effects were fully considered in the simulation by varying the contact angle for the wall adhesion effects. The effects of surface properties, channel geometries, and corner configurations on the liquid water droplet transport were studied for the high and low velocity conditions for air flow.

The results of the present study are expected to help improve the performance and safety of the PEM fuel cell, by enabling the channel designs which facilitate the liquid water exhaust and also thus reduce the possibility of the mechanical failure.

2. SIMULATION

2.1 Two-phase flow model

The two-phase water/air flow in the cathode channel of PEMFCs was modeled based on the volume of fluid (VOF) multi-phase model. The continuity equation for the mixture fluid (water + air in this study) is expressed as

\[
\frac{1}{\rho_q} \frac{\partial}{\partial t} \left( \alpha_q \rho_q \right) + \nabla \cdot \left( \alpha_q \rho_q v_q \right) = 0, \tag{1}
\]

where \( \alpha_q \), \( \rho_q \), and \( v_q \) are the volume fraction, the
density, and the velocity of the phase \( q \), respectively. For water, \( q = w \) and for air \( q = a \).

In VOF method, a single mixture velocity \( v \) common to all participating phases is used to describe the fluid motion while the interfacial effects such as the surface tension is implicitly considered as a body force. Then, the Navier-Stokes equation for the two-phase water/air flow is expressed as \[5,6\]

\[
\frac{\partial}{\partial t} (\rho v) + \nabla \cdot (\rho v v) = -\nabla \rho + \nabla \cdot \left[ \mu \left( \nabla v + \nabla v^T \right) \right] + \rho g + F_{csf}, \tag{2}
\]

where \( \rho \) is the mixture density, \( \mu \) is the mixture viscosity, and \( F_{csf} \) is the continuum surface force (CSF) corresponding to the interfacial tension between two immiscible fluids and the adhesion force between those fluids and the solid surface.

In CSF approach, \( F_{csf} \) is calculated based on the spatial gradient and curvature of the volume fraction of \( \alpha \) as \[7\]

\[
F_{csf} = \frac{2 \kappa \rho \nabla \alpha}{\rho_w + \rho_a}. \tag{3}
\]

Here, \( \sigma \) is the surface tension (0.07 N/m is used) and \( \kappa \) is the curvature computed from the divergence of the unit surface normal. The interaction of water/air two-phase flow with the solid surface is considered by the contact angle \( \theta_c \), which is the angle that liquid water makes with the wall. This contact angle is used to adjust the surface normal in cells near the wall, and with which the wall adhesion effect is considered.

![Fig. 1 Liquid water droplet morphologies on top of (a) hydrophilic and (b) hydrophobic surfaces.](image)

Two different liquid water droplet morphologies are shown in Fig. 1. When the contact angle of water on top of a surface is smaller than 90° (\( \theta_c < 90^\circ \)), the surface is called hydrophilic. On the contrary, a surface with \( \theta_c > 90^\circ \) is called hydrophobic. The GDLs for PEMFCs are generally treated with hydrophobic PTFE coating to give them better water management ability. The apparent contact angle of GDLs were measured to be about 150° and thus liquid water droplets on top of GDLs generally have rather spherical shapes. \[8-10\]

### 2.2 CFD calculation

An exemplary serpentine flow field with triple parallel-paths for PEMFCs is shown in Fig. 2. Complex meandering flow channels with many 90° and 180° corners are well observed in Fig. 2. The liquid water produced in PEMFCs generally moves in the shape of droplets through such flow channels. In this study, the liquid water transport in the cathode flow channel was studied for three-pass serpentine flow fields having two 180° corners (U-bend). Liquid water droplets were assumed to exist in a flow channel initially, and then their exhaust behaviors due to air flow were calculated.

In the CFD simulations, the channel models having sharp or curved corner configurations were considered while varying the channel width as 1 mm or 2 mm (the channel height was fixed to 1 mm). The effect of hydrophilic or hydrophobic surfaces was considered by assigning the contact angle of the channel wall as 30° (hydrophilic) or 150° (hydrophobic). Note that the contact angle for the GDL surface was fixed to 150°. The air velocities of 5 m/s and 10 m/s were assumed to study the effect of air velocity on the water transport behavior.

The simulations were conducted using a commercial CFD code (FLUENT 6.2). The explicit VOF method with the geometrical interface reconstruction approach was employed to accurately calculate the two-phase water/air flow in channels. The effects of the hydrophilic and hydrophobic surfaces were considered by specifying the relevant contact angle on each wall boundary (GDL surface or channel wall). A very small time step of \( 10^{-4} \) s was used for the stable calculation of the explicit VOF in the CFD simulations.

![Fig. 2 A serpentine flow field for PEMFCs.](image)

### 3. RESULTS

The simulated water/air two-phase flow behaviors for hydrophilic and hydrophobic channels are shown in Figs. 3–6. These figures are obtained by setting the air velocity as 5 m/s.

In general, liquid water is observed to move as liquid films attached to the wall when the channel surface is hydrophilic (Figs. 3 and 5). However, when the channel surface is hydrophobic (Figs. 4 and 6), liquid water preferentially moves in the form of liquid droplets with minimal contact with the wall. These liquid water behaviors can be easily understood by the effect of the contact angle as shown in Fig. 1. Hydrophilic and hydrophobic surfaces induce completely different liquid water morphologies, and
Fig. 3 Simulated liquid water two-phase flow in hydrophilic channels with sharp corners (1 and 2 mm)

Fig. 4 Simulated liquid water two-phase flow in hydrophobic channels with sharp corners (1 and 2 mm)

Fig. 5 Simulated liquid water two-phase flow in hydrophilic channels with curved corners (1 and 2 mm)

Fig. 6 Simulated liquid water two-phase flow in hydrophobic channels with curved corners (1 and 2 mm)
this leads to different exhaust behaviors shown in Figs. 3–6. The current CFD simulations point out that hydrophobic channel surfaces are desirable for fast exhaust of liquid water from PEMFCs over hydrophilic channel surfaces.

The effects of the 180° corner configurations, i.e. the sharp and curved corners, can be identified from the comparison of Figs. 3 and 4 with Figs. 5 and 6. Liquid water tends to be accumulated in sharp corners of the flow channels. On the contrary, liquid water is observed to be transported out of curved corners relatively easily. The flow recirculation zone is prone to develop in sharp corners, which causes liquid water to be stagnant in those reasons. Thus, curved corners are desirable for reducing the amount of residual water stagnant in PEMFCs.

Each figure in Figs. 3–6 shows the effect of different channel widths (1 mm and 2 mm) on the two-phase liquid water behaviors in flow channels. The exhaust capability of channels seems to deteriorate as the channel width increases. In addition, the amount of stagnant liquid water in corners increases as well. This is because the drag force exerted by air flow in channels decreases when the channel width (area) is expanded. Smaller channels are advantageous in exhausting liquid water by utilizing larger drag force, but also require higher pressure loss at the same time. Therefore, the channel width should be properly selected considering both the liquid water exhaust capability and the pressure drop.

The effects of the flow speed in channels were studied by changing the air velocity as 5 m/s or 10 m/s. When the air velocity becomes sufficiently high, the effects of other parameters, i.e. the surface property, corner configuration, and the channel width, are observed to be less important. Almost the same liquid water morphology, composed of very small droplets, is obtained at high flow speed irrespective of geometrical and surface properties. That is, if the air velocity is maintained at a sufficiently high level, exhaust of liquid water from PEMFCs does not need to be considered. However, higher air velocity in channels means higher consumption rate of pumping power. Thus, the air velocity should be determined to achieve fast liquid water exhaust, but not to waste excessive pumping power.

Among the channels in Figs. 3–6, hydrophobic channels with curved corners shown in Fig. 6 are expected to have the best liquid water exhaust capability. The hydrophobic channel surface induces the rather spherical droplet shapes which are easily transported by higher drag force. The curved corners reduce the flow recirculation in 180° corners (U-bend), and thus decrease the amount stagnant liquid water. In summary, the flow channels for PEMFCs are recommended to have the hydrophobic surface for fast droplet transport and the curved corners for small residual water.

4. SUMMARY

In this study, numerical simulations were conducted using a commercial CFD code (FLUENT 6.2) to clarify the effects of the surface property, corner configuration and channel width on the liquid water exhaust capability of flow channels in PEMFCs. The CFD results showed that the hydrophobic surface, cured corner, smaller channel width, and higher air velocity are generally favorable for efficient exhaust of liquid water from flow channels with small residual water. The present result is believed to provide a useful guideline for designing the flow channels for PEMFCs with optimal surface property and geometries. In addition, the possibility of the mechanical failure of PEMFCs due to the freezing of residual water in flow channels can be reduced by following the guideline.

**ACKNOWLEDGEMENT**

This work was supported by New & Renewable Energy R&D program (2006-N-HY12-P-01) under Korea Ministry of Commerce, Industry and Energy (MOCIE).

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